

# The AFLOW Library of Crystallographic Prototypes: Part 2

David Hicks<sup>a,b</sup>, Michael J. Mehl<sup>c</sup>, Eric Gossett<sup>a,b</sup>, Cormac Toher<sup>a,b</sup>, Ohad Levy<sup>a,b,d</sup>,  
Robert M. Hanson<sup>e</sup>, Gus Hart<sup>f</sup>, Stefano Curtarolo<sup>a,g,h</sup>

<sup>a</sup> Center for Materials Genomics, Duke University, Durham, NC 27708, USA

<sup>b</sup> Department of Mechanical Engineering and Materials Science, Duke University, Durham NC 27708

<sup>c</sup> Center for Materials Physics and Technology, Code 6390, U.S. Naval Research Laboratory, Washington DC 20375

<sup>d</sup> Department of Physics, NRCN, P.O. Box 9001, Beer-Sheva 84190, Israel

<sup>e</sup> Department of Chemistry, St. Olaf College, Northfield, Minnesota 55057

<sup>f</sup> Department of Physics and Astronomy, Brigham Young University, Provo UT 84602

<sup>g</sup> Materials Science, Electrical Engineering, Physics and Chemistry, Duke University, Durham, North Carolina 27708

<sup>h</sup> Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany

---

## Abstract

Materials discovery via high-throughput methods relies on the availability of structural prototypes, which are generally decorated with varying combinations of elements to produce potential new materials. To facilitate the automatic generation of these materials, we developed *The AFLOW Library of Crystallographic Prototypes* — a collection of crystal prototypes that can be rapidly decorated using the AFLOW software. Part 2 of this work introduces an additional 302 crystal structure prototypes, including at least one from each of the 138 space groups not included in Part 1. Combined with Part 1, the entire library consists of 590 unique crystallographic prototypes covering all 230 space groups. We also present discussions of enantiomorphic space groups, Wigner-Seitz cells, the two-dimensional plane groups, and the various different space group notations used throughout crystallography. All structures — from both Part 1 and Part 2 — are listed in the web version of the library available at <http://www.aflow.org/CrystalDatabase>.

**Keywords:** Crystal Structure, Space Groups, Wyckoff Positions, Lattice Vectors, Basis Vectors, Database

---

## Table of Contents

1. Introduction	7
2. Enantiomorphic Space Groups	8
3. The Wigner-Seitz Primitive Cell	9
4. Plane Groups (Two-Dimensional Space Groups)	10
4.1. The Parallelogram Crystal System	12
4.1.1. Plane Group #1: $p1$	12
4.1.2. Plane Group #2: $p2$	12
4.2. The Rectangular Crystal System	12
4.2.1. Plane Group #3: $p1m1$	12
4.2.2. Plane Group #4: $p1g1$	13
4.2.3. Plane Group #5: $c1m1$	13
4.2.4. Plane Group #6: $p2mm$	13
4.2.5. Plane Group #7: $p2mg$	14
4.2.6. Plane Group #8: $p2gg$	14
4.2.7. Plane Group #9: $c2mm$	14
4.3. The Square Crystal System	15
4.3.1. Plane Group #10: $p4$	15
4.3.2. Plane Group #11: $p4mm$	16
4.3.3. Plane Group #12: $p4gm$	16
4.4. The Trigonal Crystal System	16
4.4.1. Plane Group #13: $p3$	16
4.4.2. Plane Group #14: $p3m1$	16
4.4.3. Plane Group #15: $p31m$	17
4.5. The Hexagonal Crystal System	16
4.5.1. Plane Group #16: $p6$	17
4.5.2. Plane Group #17: $p6mm$	18
5. Space Group Notation	18
6. Conclusion	18
7. Acknowledgments	24
8. References	25
<b>Prototypes</b>	
$P\bar{1}$ (2)	
1. H <sub>2</sub> S: A2B <sub>2</sub> A <sub>6</sub> P <sub>2</sub> aei <sub>1</sub>	28
$Pm$ (6)	
1. Mo <sub>8</sub> P <sub>5</sub> : A8B <sub>5</sub> mP <sub>13</sub> 6 <sub>7</sub> a <sub>7</sub> b <sub>3</sub> a <sub>2</sub> b	30
2. FeNi: AB <sub>2</sub> mP <sub>4</sub> 6 <sub>2</sub> b <sub>2</sub> a	32
$Pc$ (7)	
1. H <sub>2</sub> S IV: A2B <sub>2</sub> mP <sub>12</sub> 7 <sub>4</sub> a <sub>2</sub> a	34
2. As <sub>2</sub> Ba: A2B <sub>2</sub> mP <sub>18</sub> 7 <sub>6</sub> a <sub>3</sub> a	36
3. $\epsilon$ -WO <sub>3</sub> : A3B <sub>3</sub> mP <sub>16</sub> 7 <sub>6</sub> a <sub>2</sub> a	38
4. Rh <sub>2</sub> Ga <sub>9</sub> : A9B <sub>2</sub> mP <sub>22</sub> 7 <sub>9</sub> a <sub>2</sub> a	40
$Cc$ (9)	
1. $\alpha$ -P <sub>3</sub> N <sub>5</sub> : A5B <sub>3</sub> mC <sub>32</sub> 9 <sub>5</sub> a <sub>3</sub> a	42
2. H <sub>3</sub> Cl: AB <sub>3</sub> mC <sub>16</sub> 9 <sub>3</sub> a	44
$P2/m$ (10)	
1. $\delta$ -PdCl <sub>2</sub> : A2B <sub>2</sub> mP <sub>6</sub> 10 <sub>mn</sub> bg	46
2. H <sub>3</sub> Cl: AB <sub>3</sub> mP <sub>16</sub> 10 <sub>mn</sub> 3m3n	48
3. Muthmannite: ABC <sub>2</sub> mP <sub>8</sub> 10 <sub>ac</sub> eh <sub>mn</sub>	50
4. LiSn: AB <sub>2</sub> mP <sub>6</sub> 10 <sub>en</sub> am	52
5. S-carbon: A <sub>2</sub> mP <sub>8</sub> 10 <sub>2m2n</sub>	54
$C2/m$ (12)	
1. Thortveitite: A7B <sub>2</sub> C <sub>2</sub> mC <sub>22</sub> 12 <sub>aij</sub> h <sub>i</sub>	56
2. M-carbon: A <sub>2</sub> mC <sub>16</sub> 12 <sub>4i</sub>	58
$P2/c$ (13)	
1. H <sub>2</sub> S: A2B <sub>2</sub> mP <sub>12</sub> 13 <sub>2g</sub> ef	60
$P2_1/c$ (14)	
1. $\gamma$ -PdCl <sub>2</sub> : A2B <sub>2</sub> mP <sub>6</sub> 14 <sub>e</sub> a	62
2. $\alpha$ -Toluene: A7B <sub>8</sub> mP <sub>120</sub> 14 <sub>14e</sub> 16e	64
$C2/c$ (15)	
1. H <sub>3</sub> Cl: AB <sub>3</sub> mC <sub>16</sub> 15 <sub>e</sub> cf	71
2. H-III: A <sub>2</sub> mC <sub>24</sub> 15 <sub>2e2f</sub>	73
$P22_2_1$ (17)	
1. $\alpha$ -Naumannite: A2B <sub>2</sub> oP <sub>12</sub> 17 <sub>abe</sub> e	75
$P2_12_12_1$ (19)	
1. H <sub>3</sub> Cl: AB <sub>3</sub> oP <sub>16</sub> 19 <sub>a</sub> 3a	77
$C222$ (21)	
1. Ta <sub>2</sub> H: AB <sub>2</sub> oC <sub>6</sub> 21 <sub>a</sub> k	79
$F222$ (22)	
1. CeRu <sub>2</sub> B <sub>2</sub> : A2BC <sub>2</sub> oF <sub>40</sub> 22 <sub>fi</sub> ad <sub>gh</sub>	81
2. FeS: AB <sub>2</sub> oF <sub>8</sub> 22 <sub>a</sub> c	83
$I222$ (23)	
1. H <sub>3</sub> S: A3B <sub>3</sub> oI <sub>32</sub> 23 <sub>ij2k</sub> k	85
2. Stannoidite: A8B <sub>2</sub> C <sub>12</sub> D <sub>2</sub> E <sub>2</sub> oI <sub>50</sub> 23 <sub>b</sub> cfk <sub>i</sub> 3k <sub>j</sub> a	87
3. NaFeS <sub>2</sub> : ABC <sub>2</sub> oI <sub>16</sub> 23 <sub>ab</sub> i <sub>k</sub>	89
4. BPS <sub>4</sub> : ABC <sub>4</sub> oI <sub>12</sub> 23 <sub>a</sub> b <sub>k</sub>	91
$I2_12_12_1$ (24)	
1. Weberite: AB <sub>7</sub> CD <sub>2</sub> oI <sub>44</sub> 24 <sub>a</sub> b <sub>3d</sub> c <sub>ac</sub>	93
$Pmc2_1$ (26)	
1. H <sub>2</sub> S*: A2B <sub>2</sub> oP <sub>12</sub> 26 <sub>abc</sub> ab	95
2. $\beta$ -SeO <sub>2</sub> *: A2B <sub>2</sub> oP <sub>12</sub> 26 <sub>abc</sub> ab	97
3. TIP <sub>5</sub> : A5B <sub>2</sub> oP <sub>24</sub> 26 <sub>3a3b2c</sub> ab	99
$Pcc2$ (27)	
1. Ca <sub>4</sub> Al <sub>6</sub> O <sub>16</sub> S: A6B <sub>4</sub> C <sub>16</sub> D <sub>2</sub> oP <sub>108</sub> 27 <sub>abcd4e</sub> 4e <sub>16e</sub> e	101
$Pca2_1$ (29)	
1. ZrO <sub>2</sub> <sup>‡</sup> : A2B <sub>2</sub> oP <sub>12</sub> 29 <sub>2a</sub> a	106
2. Pyrite <sup>‡</sup> : AB <sub>2</sub> oP <sub>12</sub> 29 <sub>a</sub> 2a	108
3. Cobaltite: ABC <sub>2</sub> oP <sub>12</sub> 29 <sub>a</sub> a	110
$Pnc2$ (30)	
1. Bi <sub>5</sub> Nb <sub>3</sub> O <sub>15</sub> : A5B <sub>3</sub> C <sub>15</sub> oP <sub>46</sub> 30 <sub>a2c</sub> bc <sub>a7c</sub>	112
2. CuBrSe <sub>3</sub> : ABC <sub>3</sub> oP <sub>20</sub> 30 <sub>2a</sub> c <sub>3c</sub>	115
$Pba2$ (32)	
1. Re <sub>2</sub> O <sub>5</sub> [SO <sub>4</sub> ] <sub>2</sub> : A13B <sub>2</sub> C <sub>2</sub> oP <sub>34</sub> 32 <sub>a6c</sub> c <sub>c</sub>	117
$Pna2_1$ (33)	

\*H<sub>2</sub>S and  $\beta$ -SeO<sub>2</sub> have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters.

<sup>‡</sup>ZrO<sub>2</sub> and Pyrite have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

1. $\kappa$ -alumina: A2B3_oP40_33_4a_6a .....	120	1. Benzene: AB_oP48_61_3c_3c .....	191
<b>Pnn2 (34)</b> .....		<b>Pnma (62)</b> .....	
1. TiAl <sub>2</sub> Br <sub>8</sub> : A2B8C_oP22_34_c_4c_a .....	123	1. Tongbaite: A2B3_oP20_62_2c_3c .....	194
2. FeSb <sub>2</sub> : AB2_oP6_34_a_c .....	125	2. Forsterite: A2B4C_oP28_62_ac_2cd_c .....	196
<b>Cmm2 (35)</b> .....		3. SrH <sub>2</sub> : A2B_oP12_62_2c_c .....	198
1. V <sub>2</sub> MoO <sub>8</sub> : AB8C2_oC22_35_a_ab3e_e .....	127	4. $\epsilon$ -NiAl <sub>3</sub> : A3B_oP16_62_cd_c .....	200
<b>Cmc2<sub>1</sub> (36)</b> .....		5. Cubanite: AB2C3_oP24_62_c_d_cd .....	202
1. HCl: AB_oC8_36_a_a .....	129	6. Molybdate: AB3_oP16_62_c_3c .....	204
<b>Ccc2 (37)</b> .....		7. Barite: AB4C_oP24_62_c_2cd_c .....	206
1. Li <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> : A2B5C2_oC36_37_d_c2d_d .....	131	8. Westerveldite: AB_oP8_62_c_c .....	208
<b>Abm2 (39)</b> .....		<b>Cmcm (63)</b> .....	
1. Ta <sub>3</sub> S <sub>2</sub> : A2B3_oC40_39_2d_2c2d .....	133	1. Rasvumite: A2BC3_oC24_63_e_c_cg .....	210
2. VPCl <sub>9</sub> : A9BC_oC44_39_3c3d_a_c .....	135	2. La <sub>43</sub> Ni <sub>17</sub> Mg <sub>5</sub> : A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h .....	212
<b>Ama2 (40)</b> .....		3. MnAl <sub>6</sub> : A6B_oC28_63_efg_c .....	218
1. K <sub>2</sub> CdPb: AB2C_oC16_40_a_2b_b .....	137	4. Post-perovskite: AB3C_oC20_63_a_cf_c .....	220
2. CeTe <sub>3</sub> : AB3_oC16_40_b_3b .....	139	5. MgSO <sub>4</sub> : AB4C_oC24_63_a_fg_c .....	222
<b>Fmm2 (42)</b> .....		6. Anhydrite: AB4C_oC24_63_c_fg_c .....	224
1. W <sub>3</sub> O <sub>10</sub> : A10B3_oF52_42_2abce_ab .....	141	<b>Cmca (64)</b> .....	
2. BN: AB_oF8_42_a_a .....	143	1. H <sub>2</sub> S: A2B_oC24_64_2f_f .....	226
<b>Iba2 (45)</b> .....		<b>Cccm (66)</b> .....	
1. MnGa <sub>2</sub> Sb <sub>2</sub> : A2BC2_oI20_45_c_b_c .....	145	1. SrAl <sub>2</sub> Se <sub>4</sub> : A2B4C_oC28_66_l_kl_a .....	228
<b>Ima2 (46)</b> .....		2. H <sub>3</sub> S: A3B_oC64_66_gi2lm_2l .....	230
1. TiFeSi: ABC_oI36_46_ac_bc_3b .....	147	3. $\beta$ -ThI <sub>3</sub> : A3B_oC64_66_kl2m_bdl .....	233
<b>Pnnn (48)</b> .....		<b>Cmma (67)</b> .....	
1. $\alpha$ -RbPr[MoO <sub>4</sub> ] <sub>2</sub> : A2B8CD_oP24_48_k_2m_d_b .....	149	1. Al <sub>2</sub> CuIr <sup>§</sup> : A2BC_oC16_67_ag_b_g .....	236
<b>Pccm (49)</b> .....		2. HoCuP <sub>2</sub> <sup>§</sup> : ABC2_oC16_67_b_g_ag .....	238
1. $\beta$ -Ta <sub>2</sub> O <sub>5</sub> : A5B2_oP14_49_dehq_ab .....	151	3. $\alpha$ -FeSe <sup>†</sup> : AB_oC8_67_a_g .....	240
2. CsPr[MoO <sub>4</sub> ] <sub>2</sub> : AB2C8D_oP24_49_g_q_2qr_e .....	153	4. $\alpha$ -PbO <sup>†</sup> : AB_oC8_67_a_g .....	242
<b>Pban (50)</b> .....		<b>Ccca (68)</b> .....	
1. La <sub>2</sub> NiO <sub>4</sub> : A2BC4_oP28_50_ij_ac_ijm .....	155	1. PdSn <sub>4</sub> : AB4_oC20_68_a_i .....	244
2. $\alpha$ -Tl <sub>2</sub> TeO <sub>3</sub> : A3BC2_oP48_50_3m_m_2m .....	157	<b>Fddd (70)</b> .....	
<b>Pnna (52)</b> .....		1. Mn <sub>2</sub> B: AB2_oF48_70_f_fg .....	246
1. GaCl <sub>2</sub> : A2B_oP24_52_2e_cd .....	160	<b>Immm (71)</b> .....	
2. Sr <sub>2</sub> Bi <sub>3</sub> : A3B2_oP20_52_de_cd .....	162	1. Ta <sub>3</sub> B <sub>4</sub> : A4B3_oI14_71_gh_cg .....	248
<b>Pmna (53)</b> .....		2. NbPS: ABC_oI12_71_h_j_g .....	250
1. TaNiTe <sub>2</sub> : ABC2_oP16_53_h_e_gh .....	164	<b>Ibca (73)</b> .....	
2. CuBrSe <sub>3</sub> : ABC3_oP20_53_e_g_hi .....	166	1. KAg[CO <sub>3</sub> ]: ABCD3_oI48_73_d_e_e_ef .....	252
<b>Pcca (54)</b> .....		<b>Imma (74)</b> .....	
1. BiGaO <sub>3</sub> : ABC3_oP20_54_e_d_cf .....	168	1. KHg <sub>2</sub> : A2B_oI12_74_h_e .....	254
<b>Pbam (55)</b> .....		2. Al <sub>4</sub> U: A4B_oI20_74_beh_e .....	256
1. GeAs <sub>2</sub> : A2B_oP24_55_2g2h_gh .....	170	<b>P4 (75)</b> .....	
2. Rh <sub>5</sub> Ge <sub>3</sub> : A3B5_oP16_55_ch_agh .....	172	1. BaCr <sub>2</sub> Ru <sub>4</sub> O <sub>12</sub> : AB2C12D4_tP76_75_2a2b_2d_12d_4d .....	258
3. R-carbon: A_oP16_55_2g2h .....	174	<b>P4<sub>1</sub> (76)</b> .....	
<b>Pnnm (58)</b> .....		1. LaRhC <sub>2</sub> : A2BC_tP16_76_2a_a_a .....	262
1. $\alpha$ -PdCl <sub>2</sub> : A2B_oP6_58_g_a .....	176		
<b>Pmmn (59)</b> .....			
1. FeOCl: ABC_oP6_59_a_b_a .....	178		
<b>Pbcn (60)</b> .....			
1. Rh <sub>2</sub> S <sub>3</sub> : A2B3_oP20_60_d_cd .....	180		
2. WO <sub>3</sub> : A3B_oP32_60_3d_d .....	182		
3. $\beta$ -Toluene: A7B8_oP120_60_7d_8d .....	185		
<b>Pbca (61)</b> .....			

<sup>§</sup>Al<sub>2</sub>CuIr and HoCuP<sub>2</sub> have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

<sup>†</sup> $\alpha$ -FeSe and  $\alpha$ -PbO have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters.

2. Cs <sub>3</sub> P <sub>7</sub> : A3B7_tP40_76_3a_7a .....	264	1. NbTe <sub>4</sub> : AB <sub>4</sub> _tP10_103_a_d .....	345
<b>P4<sub>2</sub> (77)</b> .....		<b>P4nc (104)</b> .....	
1. Pinnoite: A2B6CD7_tP64_77_2d_6d_d_ab6d .....	267	1. Ba <sub>5</sub> In <sub>4</sub> Bi <sub>5</sub> : A5B5C4_tP28_104_ac_ac_c .....	347
2. H <sub>2</sub> S III: A2B_tP48_77_8d_4d .....	270	2. Tl <sub>4</sub> HgI <sub>6</sub> : AB6C4_tP22_104_a_2ac_c .....	350
<b>P4<sub>3</sub> (78)</b> .....		<b>P4<sub>2</sub>mc (105)</b> .....	
1. Sr <sub>2</sub> As <sub>2</sub> O <sub>7</sub> : A2B7C2_tP88_78_4a_14a_4a .....	273	1. BaGe <sub>2</sub> As <sub>2</sub> : A2BC2_tP20_105_f_ac_2e .....	352
<b>I4 (79)</b> .....		<b>P4<sub>2</sub>bc (106)</b> .....	
1. TlZn <sub>2</sub> Sb <sub>2</sub> : A2BC2_tI20_79_c_2a_c .....	277	1. NaZn[OH] <sub>3</sub> : A3BC3D_tP64_106_3c_c_3c_c .....	354
<b>I4<sub>1</sub> (80)</b> .....		<b>I4mm (107)</b> .....	
1. β-NbO <sub>2</sub> : AB <sub>2</sub> _tI48_80_2b_4b .....	279	1. Co <sub>5</sub> Ge <sub>7</sub> : A5B7_tI24_107_ac_abd .....	358
<b>P<math>\bar{4}</math> (81)</b> .....		2. GeP: AB_tI4_107_a_a .....	360
1. GeSe <sub>2</sub> : AB <sub>2</sub> _tP12_81_adg_2h .....	282	<b>I4cm (108)</b> .....	
<b>I<math>\bar{4}</math> (82)</b> .....		1. Sr <sub>5</sub> Si <sub>3</sub> : A3B5_tI32_108_ac_a2c .....	362
1. Ni <sub>3</sub> P: A3B_tI32_82_3g_g .....	284	<b>I4<sub>1</sub>md (109)</b> .....	
<b>P4/m (83)</b> .....		1. LaPtSi: ABC_tI12_109_a_a_a .....	364
1. Ti <sub>2</sub> Ge <sub>3</sub> : A3B2_tP10_83_adk_j .....	286	2. NbAs: AB_tI8_109_a_a .....	366
<b>P4/n (85)</b> .....		<b>I4<sub>1</sub>cd (110)</b> .....	
1. SrBr <sub>2</sub> : A2B_tP30_85_ab2g_cg .....	288	1. Be[BH <sub>4</sub> ] <sub>2</sub> : A2BC8_tI176_110_2b_b_8b .....	368
<b>P4<sub>2</sub>/n (86)</b> .....		<b>P<math>\bar{4}</math>2m (111)</b> .....	
1. Ti <sub>3</sub> P: AB <sub>3</sub> _tP32_86_g_3g .....	291	1. MnF <sub>2</sub> : A2B_tP12_111_2n_adf .....	374
<b>I4<sub>1</sub>/a (88)</b> .....		2. NV: AB_tP8_111_n_n .....	376
1. ThCl <sub>4</sub> : A4B_tI20_88_f_a .....	294	<b>P<math>\bar{4}</math>2c (112)</b> .....	
2. α-NbO <sub>2</sub> : AB <sub>2</sub> _tI96_88_2f_4f .....	296	1. α-CuAlCl <sub>4</sub> : AB4C_tP12_112_b_n_e .....	378
<b>P422 (89)</b> .....		<b>P<math>\bar{4}</math>2<sub>1</sub>m (113)</b> .....	
1. C <sub>17</sub> FeO <sub>4</sub> Pt: A17BC4D_tP184_89_17p_p_4p_io .....	300	1. Akermanite: A2BC7D2_tP24_113_e_a_cef_e .....	380
<b>P42<sub>1</sub>2 (90)</b> .....		<b>P<math>\bar{4}</math>2<sub>1</sub>c (114)</b> .....	
1. Na <sub>4</sub> Ti <sub>2</sub> Si <sub>8</sub> O <sub>22</sub> [H <sub>2</sub> O] <sub>4</sub> : A4B2C13D_tP40_90_g_d_cef2g_c .....	307	1. SeO <sub>3</sub> : A3B_tP32_114_3e_e .....	382
2. BaCu <sub>4</sub> [VO][PO <sub>4</sub> ] <sub>4</sub> : AB4C17D4E_tP54_90_a_g_c4g_g_c .....	310	2. Pd <sub>4</sub> Se: A4B_tP10_114_e_a .....	385
<b>P4<sub>1</sub>22 (91)</b> .....		<b>P<math>\bar{4}</math>m2 (115)</b> .....	
1. ThBC: ABC_tP24_91_d_d_d .....	313	1. Rh <sub>3</sub> P <sub>2</sub> : A2B3_tP5_115_g_ag .....	387
<b>P4<sub>2</sub>22 (93)</b> .....		2. HgI <sub>2</sub> : AB <sub>2</sub> _tP12_115_j_egi .....	389
1. AsPh <sub>4</sub> CeS <sub>8</sub> P <sub>4</sub> Me <sub>8</sub> : AB32CD4E8_tP184_93_i_16p_af_2p_4p .....	315	<b>P<math>\bar{4}</math>c2 (116)</b> .....	
<b>P4<sub>2</sub>2<sub>1</sub>2 (94)</b> .....		1. Ru <sub>2</sub> Sn <sub>3</sub> : A2B3_tP20_116_bci_fj .....	391
1. Na <sub>5</sub> Fe <sub>3</sub> F <sub>14</sub> : A14B3C5_tP44_94_c3g_ad_bg .....	322	<b>P<math>\bar{4}</math>b2 (117)</b> .....	
2. Li <sub>2</sub> MoF <sub>6</sub> : A6B2C_tP18_94_eg_c_a .....	325	1. β-Bi <sub>2</sub> O <sub>3</sub> : A2B3_tP20_117_i_adgh .....	393
<b>P4<sub>3</sub>22 (95)</b> .....		<b>P<math>\bar{4}</math>n2 (118)</b> .....	
1. ThBC: ABC_tP24_95_d_d_d .....	327	1. RuIn <sub>3</sub> : A3B_tP16_118_ei_f .....	395
<b>I422 (97)</b> .....		2. Ir <sub>3</sub> Ga <sub>5</sub> : A5B3_tP32_118_g2i_aceh .....	397
1. NaGdCu <sub>2</sub> F <sub>8</sub> : A2B8CD_tI24_97_d_k_a_b .....	329	<b>I<math>\bar{4}</math>m2 (119)</b> .....	
2. Ta <sub>2</sub> Se <sub>8</sub> I: AB8C2_tI44_97_e_2k_cd .....	331	1. RbGa <sub>3</sub> : A3B_tI24_119_b2i_af .....	400
<b>I4<sub>1</sub>22 (98)</b> .....		2. GaSb: AB_tI4_119_c_a .....	402
1. CdAs <sub>2</sub> : A2B_tI12_98_f_a .....	333	<b>I<math>\bar{4}</math>c2 (120)</b> .....	
<b>P4bm (100)</b> .....		1. KAu <sub>4</sub> Sn <sub>2</sub> : A4BC2_tI28_120_i_d_e .....	404
1. Fresnoite: A2B8C2D_tP26_100_c_abcd_c_a .....	335	<b>P4/mmm (123)</b> .....	
2. Ce <sub>3</sub> Si <sub>6</sub> N <sub>11</sub> : A3B11C6_tP40_100_ac_bc2d_cd .....	337	1. CaRbFe <sub>4</sub> As <sub>4</sub> : A4BC4D_tP10_123_gh_a_i_d .....	406
<b>P4<sub>2</sub>cm (101)</b> .....		<b>P4/mcc (124)</b> .....	
1. γ-MgNiSn: A7B7C2_tP32_101_bde_ade_d .....	340	1. Nb <sub>4</sub> CoSi: AB4C_tP12_124_a_m_c .....	408
<b>P4<sub>2</sub>nm (102)</b> .....		2. NbTe <sub>4</sub> : AB <sub>4</sub> _tP10_124_a_m .....	410
1. Gd <sub>3</sub> Al <sub>2</sub> : A2B3_tP20_102_2c_b2c .....	343	<b>P4/nbm (125)</b> .....	
<b>P4cc (103)</b> .....		1. PtPb <sub>4</sub> : A4B_tP10_125_m_a .....	412
		2. KCeSe <sub>4</sub> : ABC4_tP12_125_a_b_m .....	414
		<b>P4/nnc (126)</b> .....	

1. BiAl <sub>2</sub> S <sub>4</sub> : A2BC <sub>4</sub> _tP28_126_cd_e_k .....	416	2. $\beta$ -PdCl <sub>2</sub> : A2B_hr18_148_2f_f .....	483
<b>P4/mbm (127)</b> .....		<b>P312 (149)</b> .....	
1. ThB <sub>4</sub> : A4B_tP20_127_ehj_g .....	418	1. Ti <sub>3</sub> O: AB <sub>3</sub> _hP24_149_acgi_3l .....	486
<b>P4/mnc (128)</b> .....		<b>P3<sub>2</sub>12 (153)</b> .....	
1. K <sub>2</sub> SnCl <sub>6</sub> : A6B2C_tP18_128_eh_d_b .....	420	1. CrCl <sub>3</sub> : A3B_hP24_153_3c_2b .....	488
2. FeCu <sub>2</sub> Al <sub>7</sub> : A7B2C_tP40_128_egi_h_e .....	422	<b>P3<sub>2</sub>21 (154)</b> .....	
<b>P4/ncc (130)</b> .....		1. S-II: A_hP9_154_bc .....	491
1. CuBi <sub>2</sub> O <sub>4</sub> : A2BC <sub>4</sub> _tP28_130_f_c_g .....	425	<b>P3m1 (156)</b> .....	
2. Ba <sub>5</sub> Si <sub>3</sub> : A5B3_tP32_130_cg_cf .....	427	1. CdI <sub>2</sub> : AB <sub>2</sub> _hP9_156_b2c_3a2bc .....	493
<b>P4<sub>2</sub>/mcm (132)</b> .....		2. CuI: AB_hP12_156_2ab3c_2ab3c .....	495
1. Rb <sub>2</sub> TiCu <sub>2</sub> S <sub>4</sub> : A2B2C4D_tP18_132_e_i_o_d .....	429	3. $\beta$ -CuI: AB_hP4_156_ac_ac .....	497
2. AgUF <sub>6</sub> : AB6C_tP16_132_d_io_a .....	431	<b>P31m (157)</b> .....	
<b>P4<sub>2</sub>/nbc (133)</b> .....		1. Ag <sub>5</sub> Pb <sub>2</sub> O <sub>6</sub> : A5B6C <sub>2</sub> _hP13_157_2ac_2c_b .....	499
1. $\beta$ -V <sub>3</sub> S: AB <sub>3</sub> _tP32_133_h_i2j .....	433	<b>P3c1 (158)</b> .....	
<b>P4<sub>2</sub>/mbc (135)</b> .....		1. $\beta$ -RuCl <sub>3</sub> : A3B_hP8_158_d_a .....	501
1. Downeyite: A2B_tP24_135_gh_h .....	436	<b>P31c (159)</b> .....	
2. ZnSb <sub>2</sub> O <sub>4</sub> : A4B2C_tP28_135_gh_h_d .....	438	1. Bi <sub>2</sub> O <sub>3</sub> : A2B <sub>3</sub> _hP20_159_bc_2c .....	503
<b>P4<sub>2</sub>/nmc (137)</b> .....		2. Nierite: A4B <sub>3</sub> _hP28_159_ab2c_2c .....	506
1. Zn <sub>3</sub> P <sub>2</sub> : A2B <sub>3</sub> _tP40_137_cdf_3g .....	440	3. YbBaCo <sub>4</sub> O <sub>7</sub> : AB4C7D_hP26_159_b_ac_a2c_b .....	509
2. ZrO <sub>2</sub> <sup>‡</sup> : A2B_tP6_137_d_a .....	443	<b>R3m (160)</b> .....	
3. CeCo <sub>4</sub> B <sub>4</sub> : A4BC <sub>4</sub> _tP18_137_g_b_g .....	445	1. H <sub>3</sub> S: A3B_hr4_160_b_a .....	512
4. HgI <sub>2</sub> <sup>‡</sup> : AB <sub>2</sub> _tP6_137_a_d .....	447	2. Al <sub>8</sub> Cr <sub>5</sub> : A8B <sub>5</sub> _hR26_160_a3bc_a3b .....	514
<b>P4<sub>2</sub>/ncm (138)</b> .....		3. Carbonyl Sulphide: ABC_hr3_160_a_a_a .....	517
1. C: A_tP12_138_bi .....	449	4. Moissanite-15R: AB_hr10_160_5a_5a .....	519
<b>I4/mmm (139)</b> .....		<b>P<math>\bar{3}</math>m1 (164)</b> .....	
1. Calomel: AB_tI8_139_e_e .....	451	1. La <sub>2</sub> O <sub>3</sub> : A2B <sub>3</sub> _hP5_164_d_ad .....	521
<b>I4/mcm (140)</b> .....		2. $\delta^I_H$ -NW <sub>2</sub> : AB <sub>2</sub> _hP9_164_bd_c2d .....	523
1. W <sub>5</sub> Si <sub>3</sub> : A3B <sub>5</sub> _tI32_140_ah_bk .....	453	3. CuNiSb <sub>2</sub> : ABC <sub>2</sub> _hP4_164_a_b_d .....	525
2. Cr <sub>5</sub> B <sub>3</sub> : A3B <sub>5</sub> _tI32_140_ah_cl .....	455	<b>P<math>\bar{3}</math>c1 (165)</b> .....	
<b>I4<sub>1</sub>/amd (141)</b> .....		1. Cu <sub>3</sub> P: A3B_hP24_165_bdg_f .....	527
1. $\alpha$ -ThSi <sub>2</sub> : A2B_tI12_141_e_a .....	457	<b>R<math>\bar{3}</math>m (166)</b> .....	
<b>I4<sub>1</sub>/acd (142)</b> .....		1. Al <sub>4</sub> C <sub>3</sub> : A4B <sub>3</sub> _hR7_166_2c_ac .....	530
1. S-III: A_tI16_142_f .....	459	2. SmSI: ABC_hr6_166_c_c_c .....	532
<b>P3 (143)</b> .....		<b>R<math>\bar{3}</math>c (167)</b> .....	
1. Simpsonite: A4B14C <sub>3</sub> _hP21_143_bd_ac4d_d .....	461	1. PrNiO <sub>3</sub> : AB3C_hr10_167_b_e_a .....	534
2. ScRh <sub>6</sub> P <sub>4</sub> : A4B6C_hP11_143_bd_2d_a .....	463	2. KBO <sub>2</sub> : ABC <sub>2</sub> _hR24_167_e_e_2e .....	536
3. MoS <sub>2</sub> : AB <sub>2</sub> _hP12_143_cd_ab2d .....	465	<b>P6 (168)</b> .....	
<b>P3<sub>1</sub> (144)</b> .....		1. K <sub>2</sub> Ta <sub>4</sub> O <sub>9</sub> F <sub>4</sub> : A2B13C <sub>4</sub> _hP57_168_d_c6d_2d .....	539
1. IrGe <sub>4</sub> : A4B_hP15_144_4a_a .....	467	2. Al[PO <sub>4</sub> ]: AB4C_hP72_168_2d_8d_2d .....	543
2. TeZn: AB_hP6_144_a_a .....	469	<b>P6<sub>1</sub> (169)</b> .....	
<b>P3<sub>2</sub> (145)</b> .....		1. $\alpha$ -Al <sub>2</sub> S <sub>3</sub> : A2B <sub>3</sub> _hP30_169_2a_3a .....	547
1. Sheldrickite: A2B3C3DE7_hP48_145_2a_3a_3a_a_7a .....	471	<b>P6<sub>5</sub> (170)</b> .....	
<b>R3 (146)</b> .....		1. Al <sub>2</sub> S <sub>3</sub> : A2B <sub>3</sub> _hP30_170_2a_3a .....	550
1. $\gamma$ -Ag <sub>3</sub> SI: A3BC_hr5_146_b_a_a .....	475	<b>P6<sub>2</sub> (171)</b> .....	
2. FePSe <sub>3</sub> : ABC <sub>3</sub> _hR10_146_2a_2a_2b .....	477	1. Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub> : A10B2C_hP39_171_5c_c_a .....	553
<b>R<math>\bar{3}</math> (148)</b> .....		<b>P6<sub>4</sub> (172)</b> .....	
1. Phenakite: A2B4C_hr42_148_2f_4f_f .....	479	1. Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub> : A10B2C_hP39_172_5c_c_a .....	557
		<b>P6<sub>3</sub> (173)</b> .....	
		1. PI <sub>3</sub> : A3B_hP8_173_c_b .....	560
		2. $\beta$ -Si <sub>3</sub> N <sub>4</sub> : A4B <sub>3</sub> _hP14_173_bc_c .....	562
		<b>P<math>\bar{6}</math> (174)</b> .....	
		1. Fe <sub>12</sub> Zr <sub>2</sub> P <sub>7</sub> : A12B7C <sub>2</sub> _hP21_174_2j2k_ajk_cf .....	564

<sup>‡</sup>ZrO<sub>2</sub> and HgI<sub>2</sub> have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

2. GdSI: ABC_hP12_174_cj_fk_aj .....	566	1. Mavlyanovite: A5B3_hP16_193_dg_g .....	639
<b>P6/m (175)</b> .....		<b>P6<sub>3</sub>/mmc (194)</b> .....	
1. Nb <sub>7</sub> Ru <sub>6</sub> B <sub>8</sub> : A8B7C6_hP21_175_ck_aj_k .....	568	1. Ni <sub>3</sub> Ti: A3B_hP16_194_gh_ac .....	641
2. Mg[NH]: ABC_hP36_175_jk_jk_jk .....	570	2. Co <sub>2</sub> Al <sub>5</sub> : A5B2_hP28_194_ahk_ch .....	643
<b>P6<sub>3</sub>/m (176)</b> .....		3. Al <sub>9</sub> Mn <sub>3</sub> Si: A9B3C_hP26_194_hk_h_a .....	646
1. Er <sub>3</sub> Ru <sub>2</sub> : A3B2_hP10_176_h_bd .....	573	<b>P23 (195)</b> .....	
2. Fe <sub>3</sub> Te <sub>3</sub> Tl: A3B3C_hP14_176_h_h_d .....	575	1. PrRu <sub>4</sub> P <sub>12</sub> : A12BC <sub>4</sub> _cP34_195_2j_ab_2e .....	649
3. UCl <sub>3</sub> : A3B_hP8_176_h_d .....	577	<b>F23 (196)</b> .....	
<b>P622 (177)</b> .....		1. Cu <sub>2</sub> Fe[CN] <sub>6</sub> : A12B2C_cF60_196_h_bc_a .....	652
1. SiO <sub>2</sub> : A2B_hP36_177_j2lm_n .....	579	2. MgB <sub>12</sub> H <sub>12</sub> [H <sub>2</sub> O] <sub>12</sub> : A12B36CD <sub>12</sub> _cF488_196_2h_6h_ac_fgh .....	654
<b>P6<sub>1</sub>22 (178)</b> .....		<b>P2<sub>1</sub>3 (198)</b> .....	
1. AuF <sub>3</sub> : AB3_hP24_178_b_ac .....	582	1. Sodium Chlorate: ABC <sub>3</sub> _cP20_198_a_a_b .....	661
2. Sc-V: A_hP6_178_a .....	584	<b>Pm<math>\bar{3}</math> (200)</b> .....	
<b>P6<sub>5</sub>22 (179)</b> .....		1. Mg <sub>2</sub> Zn <sub>11</sub> : A2B <sub>11</sub> _cP39_200_f_ghij .....	663
1. AuF <sub>3</sub> : AB3_hP24_179_b_ac .....	586	<b>Pn<math>\bar{3}</math> (201)</b> .....	
<b>P6<sub>4</sub>22 (181)</b> .....		1. KSbO <sub>3</sub> : AB3C_cP60_201_ce_fh_g .....	666
1. $\beta$ -SiO <sub>2</sub> : A2B_hP9_181_j_c .....	588	<b>Fm<math>\bar{3}</math> (202)</b> .....	
<b>P6mm (183)</b> .....		1. KB <sub>6</sub> H <sub>6</sub> : A6B6C_cF104_202_h_h_c .....	669
1. AuCN: ABC_hP3_183_a_a_a .....	590	2. FCC C <sub>60</sub> Buckminsterfullerine: A_cF240_202_h2i .....	671
2. CrFe <sub>3</sub> NiSn <sub>5</sub> : AB_hP6_183_c_ab .....	592	<b>Fd<math>\bar{3}</math> (203)</b> .....	
<b>P6cc (184)</b> .....		1. Pyrochlore: A2BCD3E6_cF208_203_e_c_d_f_g ...	675
1. Al[PO <sub>4</sub> ]: AB4C_hP72_184_d_4d_d .....	594	2. Tychite: A4B2C6D16E_cF232_203_e_d_f_eg_a ...	679
<b>P6<sub>3</sub>cm (185)</b> .....		3. Rb <sub>3</sub> AsSe <sub>16</sub> : AB3C16_cF160_203_b_ad_eg .....	683
1. KNiCl <sub>3</sub> : A3BC_hP30_185_cd_c_ab .....	599	<b>Pa<math>\bar{3}</math> (205)</b> .....	
2. Cu <sub>3</sub> P <sup>  </sup> : A3B_hP24_185_ab2c_c .....	602	1. Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> : A2B3C6_cP264_205_2d_ab2c2d_6d ...	687
3. $\beta$ -RuCl <sub>3</sub> : A3B_hP8_185_c_a .....	605	2. Simple Cubic C <sub>60</sub> Buckminsterfullerine: A_cP240_205_10d .....	696
4. Na <sub>3</sub> As <sup>  </sup> : AB3_hP24_185_c_ab2c .....	607	<b>Ia<math>\bar{3}</math> (206)</b> .....	
<b>P6<sub>3</sub>mc (186)</b> .....		1. AlLi <sub>3</sub> N <sub>2</sub> : AB3C2_cI96_206_c_e_ad .....	704
1. Fe <sub>3</sub> Th <sub>7</sub> : A3B7_hP20_186_c_b2c .....	610	<b>P432 (207)</b> .....	
<b>P<math>\bar{6}m2</math> (187)</b> .....		1. Pd <sub>17</sub> Se <sub>15</sub> : A17B15_cP64_207_acfk_eij .....	707
1. Re <sub>3</sub> N: AB3_hP4_187_e_fh .....	612	<b>P4<sub>2</sub>32 (208)</b> .....	
<b>P<math>\bar{6}c2</math> (188)</b> .....		1. PH <sub>3</sub> : A3B_cP16_208_j_b .....	710
1. LiScI <sub>3</sub> : A3BC_hP10_188_k_a_e .....	614	2. Cs <sub>2</sub> ZnFe[CN] <sub>6</sub> : A6B2CD6E_cP64_208_m_ad_b_m_c .....	712
2. BaSi <sub>4</sub> O <sub>9</sub> : AB9C4_hP28_188_e_kl_ak .....	616	<b>F432 (209)</b> .....	
<b>P<math>\bar{6}2m</math> (189)</b> .....		1. F <sub>6</sub> KP: A24BC_cF104_209_j_a_b .....	716
1. $\pi$ -FeMg <sub>3</sub> Al <sub>8</sub> Si <sub>6</sub> : A8BC3D6_hP18_189_bfh_a_g_i .....	619	<b>F4<sub>1</sub>32 (210)</b> .....	
2. $\pi$ -FeMg <sub>3</sub> Al <sub>9</sub> Si <sub>5</sub> : A9BC3D5_hP18_189_fi_a_g_bh .....	622	1. Te[OH] <sub>6</sub> : A12B6C_cF608_210_4h_2h_e .....	719
<b>P<math>\bar{6}2c</math> (190)</b> .....		<b>I432 (211)</b> .....	
1. Li <sub>2</sub> Sb: A2B_hP18_190_gh_bf .....	624	1. SiO <sub>2</sub> : A2B_cI72_211_hi_i .....	731
2. $\alpha$ -Sm <sub>3</sub> Ge <sub>5</sub> : A5B3_hP16_190_bdh_g .....	626	<b>P4<sub>3</sub>32 (212)</b> .....	
3. Troilite: AB_hP24_190_i_afh .....	628	1. SrSi <sub>2</sub> : A2B_cP12_212_c_a .....	734
<b>P6/mcc (192)</b> .....		<b>I4<sub>1</sub>32 (214)</b> .....	
1. Beryl: A2B3C18D6_hP58_192_c_f_lm_l .....	631	1. Ca <sub>3</sub> PI <sub>3</sub> : A3B3C_cI56_214_g_h_a .....	736
2. AlPO <sub>4</sub> : AB2_hP72_192_m_j2kl .....	635	2. Petzite: A3BC2_cI48_214_f_a_e .....	739
<b>P6<sub>3</sub>/mcm (193)</b> .....		<b>P<math>\bar{4}3m</math> (215)</b> .....	
		1. $\gamma$ -brass: A4B9_cP52_215_ei_3efgi .....	741
		<b>F<math>\bar{4}3m</math> (216)</b> .....	

<sup>||</sup>Cu<sub>3</sub>P and Na<sub>3</sub>As have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

1. Quaternary Heusler: ABCD_cF16_216_c_d_b_a .....	745
<b><math>P\bar{4}3n</math> (218)</b> .....	
1. Ag <sub>3</sub> [PO <sub>4</sub> ]: A3B4C_cP16_218_c_e_a .....	747
<b><math>F\bar{4}3c</math> (219)</b> .....	
1. Boracite: A7BC3D13_cF192_219_de_b_c_ah .....	749
<b><math>I\bar{4}3d</math> (220)</b> .....	
1. Cu <sub>15</sub> Si <sub>4</sub> : A15B4_cI76_220_ae_c .....	753
2. Th <sub>3</sub> P <sub>4</sub> : A4B3_cI28_220_c_a .....	756
<b><math>Pm\bar{3}m</math> (221)</b> .....	
1. Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> : A2B3C6_cP33_221_cd_ag_fh .....	758
<b><math>Pn\bar{3}n</math> (222)</b> .....	
1. Ce <sub>5</sub> Mo <sub>3</sub> O <sub>16</sub> : A5B3C16_cP96_222_ce_d_fi .....	761
<b><math>Fm\bar{3}m</math> (225)</b> .....	
1. Th <sub>6</sub> Mn <sub>23</sub> : A23B6_cF116_225_bd2f_e .....	766
2. K <sub>2</sub> PtCl <sub>6</sub> : A6B2C_cF36_225_e_c_a .....	769
<b><math>Fm\bar{3}c</math> (226)</b> .....	
1. NaZn <sub>13</sub> : AB13_cF112_226_a_bi .....	771
<b><math>Fd\bar{3}m</math> (227)</b> .....	
1. Pyrochlore Iridate: A2B2C7_cF88_227_c_d_af .....	774
2. Spinel: A3B4_cF56_227_ad_e .....	776
<b><math>Fd\bar{3}c</math> (228)</b> .....	
1. CuCrCl <sub>5</sub> [NH <sub>3</sub> ] <sub>6</sub> : A5BCD6_cF416_228_eg_c_b_h ..	778
2. TeO <sub>6</sub> H <sub>6</sub> : A6B_cF224_228_h_c .....	785
<b><math>Im\bar{3}m</math> (229)</b> .....	
1. $\gamma$ -brass: A3B10_cI52_229_e_fh .....	790
2. $\beta$ -Hg <sub>4</sub> Pt: A4B_cI10_229_c_a .....	793
3. Ir <sub>3</sub> Ge <sub>7</sub> : A7B3_cI40_229_df_e .....	795
<b><math>Ia\bar{3}d</math> (230)</b> .....	
1. Garnet: A2B3C12D3_cI160_230_a_c_h_d .....	797
<b>Index</b>	
1. Prototype Index .....	988
2. Pearson Symbol Index .....	991
3. Strukturbericht Designation Index .....	996
4. Duplicate AFLOW Label .....	1000
5. Similar AFLOW Label .....	1000
6. CIF Index .....	1000
7. POSCAR Index .....	1004

## 1. Introduction

The advent of high-throughput computing has paved the way for efficient and rapid exploration of materials space. Exploiting such computational frameworks has facilitated the predictions of novel materials, including metallic glasses [1], high-entropy oxides [2], candidate photovoltaic absorbers [3], rechargeable battery materials [4], and magnetic Heuslers [5]. Equipped with automated symmetry [6], mechanical [7, 8], and thermal analyses [9, 10, 11], a panoply of material properties can be readily calculated and stored in material-property repositories — such as AFLOW [12, 13, 14, 15, 16, 17, 18], *Novel Materials Discovery* (NoMaD) [19], *Materials Project* [20], and the *Open Quantum Materials Database* (OQMD) [21]. Creating new materials in these computational databases generally entails decorating structural prototypes with various atomic species. To increase the likelihood of synthesizing the conjectured materials, it is advisable to explore previously studied/observed crystal structures as the basis for developing prototype structures.

A variety of resources, such as the *Strukturbericht* series [22], *The Structure of Crystals* [23], *Pearson's Handbook* [24], and *The American Mineralogist Crystal Database* [25], have cataloged crystal structures over the past century (for a succinct historical recount of crystal structure information, see Ref. [17]). These collections are invaluable for finding crystals of certain symmetries, compositions, *Strukturbericht* designations, and other structural classifications. Furthermore, they are prime sources for structural prototypes in computational frameworks. However, until recently, much of the data was not easily accessible to the computational materials science community, hindering automatic generation of these prototypes.

A combined effort involving the U.S. Naval Research Laboratory's *Crystal Lattice Structures* web page and the AFLOW consortium yielded the construction of a new online crystal structure database: *The AFLOW Library of Crystallographic Prototypes*. The library is the result of a synergistic effort to gather crystal structure prototypes from literature and integrate them into the AFLOW computational framework for automatic generation. The first stage of this venture, Part 1, introduces 288 crystallographic prototypes from 92 different space groups [17]. Each prototype entry contains its symmetry descriptions, lattice and atomic basis vector equations, elements/compounds exhibiting the structure, and citations to the original references. With the AFLOW software, geometry files of the structure can be created in common *ab-initio* code formats, *i.e.*, VASP [26, 27, 28, 29], QUANTUM ESPRESSO [30], FHI-AIMS [31], and ABINIT [32]. Additionally, the infrastructure allows users to tune the internal degree(s) of freedom (lattice and Wyckoff parameters) and alter the atomic species of the structure, providing a robust crystal prototyping tool. The content associated with each prototype entry

is detailed in Part 1 [17].

The prototype information is also available online at the following URL: <http://www.aflow.org/CrystalDatabase>. Along with the structural information listed in the article, the website features additional functionality. An interactive Jmol applet is shown on each prototype entry page, allowing multiple viewing perspectives and differing cell representations (conventional, primitive, supercell, and Wigner-Seitz). Each page is also accompanied by a prototype generator that interfaces with the AFLOW software.

This article presents the continued work and second installment of the AFLOW Library of Crystallographic Prototypes. In Part 2, the crystallographic library is extended by 302 structure prototypes with representatives from the remaining 138 space groups not included in Part 1. The online version of the library contains all of the prototypes from Part 1 and Part 2.

The outline of this article is as follows: Section 2 highlights the enantiomorphic space groups. Section 3 discusses the Wigner-Seitz cell and showcases the Jmol functionality. Section 4 introduces the two-dimensional plane groups (or “wallpaper” groups). Section 5 describes the different space group symbols, including the Hermann-Mauguin, Hall, International, and Schönflies notations, along with the origin/setting choices used throughout the library.

## 2. Enantiomorphic Space Groups

If we look at space group  $P4_1$  (#76), we see that it has one Wyckoff position (4a), with operations [33]

$$(x, y, z) \left( -x, -y, z + \frac{1}{2} \right) \left( -y, x, z + \frac{1}{4} \right) \left( y, -x, z + \frac{3}{4} \right).$$

If we then look at space group  $P4_3$  (#78), we find it also has one (4a) Wyckoff position, with operations

$$(x, y, z) \left( -x, -y, z + \frac{1}{2} \right) \left( -y, x, z + \frac{3}{4} \right) \left( y, -x, z + \frac{1}{4} \right),$$

where the only difference is that the  $1/4$  and  $3/4$  fractions have swapped positions. We can easily show that space group #78 is a mirror reflection of #76 in the  $z = 0$  plane.

To see this more clearly, consider the  $Cs_3P_7$  structure (A3B7\_tP40\_76\_3a\_7a<sup>1</sup>). This structure was found in space group #76, but if we reflect all of the coordinates through the  $z = 0$  plane, it transforms into a structure in space group #78, as shown in the Jmol [34] rendering in Figure 1.

The distance between any pair of atoms is the same in the  $P4_3$  structure as it is in the  $P4_1$  structure, and the angle between any three atoms is the same in both structures. It

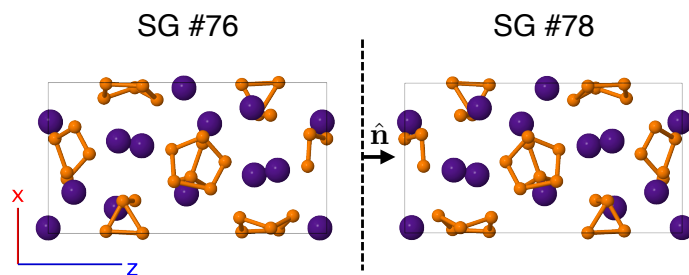


Figure 1: **Illustration of enantiomorphic structures.**  $Cs_3P_7$  in space group  $P4_1$  (#76) (left), and reflected through the  $z = 0$  plane into space group  $P4_3$  (#78) (right). The positive  $z$  direction is to the right in both figures, with the mirror plane perpendicular to the page. The figures were produced by Jmol [34].

follows that the structures are degenerate, there is no difference in energy between them, and they should be equally likely to form.

Any structure in space group  $P4_1$  can be transformed into  $P4_3$  by this method. Pairs of space groups which allow these transformations are said to be enantiomorphic [35, 36], or chiral.<sup>2</sup>

There are eleven pairs of enantiomorphic space groups [35, 36]:

- $P4_1$  (#76) and  $P4_3$  (#78),
- $P4_122$  (#91) and  $P4_322$  (#95),
- $P4_12_12$  (#92) and  $P4_32_12$  (#96),
- $P3_1$  (#144) and  $P3_2$  (#145),
- $P3_112$  (#151) and  $P3_212$  (#153),
- $P3_121$  (#152) and  $P3_221$  (#154),
- $P6_1$  (#169) and  $P6_5$  (#170),
- $P6_2$  (#171) and  $P6_4$  (#172),
- $P6_122$  (#178) and  $P6_522$  (#179),
- $P6_222$  (#180) and  $P6_422$  (#181), and
- $P4_132$  (#213) and  $P4_332$  (#212).

In addition, forty-three other space groups allow chiral crystal structures. The complete set of sixty-five space groups are known as the Sohncke groups [35].

<sup>2</sup>Formally, any object has *chirality* if it is not superposable on its mirror image [35]. Chirality is a fundamental aspect of life on Earth. All amino acids found in living organisms are left-handed [37].

<sup>1</sup>This structure can be found in the Library of Crystallographic Prototypes at [http://aflow.org/CrystalDatabase/A3B7\\_tP40\\_76\\_3a\\_7a.html](http://aflow.org/CrystalDatabase/A3B7_tP40_76_3a_7a.html).



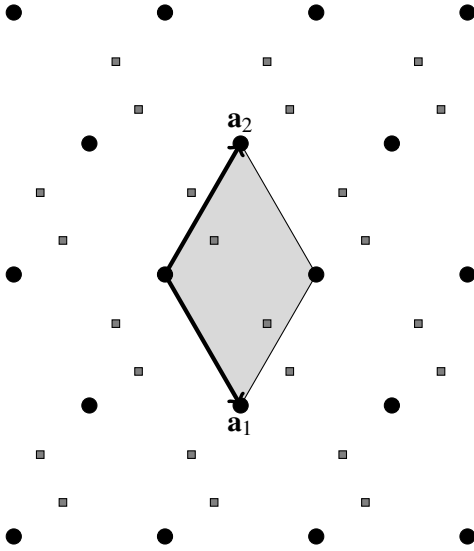


Figure 2: **A two-dimensional hexagonal lattice with basis.** The black circles show the positions of the lattice vectors,  $N_1 \mathbf{a}_1 + N_2 \mathbf{a}_2$ , where  $N_1$  and  $N_2$  are integers and  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are given by Equation (2). The gray squares are a two-site basis for this lattice.

### 3. The Wigner-Seitz Primitive Cell

Given a lattice described by a set of primitive lattice vectors,  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , and  $\mathbf{a}_3$ , we can define a *unit cell* as a volume which, when translated through every vector of the form  $N_1 \mathbf{a}_1 + N_2 \mathbf{a}_2 + N_3 \mathbf{a}_3$ , completely fills space without overlap. Even if we require that this cell have the minimum volume,

$$V = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3), \quad (1)$$

this is not a unique definition, and in fact there are an infinite number of choices for the primitive vectors.

As an example, consider the two-dimensional hexagonal lattice with primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}}. \end{aligned} \quad (2)$$

We show this lattice in Figure 2, along with a two-site basis (the gray squares). Perhaps the simplest unit cell we can construct here is a parallelogram, as seen in Figure 2. This is a unit cell, as it has the area of the primitive cell,

$$A = \frac{\sqrt{3}}{2} a^2, \quad (3)$$

each of its replicas contains two basis points, and the cell with its replicas tile the space.

The choice of unit cell is not unique. Consider, for example, an equivalent set of primitive vectors,

$$\begin{aligned} \mathbf{a}'_1 &= \frac{3}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}'_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}}, \end{aligned} \quad (4)$$

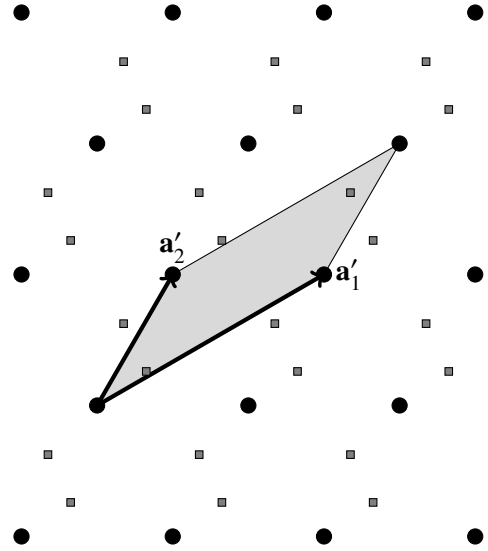


Figure 3: **A two-dimensional hexagonal lattice with non-standard primitive vectors.** This is the same hexagonal lattice from Figure 2 with primitive vectors given by Equation (4). Each unit cell still contains images of the two sites in the basis.

and the accompanying unit cell shown in Figure 3. This choice of unit cell has the proper area given by Equation (3), contains both basis points, and tiles the space. Both Figures 2 and 3 describe the same lattice plus basis, and so are both unit cells for the lattice.

Though not required, it is frequently useful to have a primitive cell which is uniquely defined and exhibits the symmetry of the lattice. Such a cell, known as the Wigner-Seitz cell [38], exists for every lattice. The Wigner-Seitz cell is defined as the locus of all points closer to a given lattice point than to any other lattice point. We have constructed the Wigner-Seitz cell for our two-dimensional hexagonal lattice as shown in Figure 4. Like all primitive cells, the Wigner-Seitz cell tiles its space, but unlike other cells it manifests the symmetry of the underlying hexagonal lattice,<sup>3</sup> in this case exhibiting the six-fold rotation symmetry characteristic of a hexagonal lattice.

By definition, all points in the Wigner-Seitz cell are closer to its origin than to any other lattice point. Since we can center the cell on a point other than the lattice points defined by Equation (1), we can use this fact to determine the nearest neighbors of a given Wyckoff position. Consider the Wigner-Seitz cell in Figure 5, where we center the cell on one of the points in the basis. Only one of the images of the other point in the basis exists in this unit cell, so these two points are nearest neighbors. The only ambiguity in this definition is when a basis point is on the boundary of

<sup>3</sup>Note that we say that the Wigner-Seitz cell has the symmetry of the lattice, not the crystal structure. Taken without a basis, the Wigner-Seitz cell in Figure 4 has a six-fold rotation axis about the origin, in agreement with the symmetry of the hexagonal lattice. With the basis, however, the cell shown in Figure 4 does *not* have full hexagonal symmetry, even though its shape is a hexagon.

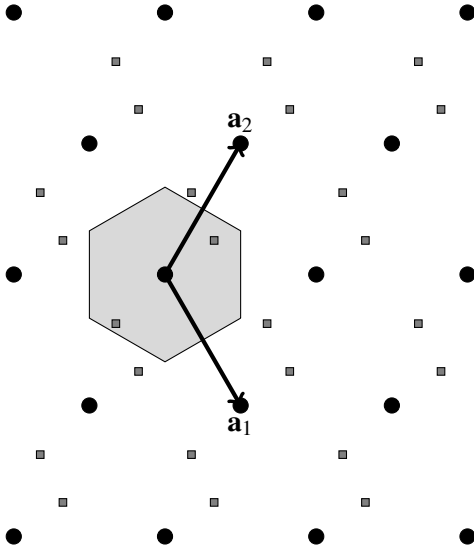


Figure 4: A two-dimensional hexagonal lattice with its corresponding Wigner-Seitz cell centered on a lattice point.

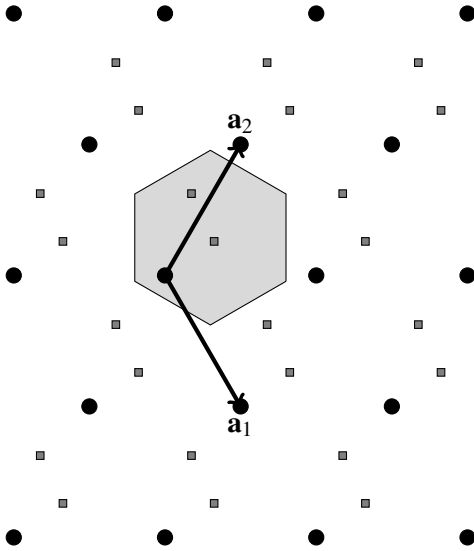


Figure 5: A two-dimensional hexagonal lattice with its corresponding Wigner-Seitz cell centered on one of the atoms.

the Wigner-Seitz zone. In this case there will be multiple copies of the basis point, all of them the same distance from the origin.

Three dimensions complicate the visualization of the Wigner-Seitz cell. We have added the ability to view the Wigner-Seitz cell to every structure in the AFLOW Library of Crystallographic Prototypes, using JSmol [39] to render the cells. As an example, consider the  $\text{SiS}_2$  structure  $\text{A2B\_oI12\_72\_j\_a}$ .<sup>4</sup> Figure 6(a) shows the primitive and conventional unit cells of this system, as well as the positions of the silicon and sulfur atoms.

Figure 6(b) shows the Wigner-Seitz cell, centered on the

<sup>4</sup>This structure can be found in the Library of Crystallographic Prototypes at [http://aflow.org/CrystalDatabase/A2B\\_oI12\\_72\\_j\\_a.html](http://aflow.org/CrystalDatabase/A2B_oI12_72_j_a.html).

origin of the lattice. One can clearly see that the unit cell contains two silicon atoms, with two sulfur atoms in the interior of the zone and two on the boundary.

We can also center the Wigner-Seitz cell on a particular atom, as shown with an silicon atom in Figure 6(c). This construction unambiguously identifies atoms which are nearest neighbors to the target silicon atom. This procedure can of course be extended to any atom in the primitive cell.

The Wigner-Seitz cell has its analog in reciprocal space. If  $\{\mathbf{R}\}$  is the set of all lattice points in three dimensional space, the reciprocal lattice is defined as the set of all vectors  $\{\mathbf{K}\}$  such that [40]

$$e^{i\mathbf{R}\cdot\mathbf{K}} = 1. \quad (5)$$

If the real-space lattice is defined by primitive vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , and  $\mathbf{a}_3$ , then the reciprocal lattice is defined by vectors

$$\mathbf{b}_i = \left(\frac{2\pi}{V}\right) \mathbf{a}_j \times \mathbf{a}_k, \quad (6)$$

where  $(i, j, k)$  are in cyclic order. The reciprocal lattice is dual to the real-space lattice, with

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}. \quad (7)$$

In matrix notation, we can write this as

$$2\pi\mathbf{B} = (\mathbf{A}^T)^{-1}, \quad (8)$$

where  $\mathbf{A}$ ,  $\mathbf{B}$  are matrices whose columns are the lattice vectors  $\mathbf{a}$  and reciprocal lattice vectors  $\mathbf{b}$ , respectively.

This reciprocal lattice has its own Wigner-Seitz cell, the *first Brillouin zone*. The relationship between real space lattices and their reciprocal space Brillouin zones are discussed in Ref. [14].

#### 4. Plane Groups (Two-Dimensional Space Groups)

Even though we live in a world with three physical dimensions, we can often achieve insight into that world by considering corresponding situations in two dimensions [41]. Two-dimensional physics is also important when we consider such materials as graphene [42],  $\text{MoS}_2$  [43], and similar materials. These systems still form periodic structures, and have symmetry operations associated with translations, rotations and reflections in two dimensions. These form the seventeen “plane groups”, often called “wallpaper groups” for obvious reasons.

Since two-dimensional figures readily translate to the page, there are numerous discussions of group properties readily available [44, 45], along with some beautiful examples of wallpaper symmetries [46].

At the atomic level, plane groups, like space groups, each possess a set of Wyckoff positions that determine allowed atomic positions in keeping with the symmetry of the group.

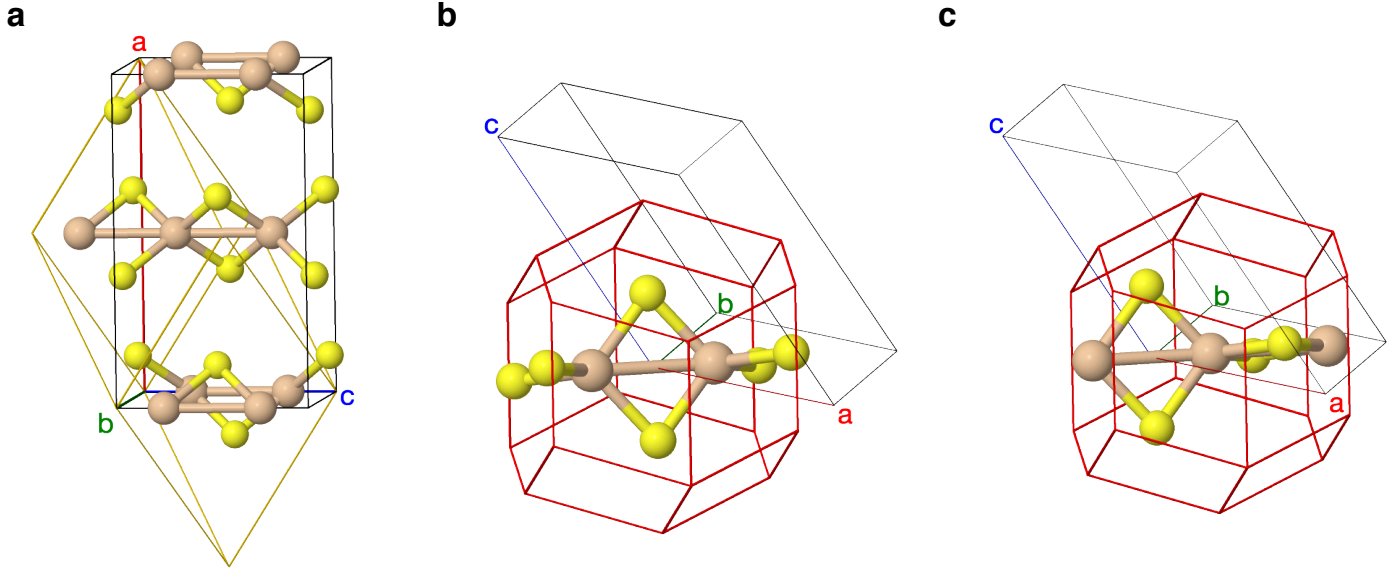


Figure 6: **Unit cell representations for body-centered orthorhombic SiS<sub>2</sub>**. The silicon and sulfur atoms are beige and yellow, respectively. (a) The primitive (yellow) and conventional (black) unit cell representations, where the axes are shown with respect to the conventional cell. (b) The Wigner-Seitz cell (red polyhedron) centered at the origin between two silicon atoms. The axes are shown with respect to the body-centered orthorhombic primitive unit cell (black) defined in Part 1 of the library [17]. (c) The Wigner-Seitz cell (red polyhedron) centered on one of the silicon atoms in the primitive cell. The axes are shown with respect to the body-centered orthorhombic primitive unit cell (black) defined in Part 1 of the library [17].

These have been tabulated in the *International Tables* [47] and online [33]. Here, we present a graphical illustration of the Wyckoff positions of each of the seventeen space groups, using the notation of the *International Tables* for each group.

Much as with three-dimensional space groups, the plane groups can be divided into crystal systems, each member of a given system having the same holohedry (rotational symmetry of the point group of the lattice).

There are five crystal systems in two dimensions:

- Simple parallelograms (plane groups #1-2): the analog to the triclinic system in three dimensions. The primitive vectors for these lattices are given by

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \cos \theta \hat{\mathbf{x}} + b \sin \theta \hat{\mathbf{y}}. \end{aligned} \quad (9)$$

The choice of  $a$ ,  $b$ , and  $\theta$  is completely arbitrary, provided that the choices do not fall into another of the crystal systems.

- Rectangles (plane groups #3-9): the system is defined by a rectangular lattice

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}}. \end{aligned} \quad (10)$$

with perpendicular lattice vectors [ $\theta = 90^\circ$  in Equation (9)]. The system contains both simple rectangular lattices, where the lattice is defined by Equation (10), and centered rectangular lattices, analogous to base-centered lattices in three dimensions. For the centered

lattices (plane groups #5 and #9), the conventional cell is defined by Equation (10), and the primitive unit cell is defined by

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}. \end{aligned} \quad (11)$$

- Squares (plane groups #10-12): special cases of the rectangular system given by Equation (10) with  $b = a$ , so that the primitive lattice is specified by the vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}}. \end{aligned} \quad (12)$$

The centered rectangular lattice Equation (11) also becomes a square lattice when  $a = b$ .

- Trigonal (plane groups #13-15): In this system the primitive vectors are of equal length and separated by an angle of  $120^\circ$ , with a three-fold rotation axis about the origin [ $b = a$  and  $\theta = 60^\circ$  is given by Equation (9), or  $b = \sqrt{3}a$  in Equation (11)]. The lattice vectors are

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}}. \end{aligned} \quad (13)$$

This can be regarded as a special case of the parallelogram in Equation (9) with  $b = a$  and  $\theta = 120^\circ$ , or of the centered rectangular lattice with  $b = \sqrt{3}a$ .

- Hexagonal (plane groups #16-17): As in the three-dimensional case, a distinction is made between the trigonal system, which has a three-fold rotational axis about the origin, and the hexagonal system, which has a six-fold rotational axis. In either case, the primitive vectors of the unit cell are given by Equation (13).

Each section below lists the primitive vectors that describe the lattice associated with the plane group, a table of Wyckoff positions allowed for the space group, and a figure showing possible Wyckoff positions, along with the Wigner-Seitz cell for the lattice.

#### 4.1. The Parallelogram Crystal System

##### 4.1.1. Plane Group #1: $p1$

This plane group has the lowest symmetry possible for a periodic lattice. The primitive lattice vectors are given by Equation (9), and the single Wyckoff position is completely general:

Label	Lattice Coordinates
(1a)	$(x, y)$

Figure 7 shows a selection of Wyckoff positions for plane group  $p1$ . It is worthwhile to note that if there is only one atom in the plane group defined by Equation (9), then we can place it at the origin, which then becomes an inversion site. This immediately promotes the structure to the higher symmetry of plane group #2,  $p2$ . If the structure contains only two identical atoms, then there is an inversion site between them, and it is once again appropriate to place the structure in space group  $p2$ .

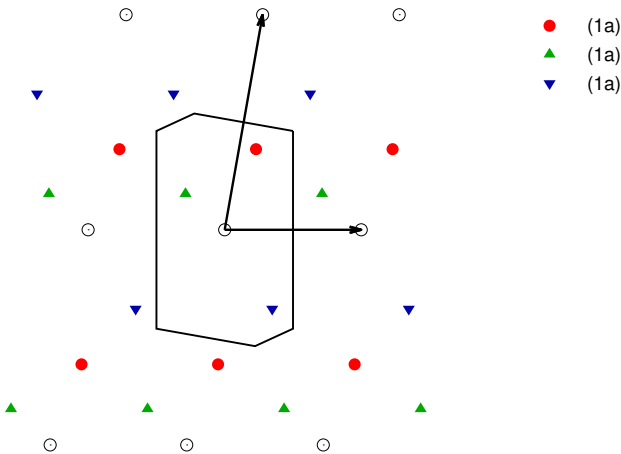


Figure 7: **Possible Wyckoff positions for plane group #1,  $p1$ .** We show multiple possible Wyckoff positions, as if only one is occupied it can be placed at the origin, and the plane group achieves the higher symmetry of plane group #2,  $p2$ . The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (9). The open circles indicate the lattice points.

##### 4.1.2. Plane Group #2: $p2$

Plane group #2,  $p2$ , has the same type of primitive lattice as  $p1$ , in Equation (9), but now inversion through the origin produces an unchanged structure. This means that any function operating in this crystal system must have the property that

$$f(x, y) = f(-x, -y). \quad (14)$$

This provides several relatively high-symmetry Wyckoff positions for single atoms, in addition to the general Wyckoff position.

Label	Lattice Coordinates
(2e)	$(x, y) (-x, -y)$
(1d)	$(1/2, 1/2)$
(1c)	$(1/2, 0)$
(1b)	$(0, 1/2)$
(1a)	$(0, 0)$

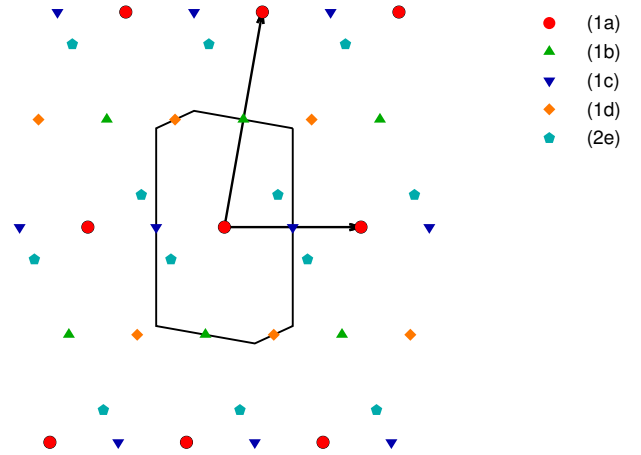


Figure 8: **Possible Wyckoff positions for plane group #2,  $p2$ .** The positions of the (1a)-(1d) sites are fixed, while the (2e) sites are arbitrary. The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (9).

#### 4.2. The Rectangular Crystal System

All of the rectangular plane groups have a conventional cell defined by the primitive vectors in Equation (10). This is also the primitive cell for space groups #3, #4, #6, #7 and #8.

##### 4.2.1. Plane Group #3: $p1m1$

This rectangular space group has primitive vectors in Equation (10) and a reflection around  $x = 0$ ; that is, any function operating in this space group must have the property that

$$f(-x, y) = f(x, y) \quad (15)$$

as well as the periodic properties

$$f(x + a, y) = f(x, y + b) = f(x, y). \quad (16)$$

The Wyckoff positions for space group #3 are given by

Label	Lattice Coordinates
(2c)	$(x, y) (-x, y)$
(1b)	$(1/2, y)$
(1a)	$(0, y)$

The plane group does not contain the inversion.

A graphical representation of the Wyckoff positions and the Wigner-Seitz cell for plane group #3 are given in Figure 9.

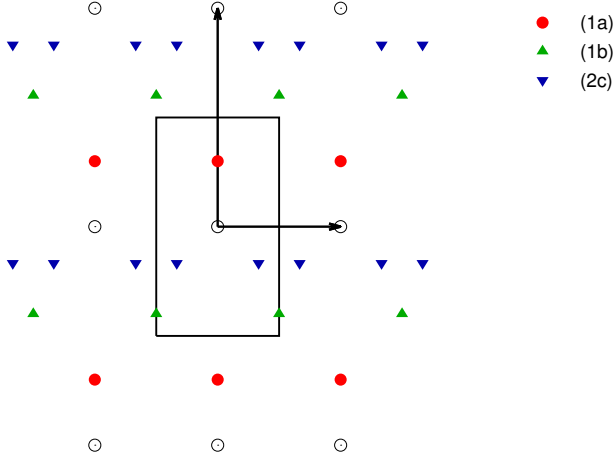


Figure 9: Possible Wyckoff positions for plane group #3,  $p1m1$ . The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (10). The open circles indicate the lattice points.

#### 4.2.2. Plane Group #4: $p1g1$

This rectangular space group has a glide reflection [44], with a reflection about  $x = 0$  combined with a translation of  $1/2 b$  along the  $y$  direction. That is, any function showing this symmetry must have the property that

$$f(x, y) = f(-x, y + 1/2) \quad (17)$$

There is only one Wyckoff position:

Label	Lattice Coordinates
(2a)	$(x, y) (-x, y + 1/2)$

There is no inversion in this crystal structure.

Figure 10 shows possible occupations of this Wyckoff position. We show two possible occupations. If only one (2a) site is occupied in this crystal system, there is an inversion between the two atoms, and we can place the origin there. In that case  $y = 1/4$ , and the system actually has the higher symmetry  $p2mg$  (#7), with atoms on the (2c) sites.

#### 4.2.3. Plane Group #5: $c1m1$

This is a centered rectangular space group, with the conventional cell given by Equation (10) and the primitive vectors given by Equation (11). Just as in space group #4, there

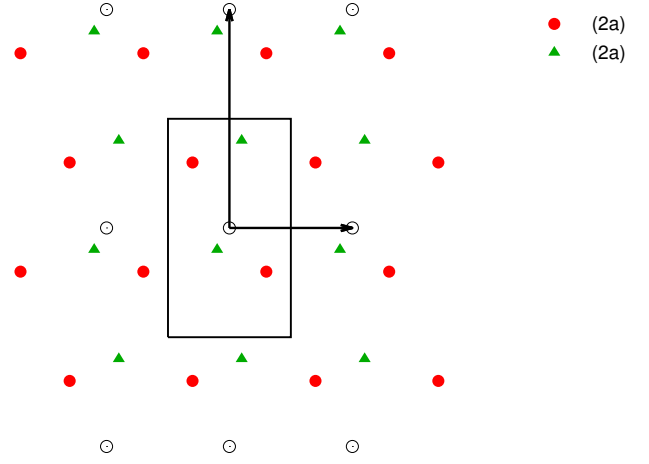


Figure 10: Possible Wyckoff positions for plane group #4,  $p1g1$ . The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (10). We show two possible occupations of the (2a) Wyckoff position to show that this is not in the higher symmetry plane group  $p2mg$  (#7). The open circles indicate the lattice points.

is a glide reflection in Equation (17). The Wyckoff positions are given by

Label	Conventional Lattice Coordinates
(4b)	$(x, y) (-x, y)$ ----- $(x + 1/2, y + 1/2) (-x + 1/2, y + 1/2)$
(2a)	$(0, y)$ ----- $(1/2, y + 1/2)$

where, following convention, we give the coordinates of the positions in terms of the conventional lattice in Equation (10), but we also explicitly show the translations due to the centered primitive cell below the dashed line. The plane group does not contain the inversion.

The Wyckoff positions for this lattice are sketched in Figure 11.

#### 4.2.4. Plane Group #6: $p2mm$

The remaining rectangular plane groups all contain the inversion given by Equation (14). Group #6 also includes a mirror reflection about  $x = 0$  in Equation (15). Combining both of these operations show us that there must also be a mirror reflection about  $y = 0$ , as well:

$$f(x, y) = f(x, -y). \quad (18)$$

This leads to several Wyckoff positions, all of which are outlined in Figure 12.

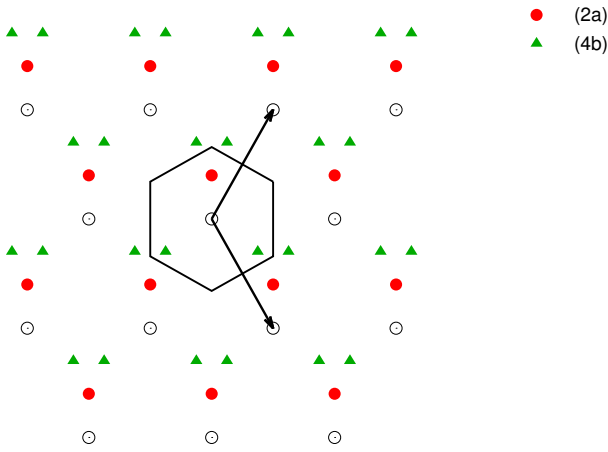


Figure 11: **Possible Wyckoff positions for plane group #5,  $c1m1$ .** The black outline represents the boundary of the Wigner-Seitz cell for the primitive cell in Equation (11). The open circles indicate the lattice points.

Label	Lattice Coordinates
(4i)	$(x, y) (-x, -y) (-x, y) (x, -y)$
(2h)	$(1/2, y) (1/2, -y)$
(2g)	$(0, y) (0, -y)$
(2f)	$(x, 1/2) (-x, 1/2)$
(2e)	$(x, 0) (-x, 0)$
(1d)	$(1/2, 1/2)$
(1c)	$(1/2, 0)$
(1b)	$(0, 1/2)$
(1a)	$(0, 0)$

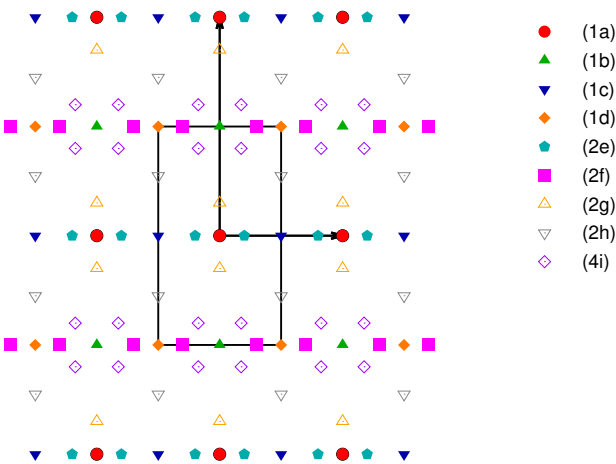


Figure 12: **Possible Wyckoff positions for plane group #6,  $p2mm$ .** The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (10). Note the mirroring about  $x = 0$  and  $y = 0$ .

#### 4.2.5. Plane Group #7: $p2mg$

In addition to the inversion, this group has a glide reflection about  $y = 0$  combined with a translation of  $1/2 a$  along the  $x$  direction:

$$f(x, y) = f(-x + 1/2, y) \quad (19)$$

The Wyckoff positions are sketched in Figure 13 and are listed below.

Label	Lattice Coordinates
(4d)	$(x, y) (-x, -y) (-x + 1/2, y) (x + 1/2, -y)$
(2c)	$(1/4, y) (3/4, -y)$
(2b)	$(0, 1/2) (1/2, 1/2)$
(2a)	$(0, 0) (1/2, 0)$

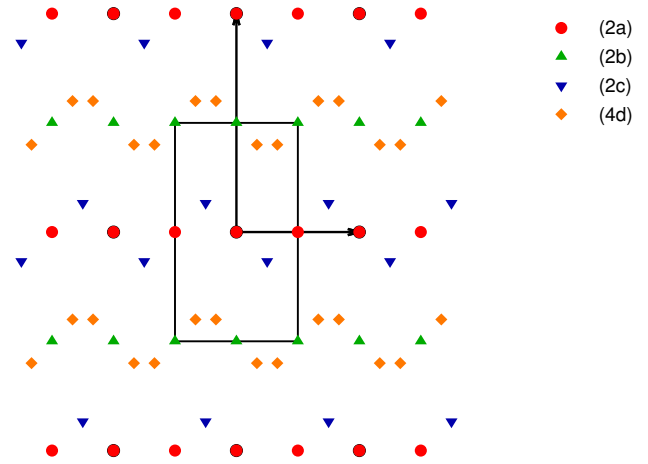


Figure 13: **Possible Wyckoff positions for plane group #7,  $p2mg$ .** The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (10). Note the mirroring about  $x = 0$  and  $y = 0$ .

#### 4.2.6. Plane Group #8: $p2gg$

This group has two glide reflections as well as the inversion. Its Wyckoff positions are shown in Figure 14 and are listed below.

Label	Lattice Coordinates
(4c)	$(x, y) (-x, -y)$ $(-x + 1/2, y + 1/2) (x + 1/2, -y + 1/2)$
(2b)	$(1/2, 0) (0, 1/2)$
(2a)	$(0, 0) (1/2, 1/2)$

#### 4.2.7. Plane Group #9: $c2mm$

Like plane group #6,  $p2mm$ , this group has mirror reflections around both  $x = 0$  and  $y = 0$ . However, it is a centered lattice, with the primitive cell defined by Equation (11) and the conventional cell defined by Equation (10). The Wyckoff positions are sketched in Figure 15 and listed below.

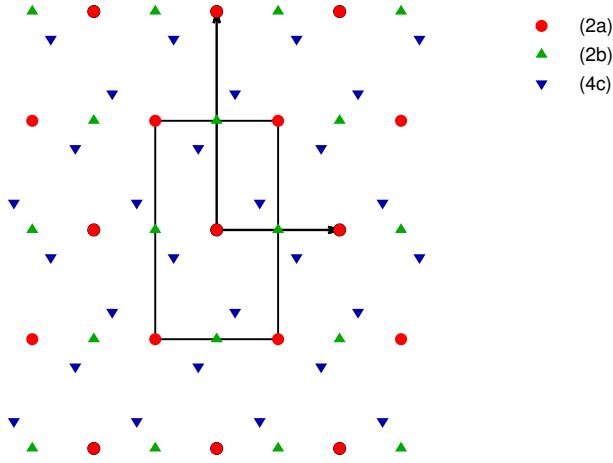


Figure 14: **Possible Wyckoff positions for plane group #8,  $p2gg$ .** The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (10).

Note that as with group  $c1m1$ , #5, we have listed the coordinates in terms of the conventional unit cell, and included the translations associated with the centered cell in the list.

Label	Conventional Lattice Coordinates
(8f)	$(x, y) (-x, -y) (-x, y) (x, -y)$
	-----
	$(x + 1/2, y + 1/2) (-x + 1/2, -y + 1/2)$ $(-x + 1/2, y + 1/2) (x + 1/2, -y + 1/2)$
(4e)	$(0, y) (0, -y)$
	-----
(4d)	$(1/2, y + 1/2) (1/2, -y + 1/2)$
	-----
(4d)	$(x, 0) (-x, 0)$
	-----
(4c)	$(x + 1/2, 1/2) (-x + 1/2, 1/2)$
	-----
(4c)	$(1/4, 1/4) (3/4, 1/4)$
	-----
(4c)	$(3/4, 3/4) (1/4, 3/4)$
	-----
(2b)	$(0, 1/2)$
	-----
(2b)	$(1/2, 0)$
	-----
(2a)	$(0, 0)$
	-----
(2a)	$(1/2, 1/2)$

### 4.3. The Square Crystal System

All of the lattices in this system remain unchanged when rotated by  $90^\circ$  about the origin, so that the crystal obeys the relationship

$$f(x, y) = f(-y, x) = f(-x, -y) = f(y, -x), \quad (20)$$

automatically including the inversion from Equation (14). They thus form perfect squares, with the primitive cell given by Equation (12).

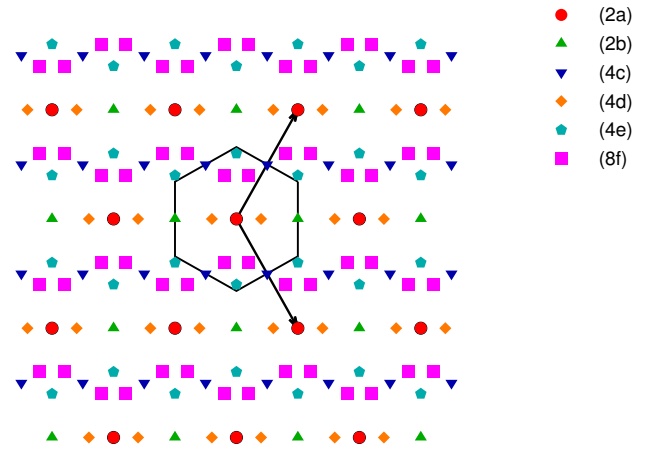


Figure 15: **Possible Wyckoff positions for plane group #9,  $c2mm$ .** The black outline represents the boundary of the Wigner-Seitz cell for the primitive cell in Equation (11). The lattice vectors and Wigner-Seitz cell for the conventional cell in Equation (10) are identical to those shown in Figure 12.

#### 4.3.1. Plane Group #10: $p4$

This is the simplest plane group, with no reflections or glide reflections. The Wyckoff positions are sketched in Figure 16 and listed below.

Label	Lattice Coordinates
(4d)	$(x, y) (-x, -y) (-y, x) (y, -x)$
(2c)	$(1/2, 0) (0, 1/2)$
(1b)	$(1/2, 1/2)$
(1a)	$(0, 0)$

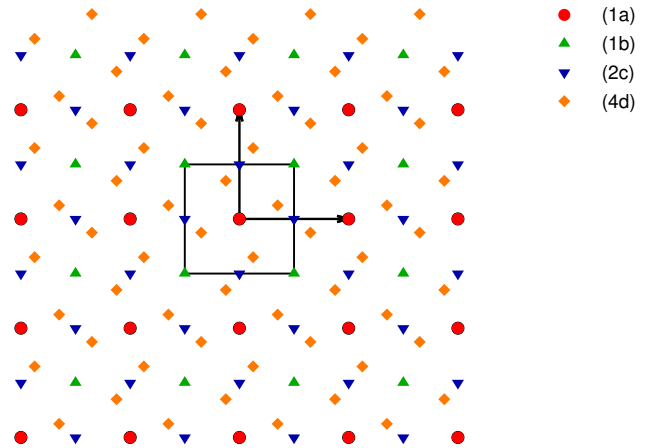


Figure 16: **Possible Wyckoff positions for plane group #10,  $p4$ .** The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (12). As with all of the square plane groups, this group is invariant with respect to a rotation of  $90^\circ$  about the origin and contains the inversion.

#### 4.3.2. Plane Group #11: $p4mm$

This square plane group includes reflections about  $x = 0$  and  $y = 0$ . When the  $90^\circ$  rotations are included, this also generates mirror reflections around the lines  $y = \pm x$ , so this group admits operations of the form

$$f(x, y) = f(-x, y) = f(x, -y) = f(y, x) = \dots \quad (21)$$

The Wyckoff positions are sketched in Figure 17 and listed below.

Label	Lattice Coordinates
(8g)	$(x, y) (-x, -y) (-y, x) (y, -x)$ $(-x, y) (x, -y) (y, x) (-y, -x)$
(4f)	$(x, x) (-x, -x) (-x, x) (x, -x)$
(4e)	$(x, 1/2) (-x, 1/2) (1/2, x) (1/2, -x)$
(4d)	$(x, 0) (-x, 0) (0, x) (0, -x)$
(2c)	$(1/2, 0) (0, 1/2)$
(1b)	$(1/2, 1/2)$
(1a)	$(0, 0)$

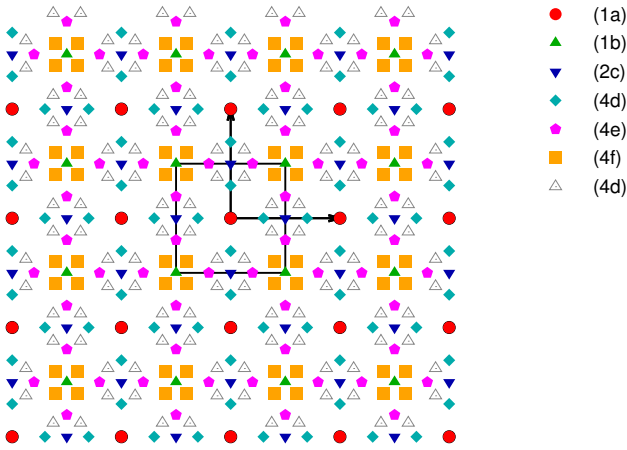


Figure 17: Possible Wyckoff positions for plane group #11,  $p4mm$ . The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (12).

#### 4.3.3. Plane Group #12: $p4gm$

This group contains reflections, but they are not centered on the center of rotation, as they are with plane group #11. The Wyckoff positions are listed below and sketched in Figure 18.

Label	Lattice Coordinates
(8d)	$(x, y) (-x, -y) (-y, x) (y, -x)$ $(-x + 1/2, y + 1/2) (x + 1/2, -y + 1/2)$ $(y + 1/2, x + 1/2) (-y + 1/2, -x + 1/2)$
(4c)	$(x, x + 1/2) (-x, -x + 1/2)$ $(-x + 1/2, x) (x + 1/2, -x)$
(2b)	$(1/2, 0) (0, 1/2)$
(2a)	$(0, 0) (1/2, 1/2)$

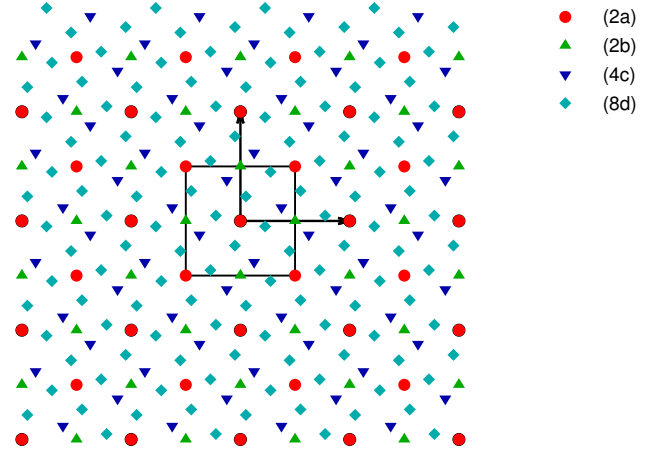


Figure 18: Possible Wyckoff positions for plane group #12,  $p4gm$ . The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (12).

### 4.4. The Trigonal Crystal System

All of the plane groups in the trigonal crystal system are described by the primitive vectors in Equation (13) and are invariant under  $120^\circ$  rotations about the origin. This system explicitly excludes groups which are invariant with respect to  $60^\circ$  rotations, and so none of these groups contains the inversion operation in Equation (14).

#### 4.4.1. Plane Group #13: $p3$

This is the simplest of the trigonal groups, with only the  $120^\circ$  symmetry operation. The Wyckoff positions are listed below, and sketched in Figure 19.

Label	Lattice Coordinates
(3d)	$(x, y) (-y, x - y) (-x + y, -x)$
(1c)	$(2/3, 1/3)$
(1b)	$(1/3, 2/3)$
(1a)	$(0, 0)$

#### 4.4.2. Plane Group #14: $p3m1$

This group includes a reflection about the Cartesian  $y$ -axis (not the  $x$  or  $y$  lattice coordinates). The Wyckoff positions are listed below, and sketched in Figure 20.

Label	Lattice Coordinates
(6e)	$(x, y) (-y, x - y) (-x + y, -x)$ $(-y, -x) (-x + y, y) (x, x - y)$
(3d)	$(x, -x) (x, 2x) (-2x, -x)$
(1c)	$(2/3, 1/3)$
(1b)	$(1/3, 2/3)$
(1a)	$(0, 0)$



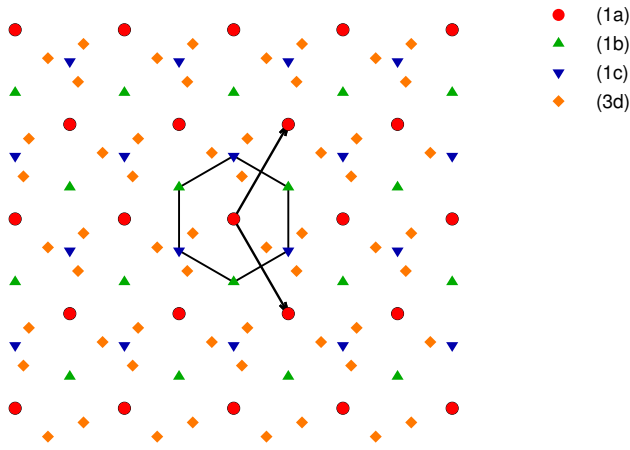


Figure 19: **Possible Wyckoff positions for plane group #13,  $p3$ .** The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (13). Note the 3-fold rotation axis about the origin.

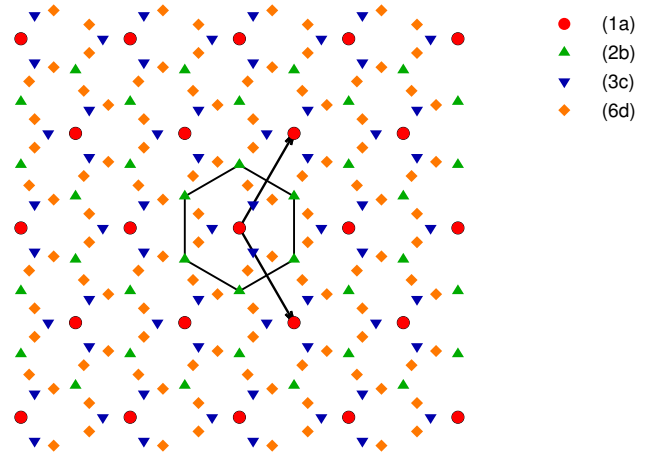


Figure 21: **Possible Wyckoff positions for plane group #15,  $p31m$ .** The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (13). Note the reflection about the Cartesian  $x$  axis.

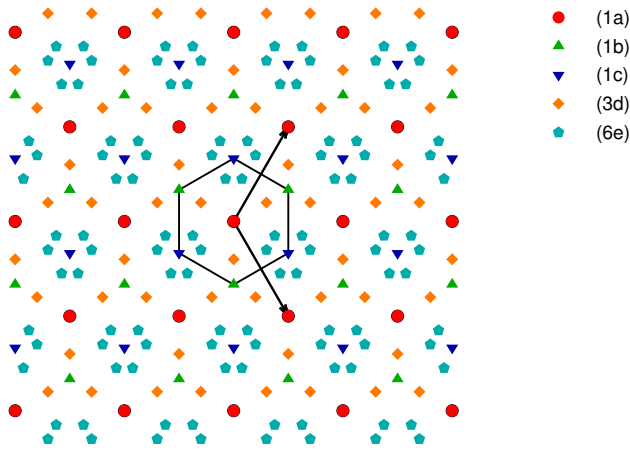


Figure 20: **Possible Wyckoff positions for plane group #14,  $p3m1$ .** The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (13). Note the reflection about the Cartesian  $y$  axis.

#### 4.4.3. Plane Group #15: $p31m$

This is similar to plane group #14, but now, instead of a reflection about the  $y$ -axis, the group includes a reflection about the Cartesian  $x$ -axis. The Wyckoff positions are listed below, and sketched in Figure 21.

Label	Lattice Coordinates
(6d)	$(x, y)$ $(-y, x - y)$ $(-x + y, -x)$ $(y, x)$ $(x - y, -y)$ $(-x, -x + y)$
(3c)	$(x, 0)$ $(0, x)$ $(-x, -x)$
(2b)	$(1/3, 2/3)$ $(2/3, 1/3)$
(1a)	$(0, 0)$

#### 4.5. The Hexagonal Crystal System

Like the trigonal crystal system, the lattice associated with the hexagonal crystal system is described by the prim-

itive vectors in Equation (13), but here both groups are invariant under a  $60^\circ$  degree rotation, and so include the inversion operation in Equation (14).

##### 4.5.1. Plane Group #16: $p6$

This group includes the  $60^\circ$  rotation operation, but no reflections. The Wyckoff positions are given below, and described graphically in Figure 22.

Label	Lattice Coordinates
(6d)	$(x, y)$ $(-y, x - y)$ $(-x + y, -x)$ $(-x, -y)$ $(y, -x + y)$ $(x - y, x)$
(3c)	$(1/2, 0)$ $(0, 1/2)$ $(1/2, 1/2)$
(2b)	$(1/3, 2/3)$ $(2/3, 1/3)$
(1a)	$(0, 0)$

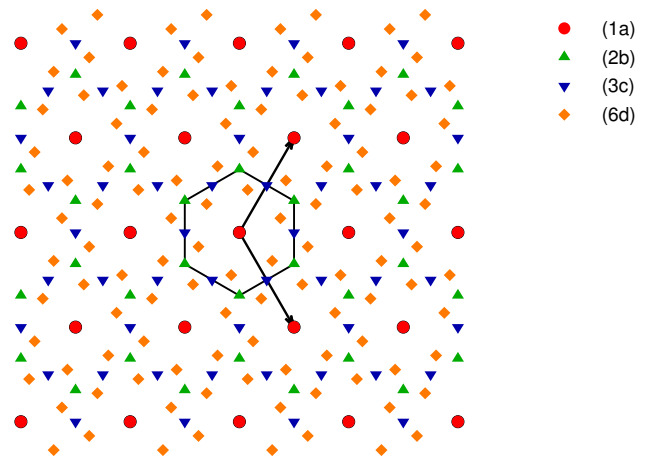


Figure 22: **Possible Wyckoff positions for plane group #16,  $p6$ .** The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (13). Note the  $60^\circ$  rotation symmetry about the origin.

#### 4.5.2. Plane Group #17: $p6mm$

The final plane group includes the  $60^\circ$  rotation operation, as well as reflections along both the Cartesian axes. The Wyckoff positions are given below, and described graphically in Figure 23.

Label	Lattice Coordinates
(12f)	$(x, y)$ $(-y, x - y)$ $(-x + y, -x)$ $(-x, -y)$ $(y, -x + y)$ $(x - y, x)$ $(-y, -x)$ $(-x + y, y)$ $(x, x - y)$ $(y, x)$ $(x - y, -y)$ $(-x, -x + y)$
(6e)	$(x, -x)$ $(x, 2x)$ $(-2x, -x)$ $(-x, x)$ $(-x, -2x)$ $(2x, x)$
(6d)	$(x, 0)$ $(0, x)$ $(-x, -x)$ $(-x, 0)$ $(0, -x)$ $(x, x)$
(3c)	$(1/2, 0)$ $(0, 1/2)$ $(1/2, 1/2)$
(2b)	$(1/3, 2/3)$ $(2/3, 1/3)$
(1a)	$(0, 0)$

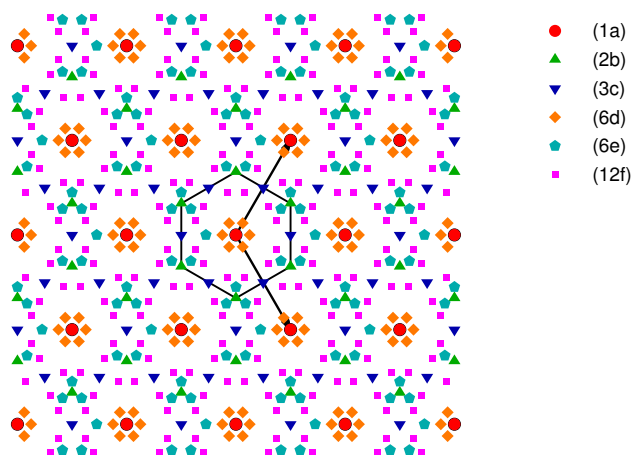


Figure 23: Possible Wyckoff positions for plane group #17,  $p6mm$ . The black outline represents the boundary of the Wigner-Seitz cell for the lattice in Equation (13). Note the  $60^\circ$  rotation symmetry about the origin as well as the reflections about the Cartesian axes.

## 5. Space Group Notation

There are a variety of space group notation methods. Each structural prototype page includes the space group number and International symbol. The Crystallographic Information Files (CIF) [48] used in the library indicates the number and the Hermann-Mauguin and Hall symbols. Lastly, the VASP POSCAR lists the number and the Hermann-Mauguin and Schönflies symbols.

The notations we use are

- Hermann-Mauguin [49, 50] (in CIF and POSCAR)
- Hall [51] (in CIF)
- “International”, a compact form of the Hermann-Mauguin notation used in the International Tables of Crystallography [52] (in entry page).

- Schönflies [53, 54] (in POSCAR)

Note that most notations provide different values for each orientation of a crystal. A complete list of orientations can be found in Hall and Grosse-Kunstleve [55]. In general we use the first space-group orientation listed for a space group on that page. There are two exceptions:

- For some space groups, *e.g.* #227, there are two settings, reflecting a choice of origin. We always take the second setting, which places the origin of the real-space coordinate system at an inversion site.
- For rhombohedral unit cells we always use the label for the full hexagonal unit cell (H) rather than the primitive rhombohedral cell (R), which follows our choice to describe the unit cell in terms of the hexagonal lattice parameters  $a$  and  $c$ , rather than the rhombohedral lattice parameters  $a$  and  $\alpha$ .

Complete listings of all space group orientations can be found at

- Concise Space Group Symbols, [http://cci.lbl.gov/sginfo/hall\\_symbols.html](http://cci.lbl.gov/sginfo/hall_symbols.html)
- Elk Spacegroup Manual, <http://elk.sourceforge.net/spacegroup.pdf>

## 6. Conclusion

Herein, we present the second part of *The AFLOW Library of Crystallographic Prototypes*. The article includes 302 crystallographic prototypes and provides the corresponding structural information for each entry. The geometry file for each structure can be generated via AFLOW to facilitate high-throughput computation of material properties. This information is also available online at <http://www.aflow.org/CrystalDatabase>, where it is combined with the prototypes listed in Part 1.

Table 1: **A list of the various space group notations.** The space group number, orientation, Hermann-Mauguin symbol, Hall symbol, International symbol, and Schönflies symbol are listed.

Number	Orientation	Hermann-Mauguin	Hall	International	Schönflies
1		P 1	P 1	$P1$	$C_1^1$
2		P -1	-P 1	$P\bar{1}$	$C_i^1$
3	b	P 1 2 1	P 2y	$P2$	$C_2^1$
4	b	P 1 21 1	P 2yb	$P2_1$	$C_2^2$
5	b1	C 1 2 1	C 2y	$C2$	$C_2^3$
6	b	P 1 m 1	P -2y	$Pm$	$C_s^1$
7	b1	P 1 c 1	P -2yc	$Pc$	$C_s^2$
8	b1	C 1 m 1	C -2y	$Cm$	$C_s^3$
9	b1	C 1 c 1	C -2yc	$Cc$	$C_s^4$
10	b	P 1 2/m 1	-P 2y	$P2/m$	$C_{2h}^1$
11	b	P 1 21/m 1	-P 2yb	$P2_1/m$	$C_{2h}^2$
12	b1	C 1 2/m 1	-C 2y	$C2/m$	$C_{2h}^3$
13	b1	P 1 2/c 1	-P 2yc	$P2/c$	$C_{2h}^4$
14	b1	P 1 21/c 1	-P 2ybc	$P2_1/c$	$C_{2h}^5$
15	b1	C 1 2/c 1	-C 2yc	$C2/c$	$C_{2h}^6$
16		P 2 2 2	P 2 2	$P222$	$D_2^1$
17		P 2 2 21	P 2c 2	$P222_1$	$D_2^2$
18		P 21 21 2	P 2 2ab	$P2_12_12$	$D_2^3$
19		P 21 21 21	P 2ac 2ab	$P2_12_12_1$	$D_2^4$
20		C 2 2 21	C 2c 2	$C222_1$	$D_2^5$
21		C 2 2 2	C 2 2	$C222$	$D_2^6$
22		F 2 2 2	F 2 2	$F222$	$D_2^7$
23		I 2 2 2	I 2 2	$I222$	$D_2^8$
24		I 21 21 21	I 2b 2c	$I2_12_12_1$	$D_2^9$
25		P m m 2	P 2 -2	$Pmm2$	$C_{2v}^1$
26		P m c 21	P 2c -2	$Pmc2_1$	$C_{2v}^2$
27		P c c 2	P 2 -2c	$Pcc2$	$C_{2v}^3$
28		P m a 2	P 2 -2a	$Pma2$	$C_{2v}^4$
29		P c a 21	P 2c -2ac	$Pca2_1$	$C_{2v}^5$
30		P n c 2	P 2 -2bc	$Pnc2$	$C_{2v}^6$
31		P m n 21	P 2ac -2	$Pmn2_1$	$C_{2v}^7$
32		P b a 2	P 2 -2ab	$Pba2$	$C_{2v}^8$
33		P n a 21	P 2c -2n	$Pna2_1$	$C_{2v}^9$
34		P n n 2	P 2 -2n	$Pnn2$	$C_{2v}^{10}$
35		C m m 2	C 2 -2	$Cmm2$	$C_{2v}^{11}$
36		C m c 21	C 2c -2	$Cmc2_1$	$C_{2v}^{12}$
37		C c c 2	C 2 -2c	$Ccc2$	$C_{2v}^{13}$
38		A m m 2	A 2 -2	$Amm2$	$C_{2v}^{14}$
39		A b m 2	A 2 -2c	$Aem2$	$C_{2v}^{15}$
40		A m a 2	A 2 -2a	$Ama2$	$C_{2v}^{16}$
41		A b a 2	A 2 -2ac	$Aea2$	$C_{2v}^{17}$
42		F m m 2	F 2 -2	$Fmm2$	$C_{2v}^{18}$
43		F d d 2	F 2 -2d	$Fdd2$	$C_{2v}^{19}$
44		I m m 2	I 2 -2	$Imm2$	$C_{2v}^{20}$
45		I b a 2	I 2 -2c	$Iba2$	$C_{2v}^{21}$
46		I m a 2	I 2 -2a	$Ima2$	$C_{2v}^{22}$

Table 1 (continued): **A list of the various space group notations.** The space group number, orientation, Hermann-Mauguin symbol, Hall symbol, International symbol, and Schönflies symbol are listed.

Number	Orientation	Hermann-Mauguin	Hall	International	Schönflies
47		P 2/m 2/m 2/m	-P 2 2	<i>Pmmm</i>	$D_{2h}^1$
48	2	P 2/n 2/n 2/n:2	-P 2ab 2bc	<i>Pnnn</i>	$D_{2h}^2$
49		P 2/c 2/c 2/m	-P 2 2c	<i>Pccm</i>	$D_{2h}^3$
50	2	P 2/b 2/a 2/n:2	-P 2ab 2b	<i>Pban</i>	$D_{2h}^4$
51		P 21/m 2/m 2/a	-P 2a 2a	<i>Pmma</i>	$D_{2h}^5$
52		P 2/n 21/n 2/a	-P 2a 2bc	<i>Pnna</i>	$D_{2h}^6$
53		P 2/m 2/n 21/a	-P 2ac 2	<i>Pmna</i>	$D_{2h}^7$
54		P 21/c 2/c 2/a	-P 2a 2ac	<i>Pcca</i>	$D_{2h}^8$
55		P 21/b 21/a 2/m	-P 2 2ab	<i>Pbam</i>	$D_{2h}^9$
56		P 21/c 21/c 2/n	-P 2ab 2ac	<i>Pccn</i>	$D_{2h}^{10}$
57		P 2/b 21/c 21/m	-P 2c 2b	<i>Pbcm</i>	$D_{2h}^{11}$
58		P 21/n 21/n 2/m	-P 2 2n	<i>Pnnm</i>	$D_{2h}^{12}$
59	2	P 21/m 21/m 2/n:2	-P 2ab 2a	<i>Pmmn</i>	$D_{2h}^{13}$
60		P 21/b 2/c 21/n	-P 2n 2ab	<i>Pbcn</i>	$D_{2h}^{14}$
61		P 21/b 21/c 21/a	-P 2ac 2ab	<i>Pbca</i>	$D_{2h}^{15}$
62		P 21/n 21/m 21/a	-P 2ac 2n	<i>Pnma</i>	$D_{2h}^{16}$
63		C 2/m 2/c 21/m	-C 2c 2	<i>Cmcm</i>	$D_{2h}^{17}$
64		C 2/m 2/c 21/a	-C 2bc 2	<i>Cmca</i>	$D_{2h}^{18}$
65		C 2/m 2/m 2/m	-C 2 2	<i>Cmmm</i>	$D_{2h}^{19}$
66		C 2/c 2/c 2/m	-C 2 2c	<i>Cccm</i>	$D_{2h}^{20}$
67		C 2/m 2/m 2/a	-C 2b 2	<i>Cmma</i>	$D_{2h}^{21}$
68	2	C 2/c 2/c 2/a:2	-C 2b 2bc	<i>Ccca</i>	$D_{2h}^{22}$
69		F 2/m 2/m 2/m	-F 2 2	<i>Fmmm</i>	$D_{2h}^{23}$
70	2	F 2/d 2/d 2/d:2	-F 2uv 2vw	<i>Fddd</i>	$D_{2h}^{24}$
71		I 2/m 2/m 2/m	-I 2 2	<i>Immm</i>	$D_{2h}^{25}$
72		I 2/b 2/a 2/m	-I 2 2c	<i>Ibam</i>	$D_{2h}^{26}$
73		I 2/b 2/c 2/a	-I 2b 2c	<i>Ibca</i>	$D_{2h}^{27}$
74		I 2/m 2/m 2/a	-I 2b 2	<i>Imma</i>	$D_{2h}^{28}$
75		P 4	P 4	<i>P4</i>	$C_4^1$
76		P 41	P 4w	<i>P4<sub>1</sub></i>	$C_4^2$
77		P 42	P 4c	<i>P4<sub>2</sub></i>	$C_4^3$
78		P 43	P 4cw	<i>P4<sub>3</sub></i>	$C_4^4$
79		I 4	I 4	<i>I4</i>	$C_4^5$
80		I 41	I 4bw	<i>I4<sub>1</sub></i>	$C_4^6$
81		P -4	P -4	$\bar{P4}$	$S_4^1$
82		I -4	I -4	$\bar{I4}$	$S_4^2$
83		P 4/m	-P 4	<i>P4/m</i>	$C_{4h}^1$
84		P 42/m	-P 4c	<i>P4<sub>2</sub>/m</i>	$C_{4h}^2$
85	2	P 4/n:2	-P 4a	<i>P4/n</i>	$C_{4h}^3$
86	2	P 42/n:2	-P 4bc	<i>P4<sub>2</sub>/n</i>	$C_{4h}^4$
87		I 4/m	-I 4	<i>I4/m</i>	$C_{4h}^5$
88	2	I 41/a:2	-I 4ad	<i>I4<sub>1</sub>/a</i>	$C_{4h}^6$
89		P 4 2 2	P 4 2	<i>P422</i>	$D_4^1$
90		P 4 21 2	P 4ab 2ab	<i>P42<sub>1</sub>2</i>	$D_4^2$
91		P 41 2 2	P 4w 2c	<i>P4<sub>1</sub>22</i>	$D_4^3$
92		P 41 21 2	P 4abw 2nw	<i>P4<sub>1</sub>2<sub>1</sub>2</i>	$D_4^4$

Table 1 (continued): **A list of the various space group notations.** The space group number, orientation, Hermann-Mauguin symbol, Hall symbol, International symbol, and Schönflies symbol are listed.

Number	Orientation	Hermann-Mauguin	Hall	International	Schönflies
93		P 42 2 2	P 4c 2	$P4_222$	$D_4^5$
94		P 42 21 2	P 4n 2n	$P4_22_12$	$D_4^6$
95		P 43 2 2	P 4cw 2c	$P4_322$	$D_4^7$
96		P 43 21 2	P 4nw 2abw	$P4_32_12$	$D_4^8$
97		I 4 2 2	I 4 2	$I422$	$D_4^9$
98		I 41 2 2	I 4bw 2bw	$I4_122$	$D_4^{10}$
99		P 4 m m	P 4 -2	$P4mm$	$C_{4v}^1$
100		P 4 b m	P 4 -2ab	$P4bm$	$C_{4v}^2$
101		P 42 c m	P 4c -2c	$P4_2cm$	$C_{4v}^3$
102		P 42 n m	P 4n -2n	$P4_2nm$	$C_{4v}^4$
103		P 4 c c	P 4 -2c	$P4cc$	$C_{4v}^5$
104		P 4 n c	P 4 -2n	$P4nc$	$C_{4v}^6$
105		P 42 m c	P 4c -2	$P4_2mc$	$C_{4v}^7$
106		P 42 b c	P 4c -2ab	$P_2bc$	$C_{4v}^8$
107		I 4 m m	I 4 -2	$I4mm$	$C_{4v}^9$
108		I 4 c m	I 4 -2c	$I4cm$	$C_{4v}^{10}$
109		I 41 m d	I 4bw -2	$I4_1md$	$C_{4v}^{11}$
110		I 41 c d	I 4bw -2c	$I4_1cd$	$C_{4v}^{12}$
111		P -4 2 m	P -4 2	$P\bar{4}2m$	$D_{2d}^1$
112		P -4 2 c	P -4 2c	$P\bar{4}2c$	$D_{2d}^2$
113		P -4 21 m	P -4 2ab	$P\bar{4}2_1m$	$D_{2d}^3$
114		P -4 21 c	P -4 2n	$P\bar{4}2_1c$	$D_{2d}^4$
115		P -4 m 2	P -4 -2	$P\bar{4}m2$	$D_{2d}^5$
116		P -4 c 2	P -4 -2c	$P\bar{4}c2$	$D_{2d}^6$
117		P -4 b 2	P -4 -2ab	$P\bar{4}b2$	$D_{2d}^7$
118		P -4 n 2	P -4 -2n	$P\bar{4}n2$	$D_{2d}^8$
119		I -4 m 2	I -4 -2	$I\bar{4}m2$	$D_{2d}^9$
120		I -4 c 2	I -4 -2c	$I\bar{4}c2$	$D_{2d}^{10}$
121		I -4 2 m	I -4 2	$I\bar{4}2m$	$D_{2d}^{11}$
122		I -4 2 d	I -4 2bw	$I\bar{4}2d$	$D_{2d}^{12}$
123		P 4/m 2/m 2/m	-P 4 2	$P4/mmm$	$D_{4h}^1$
124		P 4/m 2/c 2/c	-P 4 2c	$P4/mcc$	$D_{4h}^2$
125	2	P 4/n 2/b 2/m:2	-P 4a 2b	$P4/nbm$	$D_{4h}^3$
126	2	P 4/n 2/n 2/c:2	-P 4a 2bc	$P4/nnc$	$D_{4h}^4$
127		P 4/m 21/b 2/m	-P 4 2ab	$P4/mbm$	$D_{4h}^5$
128		P 4/m 21/n 2/c	-P 4 2n	$P4/mnc$	$D_{4h}^6$
129	2	P 4/n 21/m 2/m:2	-P 4a 2a	$P4/nmm$	$D_{4h}^7$
130	2	P 4/n 21/c 2/c:2	-P 4a 2ac	$P4/ncc$	$D_{4h}^8$
131		P 42/m 2/m 2/c	-P 4c 2	$P4_2/mmc$	$D_{4h}^9$
132		P 42/m 2/c 2/m	-P 4c 2c	$P4_2/mcm$	$D_{4h}^{10}$
133	2	P 42/n 2/b 2/c:2	-P 4ac 2b	$P4_2/nbc$	$D_{4h}^{11}$
134	2	P 42/n 2/n 2/m:2	-P 4ac 2bc	$P4_2/nnm$	$D_{4h}^{12}$
135		P 42/m 21/b 2/c	-P 4c 2ab	$P4_2/mbc$	$D_{4h}^{13}$
136		P 42/m 21/n 2/m	-P 4n 2n	$P4_2/mnm$	$D_{4h}^{14}$
137	2	P 42/n 21/m 2/c:2	-P 4ac 2a	$P4_2/nmc$	$D_{4h}^{15}$
138	2	P 42/n 21/c 2/m:2	-P 4ac 2ac	$P4_2/ncm$	$D_{4h}^{16}$

Table 1 (continued): **A list of the various space group notations.** The space group number, orientation, Hermann-Mauguin symbol, Hall symbol, International symbol, and Schönflies symbol are listed.

Number	Orientation	Hermann-Mauguin	Hall	International	Schönflies
139		I 4/m 2/m 2/m	-I 4 2	<i>I4/mmm</i>	$D_{4h}^{17}$
140		I 4/m 2/c 2/m	-I 4 2c	<i>I4/mcm</i>	$D_{4h}^{18}$
141	2	I 41/a 2/m 2/d:2	-I 4bd 2	<i>I4<sub>1</sub>/amd</i>	$D_{4h}^{19}$
142	2	I 41/a 2/c 2/d:2	-I 4bd 2c	<i>I4<sub>1</sub>/acd</i>	$D_{4h}^{20}$
143		P 3	P 3	<i>P3</i>	$C_3^1$
144		P 31	P 31	<i>P3<sub>1</sub></i>	$C_3^2$
145		P 32	P 32	<i>P3<sub>2</sub></i>	$C_3^3$
146	H	R 3:H	R 3	<i>R3</i>	$C_3^4$
147		P -3	-P 3	$\bar{P}3$	$C_{3i}^1$
148	H	R -3:H	-R 3	$\bar{R}3$	$C_{3i}^2$
149		P 3 1 2	P 3 2	<i>P312</i>	$D_3^1$
150		P 3 2 1	P 3 2''	<i>P321</i>	$D_3^2$
151		P 31 1 2	P 31 2c (0 0 1)	<i>P3<sub>1</sub>12</i>	$D_3^3$
152		P 31 2 1	P 31 2''	<i>P3<sub>1</sub>21</i>	$D_3^4$
153		P 32 1 2	P 32 2c (0 0 -1)	<i>P3<sub>2</sub>12</i>	$D_3^5$
154		P 32 2 1	P 32 2''	<i>P3<sub>2</sub>21</i>	$D_3^6$
155	H	R 32:H	R 3 2''	<i>R32</i>	$D_3^7$
156		P 3 m 1	P 3 -2''	<i>P3m1</i>	$C_{3v}^1$
157		P 3 1 m	P 3 -2	<i>P31m</i>	$C_{3v}^2$
158		P 3 c 1	P 3 -2''c	<i>P3c1</i>	$C_{3v}^3$
159		P 3 1 c	P 3 -2c	<i>P31c</i>	$C_{3v}^4$
160	H	R 3 m:H	R 3 -2''	<i>R3m</i>	$C_{3v}^5$
161	H	R 3 c:H	R 3 -2''c	<i>R3c</i>	$C_{3v}^6$
162		P -3 1 2/m	-P 3 2	$\bar{P}31m$	$D_{3d}^1$
163		P -3 1 2/c	-P 3 2c	$\bar{P}31c$	$D_{3d}^2$
164		P -3 2/m 1	-P 3 2''	$\bar{P}3m1$	$D_{3d}^3$
165		P -3 2/c 1	-P 3 2''c	$\bar{P}3c1$	$D_{3d}^4$
166	H	R -3 2/m:H	-R 3 2''	$\bar{R}3m$	$D_{3d}^5$
167	H	R -3 2/c:H	-R 3 2''c	$\bar{R}3c$	$D_{3d}^6$
168		P 6	P 6	<i>P6</i>	$C_6^1$
169		P 61	P 61	<i>P6<sub>1</sub></i>	$C_6^2$
170		P 65	P 65	<i>P6<sub>5</sub></i>	$C_6^3$
171		P 62	P 62	<i>P6<sub>2</sub></i>	$C_6^4$
172		P 64	P 64	<i>P6<sub>4</sub></i>	$C_6^5$
173		P 63	P 6c	<i>P6<sub>3</sub></i>	$C_6^6$
174		P -6	P -6	$\bar{P}6$	$C_{3h}^1$
175		P 6/m	-P 6	<i>P6/m</i>	$C_{6h}^1$
176		P 63/m	-P 6c	<i>P6<sub>3</sub>/m</i>	$C_{6h}^2$
177		P 6 2 2	P 6 2	<i>P622</i>	$D_6^1$
178		P 61 2 2	P 61 2 (0 0 -1)	<i>P6<sub>1</sub>22</i>	$D_6^2$
179		P 65 2 2	P 65 2 (0 0 1)	<i>P6<sub>5</sub>22</i>	$D_6^3$
180		P 62 2 2	P 62 2c (0 0 1)	<i>P6<sub>2</sub>22</i>	$D_6^4$
181		P 64 2 2	P 64 2c (0 0 -1)	<i>P6<sub>4</sub>22</i>	$D_6^5$
182		P 63 2 2	P 6c 2c	<i>P6<sub>3</sub>22</i>	$D_6^6$
183		P 6 m m	P 6 -2	<i>P6mm</i>	$C_{6v}^1$
184		P 6 c c	P 6 -2c	<i>P6cc</i>	$C_{6v}^2$

Table 1 (continued): **A list of the various space group notations.** The space group number, orientation, Hermann-Mauguin symbol, Hall symbol, International symbol, and Schönflies symbol are listed.

Number	Orientation	Hermann-Mauguin	Hall	International	Schönflies
185		P 63 c m	P 6c -2	$P6_3cm$	$C_{6v}^3$
186		P 63 m c	P 6c -2c	$P6_3mc$	$C_{6v}^4$
187		P -6 m 2	P -6 2	$\bar{P}6m2$	$D_{3h}^1$
188		P -6 c 2	P -6c 2	$\bar{P}6c2$	$D_{3h}^2$
189		P -6 2 m	P -6 -2	$\bar{P}6_2m$	$D_{3h}^3$
190		P -6 2 c	P -6c -2c	$\bar{P}6_2c$	$D_{3h}^4$
191		P 6/m 2/m 2/m	-P 6 2	$P6/mmm$	$D_{6h}^1$
192		P 6/m 2/c 2/c	-P 6 2c	$P6/mcc$	$D_{6h}^2$
193		P 63/m 2/c 2/m	-P 6c 2	$P6_3/mcm$	$D_{6h}^3$
194		P 63/m 2/m 2/c	-P 6c 2c	$P6_3/mmc$	$D_{6h}^4$
195		P 2 3	P 2 2 3	$P23$	$T^1$
196		F 2 3	F 2 2 3	$F23$	$T^2$
197		I 2 3	I 2 2 3	$I23$	$T^3$
198		P 21 3	P 2ac 2ab 3	$P2_13$	$T^4$
199		I 21 3	I 2b 2c 3	$I2_13$	$T^5$
200		P 2/m -3	-P 2 2 3	$Pm\bar{3}$	$T_h^1$
201	2	P 2/n -3:2	-P 2ab 2bc 3	$Pn\bar{3}$	$T_h^2$
202		F 2/m -3	-F 2 2 3	$Fm\bar{3}$	$T_h^3$
203	2	F 2/d -3:2	-F 2uv 2vw 3	$Fd\bar{3}$	$T_h^4$
204		I 2/m -3	-I 2 2 3	$Im\bar{3}$	$T_h^5$
205		P 21/a -3	-P 2ac 2ab 3	$Pa\bar{3}$	$T_h^6$
206		I 21/a -3	-I 2b 2c 3	$Ia\bar{3}$	$T_h^7$
207		P 4 3 2	P 4 2 3	$P432$	$O^1$
208		P 42 3 2	P 4n 2 3	$P4_232$	$O^2$
209		F 4 3 2	F 4 2 3	$F432$	$O^3$
210		F 41 3 2	F 4d 2 3	$F4_132$	$O^4$
211		I 4 3 2	I 4 2 3	$I432$	$O^5$
212		P 43 3 2	P 4acd 2ab 3	$P4_332$	$O^6$
213		P 41 3 2	P 4bd 2ab 3	$P4_132$	$O^7$
214		I 41 3 2	I 4bd 2c 3	$I4_132$	$O^8$
215		P -4 3 m	P -4 2 3	$\bar{P}4_3m$	$T_d^1$
216		F -4 3 m	F -4 2 3	$\bar{F}4_3m$	$T_d^2$
217		I -4 3 m	I -4 2 3	$\bar{I}4_3m$	$T_d^3$
218		P -4 3 n	P -4n 2 3	$\bar{P}4_3n$	$T_d^4$
219		F -4 3 c	F -4c 2 3	$\bar{F}4_3c$	$T_d^5$
220		I -4 3 d	I -4bd 2c 3	$\bar{I}4_3d$	$T_d^6$
221		P 4/m -3 2/m	-P 4 2 3	$Pm\bar{3}m$	$O_h^1$
222	2	P 4/n -3 2/n:2	-P 4a 2bc 3	$Pn\bar{3}n$	$O_h^2$
223		P 42/m -3 2/n	-P 4n 2 3	$Pm\bar{3}n$	$O_h^3$
224	2	P 42/n -3 2/m:2	-P 4bc 2bc 3	$Pn\bar{3}m$	$O_h^4$
225		F 4/m -3 2/m	-F 4 2 3	$Fm\bar{3}m$	$O_h^5$
226		F 4/m -3 2/c	-F 4c 2 3	$Fm\bar{3}c$	$O_h^6$
227	2	F 41/d -3 2/m:2	-F 4vw 2vw 3	$Fd\bar{3}m$	$O_h^7$
228	2	F 41/d -3 2/c:2	-F 4cvw 2vw 3	$Fd\bar{3}c$	$O_h^8$
229		I 4/m -3 2/m	-I 4 2 3	$Im\bar{3}m$	$O_h^9$
230		I 41/a -3 2/d	-I 4bd 2c 3	$Ia\bar{3}d$	$O_h^{10}$

## 7. Acknowledgments

The authors would like to thank D. A. Papaconstantopoulos, who first proposed the *Crystal Lattice Structures* database, and R. Benjamin Young, who help set up the original web site in the summer of 1995. Special thanks are due to the H. Stokes, for providing updates to the FINDSYM code, and to the librarians at the U.S. Naval Research Laboratory Ruth H. Hooker Research Library, who tracked down many dozens of research articles which are not yet available online. M. J. Mehl is supported by the Kinnear Foundation and under contract from Duke University. We also acknowledge support by the by DOD-ONR (N00014-17-1-2090, N00014-16-1-2326, N00014-15-1-2863, and N00014-16-1-2781). DH acknowledges support from the Department of Defense through the National Defense Science and Engineering Graduate (NDSEG) Fellowship Program. The AFLOW consortium would like to acknowledge the Duke University Center for Materials Genomics.



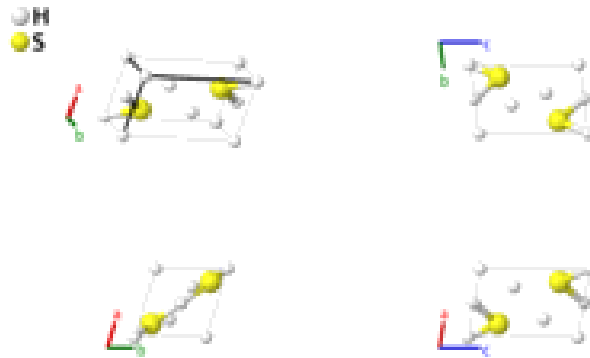
## References

- [1] E. Perim, D. Lee, Y. Liu, C. Toher, P. Gong, Y. Li, W. N. Simmons, O. Levy, J. J. Vlassak, J. Schroers, and S. Curtarolo, *Spectral descriptors for bulk metallic glasses based on the thermodynamics of competing crystalline phases*, Nat. Commun. **7**, 12315 (2016), doi:10.1038/ncomms12315.
- [2] C. M. Rost, E. Sachet, T. Borman, A. Moballeggh, E. C. Dickey, D. Hou, J. L. Jones, S. Curtarolo, and J.-P. Maria, *Entropy-stabilized oxides*, Nat. Commun. **6**, 8485 (2015), doi:10.1038/ncomms9485.
- [3] L. Yu and A. Zunger, *Identification of Potential Photovoltaic Absorbers Based on First-Principles Spectroscopic Screening of Materials*, Phys. Rev. Lett. **108**, 068701 (2012), doi:10.1103/PhysRevLett.108.068701.
- [4] G. Ceder, G. Hauthier, A. Jain, and S. P. Ong, *Recharging lithium battery research with first-principles methods*, MRS Bull. **36**, 185–191 (2011), doi:10.1557/mrs.2011.31.
- [5] S. Sanvito, C. Oses, J. Xue, A. Tiwari, M. Zic, T. Archer, P. Tozman, M. Venkatesan, J. M. D. Coey, and S. Curtarolo, *Accelerated discovery of new magnets in the Heusler alloy family*, Sci. Adv. **3**, e1602241 (2017), doi:10.1126/sciadv.1602241.
- [6] D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy, and S. Curtarolo, *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*, Acta Crystallogr. Sect. A **74**, 184–203 (2018), doi:10.1107/S2053273318003066.
- [7] C. Toher, C. Oses, J. J. Plata, D. Hicks, F. Rose, O. Levy, M. de Jong, M. D. Asta, M. Fornari, M. Buongiorno Nardelli, and S. Curtarolo, *Combining the AFLOW GIBBS and Elastic Libraries to efficiently and robustly screen thermomechanical properties of solids*, Phys. Rev. Mater. **1**, 015401 (2017), doi:10.1103/PhysRevMaterials.1.015401.
- [8] C. Toher, J. J. Plata, O. Levy, M. de Jong, M. D. Asta, M. Buongiorno Nardelli, and S. Curtarolo, *High-throughput computational screening of thermal conductivity, Debye temperature, and Grüneisen parameter using a quasiharmonic Debye model*, Phys. Rev. B **90**, 174107 (2014), doi:10.1103/PhysRevB.90.174107.
- [9] P. Nath, J. J. Plata, D. Usanmaz, R. Al Rahal Al Orabi, M. Fornari, M. Buongiorno Nardelli, C. Toher, and S. Curtarolo, *High-Throughput Prediction of Finite-Temperature Properties using the Quasi-Harmonic Approximation*, Comput. Mater. Sci. **125**, 82–91 (2016), doi:10.1016/j.commatsci.2016.07.043.
- [10] P. Nath, J. J. Plata, D. Usanmaz, C. Toher, M. Fornari, M. Buongiorno Nardelli, and S. Curtarolo, *High throughput combinatorial method for fast and robust prediction of lattice thermal conductivity*, Scr. Mater. **129**, 88–93 (2017), doi:10.1016/j.scriptamat.2016.09.034.
- [11] J. J. Plata, P. Nath, D. Usanmaz, J. Carrete, C. Toher, M. de Jong, M. D. Asta, M. Fornari, M. Buongiorno Nardelli, and S. Curtarolo, *An efficient and accurate framework for calculating lattice thermal conductivity of solids: AFLOW-AAPL Automatic Anharmonic Phonon Library*, NPJ Comput. Mater. **3**, 45 (2017), doi:10.1038/s41524-017-0046-7.
- [12] S. Curtarolo, W. Setyawan, G. L. W. Hart, M. Jahnátek, R. V. Chepulskii, R. H. Taylor, S. Wang, J. Xue, K. Yang, O. Levy, M. J. Mehl, H. T. Stokes, D. O. Demchenko, and D. Morgan, *AFLOW: An automatic framework for high-throughput materials discovery*, Comput. Mater. Sci. **58**, 218–226 (2012), doi:10.1016/j.commatsci.2012.02.005.
- [13] K. Yang, C. Oses, and S. Curtarolo, *Modeling Off-Stoichiometry Materials with a High-Throughput Ab-Initio Approach*, Chem. Mater. **28**, 6484–6492 (2016), doi:10.1021/acs.chemmater.6b01449.
- [14] W. Setyawan and S. Curtarolo, *High-throughput electronic band structure calculations: Challenges and tools*, Comput. Mater. Sci. **49**, 299–312 (2010), doi:10.1016/j.commatsci.2010.05.010.
- [15] O. Levy, G. L. W. Hart, and S. Curtarolo, *Structure maps for hcp metals from first-principles calculations*, Phys. Rev. B **81**, 174106 (2010), doi:10.1103/PhysRevB.81.174106.
- [16] G. L. W. Hart, S. Curtarolo, T. B. Massalski, and O. Levy, *Comprehensive Search for New Phases and Compounds in Binary Alloy Systems Based on Platinum-Group Metals, Using a Computational First-Principles Approach*, Phys. Rev. X **3**, 041035 (2013), doi:10.1103/PhysRevX.3.041035.
- [17] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part I*, Comput. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.
- [18] A. R. Supka, T. E. Lyons, L. S. I. Liyanage, P. D’Amico, R. Al Rahal Al Orabi, S. Mahatara,

- P. Gopal, C. Toher, D. Ceresoli, A. Calzolari, S. Curtarolo, M. Buongiorno Nardelli, and M. Fornari, *AFLOW $\pi$ : A minimalist approach to high-throughput ab initio calculations including the generation of tight-binding hamiltonians*, *Comput. Mater. Sci.* **136**, 76–84 (2017), doi:10.1016/j.commatsci.2017.03.055.
- [19] M. Scheffler, C. Draxl, and Computer Center of the Max-Planck Society, Garching, *The NoMaD Repository*, <http://nomad-repository.eu> (2014).
- [20] A. Jain, G. Hautier, C. J. Moore, S. P. Ong, C. C. Fischer, T. Mueller, K. A. Persson, and G. Ceder, *A high-throughput infrastructure for density functional theory calculations*, *Comput. Mater. Sci.* **50**, 2295–2310 (2011), doi:10.1016/j.commatsci.2011.02.023.
- [21] J. E. Saal, S. Kirklin, M. Aykol, B. Meredig, and C. Wolverton, *Materials Design and Discovery with High-Throughput Density Functional Theory: The Open Quantum Materials Database (OQMD)*, *JOM* **65**, 1501–1509 (2013), doi:10.1007/s11837-013-0755-4.
- [22] P. P. Ewald, K. Herrman, C. Herman, O. Lohrmann, H. Philipp, G. Gottfried, and F. Schossberger, eds., *Strukturbericht 1913-1939*, vol. I-VII (Akademische Verlagsgesellschaft M. B. H., 1931-1943).
- [23] R. W. G. Wyckoff, *The Structure of Crystals*, vol. I-VI (John Wiley & Sons, New York, London, Sydney, 1963 - 1971), 2<sup>nd</sup> edn.
- [24] W. B. Pearson, *A handbook of lattice spacings and structures of metals and alloys* (Pergamon Press, New York, 1958).
- [25] R. T. Downs and M. Hall-Wallace, *The American Mineralogist crystal structure database*, *Ann. Math.* **88**, 247–250 (2003).
- [26] G. Kresse and J. Hafner, *Ab initio molecular dynamics for liquid metals*, *Phys. Rev. B* **47**, 558–561 (1993), doi:10.1103/PhysRevB.47.558.
- [27] G. Kresse and J. Hafner, *Ab initio molecular-dynamics simulation of the liquid-metal-amorphous-semiconductor transition in germanium*, *Phys. Rev. B* **49**, 14251–14269 (1994), doi:10.1103/PhysRevB.49.14251.
- [28] G. Kresse and J. Furthmüller, *Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set*, *Comput. Mater. Sci.* **6**, 15–50 (1996), doi:10.1016/0927-0256(96)00008-0.
- [29] G. Kresse and J. Furthmüller, *Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set*, *Phys. Rev. B* **54**, 11169–11186 (1996), doi:10.1103/PhysRevB.54.11169.
- [30] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch, *QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials*, *J. Phys.: Condens. Matter* **21**, 395502 (2009).
- [31] V. Blum, R. Gehrke, F. Hanke, P. Havu, V. Havu, X. Ren, K. Reuter, and M. Scheffler, *Ab initio molecular simulations with numeric atom-centered orbitals*, *Comput. Phys. Commun.* **180**, 2175–2196 (2009).
- [32] X. Gonze, J. M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G. M. Rignanes, L. Sindic, M. Verstraete, G. Zerah, F. Jollet, M. Torrent, A. Roy, M. Mikami, P. Ghosez, J. Y. Raty, and D. C. Allan, *First-principles computation of material properties: the ABINIT software project*, *Comput. Mater. Sci.* **25**, 478–492 (2002), doi:10.1016/S0927-0256(02)00325-7.
- [33] M. I. Aroyo, J. M. Perez-Mato, D. Orobengoa, E. Tasci, G. de la Flor, and A. Kirov, *Crystallography online: Bilbao crystallographic server*, *Bulg. Chem. Commun.* **43**, 183–197 (2011).
- [34] *Jmol: an open-source Java viewer for chemical structures in 3D*, <http://www.jmol.org/>.
- [35] *Online Dictionary of Crystallography*. Maintained by the Commission for Crystallographic Nomenclature of the International Union of Crystallography.
- [36] T. Han, ed., *International Tables for Crystallography* (International Union of Crystallography, 2006), vol. A: Space-group symmetry, chap. 3.1.5, doi:10.1107/97809553602060000100.
- [37] D. Sedbrook, *Must the Molecules of Life Always be Left-Handed or Right-Handed?* Published online July 28, 2016.
- [38] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders College Publishing, Orlando, Florida, 1976), chap. 4, pp. 73–75.
- [39] *JSmol*, <https://sourceforge.net/projects/jsmol/>.
- [40] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders College Publishing, Orlando, Florida, 1976), chap. 5.
- [41] E. A. Abbott, *Flatland: A Romance of Many Dimensions* (Project Gutenberg, 1994).

- [42] M. J. Allen, V. C. Tung, and R. B. Kaner, *Honeycomb Carbon: A Review of Graphene*, *Chem. Rev.* **110**, 132–145 (2010), doi:10.1021/cr900070d.
- [43] X. Li and H. Zhu, *Two-dimensional MoS<sub>2</sub>: Properties, preparation, and applications*, *J. Materiomics* **1**, 33–44 (2015), doi:10.1016/j.jmat.2015.03.003.
- [44] D. E. Joyce, *Wallpaper Groups* (1997). (Plane Symmetry Groups).
- [45] P. J. Morandi, *The Classification of Wallpaper Patterns: From Group Cohomology to Escher's Tessellations* (2003). Department of Mathematical Sciences, New Mexico State University, Las Cruces, New Mexico.
- [46] D. Eck, *Wallpaper Symmetry*. Dynamic illustration of symmetries allowed in wallpaper groups.
- [47] T. Hahn, ed., *International Tables of Crystallography. Volume A: Space-group symmetry* (Kluwer Academic publishers, International Union of Crystallography, Chester, England, 2002).
- [48] S. R. Hall and B. McMahon, eds., *International Tables for Crystallography*, vol. G: Definition and exchange of crystallographic data (International Union of Crystallography, Chester, UK, 2006), doi:10.1107/97809553602060000107.
- [49] C. Hermann, XVI. *Zur systematischen Strukturtheorie. I. Eine neue Raumgruppensymbolik*, *Z. Kristallogr.* **68**, 257–287 (1928), doi:10.1524/zkri.1928.68.1.257.
- [50] C. Mauguin, *Sur le symbolisme des groupes de répétition on de symétrie des assemblages cristallins*, *Z. Kristallogr.* **76**, 542–558 (1931), doi:10.1524/zkri.1931.76.1.542.
- [51] S. R. Hall, *Space-group notation with an explicit origin*, *Acta Crystallogr. Sect. A* **37**, 517–525 (1981), doi:10.1107/S0567739481001228.
- [52] C. P. Brock, ed., *International Tables for Crystallography* (International Union of Crystallography, 2016), doi:10.1107/97809553602060000001.
- [53] A. Schönflies, *Krystallsysteme und Krystalstruktur* (B. G. Teabuer, Leipzig, 1891).
- [54] A. Schönflies, *Theorie der Krystalstruktur* (G. Borntraeger, Berlin, 1923).
- [55] S. R. Hall and R. W. Grosse-Kunstleve, *Concise Space-Group Symbols* (2015).

# H<sub>2</sub>S (90 GPa) Structure: A2B\_aP6\_2\_aei\_i

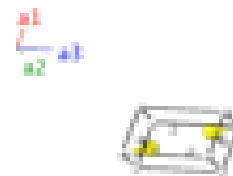


<b>Prototype</b>	:	H <sub>2</sub> S
<b>AFLOW prototype label</b>	:	A2B_aP6_2_aei_i
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	aP6
<b>Space group number</b>	:	2
<b>Space group symbol</b>	:	$P\bar{1}$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_aP6_2_aei_i --params=a, b/a, c/a, $\alpha$ , $\beta$ , $\gamma$ , $x_3$ , $y_3$ , $z_3$ , $x_4$ , $y_4$ , $z_4$

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H<sub>2</sub>S in the range 80 – 140 GPa.
- The data presented here was computed at 90 GPa.
- The original reference places H atoms on (1g), (1f) and (2i) sites, with S atoms on (2i) sites. We have changed the origin so that the H atoms are now on (1a), (1e) and (2i) sites.

## Triclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \cos \gamma \hat{\mathbf{x}} + b \sin \gamma \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c_x \hat{\mathbf{x}} + c_y \hat{\mathbf{y}} + c_z \hat{\mathbf{z}} \\ c_x &= c \cos \beta \\ c_y &= c (\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\ c_z &= \sqrt{c^2 - c_x^2 - c_y^2} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	H I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$= \frac{1}{2} (a + b \cos \gamma) \hat{\mathbf{x}} + \frac{1}{2} b \sin \gamma \hat{\mathbf{y}}$	(1e)	H II

$$\begin{aligned}
\mathbf{B}_3 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = (x_3 a + y_3 b \cos \gamma + z_3 c_x) \hat{\mathbf{x}} + (y_3 b \sin \gamma + z_3 c_y) \hat{\mathbf{y}} + z_3 c_z \hat{\mathbf{z}} & (2i) & \text{H III} \\
\mathbf{B}_4 &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = (-x_3 a - y_3 b \cos \gamma - z_3 c_x) \hat{\mathbf{x}} + (-y_3 b \sin \gamma - z_3 c_y) \hat{\mathbf{y}} - z_3 c_z \hat{\mathbf{z}} & (2i) & \text{H III} \\
\mathbf{B}_5 &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = (x_4 a + y_4 b \cos \gamma + z_4 c_x) \hat{\mathbf{x}} + (y_4 b \sin \gamma + z_4 c_y) \hat{\mathbf{y}} + z_4 c_z \hat{\mathbf{z}} & (2i) & \text{S} \\
\mathbf{B}_6 &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = (-x_4 a - y_4 b \cos \gamma - z_4 c_x) \hat{\mathbf{x}} + (-y_4 b \sin \gamma - z_4 c_y) \hat{\mathbf{y}} - z_4 c_z \hat{\mathbf{z}} & (2i) & \text{S}
\end{aligned}$$

---

**References:**

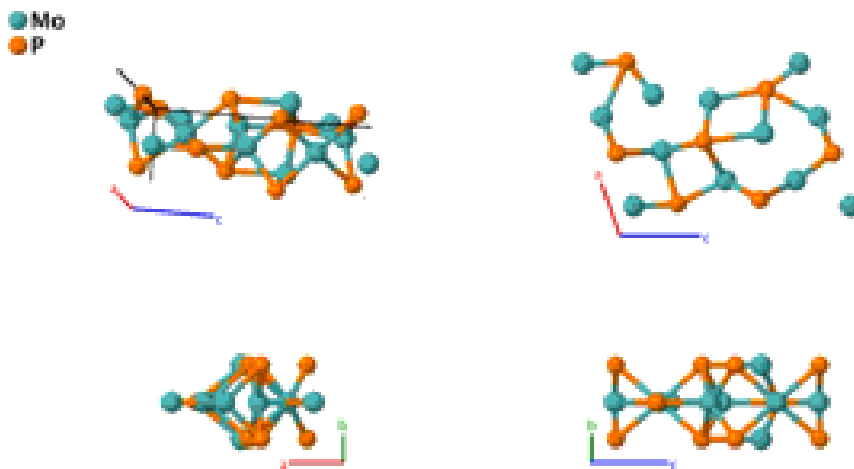
- Y. Li, J. Hao, H. Liu, Y. Li, and Y. Ma, *The metallization and superconductivity of dense hydrogen sulfide*, J. Chem. Phys. **140**, 174712 (2014), [doi:10.1063/1.4874158](https://doi.org/10.1063/1.4874158).

---

**Geometry files:**

- CIF: pp. [802](#)  
- POSCAR: pp. [802](#)

# Mo<sub>8</sub>P<sub>5</sub> (High-temperature) Structure: A8B5\_mP13\_6\_a7b\_3a2b

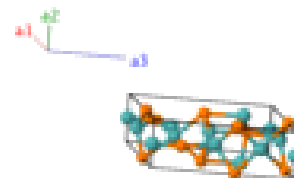


<b>Prototype</b>	:	Mo <sub>8</sub> P <sub>5</sub>
<b>AFLOW prototype label</b>	:	A8B5_mP13_6_a7b_3a2b
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mP13
<b>Space group number</b>	:	6
<b>Space group symbol</b>	:	<i>Pm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A8B5_mP13_6_a7b_3a2b --params= <i>a, b/a, c/a, β, x<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>, z<sub>9</sub>, x<sub>10</sub>, z<sub>10</sub>, x<sub>11</sub>, z<sub>11</sub>, x<sub>12</sub>, z<sub>12</sub>, x<sub>13</sub>, z<sub>13</sub></i>

- This high-temperature phase of the Mo-P system is observed between 1580°C – 1680°C (Johnsson, 1972).

## Simple Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $x_1 \mathbf{a}_1 + z_1 \mathbf{a}_3$	= $(x_1 a + z_1 c \cos \beta) \hat{\mathbf{x}} + z_1 c \sin \beta \hat{\mathbf{z}}$	(1 <i>a</i> )	Mo I
<b>B<sub>2</sub></b>	= $x_2 \mathbf{a}_1 + z_2 \mathbf{a}_3$	= $(x_2 a + z_2 c \cos \beta) \hat{\mathbf{x}} + z_2 c \sin \beta \hat{\mathbf{z}}$	(1 <i>a</i> )	P I
<b>B<sub>3</sub></b>	= $x_3 \mathbf{a}_1 + z_3 \mathbf{a}_3$	= $(x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + z_3 c \sin \beta \hat{\mathbf{z}}$	(1 <i>a</i> )	P II
<b>B<sub>4</sub></b>	= $x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3$	= $(x_4 a + z_4 c \cos \beta) \hat{\mathbf{x}} + z_4 c \sin \beta \hat{\mathbf{z}}$	(1 <i>a</i> )	P III

$$\begin{array}{llllll}
\mathbf{B}_5 & = & x_5 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_5 \mathbf{a}_3 & = & (x_5 a + z_5 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_5 c \sin \beta \hat{\mathbf{z}} & (1b) & \text{Mo II} \\
\mathbf{B}_6 & = & x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_6 \mathbf{a}_3 & = & (x_6 a + z_6 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_6 c \sin \beta \hat{\mathbf{z}} & (1b) & \text{Mo III} \\
\mathbf{B}_7 & = & x_7 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_7 \mathbf{a}_3 & = & (x_7 a + z_7 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_7 c \sin \beta \hat{\mathbf{z}} & (1b) & \text{Mo IV} \\
\mathbf{B}_8 & = & x_8 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_8 \mathbf{a}_3 & = & (x_8 a + z_8 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_8 c \sin \beta \hat{\mathbf{z}} & (1b) & \text{Mo V} \\
\mathbf{B}_9 & = & x_9 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_9 \mathbf{a}_3 & = & (x_9 a + z_9 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_9 c \sin \beta \hat{\mathbf{z}} & (1b) & \text{Mo VI} \\
\mathbf{B}_{10} & = & x_{10} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{10} \mathbf{a}_3 & = & (x_{10} a + z_{10} c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_{10} c \sin \beta \hat{\mathbf{z}} & (1b) & \text{Mo VII} \\
\mathbf{B}_{11} & = & x_{11} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{11} \mathbf{a}_3 & = & (x_{11} a + z_{11} c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_{11} c \sin \beta \hat{\mathbf{z}} & (1b) & \text{Mo VIII} \\
\mathbf{B}_{12} & = & x_{12} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{12} \mathbf{a}_3 & = & (x_{12} a + z_{12} c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_{12} c \sin \beta \hat{\mathbf{z}} & (1b) & \text{P IV} \\
\mathbf{B}_{13} & = & x_{13} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_{13} \mathbf{a}_3 & = & (x_{13} a + z_{13} c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_{13} c \sin \beta \hat{\mathbf{z}} & (1b) & \text{P V}
\end{array}$$

---

**References:**

- T. Johansson, *The crystal structure of Mo<sub>8</sub>P<sub>5</sub> from twin-crystal data*, Acta Chem. Scand. **26**, 365–382 (1972), [doi:10.3891/acta.chem.scand.26-0365](https://doi.org/10.3891/acta.chem.scand.26-0365).

**Found in:**

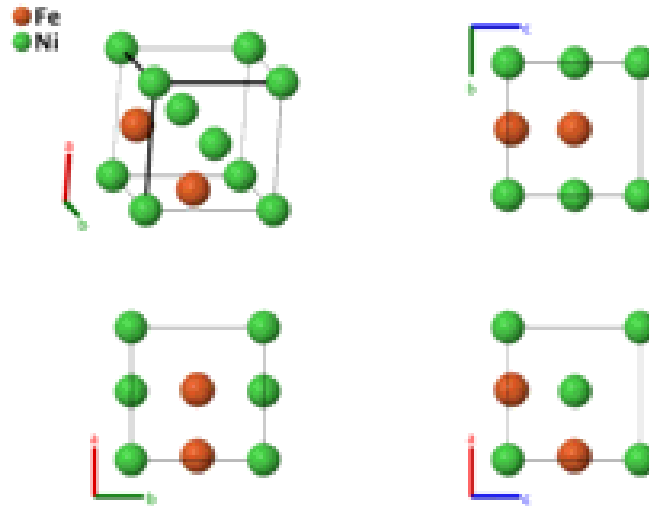
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [802](#)  
- POSCAR: pp. [802](#)

# FeNi Structure: AB\_mP4\_6\_2b\_2a

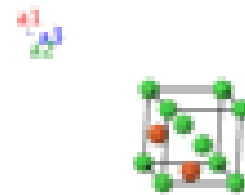


<b>Prototype</b>	:	FeNi
<b>AFLOW prototype label</b>	:	AB_mP4_6_2b_2a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mP4
<b>Space group number</b>	:	6
<b>Space group symbol</b>	:	<i>Pm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB_mP4_6_2b_2a --params= <i>a, b/a, c/a, β, x<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub></i>

- In the original the site occupations are mixed with Ni majority (0.85) on sites 1a and Fe majority on 1b.

## Simple Monoclinic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \cos\beta \hat{\mathbf{x}} + c \sin\beta \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + z_1 \mathbf{a}_3$	$(x_1 a + z_1 c \cos\beta) \hat{\mathbf{x}} + z_1 c \sin\beta \hat{\mathbf{z}}$	(1a)	Ni I
$\mathbf{B}_2$	$x_2 \mathbf{a}_1 + z_2 \mathbf{a}_3$	$(x_2 a + z_2 c \cos\beta) \hat{\mathbf{x}} + z_2 c \sin\beta \hat{\mathbf{z}}$	(1a)	Ni II
$\mathbf{B}_3$	$x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$(x_3 a + z_3 c \cos\beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_3 c \sin\beta \hat{\mathbf{z}}$	(1b)	Fe I
$\mathbf{B}_4$	$x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$(x_4 a + z_4 c \cos\beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_4 c \sin\beta \hat{\mathbf{z}}$	(1b)	Fe II



---

**References:**

- T. Tagai, H. Takeda, and T. Fukuda, *Superstructure of tetrataenite from the Saint Severin meteorite*, *Zeitschrift für Kristallographie - Crystalline Materials* **210**, 14–18 (1995), doi:[10.1524/zkri.1995.210.1.14](https://doi.org/10.1524/zkri.1995.210.1.14).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

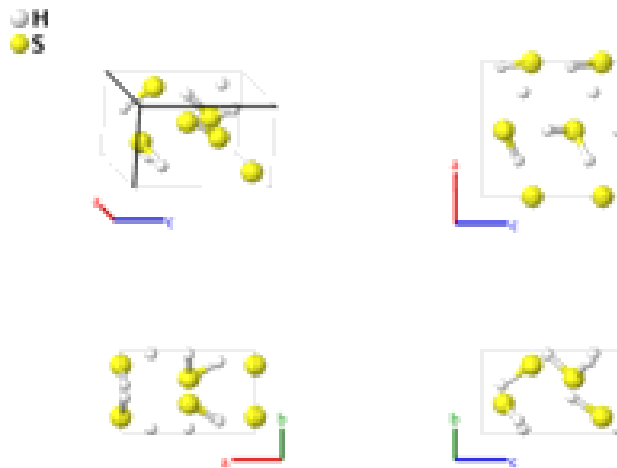
---

**Geometry files:**

- CIF: pp. [802](#)

- POSCAR: pp. [803](#)

# H<sub>2</sub>S IV Structure: A2B\_mP12\_7\_4a\_2a

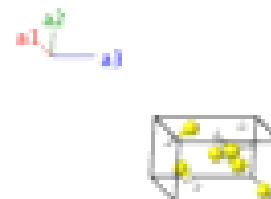


<b>Prototype</b>	:	H <sub>2</sub> S
<b>AFLOW prototype label</b>	:	A2B_mP12_7_4a_2a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mP12
<b>Space group number</b>	:	7
<b>Space group symbol</b>	:	<i>Pc</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_mP12_7_4a_2a --params= <i>a, b/a, c/a, β, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub></i>

- The H<sub>2</sub>S-IV phase is stable at pressures greater than 5 GPa and temperatures below 150 K, and is stable at higher pressures for higher temperatures. Shimizu *et al.* (Shimizu, 1995) determined the phase diagram. Endo *et al.* (Endo, 1998) found the crystal structure at 11.4 GPa, but could not determine the positions of the hydrogen atoms. Here we use the predicted structure from Li *et al.* at 30 GPa.

## Simple Monoclinic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$(x_1 a + z_1 c \cos \beta) \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \sin \beta \hat{\mathbf{z}}$	(2a)	H I
<b>B<sub>2</sub></b>	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\left(\frac{1}{2} c \cos \beta + x_1 a + z_1 c \cos \beta\right) \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \sin \beta \hat{\mathbf{z}}$	(2a)	H I

$$\begin{aligned}
\mathbf{B}_3 &= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 = (x_2 a + z_2 c \cos \beta) \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{H II} \\
\mathbf{B}_4 &= x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_2 a + z_2 c \cos \beta\right) \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{H II} \\
\mathbf{B}_5 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = (x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{H III} \\
\mathbf{B}_6 &= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_3 a + z_3 c \cos \beta\right) \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{H III} \\
\mathbf{B}_7 &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = (x_4 a + z_4 c \cos \beta) \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{H IV} \\
\mathbf{B}_8 &= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_4 a + z_4 c \cos \beta\right) \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{H IV} \\
\mathbf{B}_9 &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = (x_5 a + z_5 c \cos \beta) \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{S I} \\
\mathbf{B}_{10} &= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_5 a + z_5 c \cos \beta\right) \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{S I} \\
\mathbf{B}_{11} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = (x_6 a + z_6 c \cos \beta) \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{S II} \\
\mathbf{B}_{12} &= x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_6 a + z_6 c \cos \beta\right) \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{S II}
\end{aligned}$$

---

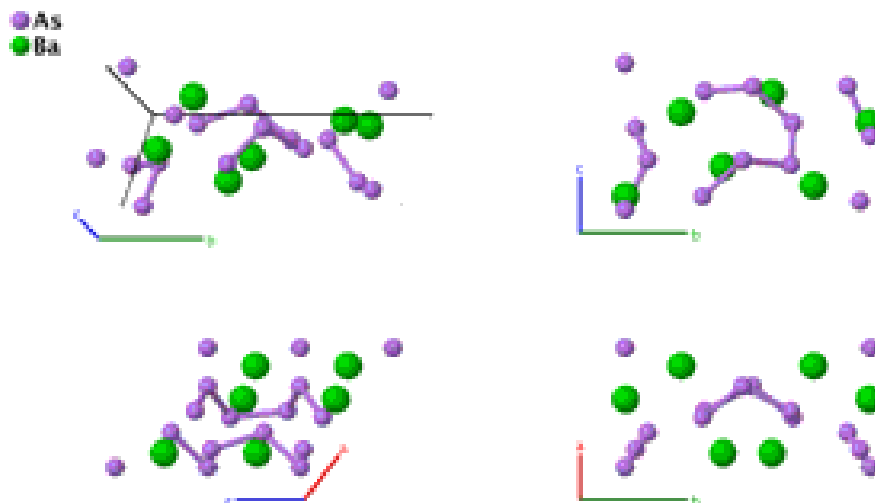
#### References:

- Y. Li, J. Hao, H. Liu, Y. Li, and Y. Ma, *The metallization and superconductivity of dense hydrogen sulfide*, J. Chem. Phys. **140**, 174712 (2014), doi:10.1063/1.4874158.
  - H. Shimizu, H. Yamaguchi, S. Sasaki, A. Honda, S. Endo, and M. Kobayashi, *Pressure-temperature phase diagram of solid hydrogen sulfide determined by Raman spectroscopy*, Phys. Rev. B **51**, 9391–9394 (1995), doi:10.1103/PhysRevB.51.9391.
  - S. Endo, A. Honda, K. Koto, O. Shimomura, T. Kikegawa, and N. Hamaya, *Crystal structure of high-pressure phase-IV solid hydrogen sulfide*, Phys. Rev. B **57**, 5699–5703 (1998), doi:10.1103/PhysRevB.57.5699.
- 

#### Geometry files:

- CIF: pp. 803
- POSCAR: pp. 803

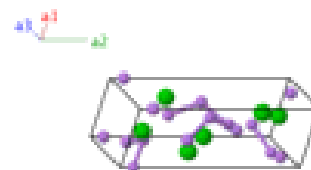
# As<sub>2</sub>Ba Structure: A2B\_mP18\_7\_6a\_3a



<b>Prototype</b>	:	As <sub>2</sub> Ba
<b>AFLOW prototype label</b>	:	A2B_mP18_7_6a_3a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mP18
<b>Space group number</b>	:	7
<b>Space group symbol</b>	:	<i>Pc</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_mP18_7_6a_3a --params= <i>a, b/a, c/a, β, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>, y<sub>9</sub>, z<sub>9</sub></i>

## Simple Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos\beta \hat{\mathbf{x}} + c \sin\beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$(x_1 a + z_1 c \cos\beta) \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \sin\beta \hat{\mathbf{z}}$	(2 <i>a</i> )	As I
<b>B<sub>2</sub></b>	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\left(\frac{1}{2} c \cos\beta + x_1 a + z_1 c \cos\beta\right) \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \sin\beta \hat{\mathbf{z}}$	(2 <i>a</i> )	As I
<b>B<sub>3</sub></b>	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$(x_2 a + z_2 c \cos\beta) \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \sin\beta \hat{\mathbf{z}}$	(2 <i>a</i> )	As II
<b>B<sub>4</sub></b>	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$\left(\frac{1}{2} c \cos\beta + x_2 a + z_2 c \cos\beta\right) \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \sin\beta \hat{\mathbf{z}}$	(2 <i>a</i> )	As II
<b>B<sub>5</sub></b>	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$(x_3 a + z_3 c \cos\beta) \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \sin\beta \hat{\mathbf{z}}$	(2 <i>a</i> )	As III

$$\begin{aligned}
\mathbf{B}_6 &= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_3a + z_3c \cos \beta\right) \hat{\mathbf{x}} - y_3b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right)c \sin \beta \hat{\mathbf{z}} & (2a) & \text{As III} \\
\mathbf{B}_7 &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = (x_4a + z_4c \cos \beta) \hat{\mathbf{x}} + y_4b \hat{\mathbf{y}} + z_4c \sin \beta \hat{\mathbf{z}} & (2a) & \text{As IV} \\
\mathbf{B}_8 &= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_4a + z_4c \cos \beta\right) \hat{\mathbf{x}} - y_4b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right)c \sin \beta \hat{\mathbf{z}} & (2a) & \text{As IV} \\
\mathbf{B}_9 &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = (x_5a + z_5c \cos \beta) \hat{\mathbf{x}} + y_5b \hat{\mathbf{y}} + z_5c \sin \beta \hat{\mathbf{z}} & (2a) & \text{As V} \\
\mathbf{B}_{10} &= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_5a + z_5c \cos \beta\right) \hat{\mathbf{x}} - y_5b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right)c \sin \beta \hat{\mathbf{z}} & (2a) & \text{As V} \\
\mathbf{B}_{11} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = (x_6a + z_6c \cos \beta) \hat{\mathbf{x}} + y_6b \hat{\mathbf{y}} + z_6c \sin \beta \hat{\mathbf{z}} & (2a) & \text{As VI} \\
\mathbf{B}_{12} &= x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_6a + z_6c \cos \beta\right) \hat{\mathbf{x}} - y_6b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right)c \sin \beta \hat{\mathbf{z}} & (2a) & \text{As VI} \\
\mathbf{B}_{13} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = (x_7a + z_7c \cos \beta) \hat{\mathbf{x}} + y_7b \hat{\mathbf{y}} + z_7c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ba I} \\
\mathbf{B}_{14} &= x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_7a + z_7c \cos \beta\right) \hat{\mathbf{x}} - y_7b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right)c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ba I} \\
\mathbf{B}_{15} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = (x_8a + z_8c \cos \beta) \hat{\mathbf{x}} + y_8b \hat{\mathbf{y}} + z_8c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ba II} \\
\mathbf{B}_{16} &= x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_8a + z_8c \cos \beta\right) \hat{\mathbf{x}} - y_8b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right)c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ba II} \\
\mathbf{B}_{17} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = (x_9a + z_9c \cos \beta) \hat{\mathbf{x}} + y_9b \hat{\mathbf{y}} + z_9c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ba III} \\
\mathbf{B}_{18} &= x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_9a + z_9c \cos \beta\right) \hat{\mathbf{x}} - y_9b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right)c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ba III}
\end{aligned}$$

---

#### References:

- F. Emmerling, D. Petri, and C. Röhr, *Neue Arsenide mit As<sup>-</sup>-Ketten und -Ringen: BaAs<sub>2</sub> und A<sup>I</sup>Ba<sub>2</sub>As<sub>5</sub> (A<sup>I</sup> = K, Rb)*, *Z. Anorg. Allg. Chem.* **630**, 2490–2501 (2004), doi:10.1002/zaac.200400257.

#### Found in:

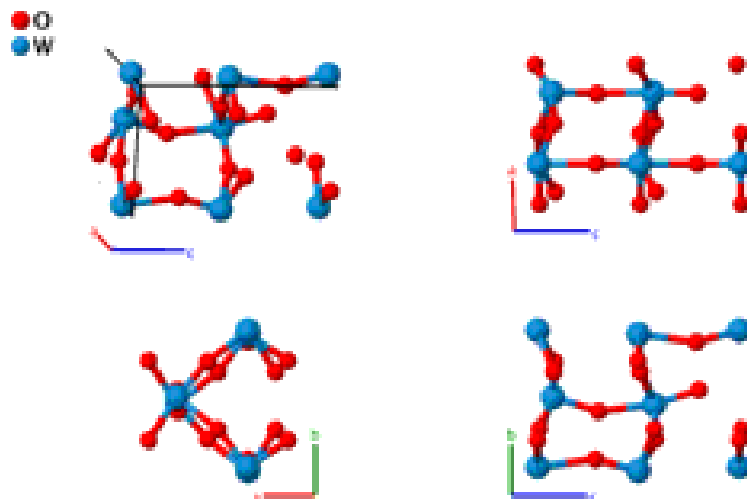
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 803  
- POSCAR: pp. 804

# $\epsilon$ -WO<sub>3</sub> (Low-temperature) Structure: A3B\_mP16\_7\_6a\_2a

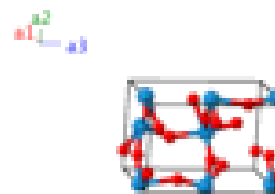


<b>Prototype</b>	:	$\epsilon$ -WO <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B_mP16_7_6a_2a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mP16
<b>Space group number</b>	:	7
<b>Space group symbol</b>	:	<i>Pc</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3B_mP16_7_6a_2a --params= <i>a, b/a, c/a, <math>\beta</math>, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub></i>

- This is a low-temperature phase of tungsten trioxide (WO<sub>3</sub>), which was observed at 15 K (Woodward, 1997).

## Simple Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$(x_1 a + z_1 c \cos \beta) \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \sin \beta \hat{\mathbf{z}}$	(2a)	O I
<b>B<sub>2</sub></b>	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\left(\frac{1}{2} c \cos \beta + x_1 a + z_1 c \cos \beta\right) \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \sin \beta \hat{\mathbf{z}}$	(2a)	O I
<b>B<sub>3</sub></b>	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$(x_2 a + z_2 c \cos \beta) \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \sin \beta \hat{\mathbf{z}}$	(2a)	O II
<b>B<sub>4</sub></b>	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$\left(\frac{1}{2} c \cos \beta + x_2 a + z_2 c \cos \beta\right) \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \sin \beta \hat{\mathbf{z}}$	(2a)	O II

$$\begin{aligned}
\mathbf{B}_5 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = (x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{O III} \\
\mathbf{B}_6 &= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_3 a + z_3 c \cos \beta\right) \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{O III} \\
\mathbf{B}_7 &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = (x_4 a + z_4 c \cos \beta) \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{O IV} \\
\mathbf{B}_8 &= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_4 a + z_4 c \cos \beta\right) \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{O IV} \\
\mathbf{B}_9 &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = (x_5 a + z_5 c \cos \beta) \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{O V} \\
\mathbf{B}_{10} &= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_5 a + z_5 c \cos \beta\right) \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{O V} \\
\mathbf{B}_{11} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = (x_6 a + z_6 c \cos \beta) \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{O VI} \\
\mathbf{B}_{12} &= x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_6 a + z_6 c \cos \beta\right) \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{O VI} \\
\mathbf{B}_{13} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = (x_7 a + z_7 c \cos \beta) \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{W I} \\
\mathbf{B}_{14} &= x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_7 a + z_7 c \cos \beta\right) \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{W I} \\
\mathbf{B}_{15} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = (x_8 a + z_8 c \cos \beta) \hat{\mathbf{x}} + y_8 b \hat{\mathbf{y}} + z_8 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{W II} \\
\mathbf{B}_{16} &= x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_8 a + z_8 c \cos \beta\right) \hat{\mathbf{x}} - y_8 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{W II}
\end{aligned}$$

---

#### References:

- P. M. Woodward, A. W. Sleight, and T. Vogt, *Ferroelectric tungsten trioxide*, J. Solid State Chem. **131**, 9–17 (1997), [doi:10.1006/jssc.1997.7268](https://doi.org/10.1006/jssc.1997.7268).

#### Found in:

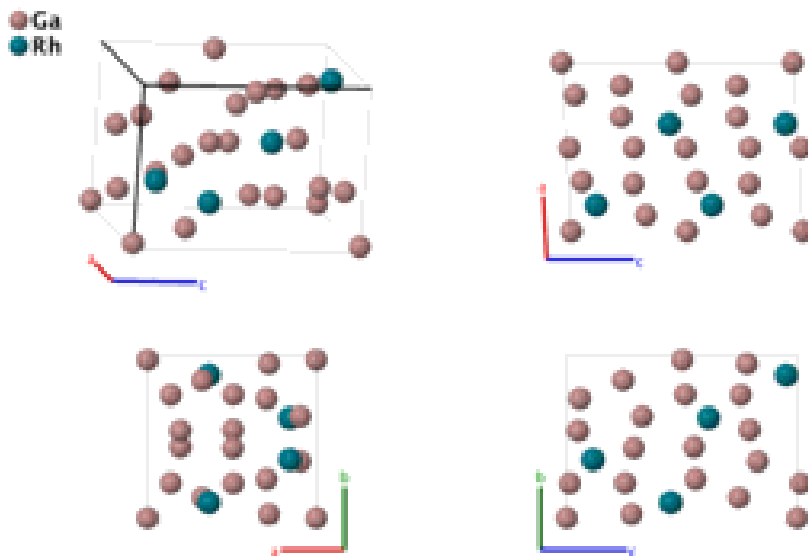
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 804  
- POSCAR: pp. 804

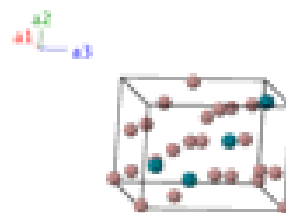
# Rh<sub>2</sub>Ga<sub>9</sub> Structure: A9B2\_mP22\_7\_9a\_2a



**Prototype** : Rh<sub>2</sub>Ga<sub>9</sub>  
**AFLOW prototype label** : A9B2\_mP22\_7\_9a\_2a  
**Strukturbericht designation** : None  
**Pearson symbol** : mP22  
**Space group number** : 7  
**Space group symbol** : *Pc*  
**AFLOW prototype command** : `aflow --proto=A9B2_mP22_7_9a_2a`  
`--params=a, b/a, c/a, β, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11`

## Simple Monoclinic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$(x_1 a + z_1 c \cos \beta) \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \sin \beta \hat{\mathbf{z}}$	(2a)	Ga I
<b>B<sub>2</sub></b>	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\left(\frac{1}{2} c \cos \beta + x_1 a + z_1 c \cos \beta\right) \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \sin \beta \hat{\mathbf{z}}$	(2a)	Ga I
<b>B<sub>3</sub></b>	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$(x_2 a + z_2 c \cos \beta) \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \sin \beta \hat{\mathbf{z}}$	(2a)	Ga II
<b>B<sub>4</sub></b>	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$\left(\frac{1}{2} c \cos \beta + x_2 a + z_2 c \cos \beta\right) \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \sin \beta \hat{\mathbf{z}}$	(2a)	Ga II



$$\begin{aligned}
\mathbf{B}_5 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = (x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga III} \\
\mathbf{B}_6 &= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_3 a + z_3 c \cos \beta\right) \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga III} \\
\mathbf{B}_7 &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = (x_4 a + z_4 c \cos \beta) \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga IV} \\
\mathbf{B}_8 &= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_4 a + z_4 c \cos \beta\right) \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga IV} \\
\mathbf{B}_9 &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = (x_5 a + z_5 c \cos \beta) \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga V} \\
\mathbf{B}_{10} &= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_5 a + z_5 c \cos \beta\right) \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga V} \\
\mathbf{B}_{11} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = (x_6 a + z_6 c \cos \beta) \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga VI} \\
\mathbf{B}_{12} &= x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_6 a + z_6 c \cos \beta\right) \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga VI} \\
\mathbf{B}_{13} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = (x_7 a + z_7 c \cos \beta) \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga VII} \\
\mathbf{B}_{14} &= x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_7 a + z_7 c \cos \beta\right) \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga VII} \\
\mathbf{B}_{15} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = (x_8 a + z_8 c \cos \beta) \hat{\mathbf{x}} + y_8 b \hat{\mathbf{y}} + z_8 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga VIII} \\
\mathbf{B}_{16} &= x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_8 a + z_8 c \cos \beta\right) \hat{\mathbf{x}} - y_8 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga VIII} \\
\mathbf{B}_{17} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = (x_9 a + z_9 c \cos \beta) \hat{\mathbf{x}} + y_9 b \hat{\mathbf{y}} + z_9 c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga IX} \\
\mathbf{B}_{18} &= x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_9 a + z_9 c \cos \beta\right) \hat{\mathbf{x}} - y_9 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Ga IX} \\
\mathbf{B}_{19} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = (x_{10} a + z_{10} c \cos \beta) \hat{\mathbf{x}} + y_{10} b \hat{\mathbf{y}} + z_{10} c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Rh I} \\
\mathbf{B}_{20} &= x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_{10} a + z_{10} c \cos \beta\right) \hat{\mathbf{x}} - y_{10} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Rh I} \\
\mathbf{B}_{21} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = (x_{11} a + z_{11} c \cos \beta) \hat{\mathbf{x}} + y_{11} b \hat{\mathbf{y}} + z_{11} c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Rh II} \\
\mathbf{B}_{22} &= x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + \left(\frac{1}{2} + z_{11}\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_{11} a + z_{11} c \cos \beta\right) \hat{\mathbf{x}} - y_{11} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{11}\right) c \sin \beta \hat{\mathbf{z}} & (2a) & \text{Rh II}
\end{aligned}$$

---

### References:

- M. Boström, H. Rosner, Y. Prots, U. Burkhardt, and Y. Grin, *The Co<sub>2</sub>Al<sub>9</sub> structure type revisited*, *Z. Anorg. Allg. Chem.* **631**, 534–541 (2005), [doi:10.1002/zaac.200400418](https://doi.org/10.1002/zaac.200400418).

### Found in:

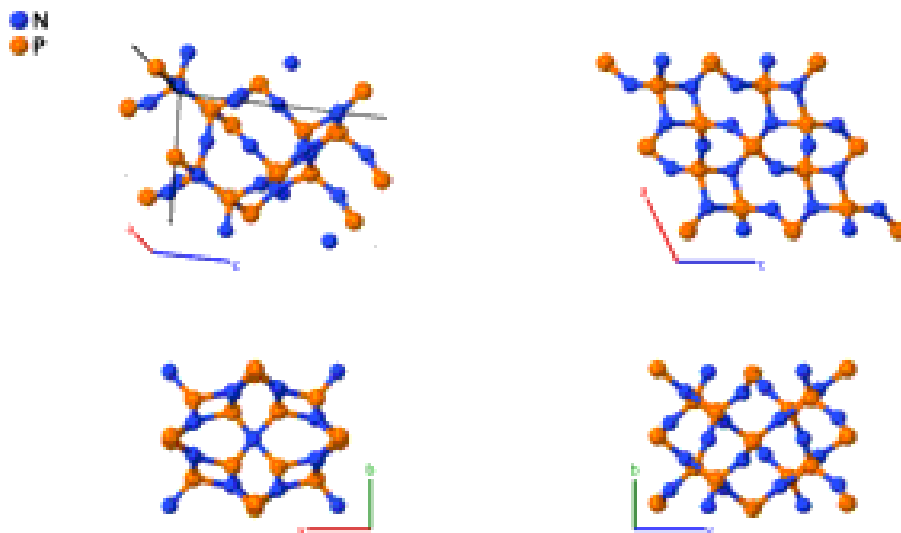
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. [804](#)  
- POSCAR: pp. [805](#)

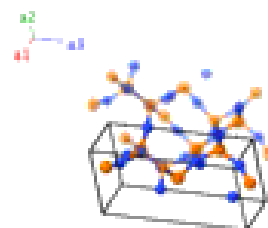
# $\alpha$ -P<sub>3</sub>N<sub>5</sub> Structure: A5B3\_mC32\_9\_5a\_3a



<b>Prototype</b>	:	$\alpha$ -P <sub>3</sub> N <sub>5</sub>
<b>AFLOW prototype label</b>	:	A5B3_mC32_9_5a_3a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mC32
<b>Space group number</b>	:	9
<b>Space group symbol</b>	:	<i>Cc</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A5B3_mC32_9_5a_3a</code> <code>--params=a, b/a, c/a, <math>\beta</math>, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub></code>

## Base-centered Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$(x_1 - y_1) \mathbf{a}_1 + (x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$(x_1 a + z_1 c \cos \beta) \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \sin \beta \hat{\mathbf{z}}$	(4a)	N I
$\mathbf{B}_2$	$(x_1 + y_1) \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\left(\frac{1}{2} c \cos \beta + x_1 a + z_1 c \cos \beta\right) \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \sin \beta \hat{\mathbf{z}}$	(4a)	N I
$\mathbf{B}_3$	$(x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$(x_2 a + z_2 c \cos \beta) \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \sin \beta \hat{\mathbf{z}}$	(4a)	N II
$\mathbf{B}_4$	$(x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$\left(\frac{1}{2} c \cos \beta + x_2 a + z_2 c \cos \beta\right) \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \sin \beta \hat{\mathbf{z}}$	(4a)	N II

$$\begin{aligned}
\mathbf{B}_5 &= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3 = (x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \sin \beta \hat{\mathbf{z}} & (4a) & \text{N III} \\
\mathbf{B}_6 &= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_3 a + z_3 c \cos \beta\right) \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \sin \beta \hat{\mathbf{z}} & (4a) & \text{N III} \\
\mathbf{B}_7 &= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 = (x_4 a + z_4 c \cos \beta) \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \sin \beta \hat{\mathbf{z}} & (4a) & \text{N IV} \\
\mathbf{B}_8 &= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_4 a + z_4 c \cos \beta\right) \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \sin \beta \hat{\mathbf{z}} & (4a) & \text{N IV} \\
\mathbf{B}_9 &= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 = (x_5 a + z_5 c \cos \beta) \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \sin \beta \hat{\mathbf{z}} & (4a) & \text{N V} \\
\mathbf{B}_{10} &= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_5 a + z_5 c \cos \beta\right) \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \sin \beta \hat{\mathbf{z}} & (4a) & \text{N V} \\
\mathbf{B}_{11} &= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3 = (x_6 a + z_6 c \cos \beta) \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \sin \beta \hat{\mathbf{z}} & (4a) & \text{P I} \\
\mathbf{B}_{12} &= (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_6 a + z_6 c \cos \beta\right) \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \sin \beta \hat{\mathbf{z}} & (4a) & \text{P I} \\
\mathbf{B}_{13} &= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3 = (x_7 a + z_7 c \cos \beta) \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \sin \beta \hat{\mathbf{z}} & (4a) & \text{P II} \\
\mathbf{B}_{14} &= (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_7 a + z_7 c \cos \beta\right) \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \sin \beta \hat{\mathbf{z}} & (4a) & \text{P II} \\
\mathbf{B}_{15} &= (x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3 = (x_8 a + z_8 c \cos \beta) \hat{\mathbf{x}} + y_8 b \hat{\mathbf{y}} + z_8 c \sin \beta \hat{\mathbf{z}} & (4a) & \text{P III} \\
\mathbf{B}_{16} &= (x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_8 a + z_8 c \cos \beta\right) \hat{\mathbf{x}} - y_8 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \sin \beta \hat{\mathbf{z}} & (4a) & \text{P III}
\end{aligned}$$

---

### References:

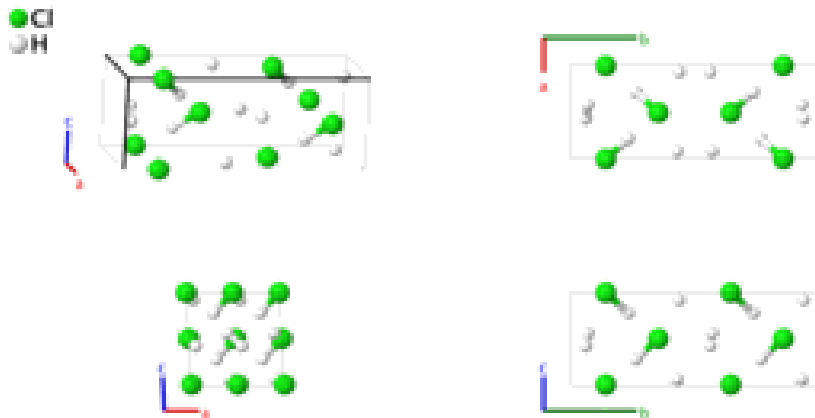
- S. Horstmann, E. Irran, and W. Schnick, *Synthesis and Crystal Structure of Phosphorus(V) Nitride  $\alpha$ -P<sub>3</sub>N<sub>5</sub>*, *Angew. Chem. Int. Ed.* **36**, 1873–1875 (1997), [doi:10.1002/anie.199718731](https://doi.org/10.1002/anie.199718731).

---

### Geometry files:

- CIF: pp. 805  
- POSCAR: pp. 805

# H<sub>3</sub>Cl (20 GPa) Structure: AB3\_mC16\_9\_a\_3a

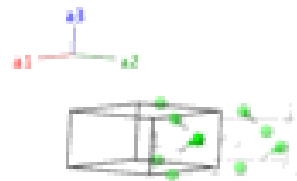


<b>Prototype</b>	:	H <sub>3</sub> Cl
<b>AFLOW prototype label</b>	:	AB3_mC16_9_a_3a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mC16
<b>Space group number</b>	:	9
<b>Space group symbol</b>	:	<i>Cc</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB3_mC16_9_a_3a --params= <i>a, b/a, c/a, β, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub></i>

- This structure was found via first-principles calculations. The data presented here was computed at a pressure of 20 GPa.

## Base-centered Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$(x_1 - y_1) \mathbf{a}_1 + (x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$(x_1 a + z_1 c \cos \beta) \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \sin \beta \hat{\mathbf{z}}$	(4a)	Cl
<b>B<sub>2</sub></b>	$(x_1 + y_1) \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\left(\frac{1}{2} c \cos \beta + x_1 a + z_1 c \cos \beta\right) \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \sin \beta \hat{\mathbf{z}}$	(4a)	Cl
<b>B<sub>3</sub></b>	$(x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$(x_2 a + z_2 c \cos \beta) \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \sin \beta \hat{\mathbf{z}}$	(4a)	H I
<b>B<sub>4</sub></b>	$(x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$\left(\frac{1}{2} c \cos \beta + x_2 a + z_2 c \cos \beta\right) \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \sin \beta \hat{\mathbf{z}}$	(4a)	H I
<b>B<sub>5</sub></b>	$(x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$(x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \sin \beta \hat{\mathbf{z}}$	(4a)	H II

$$\mathbf{B}_6 = \begin{matrix} (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \\ \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 \end{matrix} = \begin{matrix} \left(\frac{1}{2}c \cos\beta + x_3a + z_3c \cos\beta\right) \hat{\mathbf{x}} - \\ y_3b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right)c \sin\beta \hat{\mathbf{z}} \end{matrix} \quad (4a) \quad \text{H II}$$

$$\mathbf{B}_7 = (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 = \begin{matrix} (x_4a + z_4c \cos\beta) \hat{\mathbf{x}} + y_4b \hat{\mathbf{y}} + \\ z_4c \sin\beta \hat{\mathbf{z}} \end{matrix} \quad (4a) \quad \text{H III}$$

$$\mathbf{B}_8 = \begin{matrix} (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \\ \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 \end{matrix} = \begin{matrix} \left(\frac{1}{2}c \cos\beta + x_4a + z_4c \cos\beta\right) \hat{\mathbf{x}} - \\ y_4b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right)c \sin\beta \hat{\mathbf{z}} \end{matrix} \quad (4a) \quad \text{H III}$$

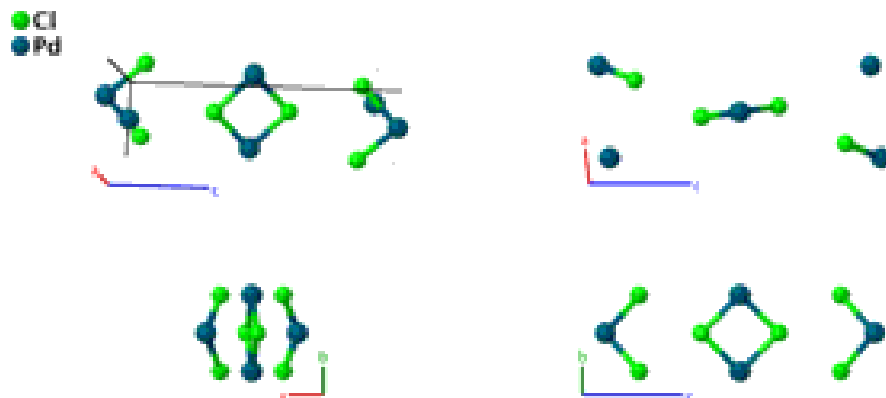
### References:

- D. Duan, X. Huang, F. Tian, Y. Liu, D. Li, H. Yu, B. Liu, W. Tian, and T. Cui, *Predicted Formation of  $H_3^+$  in Solid Halogen Polyhydrides at High Pressures*, J. Phys. Chem. A **119**, 11059–11065 (2015), [doi:10.1021/acs.jpca.5b08183](https://doi.org/10.1021/acs.jpca.5b08183).

### Geometry files:

- CIF: pp. [806](#)
- POSCAR: pp. [806](#)

# $\delta$ -PdCl<sub>2</sub> Structure: A2B\_mP6\_10\_mn\_bg

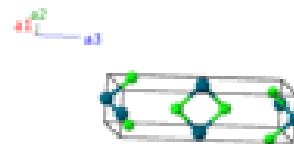


<b>Prototype</b>	:	$\delta$ -PdCl <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_mP6_10_mn_bg
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mP6
<b>Space group number</b>	:	10
<b>Space group symbol</b>	:	$P2/m$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A2B_mP6_10_mn_bg</code> <code>--params=a, b/a, c/a, <math>\beta</math>, <math>x_3</math>, <math>z_3</math>, <math>x_4</math>, <math>z_4</math></code>

- (Evers, 2010) use the unique-axis  $c$  setting of space group  $P2/m$ . We have switched this to our standard unique-axis  $b$  setting. The data was taken at 793 K.

## Simple Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2$	$= \frac{1}{2} b \hat{\mathbf{y}}$	(1b)	Pd I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} (a + c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(1g)	Pd II
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_3$	$= (x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + z_3 c \sin \beta \hat{\mathbf{z}}$	(2m)	Cl I
$\mathbf{B}_4$	$= -x_3 \mathbf{a}_1 + -z_3 \mathbf{a}_3$	$= (-x_3 a - z_3 c \cos \beta) \hat{\mathbf{x}} + -z_3 c \sin \beta \hat{\mathbf{z}}$	(2m)	Cl I
$\mathbf{B}_5$	$= x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= (x_4 a + z_4 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_4 c \sin \beta \hat{\mathbf{z}}$	(2n)	Cl II
$\mathbf{B}_6$	$= -x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$= (-x_4 a - z_4 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - z_4 c \sin \beta \hat{\mathbf{z}}$	(2n)	Cl II

## References:

- J. Evers, W. Beck, M. Göbel, S. Jakob, P. Mayer, G. Oehlinger, M. Rotter, and T. M. Klapötke, *The Structures of  $\delta$ -PdCl<sub>2</sub> and  $\gamma$ -PdCl<sub>2</sub>: Phases with Negative Thermal Expansion in One Direction*, *Angew. Chem. Int. Ed.* **49**, 5677–5682 (2010), [doi:10.1002/anie.201000680](https://doi.org/10.1002/anie.201000680).

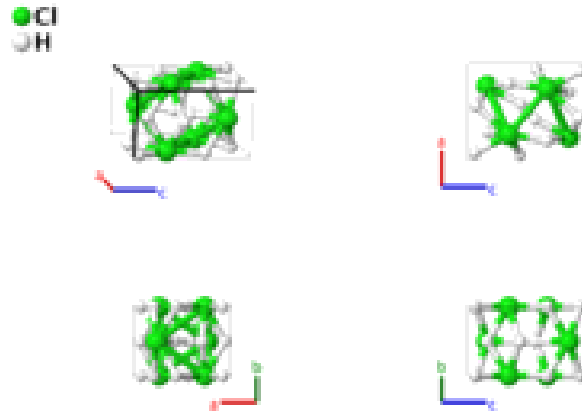
---

**Geometry files:**

- CIF: pp. [806](#)

- POSCAR: pp. [806](#)

# H<sub>3</sub>Cl (400 GPa) Structure: AB3\_mP16\_10\_mn\_3m3n

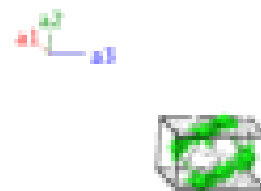


<b>Prototype</b>	:	H <sub>3</sub> Cl
<b>AFLOW prototype label</b>	:	AB3_mP16_10_mn_3m3n
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mP16
<b>Space group number</b>	:	10
<b>Space group symbol</b>	:	<i>P2/m</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB3_mP16_10_mn_3m3n</code> <code>--params=a, b/a, c/a, <math>\beta</math>, x<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, z<sub>8</sub></code>

- This structure was found via first-principles calculations. The data presented here was computed at a pressure of 400 GPa.

## Simple Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= x_1 \mathbf{a}_1 + z_1 \mathbf{a}_3$	$= (x_1 a + z_1 c \cos \beta) \hat{\mathbf{x}} + z_1 c \sin \beta \hat{\mathbf{z}}$	(2 <i>m</i> )	Cl I
<b>B<sub>2</sub></b>	$= -x_1 \mathbf{a}_1 + -z_1 \mathbf{a}_3$	$= (-x_1 a - z_1 c \cos \beta) \hat{\mathbf{x}} + -z_1 c \sin \beta \hat{\mathbf{z}}$	(2 <i>m</i> )	Cl I
<b>B<sub>3</sub></b>	$= x_2 \mathbf{a}_1 + z_2 \mathbf{a}_3$	$= (x_2 a + z_2 c \cos \beta) \hat{\mathbf{x}} + z_2 c \sin \beta \hat{\mathbf{z}}$	(2 <i>m</i> )	H I
<b>B<sub>4</sub></b>	$= -x_2 \mathbf{a}_1 + -z_2 \mathbf{a}_3$	$= (-x_2 a - z_2 c \cos \beta) \hat{\mathbf{x}} + -z_2 c \sin \beta \hat{\mathbf{z}}$	(2 <i>m</i> )	H I
<b>B<sub>5</sub></b>	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_3$	$= (x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + z_3 c \sin \beta \hat{\mathbf{z}}$	(2 <i>m</i> )	H II
<b>B<sub>6</sub></b>	$= -x_3 \mathbf{a}_1 + -z_3 \mathbf{a}_3$	$= (-x_3 a - z_3 c \cos \beta) \hat{\mathbf{x}} + -z_3 c \sin \beta \hat{\mathbf{z}}$	(2 <i>m</i> )	H II



$$\begin{aligned}
\mathbf{B}_7 &= x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3 = (x_4 a + z_4 c \cos \beta) \hat{\mathbf{x}} + z_4 c \sin \beta \hat{\mathbf{z}} & (2m) & \text{H III} \\
\mathbf{B}_8 &= -x_4 \mathbf{a}_1 + -z_4 \mathbf{a}_3 = (-x_4 a - z_4 c \cos \beta) \hat{\mathbf{x}} + -z_4 c \sin \beta \hat{\mathbf{z}} & (2m) & \text{H III} \\
\mathbf{B}_9 &= x_5 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_5 \mathbf{a}_3 = (x_5 a + z_5 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_5 c \sin \beta \hat{\mathbf{z}} & (2n) & \text{Cl II} \\
\mathbf{B}_{10} &= -x_5 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_5 \mathbf{a}_3 = (-x_5 a - z_5 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - z_5 c \sin \beta \hat{\mathbf{z}} & (2n) & \text{Cl II} \\
\mathbf{B}_{11} &= x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_6 \mathbf{a}_3 = (x_6 a + z_6 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_6 c \sin \beta \hat{\mathbf{z}} & (2n) & \text{H IV} \\
\mathbf{B}_{12} &= -x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_6 \mathbf{a}_3 = (-x_6 a - z_6 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - z_6 c \sin \beta \hat{\mathbf{z}} & (2n) & \text{H IV} \\
\mathbf{B}_{13} &= x_7 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_7 \mathbf{a}_3 = (x_7 a + z_7 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_7 c \sin \beta \hat{\mathbf{z}} & (2n) & \text{H V} \\
\mathbf{B}_{14} &= -x_7 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_7 \mathbf{a}_3 = (-x_7 a - z_7 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - z_7 c \sin \beta \hat{\mathbf{z}} & (2n) & \text{H V} \\
\mathbf{B}_{15} &= x_8 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_8 \mathbf{a}_3 = (x_8 a + z_8 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_8 c \sin \beta \hat{\mathbf{z}} & (2n) & \text{H VI} \\
\mathbf{B}_{16} &= -x_8 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_8 \mathbf{a}_3 = (-x_8 a - z_8 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - z_8 c \sin \beta \hat{\mathbf{z}} & (2n) & \text{H VI}
\end{aligned}$$

---

### References:

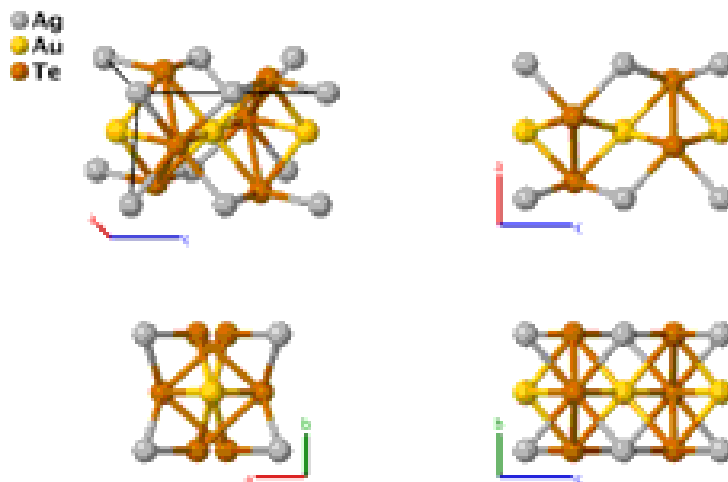
- Q. Zeng, S. Yu, D. Li, A. R. Oganov, and G. Frapper, *Emergence of novel hydrogen chlorides under high pressure*, Phys. Chem. Chem. Phys. **19**, 8236–8242 (2017), [doi:10.1039/C6CP08708F](https://doi.org/10.1039/C6CP08708F).

---

### Geometry files:

- CIF: pp. [806](#)  
- POSCAR: pp. [807](#)

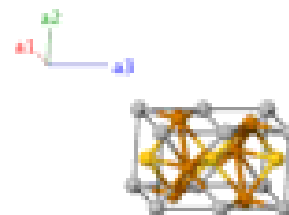
# Muthmannite (AuAgTe<sub>2</sub>) Structure: ABC2\_mP8\_10\_ac\_eh\_mn



<b>Prototype</b>	:	AuAgTe <sub>2</sub>
<b>AFLOW prototype label</b>	:	ABC2_mP8_10_ac_eh_mn
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mP8
<b>Space group number</b>	:	10
<b>Space group symbol</b>	:	<i>P2/m</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=ABC2_mP8_10_ac_eh_mn --params=a, b/a, c/a, β, x<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, z<sub>6</sub></code>

## Simple Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos\beta \hat{\mathbf{x}} + c \sin\beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Ag I
<b>B<sub>2</sub></b>	$\frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} c \cos\beta \hat{\mathbf{x}} + \frac{1}{2} c \sin\beta \hat{\mathbf{z}}$	(1c)	Ag II
<b>B<sub>3</sub></b>	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(1e)	Au I
<b>B<sub>4</sub></b>	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} (a + c \cos\beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin\beta \hat{\mathbf{z}}$	(1h)	Au II
<b>B<sub>5</sub></b>	$x_5 \mathbf{a}_1 + z_5 \mathbf{a}_3$	$(x_5 a + z_5 c \cos\beta) \hat{\mathbf{x}} + z_5 c \sin\beta \hat{\mathbf{z}}$	(2m)	Te I
<b>B<sub>6</sub></b>	$-x_5 \mathbf{a}_1 + -z_5 \mathbf{a}_3$	$(-x_5 a - z_5 c \cos\beta) \hat{\mathbf{x}} + -z_5 c \sin\beta \hat{\mathbf{z}}$	(2m)	Te I

$$\mathbf{B}_7 = x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_6 \mathbf{a}_3 = (x_6 a + z_6 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_6 c \sin \beta \hat{\mathbf{z}} \quad (2n) \quad \text{Te II}$$

$$\mathbf{B}_8 = -x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_6 \mathbf{a}_3 = (-x_6 a - z_6 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - z_6 c \sin \beta \hat{\mathbf{z}} \quad (2n) \quad \text{Te II}$$

---

**References:**

- L. Bindi, *Commensurate-incommensurate phase transition in muthmannite, AuAgTe<sub>2</sub>: first evidence of a modulated structure at low temperature*, Philos. Mag. Lett. **88**, 533–541 (2008), [doi:10.1080/09500830802311072](https://doi.org/10.1080/09500830802311072).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

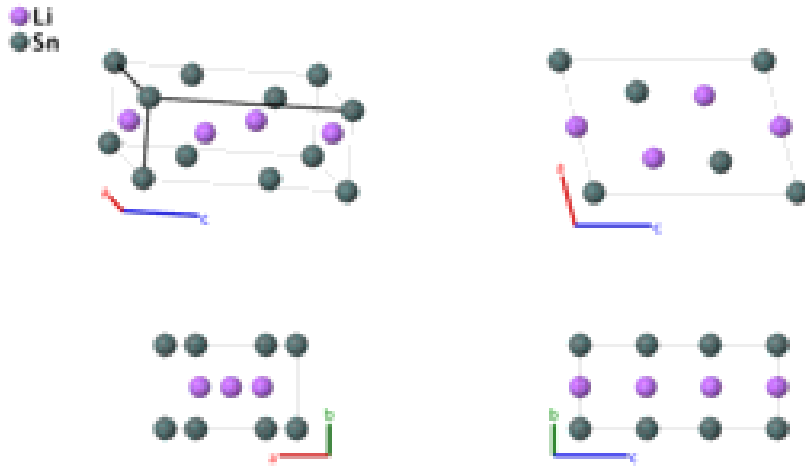
---

**Geometry files:**

- CIF: pp. [807](#)

- POSCAR: pp. [807](#)

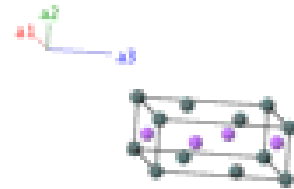
# LiSn Structure: AB\_mP6\_10\_en\_am



<b>Prototype</b>	:	LiSn
<b>AFLOW prototype label</b>	:	AB_mP6_10_en_am
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mP6
<b>Space group number</b>	:	10
<b>Space group symbol</b>	:	$P2/m$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB_mP6_10_en_am --params=a, b/a, c/a, <math>\beta</math>, <math>x_3</math>, <math>z_3</math>, <math>x_4</math>, <math>z_4</math></code>

## Simple Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos\beta \hat{\mathbf{x}} + c \sin\beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Sn I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(1e)	Li I
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_3$	$= (x_3 a + z_3 c \cos\beta) \hat{\mathbf{x}} + z_3 c \sin\beta \hat{\mathbf{z}}$	(2m)	Sn II
$\mathbf{B}_4$	$= -x_3 \mathbf{a}_1 + -z_3 \mathbf{a}_3$	$= (-x_3 a - z_3 c \cos\beta) \hat{\mathbf{x}} + -z_3 c \sin\beta \hat{\mathbf{z}}$	(2m)	Sn II
$\mathbf{B}_5$	$= x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= (x_4 a + z_4 c \cos\beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_4 c \sin\beta \hat{\mathbf{z}}$	(2n)	Li II
$\mathbf{B}_6$	$= -x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$= (-x_4 a - z_4 c \cos\beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - z_4 c \sin\beta \hat{\mathbf{z}}$	(2n)	Li II

## References:

- W. Müller and H. Schäfer, *Die Kristallstruktur der Phase LiSn*, Z. Naturforsch. B **28**, 246–248 (1973),  
[doi:10.1515/znb-1973-5-604](https://doi.org/10.1515/znb-1973-5-604).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

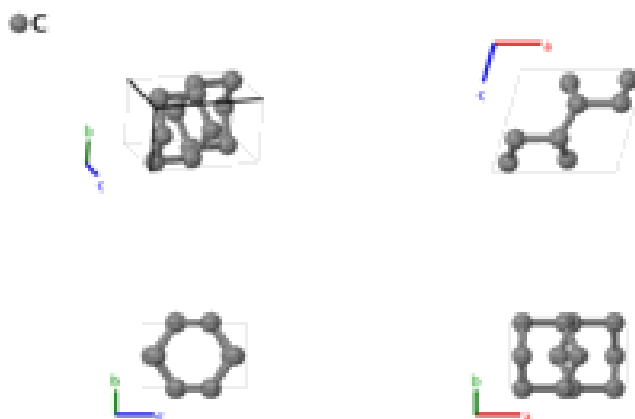
---

**Geometry files:**

- CIF: pp. [807](#)

- POSCAR: pp. [808](#)

# S-carbon Structure: A\_mP8\_10\_2m2n

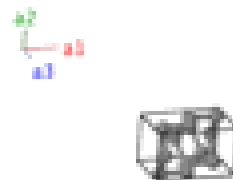


<b>Prototype</b>	:	C
<b>AFLOW prototype label</b>	:	A_mP8_10_2m2n
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mP8
<b>Space group number</b>	:	10
<b>Space group symbol</b>	:	$P2/m$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A_mP8_10_2m2n --params=a, b/a, c/a, <math>\beta</math>, <math>x_1</math>, <math>z_1</math>, <math>x_2</math>, <math>z_2</math>, <math>x_3</math>, <math>z_3</math>, <math>x_4</math>, <math>z_4</math></code>

- This is a predicted “superhard” allotrope of carbon. Shortly after this paper was published, two other papers predicted similar structures, differentiated mainly by an origin shift:
  - F-carbon (Tian, 2012): the origin is shifted by  $1/2 \mathbf{a}_3$ .
  - J-carbon (Wang, 2012): the origin is shifted by  $1/2 (\mathbf{a}_1 + \mathbf{a}_3)$ .
- This is *not* the orthorhombic phase, also denoted S-carbon, found by He *et al.* (He, 2012)

## Simple Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + z_1 \mathbf{a}_3$	$= (x_1 a + z_1 c \cos \beta) \hat{\mathbf{x}} + z_1 c \sin \beta \hat{\mathbf{z}}$	(2m)	C I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 + -z_1 \mathbf{a}_3$	$= (-x_1 a - z_1 c \cos \beta) \hat{\mathbf{x}} + -z_1 c \sin \beta \hat{\mathbf{z}}$	(2m)	C I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + z_2 \mathbf{a}_3$	$= (x_2 a + z_2 c \cos \beta) \hat{\mathbf{x}} + z_2 c \sin \beta \hat{\mathbf{z}}$	(2m)	C II

$$\begin{aligned}
\mathbf{B}_4 &= -x_2 \mathbf{a}_1 + -z_2 \mathbf{a}_3 = (-x_2 a - z_2 c \cos \beta) \hat{\mathbf{x}} + -z_2 c \sin \beta \hat{\mathbf{z}} & (2m) & \text{C II} \\
\mathbf{B}_5 &= x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3 = (x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_3 c \sin \beta \hat{\mathbf{z}} & (2n) & \text{C III} \\
\mathbf{B}_6 &= -x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_3 \mathbf{a}_3 = (-x_3 a - z_3 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - z_3 c \sin \beta \hat{\mathbf{z}} & (2n) & \text{C III} \\
\mathbf{B}_7 &= x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3 = (x_4 a + z_4 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_4 c \sin \beta \hat{\mathbf{z}} & (2n) & \text{C IV} \\
\mathbf{B}_8 &= -x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_4 \mathbf{a}_3 = (-x_4 a - z_4 c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - z_4 c \sin \beta \hat{\mathbf{z}} & (2n) & \text{C IV}
\end{aligned}$$

---

### References:

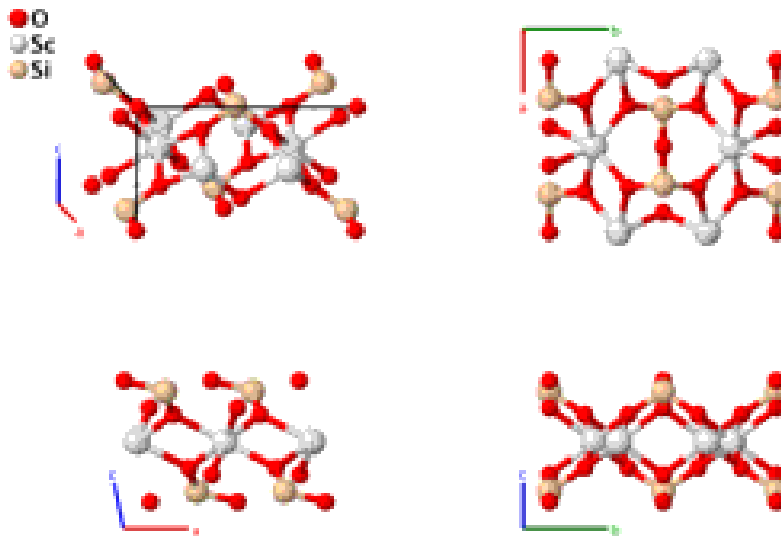
- H. Niu, X.-Q. Chen, S. Wang, D. Li, W. L. Mao, and Y. Li, *Families of Superhard Crystalline Carbon Allotropes Constructed via Cold Compression of Graphite and Nanotubes*, Phys. Rev. Lett. **108**, 135501 (2012), [doi:10.1103/PhysRevLett.108.135501](https://doi.org/10.1103/PhysRevLett.108.135501).
- F. Tian, X. Dong, Z. Zhao, J. He, and H.-T. Wang, *Superhard F-carbon predicted by ab initio particle-swarm optimization methodology*, J. Phys.: Condens. Matter **24**, 165504 (2012), [doi:10.1088/0953-8984/24/16/165504](https://doi.org/10.1088/0953-8984/24/16/165504).
- J.-T. Wang, C. Chen, and Y. Kawazoe, *Phase conversion from graphite toward a simple monoclinic sp<sup>3</sup>-carbon allotrope*, J. Chem. Phys. **137**, 024502 (2012), [doi:10.1063/1.4732538](https://doi.org/10.1063/1.4732538).
- C. He, L. Sun, C. Zhang, X. Peng, K. Zhang, and J. Zhong, *New superhard carbon phases between graphite and diamond*, Solid State Commun. **152**, 1560–1563 (2012), [doi:10.1016/j.ssc.2012.05.022](https://doi.org/10.1016/j.ssc.2012.05.022).
- C. He, L. Z. Sun, and J. Zhong, *Prediction of superhard carbon allotropes from the segment combination method*, J. Superhard Mater. **34**, 386–399 (2012), [doi:10.3103/S1063457612060123](https://doi.org/10.3103/S1063457612060123).

---

### Geometry files:

- CIF: pp. 808
- POSCAR: pp. 808

# Thortveitite ( $[\text{Sc}, \text{Y}]_2\text{Si}_2\text{O}_7$ , $S 2_1$ ) Structure: A7B2C2\_mC22\_12\_aj\_h\_i

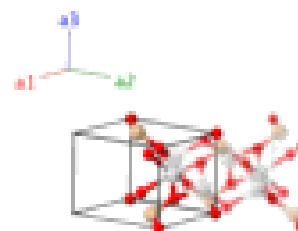


<b>Prototype</b>	:	$[\text{Sc}, \text{Y}]_2\text{Si}_2\text{O}_7$
<b>AFLOW prototype label</b>	:	A7B2C2_mC22_12_aj_h_i
<b>Strukturbericht designation</b>	:	$S 2_1$
<b>Pearson symbol</b>	:	mC22
<b>Space group number</b>	:	12
<b>Space group symbol</b>	:	$C2/m$
<b>AFLOW prototype command</b>	:	aflow --proto=A7B2C2_mC22_12_aj_h_i --params=a, b/a, c/a, $\beta$ , $y_2$ , $x_3$ , $z_3$ , $x_4$ , $z_4$ , $x_5$ , $y_5$ , $z_5$

- Thortveitite is the primary source of scandium, and is one of the simplest sorosilicates, minerals with isolated  $\text{Si}_2\text{O}_7$  groups (Bianchi, 1988).
- Although the (4h) Wyckoff position is randomly occupied by both Sc and Y atoms, we use Sc to represent the site.
- (Bianchi, 1988) gives structural information for several samples of thortveitite. We use the data from sample 1, collected in Iveland, Norway.

## Base-centered Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:



	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_2$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Sc
$\mathbf{B}_3$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Sc
$\mathbf{B}_4$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + z_3 c \sin \beta \hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B}_5$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$(-x_3 a - z_3 c \cos \beta) \hat{\mathbf{x}} - z_3 c \sin \beta \hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B}_6$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(x_4 a + z_4 c \cos \beta) \hat{\mathbf{x}} + z_4 c \sin \beta \hat{\mathbf{z}}$	(4i)	Si
$\mathbf{B}_7$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$(-x_4 a - z_4 c \cos \beta) \hat{\mathbf{x}} - z_4 c \sin \beta \hat{\mathbf{z}}$	(4i)	Si
$\mathbf{B}_8$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(x_5 a + z_5 c \cos \beta) \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \sin \beta \hat{\mathbf{z}}$	(8j)	O III
$\mathbf{B}_9$	$= (-x_5 - y_5) \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$(-x_5 a - z_5 c \cos \beta) \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} - z_5 c \sin \beta \hat{\mathbf{z}}$	(8j)	O III
$\mathbf{B}_{10}$	$= (-x_5 + y_5) \mathbf{a}_1 + (-x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$(-x_5 a - z_5 c \cos \beta) \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} - z_5 c \sin \beta \hat{\mathbf{z}}$	(8j)	O III
$\mathbf{B}_{11}$	$= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(x_5 a + z_5 c \cos \beta) \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + z_5 c \sin \beta \hat{\mathbf{z}}$	(8j)	O III

---

#### References:

- R. Bianchi, T. Pilati, V. Diella, C. M. Gramaccioli, and G. Mannucci, *A re-examination of thortveitite*, *Am. Mineral.* **73**, 601–607 (1988).

#### Found in:

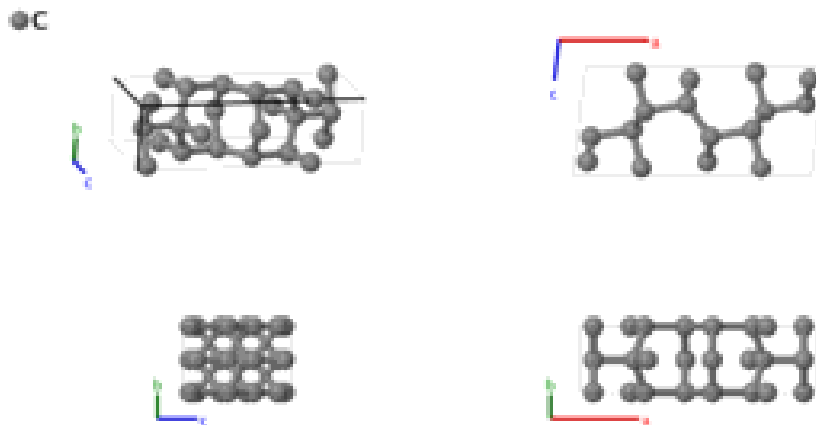
- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, *Am. Mineral.* **88**, 247–250 (2003).

---

#### Geometry files:

- CIF: pp. [808](#)
- POSCAR: pp. [809](#)

# M-carbon Structure: A\_mC16\_12\_4i

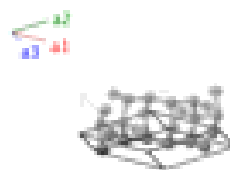


<b>Prototype</b>	:	C
<b>AFLOW prototype label</b>	:	A_mC16_12_4i
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mC16
<b>Space group number</b>	:	12
<b>Space group symbol</b>	:	$C2/m$
<b>AFLOW prototype command</b>	:	aflow --proto=A_mC16_12_4i --params=a, b/a, c/a, $\beta$ , $x_1$ , $z_1$ , $x_2$ , $z_2$ , $x_3$ , $z_3$ , $x_4$ , $z_4$

- This structure was originally found by Oganov and Glass, (Oganov, 2006) and was refined and designated M-Carbon by Li *et al.* (Li, 2009)

## Base-centered Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= (x_1 a + z_1 c \cos \beta) \hat{\mathbf{x}} + z_1 c \sin \beta \hat{\mathbf{z}}$	(4i)	C I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= (-x_1 a - z_1 c \cos \beta) \hat{\mathbf{x}} - z_1 c \sin \beta \hat{\mathbf{z}}$	(4i)	C I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= (x_2 a + z_2 c \cos \beta) \hat{\mathbf{x}} + z_2 c \sin \beta \hat{\mathbf{z}}$	(4i)	C II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$= (-x_2 a - z_2 c \cos \beta) \hat{\mathbf{x}} - z_2 c \sin \beta \hat{\mathbf{z}}$	(4i)	C II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= (x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + z_3 c \sin \beta \hat{\mathbf{z}}$	(4i)	C III
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$= (-x_3 a - z_3 c \cos \beta) \hat{\mathbf{x}} - z_3 c \sin \beta \hat{\mathbf{z}}$	(4i)	C III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= (x_4 a + z_4 c \cos \beta) \hat{\mathbf{x}} + z_4 c \sin \beta \hat{\mathbf{z}}$	(4i)	C IV
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$= (-x_4 a - z_4 c \cos \beta) \hat{\mathbf{x}} - z_4 c \sin \beta \hat{\mathbf{z}}$	(4i)	C IV

---

**References:**

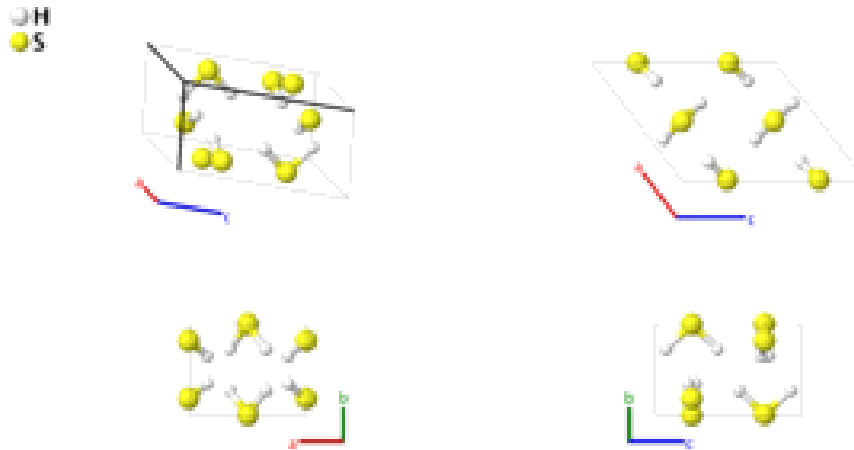
- Q. Li, Y. Ma, A. R. Oganov, H. Wang, H. Wang, Y. Xu, T. Cui, H.-K. Mao, and G. Zou, *Superhard Monoclinic Polymorph of Carbon*, Phys. Rev. Lett. **102**, 175506 (2009), doi:[10.1103/PhysRevLett.102.175506](https://doi.org/10.1103/PhysRevLett.102.175506).
- A. R. Oganov and C. W. Glass, *Crystal structure prediction using ab initio evolutionary techniques: Principles and applications*, J. Chem. Phys. **124**, 244704 (2006), doi:[10.1063/1.2210932](https://doi.org/10.1063/1.2210932).

---

**Geometry files:**

- CIF: pp. [809](#)
- POSCAR: pp. [809](#)

# H<sub>2</sub>S (15 GPa) Structure: A2B\_mP12\_13\_2g\_ef

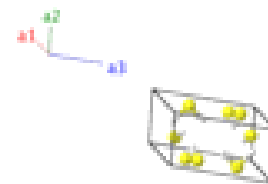


<b>Prototype</b>	:	H <sub>2</sub> S
<b>AFLOW prototype label</b>	:	A2B_mP12_13_2g_ef
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mP12
<b>Space group number</b>	:	13
<b>Space group symbol</b>	:	<i>P2/c</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_mP12_13_2g_ef --params= <i>a, b/a, c/a, β, y<sub>1</sub>, y<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub></i>

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H<sub>2</sub>S in the range 10 – 30 GPa, which does not agree with the experimental phase diagram. (Shimizu, 1995)
- The data presented here was computed at 15 GPa.

## Simple Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(2e)	S I
<b>B<sub>2</sub></b>	$-y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(2e)	S I
<b>B<sub>3</sub></b>	$\frac{1}{2} \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\left(\frac{1}{2}a + \frac{1}{4}c \cos \beta\right) \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(2f)	S II
<b>B<sub>4</sub></b>	$\frac{1}{2} \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\left(\frac{1}{2}a + \frac{3}{4}c \cos \beta\right) \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(2f)	S II
<b>B<sub>5</sub></b>	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$(x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \sin \beta \hat{\mathbf{z}}$	(4g)	H I

$$\begin{aligned}
\mathbf{B}_6 &= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta - x_3a - z_3c \cos \beta\right) \hat{\mathbf{x}} + y_3b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \sin \beta \hat{\mathbf{z}} & (4g) & \text{H I} \\
\mathbf{B}_7 &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = (-x_3a - z_3c \cos \beta) \hat{\mathbf{x}} - y_3b \hat{\mathbf{y}} - z_3c \sin \beta \hat{\mathbf{z}} & (4g) & \text{H I} \\
\mathbf{B}_8 &= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_3a + z_3c \cos \beta\right) \hat{\mathbf{x}} - y_3b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \sin \beta \hat{\mathbf{z}} & (4g) & \text{H I} \\
\mathbf{B}_9 &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = (x_4a + z_4c \cos \beta) \hat{\mathbf{x}} + y_4b \hat{\mathbf{y}} + z_4c \sin \beta \hat{\mathbf{z}} & (4g) & \text{H II} \\
\mathbf{B}_{10} &= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta - x_4a - z_4c \cos \beta\right) \hat{\mathbf{x}} + y_4b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \sin \beta \hat{\mathbf{z}} & (4g) & \text{H II} \\
\mathbf{B}_{11} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = (-x_4a - z_4c \cos \beta) \hat{\mathbf{x}} - y_4b \hat{\mathbf{y}} - z_4c \sin \beta \hat{\mathbf{z}} & (4g) & \text{H II} \\
\mathbf{B}_{12} &= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_4a + z_4c \cos \beta\right) \hat{\mathbf{x}} - y_4b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \sin \beta \hat{\mathbf{z}} & (4g) & \text{H II}
\end{aligned}$$

---

### References:

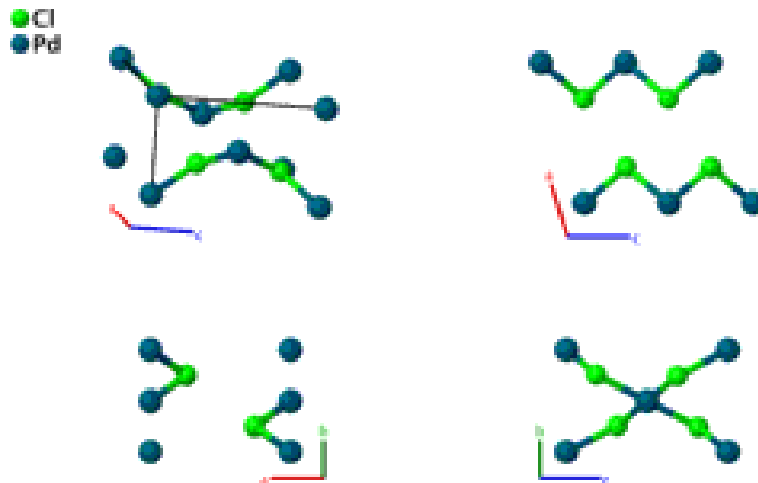
- Y. Li, J. Hao, H. Liu, Y. Li, and Y. Ma, *The metallization and superconductivity of dense hydrogen sulfide*, J. Chem. Phys. **140**, 174712 (2014), [doi:10.1063/1.4874158](https://doi.org/10.1063/1.4874158).
- H. Shimizu, H. Yamaguchi, S. Sasaki, A. Honda, S. Endo, and M. Kobayashi, *Pressure-temperature phase diagram of solid hydrogen sulfide determined by Raman spectroscopy*, Phys. Rev. B **51**, 9391–9394 (1995), [doi:10.1103/PhysRevB.51.9391](https://doi.org/10.1103/PhysRevB.51.9391).

---

### Geometry files:

- CIF: pp. [809](#)
- POSCAR: pp. [810](#)

# $\gamma$ -PdCl<sub>2</sub> Structure: A2B\_mP6\_14\_e\_a

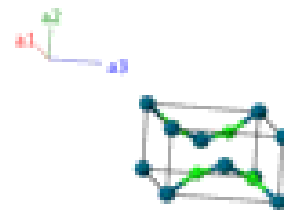


**Prototype** :  $\gamma$ -PdCl<sub>2</sub>  
**AFLOW prototype label** : A2B\_mP6\_14\_e\_a  
**Strukturbericht designation** : None  
**Pearson symbol** : mP6  
**Space group number** : 14  
**Space group symbol** :  $P2_1/c$   
**AFLOW prototype command** : `aflow --proto=A2B_mP6_14_e_a`  
                                   `--params=a, b/a, c/a,  $\beta$ ,  $x_2$ ,  $y_2$ ,  $z_2$`

- (Evers, 2010) place the Pd atoms on the (2c) Wyckoff position. We have shifted the origin so that the Pd atoms are at the (2a) position.
- Data was taken at 300 K.

## Simple Monoclinic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	Pd
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} c \cos \beta \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(2a)	Pd
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$(x_2 a + z_2 c \cos \beta) \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \sin \beta \hat{\mathbf{z}}$	(4e)	Cl

$$\mathbf{B}_4 = -x_2 \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta - x_2a - z_2c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right)c \sin \beta \hat{\mathbf{z}} \quad (4e) \quad \text{Cl}$$

$$\mathbf{B}_5 = -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3 = (-x_2a - z_2c \cos \beta) \hat{\mathbf{x}} - y_2b \hat{\mathbf{y}} - z_2c \sin \beta \hat{\mathbf{z}} \quad (4e) \quad \text{Cl}$$

$$\mathbf{B}_6 = x_2 \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_2a + z_2c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right)c \sin \beta \hat{\mathbf{z}} \quad (4e) \quad \text{Cl}$$

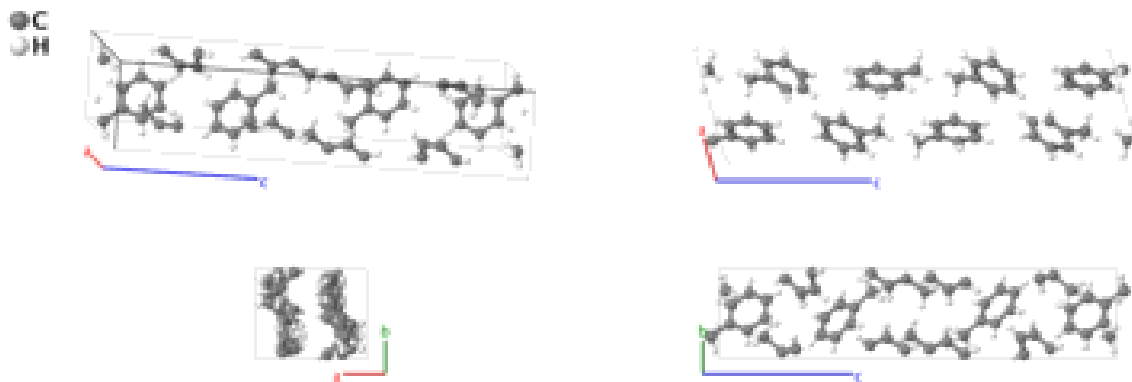
### References:

- J. Evers, W. Beck, M. Göbel, S. Jakob, P. Mayer, G. Oehlinger, M. Rotter, and T. M. Klapötke, *The Structures of  $\delta$ -PdCl<sub>2</sub> and  $\gamma$ -PdCl<sub>2</sub>: Phases with Negative Thermal Expansion in One Direction*, *Angew. Chem. Int. Ed.* **49**, 5677–5682 (2010), [doi:10.1002/anie.201000680](https://doi.org/10.1002/anie.201000680).

### Geometry files:

- CIF: pp. [810](#)
- POSCAR: pp. [810](#)

# $\alpha$ -Toluene Structure: A7B8\_mP120\_14\_14e\_16e

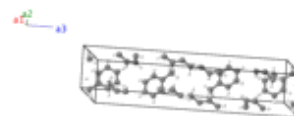


<b>Prototype</b>	:	$\alpha$ -C <sub>7</sub> H <sub>8</sub>
<b>AFLOW prototype label</b>	:	A7B8_mP120_14_14e_16e
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mP120
<b>Space group number</b>	:	14
<b>Space group symbol</b>	:	$P2_1/c$
<b>AFLOW prototype command</b>	:	<pre>aflow --proto=A7B8_mP120_14_14e_16e --params=a, b/a, c/a, <math>\beta</math>, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>, y<sub>9</sub>, z<sub>9</sub>, x<sub>10</sub>, y<sub>10</sub>, z<sub>10</sub>, x<sub>11</sub>, y<sub>11</sub>, z<sub>11</sub>, x<sub>12</sub>, y<sub>12</sub>, z<sub>12</sub>, x<sub>13</sub>, y<sub>13</sub>, z<sub>13</sub>, x<sub>14</sub>, y<sub>14</sub>, z<sub>14</sub>, x<sub>15</sub>, y<sub>15</sub>, z<sub>15</sub>, x<sub>16</sub>, y<sub>16</sub>, z<sub>16</sub>, x<sub>17</sub>, y<sub>17</sub>, z<sub>17</sub>, x<sub>18</sub>, y<sub>18</sub>, z<sub>18</sub>, x<sub>19</sub>, y<sub>19</sub>, z<sub>19</sub>, x<sub>20</sub>, y<sub>20</sub>, z<sub>20</sub>, x<sub>21</sub>, y<sub>21</sub>, z<sub>21</sub>, x<sub>22</sub>, y<sub>22</sub>, z<sub>22</sub>, x<sub>23</sub>, y<sub>23</sub>, z<sub>23</sub>, x<sub>24</sub>, y<sub>24</sub>, z<sub>24</sub>, x<sub>25</sub>, y<sub>25</sub>, z<sub>25</sub>, x<sub>26</sub>, y<sub>26</sub>, z<sub>26</sub>, x<sub>27</sub>, y<sub>27</sub>, z<sub>27</sub>, x<sub>28</sub>, y<sub>28</sub>, z<sub>28</sub>, x<sub>29</sub>, y<sub>29</sub>, z<sub>29</sub>, x<sub>30</sub>, y<sub>30</sub>, z<sub>30</sub></pre>

- $\alpha$ -Toluene is the stable low-temperature crystalline structure of the toluene molecule, C<sub>7</sub>H<sub>8</sub>, which crystallizes below 178 K. This data was constructed from experiments at 150 K.
- The hydrogen atomic positions were approximated to agree with the chemistry of the toluene molecule.

## Simple Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$(x_1 a + z_1 c \cos \beta) \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \sin \beta \hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$\left(\frac{1}{2} c \cos \beta - x_1 a - z_1 c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \sin \beta \hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$(-x_1 a - z_1 c \cos \beta) \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} - z_1 c \sin \beta \hat{\mathbf{z}}$	(4e)	C I





$$\begin{aligned}
\mathbf{B}_{26} &= -x_7 \mathbf{a}_1 + \left(\frac{1}{2} + y_7\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_7\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta - x_7a - z_7c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} + y_7\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_7\right)c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C VII} \\
\mathbf{B}_{27} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 = (-x_7a - z_7c \cos \beta) \hat{\mathbf{x}} - y_7b \hat{\mathbf{y}} - z_7c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C VII} \\
\mathbf{B}_{28} &= x_7 \mathbf{a}_1 + \left(\frac{1}{2} - y_7\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_7a + z_7c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} - y_7\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right)c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C VII} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = (x_8a + z_8c \cos \beta) \hat{\mathbf{x}} + y_8b \hat{\mathbf{y}} + z_8c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C VIII} \\
\mathbf{B}_{30} &= -x_8 \mathbf{a}_1 + \left(\frac{1}{2} + y_8\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_8\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta - x_8a - z_8c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} + y_8\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_8\right)c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C VIII} \\
\mathbf{B}_{31} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 = (-x_8a - z_8c \cos \beta) \hat{\mathbf{x}} - y_8b \hat{\mathbf{y}} - z_8c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C VIII} \\
\mathbf{B}_{32} &= x_8 \mathbf{a}_1 + \left(\frac{1}{2} - y_8\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_8a + z_8c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} - y_8\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right)c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C VIII} \\
\mathbf{B}_{33} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = (x_9a + z_9c \cos \beta) \hat{\mathbf{x}} + y_9b \hat{\mathbf{y}} + z_9c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C IX} \\
\mathbf{B}_{34} &= -x_9 \mathbf{a}_1 + \left(\frac{1}{2} + y_9\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_9\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta - x_9a - z_9c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} + y_9\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_9\right)c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C IX} \\
\mathbf{B}_{35} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 = (-x_9a - z_9c \cos \beta) \hat{\mathbf{x}} - y_9b \hat{\mathbf{y}} - z_9c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C IX} \\
\mathbf{B}_{36} &= x_9 \mathbf{a}_1 + \left(\frac{1}{2} - y_9\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_9a + z_9c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} - y_9\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right)c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C IX} \\
\mathbf{B}_{37} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = (x_{10}a + z_{10}c \cos \beta) \hat{\mathbf{x}} + y_{10}b \hat{\mathbf{y}} + z_{10}c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C X} \\
\mathbf{B}_{38} &= -x_{10} \mathbf{a}_1 + \left(\frac{1}{2} + y_{10}\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_{10}\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta - x_{10}a - z_{10}c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} + y_{10}\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{10}\right)c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C X} \\
\mathbf{B}_{39} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 = (-x_{10}a - z_{10}c \cos \beta) \hat{\mathbf{x}} - y_{10}b \hat{\mathbf{y}} - z_{10}c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C X} \\
\mathbf{B}_{40} &= x_{10} \mathbf{a}_1 + \left(\frac{1}{2} - y_{10}\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_{10}a + z_{10}c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} - y_{10}\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right)c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C X} \\
\mathbf{B}_{41} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = (x_{11}a + z_{11}c \cos \beta) \hat{\mathbf{x}} + y_{11}b \hat{\mathbf{y}} + z_{11}c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C XI} \\
\mathbf{B}_{42} &= -x_{11} \mathbf{a}_1 + \left(\frac{1}{2} + y_{11}\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_{11}\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta - x_{11}a - z_{11}c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} + y_{11}\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{11}\right)c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C XI} \\
\mathbf{B}_{43} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 = (-x_{11}a - z_{11}c \cos \beta) \hat{\mathbf{x}} - y_{11}b \hat{\mathbf{y}} - z_{11}c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C XI} \\
\mathbf{B}_{44} &= x_{11} \mathbf{a}_1 + \left(\frac{1}{2} - y_{11}\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_{11}\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta + x_{11}a + z_{11}c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} - y_{11}\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{11}\right)c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C XI} \\
\mathbf{B}_{45} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = (x_{12}a + z_{12}c \cos \beta) \hat{\mathbf{x}} + y_{12}b \hat{\mathbf{y}} + z_{12}c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C XII} \\
\mathbf{B}_{46} &= -x_{12} \mathbf{a}_1 + \left(\frac{1}{2} + y_{12}\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_{12}\right) \mathbf{a}_3 = \left(\frac{1}{2}c \cos \beta - x_{12}a - z_{12}c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} + y_{12}\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{12}\right)c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C XII} \\
\mathbf{B}_{47} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 = (-x_{12}a - z_{12}c \cos \beta) \hat{\mathbf{x}} - y_{12}b \hat{\mathbf{y}} - z_{12}c \sin \beta \hat{\mathbf{z}} & (4e) & \text{C XII}
\end{aligned}$$







$$\begin{aligned}
\mathbf{B}_{114} &= -x_{29} \mathbf{a}_1 + \left(\frac{1}{2} + y_{29}\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_{29}\right) \mathbf{a}_3 &= \left(\frac{1}{2}c \cos \beta - x_{29}a - z_{29}c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} + y_{29}\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{29}\right)c \sin \beta \hat{\mathbf{z}} &(4e) & \text{H XV} \\
\mathbf{B}_{115} &= -x_{29} \mathbf{a}_1 - y_{29} \mathbf{a}_2 - z_{29} \mathbf{a}_3 &= (-x_{29}a - z_{29}c \cos \beta) \hat{\mathbf{x}} - y_{29}b \hat{\mathbf{y}} - z_{29}c \sin \beta \hat{\mathbf{z}} &(4e) & \text{H XV} \\
\mathbf{B}_{116} &= x_{29} \mathbf{a}_1 + \left(\frac{1}{2} - y_{29}\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_{29}\right) \mathbf{a}_3 &= \left(\frac{1}{2}c \cos \beta + x_{29}a + z_{29}c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} - y_{29}\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{29}\right)c \sin \beta \hat{\mathbf{z}} &(4e) & \text{H XV} \\
\mathbf{B}_{117} &= x_{30} \mathbf{a}_1 + y_{30} \mathbf{a}_2 + z_{30} \mathbf{a}_3 &= (x_{30}a + z_{30}c \cos \beta) \hat{\mathbf{x}} + y_{30}b \hat{\mathbf{y}} + z_{30}c \sin \beta \hat{\mathbf{z}} &(4e) & \text{H XVI} \\
\mathbf{B}_{118} &= -x_{30} \mathbf{a}_1 + \left(\frac{1}{2} + y_{30}\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_{30}\right) \mathbf{a}_3 &= \left(\frac{1}{2}c \cos \beta - x_{30}a - z_{30}c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} + y_{30}\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{30}\right)c \sin \beta \hat{\mathbf{z}} &(4e) & \text{H XVI} \\
\mathbf{B}_{119} &= -x_{30} \mathbf{a}_1 - y_{30} \mathbf{a}_2 - z_{30} \mathbf{a}_3 &= (-x_{30}a - z_{30}c \cos \beta) \hat{\mathbf{x}} - y_{30}b \hat{\mathbf{y}} - z_{30}c \sin \beta \hat{\mathbf{z}} &(4e) & \text{H XVI} \\
\mathbf{B}_{120} &= x_{30} \mathbf{a}_1 + \left(\frac{1}{2} - y_{30}\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_{30}\right) \mathbf{a}_3 &= \left(\frac{1}{2}c \cos \beta + x_{30}a + z_{30}c \cos \beta\right) \hat{\mathbf{x}} + \left(\frac{1}{2} - y_{30}\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{30}\right)c \sin \beta \hat{\mathbf{z}} &(4e) & \text{H XVI}
\end{aligned}$$

---

### References:

- S. K. Nayak, R. Sathishkumar, and T. N. Guru Row, *Directing role of functional groups in selective generation of C-H- $\pi$  interactions: In situ cryo-crystallographic studies on benzyl derivatives*, *CrystEngComm* **12**, 3112–3118 (2010), [doi:10.1039/C001190H](https://doi.org/10.1039/C001190H).

### Found in:

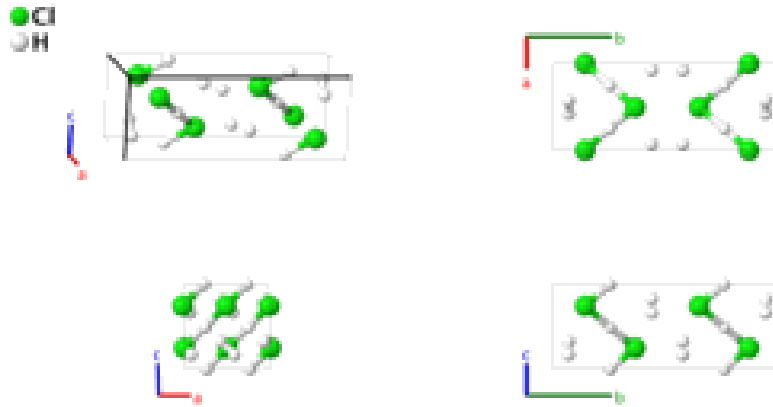
- *Cambridge Structural Database*. CSD Entry: TOLUEN03.

---

### Geometry files:

- CIF: pp. [810](#)  
- POSCAR: pp. [811](#)

# H<sub>3</sub>Cl (50 GPa) Structure: AB3\_mC16\_15\_e\_cf

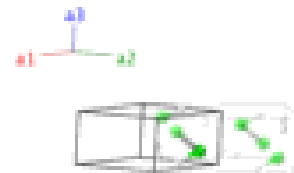


<b>Prototype</b>	:	H <sub>3</sub> Cl
<b>AFLOW prototype label</b>	:	AB3_mC16_15_e_cf
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mC16
<b>Space group number</b>	:	15
<b>Space group symbol</b>	:	C2/c
<b>AFLOW prototype command</b>	:	aflow --proto=AB3_mC16_15_e_cf --params=a, b/a, c/a, $\beta$ , y <sub>2</sub> , x <sub>3</sub> , y <sub>3</sub> , z <sub>3</sub>

- This structure was found via first-principles calculations. The data presented here was computed at a pressure of 50 GPa.

## Base-centered Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}}$	(4c)	H I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$= \left( \frac{1}{4} a + \frac{1}{2} c \cos \beta \right) \hat{\mathbf{x}} - \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{4} c \cos \beta \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \frac{1}{4} c \sin \beta \hat{\mathbf{z}}$	(4e)	Cl
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{3}{4} c \cos \beta \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \frac{3}{4} c \sin \beta \hat{\mathbf{z}}$	(4e)	Cl
$\mathbf{B}_5$	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= (x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \sin \beta \hat{\mathbf{z}}$	(8f)	H II
$\mathbf{B}_6$	$= (-x_3 - y_3) \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left( \frac{1}{2} - z_3 \right) \mathbf{a}_3$	$= \left( \frac{1}{2} c \cos \beta - x_3 a - z_3 c \cos \beta \right) \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left( \frac{1}{2} - z_3 \right) c \sin \beta \hat{\mathbf{z}}$	(8f)	H II

$$\mathbf{B}_7 = (-x_3 + y_3) \mathbf{a}_1 + (-x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3 = \begin{pmatrix} -x_3 a - z_3 c \cos \beta \\ z_3 c \sin \beta \\ -y_3 b \end{pmatrix} \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} - z_3 c \sin \beta \hat{\mathbf{z}} \quad (8f) \quad \text{H II}$$

$$\mathbf{B}_8 = \begin{pmatrix} (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \\ (\frac{1}{2} + z_3) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} c \cos \beta + x_3 a + z_3 c \cos \beta \\ y_3 b \\ (\frac{1}{2} + z_3) c \sin \beta \end{pmatrix} \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + (\frac{1}{2} + z_3) c \sin \beta \hat{\mathbf{z}} \quad (8f) \quad \text{H II}$$

### References:

- D. Duan, X. Huang, F. Tian, Y. Liu, D. Li, H. Yu, B. Liu, W. Tian, and T. Cui, *Predicted Formation of  $H_3^+$  in Solid Halogen Polyhydrides at High Pressures*, J. Phys. Chem. A **119**, 11059–11065 (2015), [doi:10.1021/acs.jpca.5b08183](https://doi.org/10.1021/acs.jpca.5b08183).

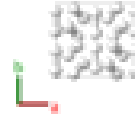
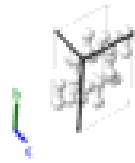
### Geometry files:

- CIF: pp. [811](#)
- POSCAR: pp. [812](#)



# H-III (300 GPa) Structure: A\_mC24\_15\_2e2f

OH



<b>Prototype</b>	:	H
<b>AFLOW prototype label</b>	:	A_mC24_15_2e2f
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	mC24
<b>Space group number</b>	:	15
<b>Space group symbol</b>	:	$C2/c$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A_mC24_15_2e2f</code> <code>--params=a, b/a, c/a, <math>\beta</math>, <math>y_1</math>, <math>y_2</math>, <math>x_3</math>, <math>y_3</math>, <math>z_3</math>, <math>x_4</math>, <math>y_4</math>, <math>z_4</math></code>

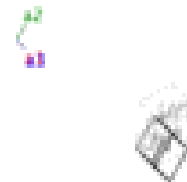
- This structure was determined by density functional simulations. The authors claim it is in good agreement with experimental data for H-III, and is the lowest energy structure at pressures from approximately 100-250 GPa, including zero-point motion. The data presented here was computed at 300 GPa. If we change our description of the unit cell so that

$$\mathbf{a}_3 \rightarrow \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$$

then all of the primitive vectors for the base-centered orthorhombic structure have approximately equal lengths, and the angles between them are approximately  $60^\circ$ . This structure is very close to exhibiting a face-centered cubic lattice.

## Base-centered Monoclinic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{4} c \cos \beta \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + \frac{1}{4} c \sin \beta \hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{3}{4} c \cos \beta \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \frac{3}{4} c \sin \beta \hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{4} c \cos \beta \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \frac{1}{4} c \sin \beta \hat{\mathbf{z}}$	(4e)	H II
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{3}{4} c \cos \beta \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \frac{3}{4} c \sin \beta \hat{\mathbf{z}}$	(4e)	H II

$$\begin{aligned}
\mathbf{B}_5 &= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3 = (x_3 a + z_3 c \cos \beta) \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \sin \beta \hat{\mathbf{z}} & (8f) & \text{H III} \\
\mathbf{B}_6 &= (-x_3 - y_3) \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta - x_3 a - z_3 c \cos \beta\right) \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \sin \beta \hat{\mathbf{z}} & (8f) & \text{H III} \\
\mathbf{B}_7 &= (-x_3 + y_3) \mathbf{a}_1 + (-x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3 = (-x_3 a - z_3 c \cos \beta) \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} - z_3 c \sin \beta \hat{\mathbf{z}} & (8f) & \text{H III} \\
\mathbf{B}_8 &= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_3 a + z_3 c \cos \beta\right) \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \sin \beta \hat{\mathbf{z}} & (8f) & \text{H III} \\
\mathbf{B}_9 &= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 = (x_4 a + z_4 c \cos \beta) \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \sin \beta \hat{\mathbf{z}} & (8f) & \text{H IV} \\
\mathbf{B}_{10} &= (-x_4 - y_4) \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta - x_4 a - z_4 c \cos \beta\right) \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \sin \beta \hat{\mathbf{z}} & (8f) & \text{H IV} \\
\mathbf{B}_{11} &= (-x_4 + y_4) \mathbf{a}_1 + (-x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3 = (-x_4 a - z_4 c \cos \beta) \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} - z_4 c \sin \beta \hat{\mathbf{z}} & (8f) & \text{H IV} \\
\mathbf{B}_{12} &= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} c \cos \beta + x_4 a + z_4 c \cos \beta\right) \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \sin \beta \hat{\mathbf{z}} & (8f) & \text{H IV}
\end{aligned}$$

---

#### References:

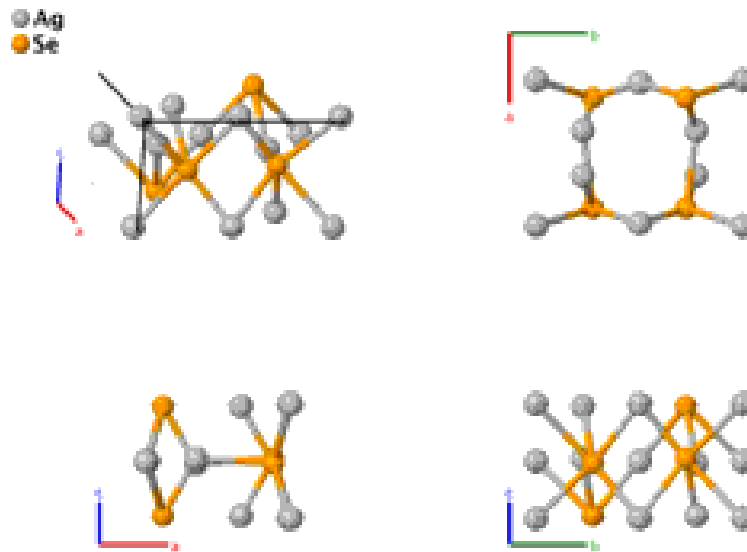
- C. J. Pickard and R. J. Needs, *Structure of phase III of solid hydrogen*, Nat. Phys. **3**, 473–476 (2007), [doi:10.1038/nphys625](https://doi.org/10.1038/nphys625).

---

#### Geometry files:

- CIF: pp. 812  
- POSCAR: pp. 812

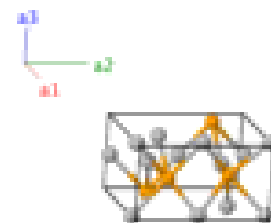
# $\alpha$ -Naumannite (Ag<sub>2</sub>Se) Structure: A2B\_oP12\_17\_abe\_e



**Prototype** :  $\alpha$ -Ag<sub>2</sub>Se  
**AFLOW prototype label** : A2B\_oP12\_17\_abe\_e  
**Strukturbericht designation** : None  
**Pearson symbol** : oP12  
**Space group number** : 17  
**Space group symbol** :  $P222_1$   
**AFLOW prototype command** : aflow --proto=A2B\_oP12\_17\_abe\_e  
 --params=a, b/a, c/a, x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>

**Simple Orthorhombic primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1$	$=$	$x_1 a \hat{\mathbf{x}}$	(2a)	Ag I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_1 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Ag I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$x_2 a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(2b)	Ag II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_2 a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2b)	Ag II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4e)	Ag III

$$\begin{aligned}
\mathbf{B}_6 &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} && (4e) && \text{Ag III} \\
\mathbf{B}_7 &= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} && (4e) && \text{Ag III} \\
\mathbf{B}_8 &= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} && (4e) && \text{Ag III} \\
\mathbf{B}_9 &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (4e) && \text{Se} \\
\mathbf{B}_{10} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} && (4e) && \text{Se} \\
\mathbf{B}_{11} &= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} && (4e) && \text{Se} \\
\mathbf{B}_{12} &= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (4e) && \text{Se}
\end{aligned}$$

**References:**

- Z. G. Pinsker, C. Ching-liang, R. M. Imamov, and E. L. Lapidus, *Determination of the crystal structure of the low-temperature phase  $\alpha$ -Ag<sub>2</sub>Se*, Sov. Phys. Crystallogr. **10**, 225–231 (1965).

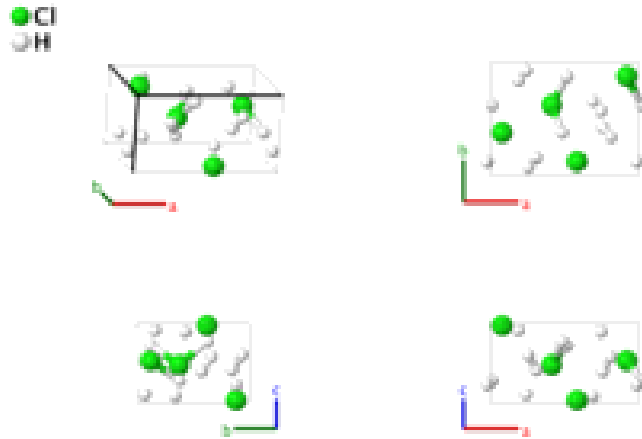
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [812](#)  
- POSCAR: pp. [813](#)

# H<sub>3</sub>Cl (100 GPa) Structure: AB3\_oP16\_19\_a\_3a



<b>Prototype</b>	:	H <sub>3</sub> Cl
<b>AFLOW prototype label</b>	:	AB3_oP16_19_a_3a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP16
<b>Space group number</b>	:	19
<b>Space group symbol</b>	:	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
<b>AFLOW prototype command</b>	:	aflow --proto=AB3_oP16_19_a_3a --params= <i>a, b/a, c/a, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub></i>

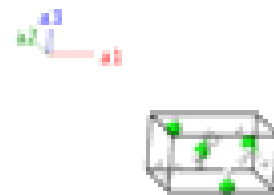
- This structure was found via first-principles calculations. The data presented here was computed at a pressure of 100 GPa.

## Simple Orthorhombic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	= $x_1 a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4 <i>a</i> )	Cl
<b>B<sub>2</sub></b>	= $(\frac{1}{2} - x_1) \mathbf{a}_1 - y_1 \mathbf{a}_2 + (\frac{1}{2} + z_1) \mathbf{a}_3$	= $(\frac{1}{2} - x_1) a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + (\frac{1}{2} + z_1) c \hat{\mathbf{z}}$	(4 <i>a</i> )	Cl
<b>B<sub>3</sub></b>	= $-x_1 \mathbf{a}_1 + (\frac{1}{2} + y_1) \mathbf{a}_2 + (\frac{1}{2} - z_1) \mathbf{a}_3$	= $-x_1 a \hat{\mathbf{x}} + (\frac{1}{2} + y_1) b \hat{\mathbf{y}} + (\frac{1}{2} - z_1) c \hat{\mathbf{z}}$	(4 <i>a</i> )	Cl
<b>B<sub>4</sub></b>	= $(\frac{1}{2} + x_1) \mathbf{a}_1 + (\frac{1}{2} - y_1) \mathbf{a}_2 - z_1 \mathbf{a}_3$	= $(\frac{1}{2} + x_1) a \hat{\mathbf{x}} + (\frac{1}{2} - y_1) b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(4 <i>a</i> )	Cl
<b>B<sub>5</sub></b>	= $x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	= $x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4 <i>a</i> )	H I

$$\begin{aligned}
\mathbf{B}_6 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4a) & \text{H I} \\
\mathbf{B}_7 &= -x_2 \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} & (4a) & \text{H I} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 - z_2 \mathbf{a}_3 = \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} & (4a) & \text{H I} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4a) & \text{H II} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4a) & \text{H II} \\
\mathbf{B}_{11} &= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = -x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (4a) & \text{H II} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 = \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (4a) & \text{H II} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (4a) & \text{H III} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (4a) & \text{H III} \\
\mathbf{B}_{15} &= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 = -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (4a) & \text{H III} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 - z_4 \mathbf{a}_3 = \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (4a) & \text{H III}
\end{aligned}$$

---

### References:

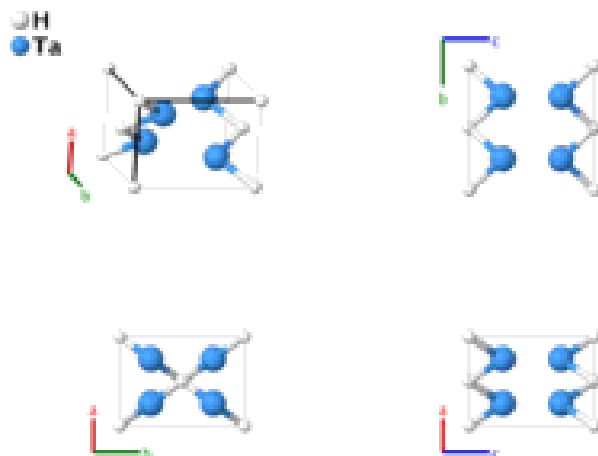
- D. Duan, X. Huang, F. Tian, Y. Liu, D. Li, H. Yu, B. Liu, W. Tian, and T. Cui, *Predicted Formation of  $H_3^+$  in Solid Halogen Polyhydrides at High Pressures*, J. Phys. Chem. A **119**, 11059–11065 (2015), doi:10.1021/acs.jpca.5b08183.

---

### Geometry files:

- CIF: pp. 813  
- POSCAR: pp. 813

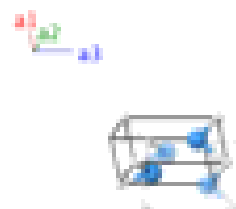
# Ta<sub>2</sub>H Structure: AB2\_oC6\_21\_a\_k



<b>Prototype</b>	:	Ta <sub>2</sub> H
<b>AFLOW prototype label</b>	:	AB2_oC6_21_a_k
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC6
<b>Space group number</b>	:	21
<b>Space group symbol</b>	:	C222
<b>AFLOW prototype command</b>	:	aflow --proto=AB2_oC6_21_a_k --params=a,b/a,c/a,z <sub>2</sub>

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	H
<b>B<sub>2</sub></b>	$\frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4k)	Ta
<b>B<sub>3</sub></b>	$\frac{1}{2} \mathbf{a}_1 + -z_2 \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} - \frac{1}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(4k)	Ta

## References:

- H. Asano, Y. Ishikawa, and M. Hirabayashi, *Single-crystal X-ray diffraction study on the hydrogen ordering in Ta<sub>2</sub>H*, J. Appl. Crystallogr. **11**, 681–683 (1978), doi:10.1107/S0021889878014260.

## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

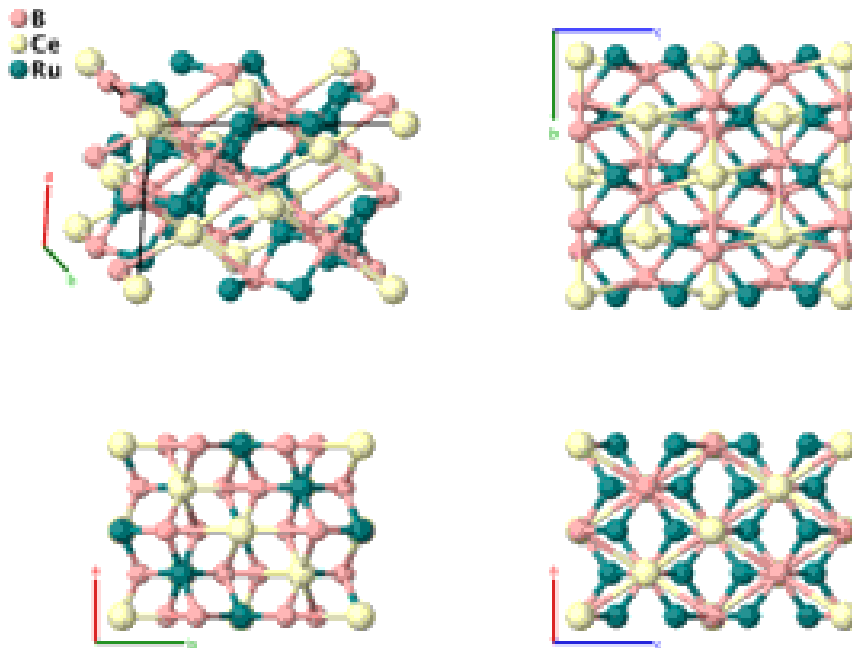
**Geometry files:**

- CIF: pp. [813](#)

- POSCAR: pp. [814](#)



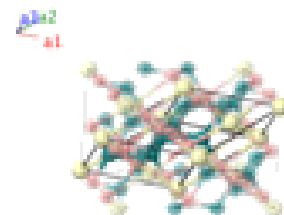
# CeRu<sub>2</sub>B<sub>2</sub> Structure: A2BC2\_oF40\_22\_fi\_ad\_gh



<b>Prototype</b>	:	CeRu <sub>2</sub> B <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2BC2_oF40_22_fi_ad_gh
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oF40
<b>Space group number</b>	:	22
<b>Space group symbol</b>	:	<i>F222</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2BC2_oF40_22_fi_ad_gh --params= <i>a, b/a, c/a, y<sub>3</sub>, z<sub>4</sub>, z<sub>5</sub>, y<sub>6</sub></i>

**Face-centered Orthorhombic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(4 <i>a</i> )	Ce I
<b>B<sub>2</sub></b> =	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4 <i>d</i> )	Ce II
<b>B<sub>3</sub></b> =	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	=	$y_3 b \hat{\mathbf{y}}$	(8 <i>f</i> )	B I

$$\begin{aligned} \mathbf{B}_4 &= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - y_3 \mathbf{a}_3 &= -y_3 b \hat{\mathbf{y}} & (8f) & \text{B I} \\ \mathbf{B}_5 &= z_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= z_4 c \hat{\mathbf{z}} & (8g) & \text{Ru I} \\ \mathbf{B}_6 &= -z_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= -z_4 c \hat{\mathbf{z}} & (8g) & \text{Ru I} \\ \mathbf{B}_7 &= z_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8h) & \text{Ru II} \\ \mathbf{B}_8 &= \left(\frac{1}{2} - z_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} & (8h) & \text{Ru II} \\ \mathbf{B}_9 &= y_6 \mathbf{a}_1 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_2 + y_6 \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8i) & \text{B II} \\ \mathbf{B}_{10} &= \left(\frac{1}{2} - y_6\right) \mathbf{a}_1 + y_6 \mathbf{a}_2 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8i) & \text{B II} \end{aligned}$$

#### References:

- P. Rogl, *Structural chemistry and phase equilibria of ternary rare earth-platinum metal borides*, J. Less-Common Met. **110**, 283–294 (1985), [doi:10.1016/0022-5088\(85\)90334-0](https://doi.org/10.1016/0022-5088(85)90334-0).

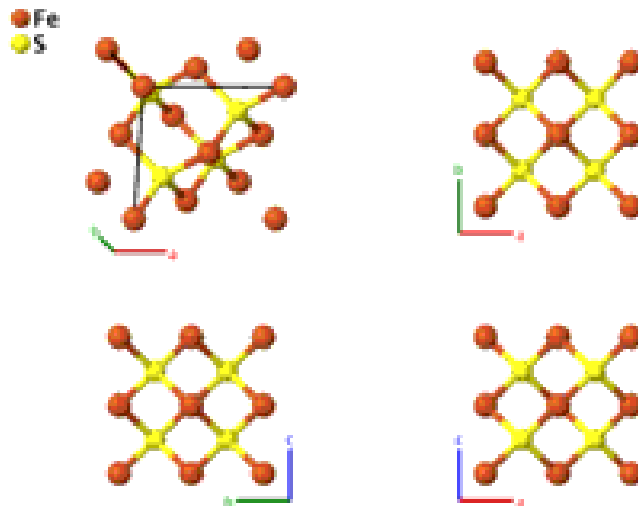
#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. [814](#)  
 - POSCAR: pp. [814](#)

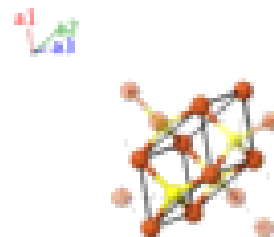
# FeS (Low-temperature) Structure: AB\_oF8\_22\_a\_c



<b>Prototype</b>	:	FeS
<b>AFLOW prototype label</b>	:	AB_oF8_22_a_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oF8
<b>Space group number</b>	:	22
<b>Space group symbol</b>	:	$F222$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB_oF8_22_a_c --params=a,b/a,c/a</code>

## Face-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(4a)	Fe
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	S

## References:

- M. Wintenberger, B. Srouf, C. Meyer, F. Hartmannboutron, Y. Gros, and J. L. Buevoz, *First order transitions and magnetic-structure of zincblende-type iron sulfide*, Acta Crystallogr. Sect. A **34**, S318–S318 (1978).

## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

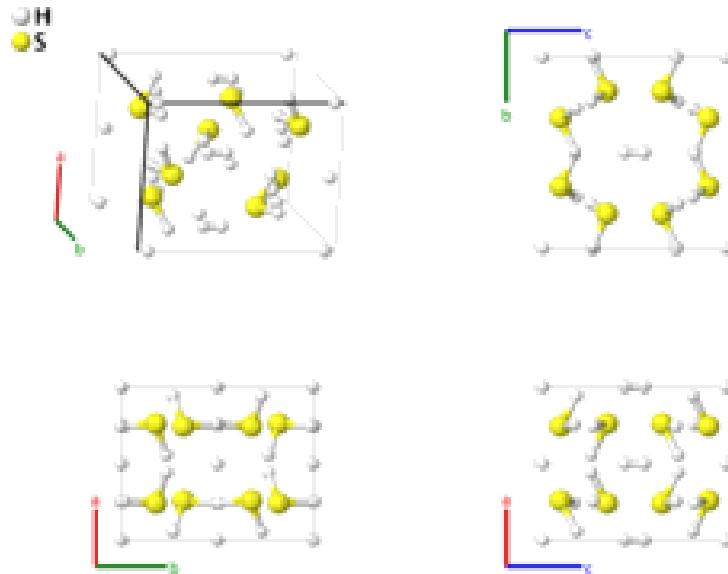
---

**Geometry files:**

- CIF: pp. [814](#)

- POSCAR: pp. [815](#)

# H<sub>3</sub>S (5 GPa) Structure: A3B\_oI32\_23\_ij2k\_k

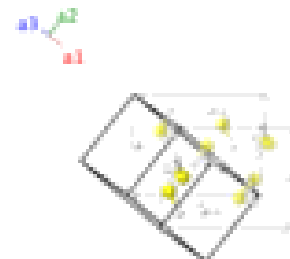


<b>Prototype</b>	:	H <sub>3</sub> S
<b>AFLOW prototype label</b>	:	A3B_oI32_23_ij2k_k
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oI32
<b>Space group number</b>	:	23
<b>Space group symbol</b>	:	<i>I</i> 222
<b>AFLOW prototype command</b>	:	aflow --proto=A3B_oI32_23_ij2k_k --params=a, b/a, c/a, z <sub>1</sub> , z <sub>2</sub> , x <sub>3</sub> , y <sub>3</sub> , z <sub>3</sub> , x <sub>4</sub> , y <sub>4</sub> , z <sub>4</sub> , x <sub>5</sub> , y <sub>5</sub> , z <sub>5</sub>

- This structure is found in H<sub>3</sub>S in the pressure range 3.5-17 GPa. The data presented here was taken at 5 GPa.

## Body-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2$	$z_1 c \hat{\mathbf{z}}$	(4 <i>i</i> )	H I
<b>B<sub>2</sub></b> =	$-z_1 \mathbf{a}_1 - z_1 \mathbf{a}_2$	$-z_1 c \hat{\mathbf{z}}$	(4 <i>i</i> )	H I
<b>B<sub>3</sub></b> =	$\left(\frac{1}{2} + z_2\right) \mathbf{a}_1 + z_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2}b\hat{\mathbf{y}} + z_2c\hat{\mathbf{z}}$	(4 <i>j</i> )	H II

$$\begin{aligned}
\mathbf{B}_4 &= \left(\frac{1}{2} - z_2\right) \mathbf{a}_1 - z_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \frac{1}{2} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} &(4j) & \text{H II} \\
\mathbf{B}_5 &= (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} &(8k) & \text{H III} \\
\mathbf{B}_6 &= (-y_3 + z_3) \mathbf{a}_1 + (-x_3 + z_3) \mathbf{a}_2 + (-x_3 - y_3) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} &(8k) & \text{H III} \\
\mathbf{B}_7 &= (y_3 - z_3) \mathbf{a}_1 + (-x_3 - z_3) \mathbf{a}_2 + (-x_3 + y_3) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} &(8k) & \text{H III} \\
\mathbf{B}_8 &= (-y_3 - z_3) \mathbf{a}_1 + (x_3 - z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} &(8k) & \text{H III} \\
\mathbf{B}_9 &= (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} &(8k) & \text{H IV} \\
\mathbf{B}_{10} &= (-y_4 + z_4) \mathbf{a}_1 + (-x_4 + z_4) \mathbf{a}_2 + (-x_4 - y_4) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} &(8k) & \text{H IV} \\
\mathbf{B}_{11} &= (y_4 - z_4) \mathbf{a}_1 + (-x_4 - z_4) \mathbf{a}_2 + (-x_4 + y_4) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} &(8k) & \text{H IV} \\
\mathbf{B}_{12} &= (-y_4 - z_4) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} &(8k) & \text{H IV} \\
\mathbf{B}_{13} &= (y_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + (x_5 + y_5) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} &(8k) & \text{S} \\
\mathbf{B}_{14} &= (-y_5 + z_5) \mathbf{a}_1 + (-x_5 + z_5) \mathbf{a}_2 + (-x_5 - y_5) \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} &(8k) & \text{S} \\
\mathbf{B}_{15} &= (y_5 - z_5) \mathbf{a}_1 + (-x_5 - z_5) \mathbf{a}_2 + (-x_5 + y_5) \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} &(8k) & \text{S} \\
\mathbf{B}_{16} &= (-y_5 - z_5) \mathbf{a}_1 + (x_5 - z_5) \mathbf{a}_2 + (x_5 - y_5) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} &(8k) & \text{S}
\end{aligned}$$

---

**References:**

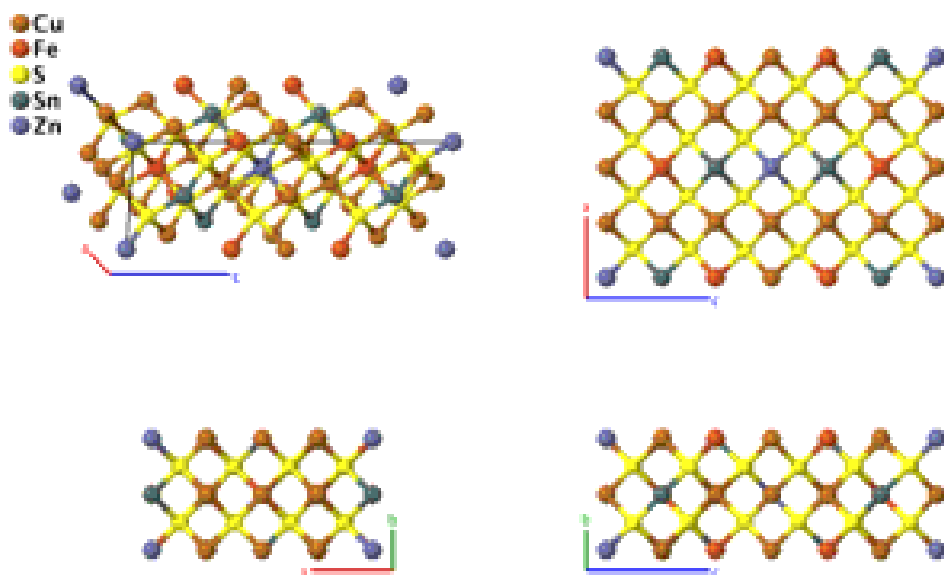
- T. A. Strobel, P. Ganesh, M. Somayazulu, P. R. C. Kent, and R. J. Hemley, *Novel Cooperative Interactions and Structural Ordering in  $H_2S-H_2$* , Phys. Rev. Lett. **107**, 255503 (2011), doi:[10.1103/PhysRevLett.107.255503](https://doi.org/10.1103/PhysRevLett.107.255503).

---

**Geometry files:**

- CIF: pp. [815](#)  
- POSCAR: pp. [815](#)

# Stannoidite ( $\text{Cu}_8(\text{Fe,Zn})_3\text{Sn}_2\text{S}_{12}$ ) Structure: A8B2C12D2E\_oI50\_23\_bcfk\_i\_3k\_j\_a

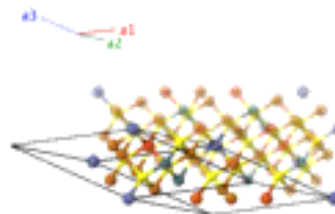


<b>Prototype</b>	:	$\text{Cu}_8(\text{Fe, Zn})_3\text{Sn}_2\text{S}_{12}$
<b>AFLOW prototype label</b>	:	A8B2C12D2E_oI50_23_bcfk_i_3k_j_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oI50
<b>Space group number</b>	:	23
<b>Space group symbol</b>	:	$I222$
<b>AFLOW prototype command</b>	:	aflow --proto=A8B2C12D2E_oI50_23_bcfk_i_3k_j_a --params=a, b/a, c/a, x4, z5, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10

- The composition of the Zn (2a) site is actually  $\text{Zn}_{0.85}\text{Fe}_{0.15}$ .

## Body-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	Zn
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(2b)	Cu I

$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Cu III
$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Cu III
$\mathbf{B}_6$	$=$	$z_5 \mathbf{a}_1 + z_5 \mathbf{a}_2$	$=$	$z_5 c \hat{\mathbf{z}}$	(4i)	Fe
$\mathbf{B}_7$	$=$	$-z_5 \mathbf{a}_1 - z_5 \mathbf{a}_2$	$=$	$-z_5 c \hat{\mathbf{z}}$	(4i)	Fe
$\mathbf{B}_8$	$=$	$\left(\frac{1}{2} + z_6\right) \mathbf{a}_1 + z_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4j)	Sn
$\mathbf{B}_9$	$=$	$\left(\frac{1}{2} - z_6\right) \mathbf{a}_1 - z_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(4j)	Sn
$\mathbf{B}_{10}$	$=$	$(y_7 + z_7) \mathbf{a}_1 + (x_7 + z_7) \mathbf{a}_2 + (x_7 + y_7) \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8k)	Cu IV
$\mathbf{B}_{11}$	$=$	$(-y_7 + z_7) \mathbf{a}_1 + (-x_7 + z_7) \mathbf{a}_2 + (-x_7 - y_7) \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8k)	Cu IV
$\mathbf{B}_{12}$	$=$	$(y_7 - z_7) \mathbf{a}_1 + (-x_7 - z_7) \mathbf{a}_2 + (-x_7 + y_7) \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}}$	(8k)	Cu IV
$\mathbf{B}_{13}$	$=$	$(-y_7 - z_7) \mathbf{a}_1 + (x_7 - z_7) \mathbf{a}_2 + (x_7 - y_7) \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}}$	(8k)	Cu IV
$\mathbf{B}_{14}$	$=$	$(y_8 + z_8) \mathbf{a}_1 + (x_8 + z_8) \mathbf{a}_2 + (x_8 + y_8) \mathbf{a}_3$	$=$	$x_8 a \hat{\mathbf{x}} + y_8 b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(8k)	S I
$\mathbf{B}_{15}$	$=$	$(-y_8 + z_8) \mathbf{a}_1 + (-x_8 + z_8) \mathbf{a}_2 + (-x_8 - y_8) \mathbf{a}_3$	$=$	$-x_8 a \hat{\mathbf{x}} - y_8 b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(8k)	S I
$\mathbf{B}_{16}$	$=$	$(y_8 - z_8) \mathbf{a}_1 + (-x_8 - z_8) \mathbf{a}_2 + (-x_8 + y_8) \mathbf{a}_3$	$=$	$-x_8 a \hat{\mathbf{x}} + y_8 b \hat{\mathbf{y}} - z_8 c \hat{\mathbf{z}}$	(8k)	S I
$\mathbf{B}_{17}$	$=$	$(-y_8 - z_8) \mathbf{a}_1 + (x_8 - z_8) \mathbf{a}_2 + (x_8 - y_8) \mathbf{a}_3$	$=$	$x_8 a \hat{\mathbf{x}} - y_8 b \hat{\mathbf{y}} - z_8 c \hat{\mathbf{z}}$	(8k)	S I
$\mathbf{B}_{18}$	$=$	$(y_9 + z_9) \mathbf{a}_1 + (x_9 + z_9) \mathbf{a}_2 + (x_9 + y_9) \mathbf{a}_3$	$=$	$x_9 a \hat{\mathbf{x}} + y_9 b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(8k)	S II
$\mathbf{B}_{19}$	$=$	$(-y_9 + z_9) \mathbf{a}_1 + (-x_9 + z_9) \mathbf{a}_2 + (-x_9 - y_9) \mathbf{a}_3$	$=$	$-x_9 a \hat{\mathbf{x}} - y_9 b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(8k)	S II
$\mathbf{B}_{20}$	$=$	$(y_9 - z_9) \mathbf{a}_1 + (-x_9 - z_9) \mathbf{a}_2 + (-x_9 + y_9) \mathbf{a}_3$	$=$	$-x_9 a \hat{\mathbf{x}} + y_9 b \hat{\mathbf{y}} - z_9 c \hat{\mathbf{z}}$	(8k)	S II
$\mathbf{B}_{21}$	$=$	$(-y_9 - z_9) \mathbf{a}_1 + (x_9 - z_9) \mathbf{a}_2 + (x_9 - y_9) \mathbf{a}_3$	$=$	$x_9 a \hat{\mathbf{x}} - y_9 b \hat{\mathbf{y}} - z_9 c \hat{\mathbf{z}}$	(8k)	S II
$\mathbf{B}_{22}$	$=$	$(y_{10} + z_{10}) \mathbf{a}_1 + (x_{10} + z_{10}) \mathbf{a}_2 + (x_{10} + y_{10}) \mathbf{a}_3$	$=$	$x_{10} a \hat{\mathbf{x}} + y_{10} b \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(8k)	S III
$\mathbf{B}_{23}$	$=$	$(-y_{10} + z_{10}) \mathbf{a}_1 + (-x_{10} + z_{10}) \mathbf{a}_2 +$ $(-x_{10} - y_{10}) \mathbf{a}_3$	$=$	$-x_{10} a \hat{\mathbf{x}} - y_{10} b \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(8k)	S III
$\mathbf{B}_{24}$	$=$	$(y_{10} - z_{10}) \mathbf{a}_1 + (-x_{10} - z_{10}) \mathbf{a}_2 +$ $(-x_{10} + y_{10}) \mathbf{a}_3$	$=$	$-x_{10} a \hat{\mathbf{x}} + y_{10} b \hat{\mathbf{y}} - z_{10} c \hat{\mathbf{z}}$	(8k)	S III
$\mathbf{B}_{25}$	$=$	$(-y_{10} - z_{10}) \mathbf{a}_1 + (x_{10} - z_{10}) \mathbf{a}_2 +$ $(x_{10} - y_{10}) \mathbf{a}_3$	$=$	$x_{10} a \hat{\mathbf{x}} - y_{10} b \hat{\mathbf{y}} - z_{10} c \hat{\mathbf{z}}$	(8k)	S III

---

#### References:

- Y. Kudoh and Y. Takéuchi, *The superstructure of stannoidite*, *Zeitschrift für Kristallographie - Crystalline Materials* **144**, 145–160 (1976), doi:10.1524/zkri.1976.144.16.145.

---

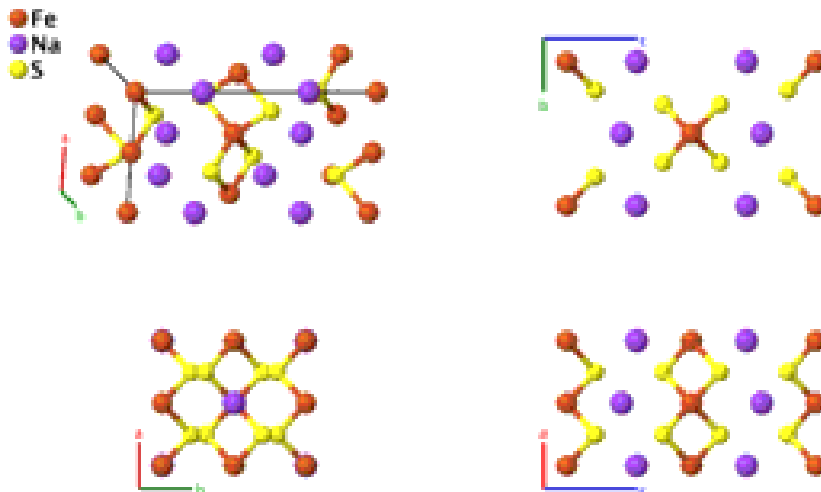
#### Geometry files:

- CIF: pp. 815

- POSCAR: pp. 816



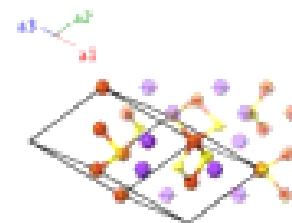
# NaFeS<sub>2</sub> Structure: ABC2\_oI16\_23\_ab\_i\_k



**Prototype** : NaFeS<sub>2</sub>  
**AFLOW prototype label** : ABC2\_oI16\_23\_ab\_i\_k  
**Strukturbericht designation** : None  
**Pearson symbol** : oI16  
**Space group number** : 23  
**Space group symbol** : *I*222  
**AFLOW prototype command** : aflow --proto=ABC2\_oI16\_23\_ab\_i\_k  
 --params=*a, b/a, c/a, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>*

**Body-centered Orthorhombic primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\
 \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub> =	$0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$	$0\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}}$	(2 <i>a</i> )	Fe I
<b>B</b> <sub>2</sub> =	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$\frac{1}{2}a\hat{\mathbf{x}}$	(2 <i>b</i> )	Fe II
<b>B</b> <sub>3</sub> =	$z_3\mathbf{a}_1 + z_3\mathbf{a}_2$	$z_3c\hat{\mathbf{z}}$	(4 <i>i</i> )	Na
<b>B</b> <sub>4</sub> =	$-z_3\mathbf{a}_1 - z_3\mathbf{a}_2$	$-z_3c\hat{\mathbf{z}}$	(4 <i>i</i> )	Na
<b>B</b> <sub>5</sub> =	$(y_4 + z_4)\mathbf{a}_1 + (x_4 + z_4)\mathbf{a}_2 + (x_4 + y_4)\mathbf{a}_3$	$x_4a\hat{\mathbf{x}} + y_4b\hat{\mathbf{y}} + z_4c\hat{\mathbf{z}}$	(8 <i>k</i> )	S
<b>B</b> <sub>6</sub> =	$(-y_4 + z_4)\mathbf{a}_1 + (-x_4 + z_4)\mathbf{a}_2 + (-x_4 - y_4)\mathbf{a}_3$	$-x_4a\hat{\mathbf{x}} - y_4b\hat{\mathbf{y}} + z_4c\hat{\mathbf{z}}$	(8 <i>k</i> )	S
<b>B</b> <sub>7</sub> =	$(y_4 - z_4)\mathbf{a}_1 + (-x_4 - z_4)\mathbf{a}_2 + (-x_4 + y_4)\mathbf{a}_3$	$-x_4a\hat{\mathbf{x}} + y_4b\hat{\mathbf{y}} - z_4c\hat{\mathbf{z}}$	(8 <i>k</i> )	S
<b>B</b> <sub>8</sub> =	$(-y_4 - z_4)\mathbf{a}_1 + (x_4 - z_4)\mathbf{a}_2 + (x_4 - y_4)\mathbf{a}_3$	$x_4a\hat{\mathbf{x}} - y_4b\hat{\mathbf{y}} - z_4c\hat{\mathbf{z}}$	(8 <i>k</i> )	S

---

**References:**

- H. Boller and H. Blaha, *Zur Kenntnis des Natriumthioferrates (III)*, *Monatsh. Chem.* **114**, 145–154 (1983),  
[doi:10.1007/BF00798319](https://doi.org/10.1007/BF00798319).

**Found in:**

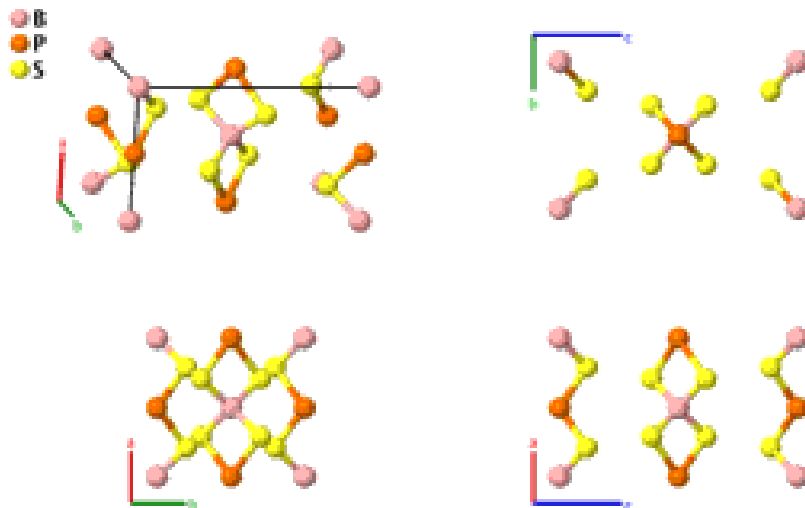
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [816](#)  
- POSCAR: pp. [816](#)

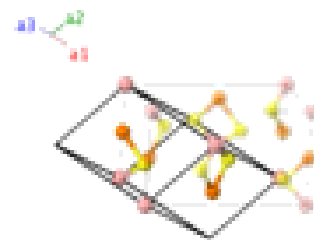
# BPS<sub>4</sub> Structure: ABC<sub>4</sub>\_oI12\_23\_a\_b\_k



<b>Prototype</b>	:	BPS <sub>4</sub>
<b>AFLOW prototype label</b>	:	ABC <sub>4</sub> _oI12_23_a_b_k
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oI12
<b>Space group number</b>	:	23
<b>Space group symbol</b>	:	<i>I</i> 222
<b>AFLOW prototype command</b>	:	aflow --proto=ABC <sub>4</sub> _oI12_23_a_b_k --params= <i>a, b/a, c/a, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub></i>

## Body-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2 <i>a</i> )	B
<b>B</b> <sub>2</sub>	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}}$	(2 <i>b</i> )	P
<b>B</b> <sub>3</sub>	$(y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8 <i>k</i> )	S
<b>B</b> <sub>4</sub>	$(-y_3 + z_3) \mathbf{a}_1 + (-x_3 + z_3) \mathbf{a}_2 + (-x_3 - y_3) \mathbf{a}_3$	$-x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8 <i>k</i> )	S
<b>B</b> <sub>5</sub>	$(y_3 - z_3) \mathbf{a}_1 + (-x_3 - z_3) \mathbf{a}_2 + (-x_3 + y_3) \mathbf{a}_3$	$-x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(8 <i>k</i> )	S
<b>B</b> <sub>6</sub>	$(-y_3 - z_3) \mathbf{a}_1 + (x_3 - z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(8 <i>k</i> )	S

**References:**

- A. Weiss and H. Schäfer, *Zur Kenntnis von Bortetrathiophosphat BPS<sub>4</sub>*, Z. Naturforsch. B **18**, 81–82 (1963), [doi:10.1515/znb-1963-0117](https://doi.org/10.1515/znb-1963-0117).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

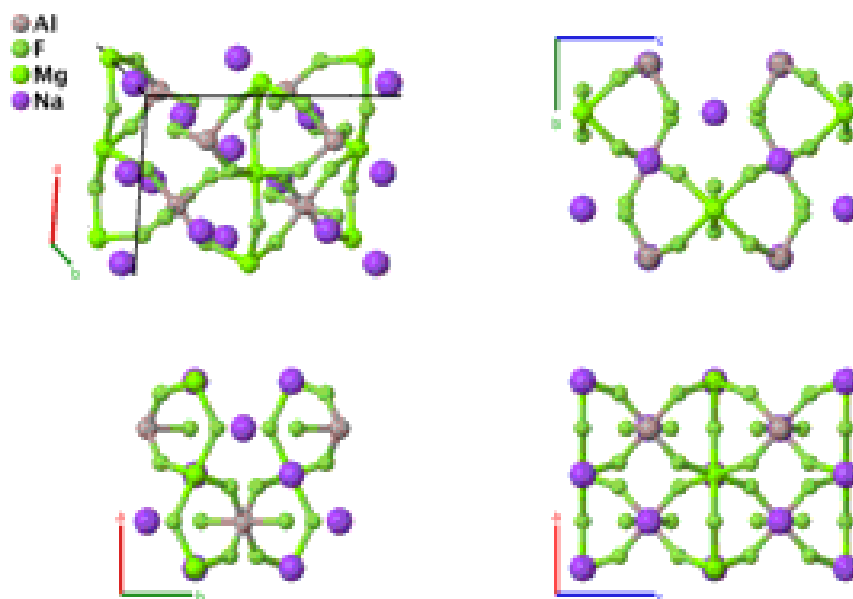
---

**Geometry files:**

- CIF: pp. [816](#)

- POSCAR: pp. [817](#)

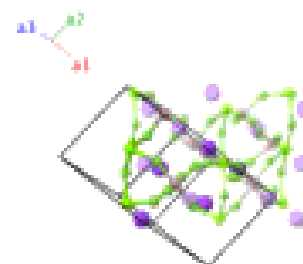
# Weberite ( $\text{Na}_2\text{MgAlF}_7$ ) Structure: AB7CD2\_oI44\_24\_a\_b3d\_c\_ac



<b>Prototype</b>	:	$\text{Na}_2\text{MgAlF}_7$
<b>AFLOW prototype label</b>	:	AB7CD2_oI44_24_a_b3d_c_ac
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oI44
<b>Space group number</b>	:	24
<b>Space group symbol</b>	:	$I2_12_12_1$
<b>AFLOW prototype command</b>	:	aflow --proto=AB7CD2_oI44_24_a_b3d_c_ac --params=a, b/a, c/a, $x_1, x_2, y_3, z_4, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

## Body-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{x} + \frac{1}{2}b\hat{y} + \frac{1}{2}c\hat{z} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{x} - \frac{1}{2}b\hat{y} + \frac{1}{2}c\hat{z} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{x} + \frac{1}{2}b\hat{y} - \frac{1}{2}c\hat{z} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_1 + \left(\frac{1}{4} + x_1\right)\mathbf{a}_2 + x_1\mathbf{a}_3$	$= x_1a\hat{x} + \frac{1}{4}c\hat{z}$	(4a)	Al
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_1 + \left(\frac{1}{4} - x_1\right)\mathbf{a}_2 + \left(\frac{1}{2} - x_1\right)\mathbf{a}_3$	$= -x_1a\hat{x} + \frac{1}{2}b\hat{y} + \frac{1}{4}c\hat{z}$	(4a)	Al
$\mathbf{B}_3$	$= \frac{1}{4}\mathbf{a}_1 + \left(\frac{1}{4} + x_2\right)\mathbf{a}_2 + x_2\mathbf{a}_3$	$= x_2a\hat{x} + \frac{1}{4}c\hat{z}$	(4a)	Na I
$\mathbf{B}_4$	$= \frac{3}{4}\mathbf{a}_1 + \left(\frac{1}{4} - x_2\right)\mathbf{a}_2 + \left(\frac{1}{2} - x_2\right)\mathbf{a}_3$	$= -x_2a\hat{x} + \frac{1}{2}b\hat{y} + \frac{1}{4}c\hat{z}$	(4a)	Na I

$$\begin{aligned}
\mathbf{B}_5 &= y_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{4} + y_3\right) \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} && (4b) && \text{F I} \\
\mathbf{B}_6 &= \left(\frac{1}{2} - y_3\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{4} - y_3\right) \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} && (4b) && \text{F I} \\
\mathbf{B}_7 &= \left(\frac{1}{4} + z_4\right) \mathbf{a}_1 + z_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{4} b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (4c) && \text{Mg} \\
\mathbf{B}_8 &= \left(\frac{1}{4} - z_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (4c) && \text{Mg} \\
\mathbf{B}_9 &= \left(\frac{1}{4} + z_5\right) \mathbf{a}_1 + z_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{4} b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (4c) && \text{Na II} \\
\mathbf{B}_{10} &= \left(\frac{1}{4} - z_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} && (4c) && \text{Na II} \\
\mathbf{B}_{11} &= (y_6 + z_6) \mathbf{a}_1 + (x_6 + z_6) \mathbf{a}_2 + (x_6 + y_6) \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} && (8d) && \text{F II} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} - y_6 + z_6\right) \mathbf{a}_1 + (-x_6 + z_6) \mathbf{a}_2 + &= -x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} && (8d) && \text{F II} \\
&\quad \left(\frac{1}{2} - x_6 - y_6\right) \mathbf{a}_3 \\
\mathbf{B}_{13} &= (y_6 - z_6) \mathbf{a}_1 + \left(\frac{1}{2} - x_6 - z_6\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} && (8d) && \text{F II} \\
&\quad \left(\frac{1}{2} - x_6 + y_6\right) \mathbf{a}_3 \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - y_6 - z_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_6 - z_6\right) \mathbf{a}_2 + &= x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}} && (8d) && \text{F II} \\
&\quad (x_6 - y_6) \mathbf{a}_3 \\
\mathbf{B}_{15} &= (y_7 + z_7) \mathbf{a}_1 + (x_7 + z_7) \mathbf{a}_2 + (x_7 + y_7) \mathbf{a}_3 &= x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} && (8d) && \text{F III} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} - y_7 + z_7\right) \mathbf{a}_1 + (-x_7 + z_7) \mathbf{a}_2 + &= -x_7 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_7\right) b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} && (8d) && \text{F III} \\
&\quad \left(\frac{1}{2} - x_7 - y_7\right) \mathbf{a}_3 \\
\mathbf{B}_{17} &= (y_7 - z_7) \mathbf{a}_1 + \left(\frac{1}{2} - x_7 - z_7\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_7\right) a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} && (8d) && \text{F III} \\
&\quad \left(\frac{1}{2} - x_7 + y_7\right) \mathbf{a}_3 \\
\mathbf{B}_{18} &= \left(\frac{1}{2} - y_7 - z_7\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_7 - z_7\right) \mathbf{a}_2 + &= x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_7\right) c \hat{\mathbf{z}} && (8d) && \text{F III} \\
&\quad (x_7 - y_7) \mathbf{a}_3 \\
\mathbf{B}_{19} &= (y_8 + z_8) \mathbf{a}_1 + (x_8 + z_8) \mathbf{a}_2 + (x_8 + y_8) \mathbf{a}_3 &= x_8 a \hat{\mathbf{x}} + y_8 b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} && (8d) && \text{F IV} \\
\mathbf{B}_{20} &= \left(\frac{1}{2} - y_8 + z_8\right) \mathbf{a}_1 + (-x_8 + z_8) \mathbf{a}_2 + &= -x_8 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_8\right) b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} && (8d) && \text{F IV} \\
&\quad \left(\frac{1}{2} - x_8 - y_8\right) \mathbf{a}_3 \\
\mathbf{B}_{21} &= (y_8 - z_8) \mathbf{a}_1 + \left(\frac{1}{2} - x_8 - z_8\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_8\right) a \hat{\mathbf{x}} + y_8 b \hat{\mathbf{y}} - z_8 c \hat{\mathbf{z}} && (8d) && \text{F IV} \\
&\quad \left(\frac{1}{2} - x_8 + y_8\right) \mathbf{a}_3 \\
\mathbf{B}_{22} &= \left(\frac{1}{2} - y_8 - z_8\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_8 - z_8\right) \mathbf{a}_2 + &= x_8 a \hat{\mathbf{x}} - y_8 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_8\right) c \hat{\mathbf{z}} && (8d) && \text{F IV} \\
&\quad (x_8 - y_8) \mathbf{a}_3
\end{aligned}$$

---

#### References:

- O. Knop, T. S. Cameron, and K. Jochem, *What is the true space group of weberite?*, J. Solid State Chem. **43**, 213–221 (1982), doi:[10.1016/0022-4596\(82\)90231-6](https://doi.org/10.1016/0022-4596(82)90231-6).

#### Found in:

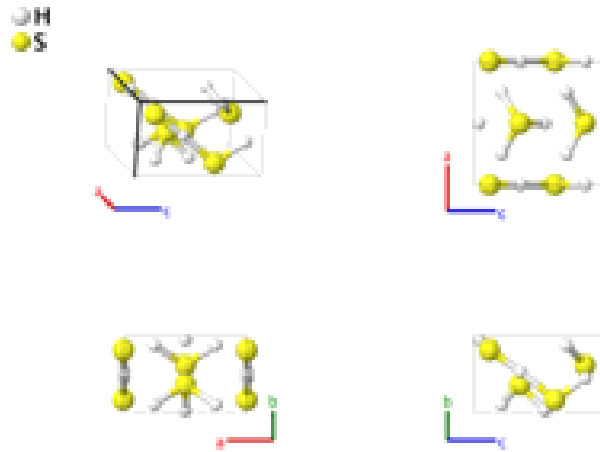
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [817](#)  
- POSCAR: pp. [817](#)

# H<sub>2</sub>S (70 GPa) Structure: A2B\_oP12\_26\_abc\_ab



**Prototype** : H<sub>2</sub>S  
**AFLOW prototype label** : A2B\_oP12\_26\_abc\_ab  
**Strukturbericht designation** : None  
**Pearson symbol** : oP12  
**Space group number** : 26  
**Space group symbol** : *Pmc*2<sub>1</sub>  
**AFLOW prototype command** : `aflow --proto=A2B_oP12_26_abc_ab`  
`--params=a, b/a, c/a, y1, z1, y2, z2, y3, z3, y4, z4, x5, y5, z5`

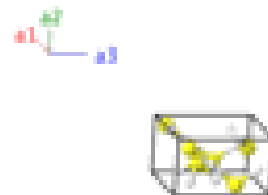
- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H<sub>2</sub>S in the range 40 – 80 GPa. The data presented here was computed at 70 GPa. H<sub>2</sub>S (pp. 95) and β-SeO<sub>2</sub> (pp. 97) have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

## Simple Orthorhombic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub> =	$y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(2a)	HI
<b>B</b> <sub>2</sub> =	$-y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$-y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	HI
<b>B</b> <sub>3</sub> =	$y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2a)	SI

$$\begin{aligned}
\mathbf{B}_4 &= -y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= -y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (2a) & \text{S I} \\
\mathbf{B}_5 &= \frac{1}{2} \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (2b) & \text{H II} \\
\mathbf{B}_6 &= \frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (2b) & \text{H II} \\
\mathbf{B}_7 &= \frac{1}{2} \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (2b) & \text{S II} \\
\mathbf{B}_8 &= \frac{1}{2} \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (2b) & \text{S II} \\
\mathbf{B}_9 &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (4c) & \text{H III} \\
\mathbf{B}_{10} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (4c) & \text{H III} \\
\mathbf{B}_{11} &= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (4c) & \text{H III} \\
\mathbf{B}_{12} &= -x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (4c) & \text{H III}
\end{aligned}$$

---

**References:**

- Y. Li, J. Hao, H. Liu, Y. Li, and Y. Ma, *The metallization and superconductivity of dense hydrogen sulfide*, J. Chem. Phys. **140**, 174712 (2014), doi:10.1063/1.4874158.

---

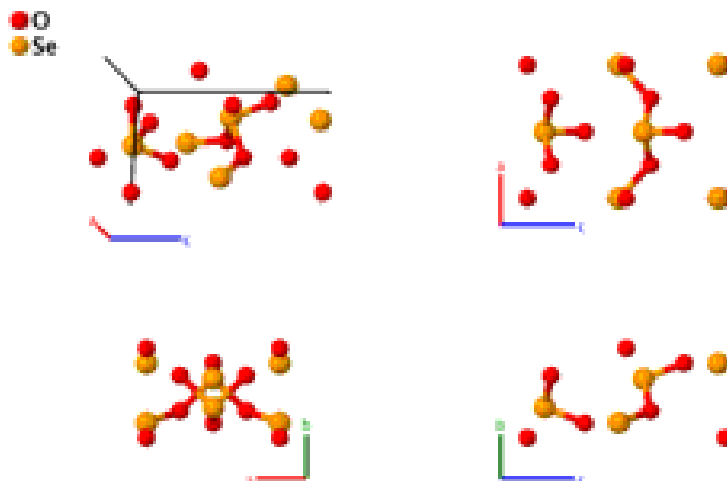
**Geometry files:**

- CIF: pp. [817](#)

- POSCAR: pp. [818](#)



# $\beta$ -SeO<sub>2</sub> Structure: A2B\_oP12\_26\_abc\_ab

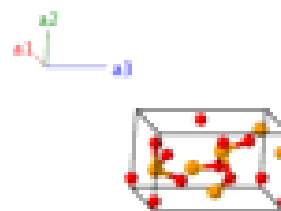


<b>Prototype</b>	:	$\beta$ -SeO <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_oP12_26_abc_ab
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP12
<b>Space group number</b>	:	26
<b>Space group symbol</b>	:	$Pmc2_1$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_oP12_26_abc_ab --params= $a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4, x_5, y_5, z_5$

- H<sub>2</sub>S (pp. 95) and  $\beta$ -SeO<sub>2</sub> (pp. 97) have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters (--params) specified in their corresponding CIF files.

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_2$	$= -y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$-y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_3$	$= y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2a)	Se I
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	=	$-y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(2a)	Se I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2b)	O II

$$\begin{aligned}
\mathbf{B}_6 &= \frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} && (2b) && \text{O II} \\
\mathbf{B}_7 &= \frac{1}{2} \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (2b) && \text{Se II} \\
\mathbf{B}_8 &= \frac{1}{2} \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} && (2b) && \text{Se II} \\
\mathbf{B}_9 &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (4c) && \text{O III} \\
\mathbf{B}_{10} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} && (4c) && \text{O III} \\
\mathbf{B}_{11} &= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} && (4c) && \text{O III} \\
\mathbf{B}_{12} &= -x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (4c) && \text{O III}
\end{aligned}$$

**References:**

- D. Orosel, O. Leynaud, P. Balog, and M. Jansen, *Pressure-temperature phase diagram of SeO<sub>2</sub>. Characterization of new phases*, J. Solid State Chem. **177**, 1631–1638 (2004), doi:[10.1016/j.jssc.2003.12.028](https://doi.org/10.1016/j.jssc.2003.12.028).

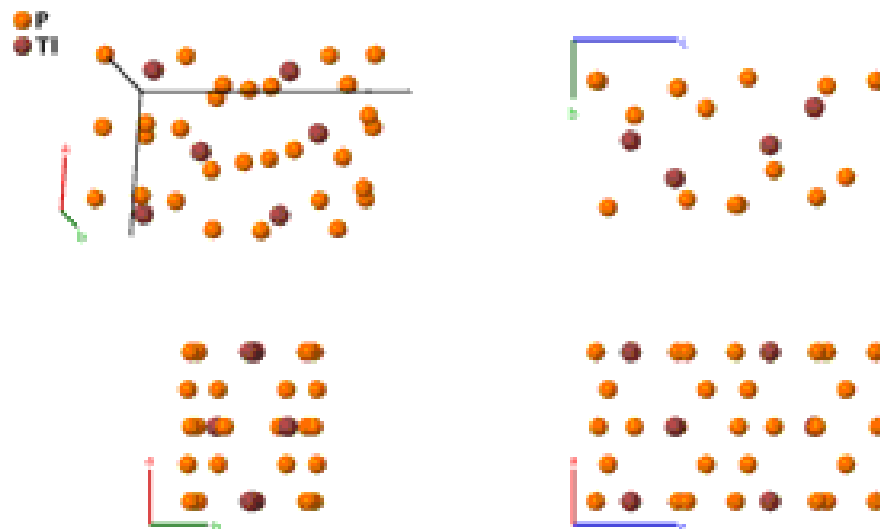
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [818](#)
- POSCAR: pp. [818](#)

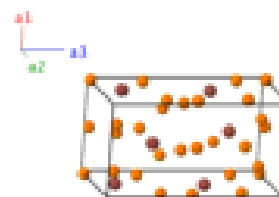
# TIP<sub>5</sub> Structure: A5B\_oP24\_26\_3a3b2c\_ab



**Prototype** : TIP<sub>5</sub>  
**AFLOW prototype label** : A5B\_oP24\_26\_3a3b2c\_ab  
**Strukturbericht designation** : None  
**Pearson symbol** : oP24  
**Space group number** : 26  
**Space group symbol** :  $Pmc2_1$   
**AFLOW prototype command** : `aflow --proto=A5B_oP24_26_3a3b2c_ab`  
`--params=a, b/a, c/a, y1, z1, y2, z2, y3, z3, y4, z4, y5, z5, y6, z6, y7, z7, y8, z8, x9,`  
`y9, z9, x10, y10, z10`

## Simple Orthorhombic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(2a)	P I
$\mathbf{B}_2$	$= -y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$=$	$-y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	P I
$\mathbf{B}_3$	$= y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2a)	P II
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$-y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(2a)	P II
$\mathbf{B}_5$	$= y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2a)	P III
$\mathbf{B}_6$	$= -y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$-y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(2a)	P III
$\mathbf{B}_7$	$= y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(2a)	Tl I

$\mathbf{B}_8$	$=$	$-y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$-y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(2a)	TI I
$\mathbf{B}_9$	$=$	$\frac{1}{2} \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(2b)	P IV
$\mathbf{B}_{10}$	$=$	$\frac{1}{2} \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(2b)	P IV
$\mathbf{B}_{11}$	$=$	$\frac{1}{2} \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(2b)	P V
$\mathbf{B}_{12}$	$=$	$\frac{1}{2} \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(2b)	P V
$\mathbf{B}_{13}$	$=$	$\frac{1}{2} \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(2b)	P VI
$\mathbf{B}_{14}$	$=$	$\frac{1}{2} \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(2b)	P VI
$\mathbf{B}_{15}$	$=$	$\frac{1}{2} \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + y_8 b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(2b)	TI II
$\mathbf{B}_{16}$	$=$	$\frac{1}{2} \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - y_8 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \hat{\mathbf{z}}$	(2b)	TI II
$\mathbf{B}_{17}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$x_9 a \hat{\mathbf{x}} + y_9 b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4c)	P VII
$\mathbf{B}_{18}$	$=$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3$	$=$	$-x_9 a \hat{\mathbf{x}} - y_9 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}}$	(4c)	P VII
$\mathbf{B}_{19}$	$=$	$x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3$	$=$	$x_9 a \hat{\mathbf{x}} - y_9 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}}$	(4c)	P VII
$\mathbf{B}_{20}$	$=$	$-x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-x_9 a \hat{\mathbf{x}} + y_9 b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4c)	P VII
$\mathbf{B}_{21}$	$=$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$x_{10} a \hat{\mathbf{x}} + y_{10} b \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(4c)	P VIII
$\mathbf{B}_{22}$	$=$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3$	$=$	$-x_{10} a \hat{\mathbf{x}} - y_{10} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}}$	(4c)	P VIII
$\mathbf{B}_{23}$	$=$	$x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3$	$=$	$x_{10} a \hat{\mathbf{x}} - y_{10} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}}$	(4c)	P VIII
$\mathbf{B}_{24}$	$=$	$-x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-x_{10} a \hat{\mathbf{x}} + y_{10} b \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(4c)	P VIII

---

#### References:

- O. Olofsson and J. Gullman, *The crystal structure of TIP<sub>5</sub>*, Acta Chem. Scand. **25**, 1327–1337 (1971), [doi:10.3891/acta.chem.scand.25-1327](https://doi.org/10.3891/acta.chem.scand.25-1327).

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

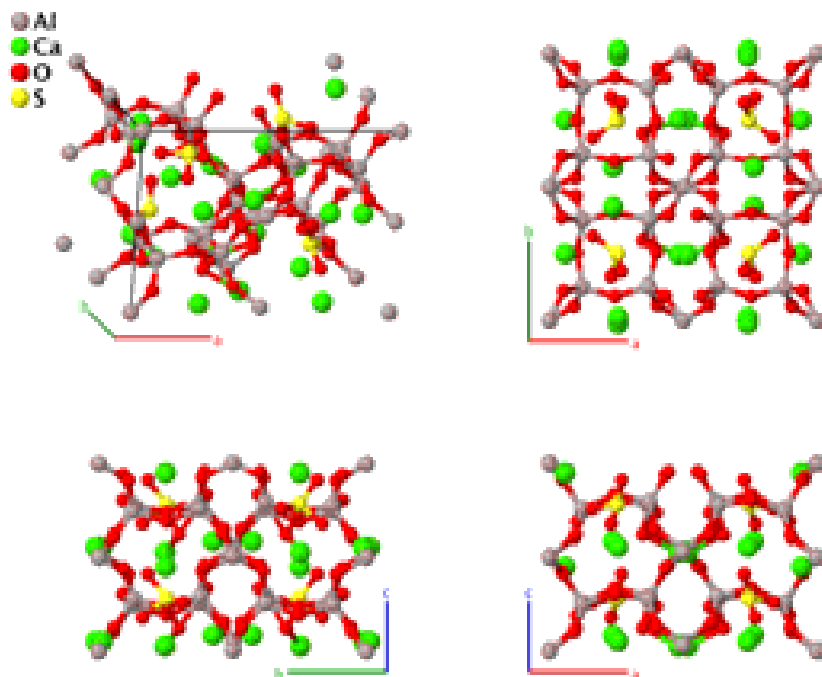
---

#### Geometry files:

- CIF: pp. [818](#)  
- POSCAR: pp. [819](#)

# Ca<sub>4</sub>Al<sub>6</sub>O<sub>16</sub>S Structure:

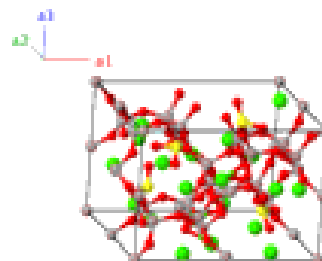
## A6B4C16D\_oP108\_27\_abcd4e\_4e\_16e\_e



<b>Prototype</b>	:	Ca <sub>4</sub> Al <sub>6</sub> O <sub>16</sub> S
<b>AFLOW prototype label</b>	:	A6B4C16D_oP108_27_abcd4e_4e_16e_e
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP108
<b>Space group number</b>	:	27
<b>Space group symbol</b>	:	<i>Pcc2</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A6B4C16D_oP108_27_abcd4e_4e_16e_e --params= <i>a, b/a, c/a, z1, z2, z3, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18, y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22, x23, y23, z23, x24, y24, z24, x25, y25, z25, x26, y26, z26, x27, y27, z27, x28, y28, z28, x29, y29, z29</i>

**Simple Orthorhombic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= b \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(2a)	Al I
<b>B</b> <sub>2</sub>	= $\left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$\left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Al I
<b>B</b> <sub>3</sub>	= $\frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2b)	Al II
<b>B</b> <sub>4</sub>	= $\frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	=	$\frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(2b)	Al II
<b>B</b> <sub>5</sub>	= $\frac{1}{2} \mathbf{a}_1 + z_3 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + z_3 c \hat{\mathbf{z}}$	(2c)	Al III
<b>B</b> <sub>6</sub>	= $\frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(2c)	Al III
<b>B</b> <sub>7</sub>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(2d)	Al IV
<b>B</b> <sub>8</sub>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(2d)	Al IV
<b>B</b> <sub>9</sub>	= $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4e)	Al V
<b>B</b> <sub>10</sub>	= $-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$-x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4e)	Al V
<b>B</b> <sub>11</sub>	= $x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	=	$x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(4e)	Al V
<b>B</b> <sub>12</sub>	= $-x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	=	$-x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(4e)	Al V
<b>B</b> <sub>13</sub>	= $x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4e)	Al VI
<b>B</b> <sub>14</sub>	= $-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$-x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4e)	Al VI
<b>B</b> <sub>15</sub>	= $x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	=	$x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(4e)	Al VI
<b>B</b> <sub>16</sub>	= $-x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	=	$-x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(4e)	Al VI
<b>B</b> <sub>17</sub>	= $x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4e)	Al VII
<b>B</b> <sub>18</sub>	= $-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4e)	Al VII
<b>B</b> <sub>19</sub>	= $x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(4e)	Al VII
<b>B</b> <sub>20</sub>	= $-x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(4e)	Al VII
<b>B</b> <sub>21</sub>	= $x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$x_8 a \hat{\mathbf{x}} + y_8 b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4e)	Al VIII
<b>B</b> <sub>22</sub>	= $-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$-x_8 a \hat{\mathbf{x}} - y_8 b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4e)	Al VIII
<b>B</b> <sub>23</sub>	= $x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3$	=	$x_8 a \hat{\mathbf{x}} - y_8 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \hat{\mathbf{z}}$	(4e)	Al VIII
<b>B</b> <sub>24</sub>	= $-x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3$	=	$-x_8 a \hat{\mathbf{x}} + y_8 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \hat{\mathbf{z}}$	(4e)	Al VIII
<b>B</b> <sub>25</sub>	= $x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$x_9 a \hat{\mathbf{x}} + y_9 b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4e)	Ca I
<b>B</b> <sub>26</sub>	= $-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$-x_9 a \hat{\mathbf{x}} - y_9 b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4e)	Ca I
<b>B</b> <sub>27</sub>	= $x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3$	=	$x_9 a \hat{\mathbf{x}} - y_9 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}}$	(4e)	Ca I
<b>B</b> <sub>28</sub>	= $-x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3$	=	$-x_9 a \hat{\mathbf{x}} + y_9 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}}$	(4e)	Ca I
<b>B</b> <sub>29</sub>	= $x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$x_{10} a \hat{\mathbf{x}} + y_{10} b \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(4e)	Ca II
<b>B</b> <sub>30</sub>	= $-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$-x_{10} a \hat{\mathbf{x}} - y_{10} b \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(4e)	Ca II
<b>B</b> <sub>31</sub>	= $x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3$	=	$x_{10} a \hat{\mathbf{x}} - y_{10} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}}$	(4e)	Ca II
<b>B</b> <sub>32</sub>	= $-x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3$	=	$-x_{10} a \hat{\mathbf{x}} + y_{10} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}}$	(4e)	Ca II
<b>B</b> <sub>33</sub>	= $x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	=	$x_{11} a \hat{\mathbf{x}} + y_{11} b \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}}$	(4e)	Ca III
<b>B</b> <sub>34</sub>	= $-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	=	$-x_{11} a \hat{\mathbf{x}} - y_{11} b \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}}$	(4e)	Ca III
<b>B</b> <sub>35</sub>	= $x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + \left(\frac{1}{2} + z_{11}\right) \mathbf{a}_3$	=	$x_{11} a \hat{\mathbf{x}} - y_{11} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{11}\right) c \hat{\mathbf{z}}$	(4e)	Ca III







$$\mathbf{B}_{108} = -x_{29} \mathbf{a}_1 + y_{29} \mathbf{a}_2 + \left(\frac{1}{2} + z_{29}\right) \mathbf{a}_3 = -x_{29}a \hat{\mathbf{x}} + y_{29}b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{29}\right)c \hat{\mathbf{z}} \quad (4e) \quad \text{S}$$

---

**References:**

- N. J. Calos, C. H. L. Kennard, A. K. Whittaker, and R. L. Davis, *Structure of calcium aluminate sulfate  $\text{Ca}_4\text{Al}_6\text{O}_{16}\text{S}$* , J. Solid State Chem. **119**, 1–7 (1995), doi:10.1016/0022-4596(95)80002-7.

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

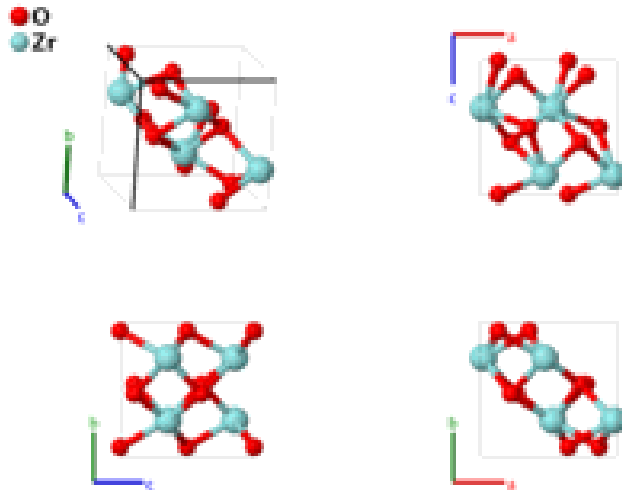
---

**Geometry files:**

- CIF: pp. [819](#)

- POSCAR: pp. [819](#)

# ZrO<sub>2</sub> Structure: A2B\_oP12\_29\_2a\_a

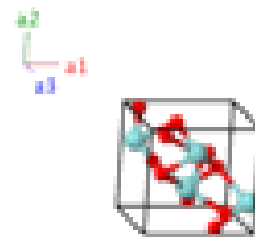


<b>Prototype</b>	:	ZrO <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_oP12_29_2a_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP12
<b>Space group number</b>	:	29
<b>Space group symbol</b>	:	<i>Pca</i> 2 <sub>1</sub>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_oP12_29_2a_a --params= <i>a, b/a, c/a, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub></i>

- ZrO<sub>2</sub> (pp. 106) and Pyrite (pp. 108) have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4a)	O I
<b>B<sub>2</sub></b>	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4a)	O I
<b>B<sub>3</sub></b>	$\left(\frac{1}{2} + x_1\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$\left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4a)	O I
<b>B<sub>4</sub></b>	$\left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4a)	O I

$$\begin{aligned}
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (4a) & \text{O II} \\
\mathbf{B}_6 &= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4a) & \text{O II} \\
\mathbf{B}_7 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (4a) & \text{O II} \\
\mathbf{B}_8 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4a) & \text{O II} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4a) & \text{Zr} \\
\mathbf{B}_{10} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4a) & \text{Zr} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4a) & \text{Zr} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4a) & \text{Zr}
\end{aligned}$$

---

### References:

- J. Grins, P.-O. Käll, and G. Svensson, *Phases in the  $Zr_xTa_{1-x}(O,N)_y$  system, formed by ammonolysis of Zr-Ta gels: Preparation of a baddeleyite-type solid solution phase  $Zr_xTa_{1-x}O_{1+x}N_{1-x}$ ,  $0 \leq x \leq 1$* , J. Mater. Chem. **4**, 1293–1301 (1994), doi:[10.1039/JM9940401293](https://doi.org/10.1039/JM9940401293).

### Found in:

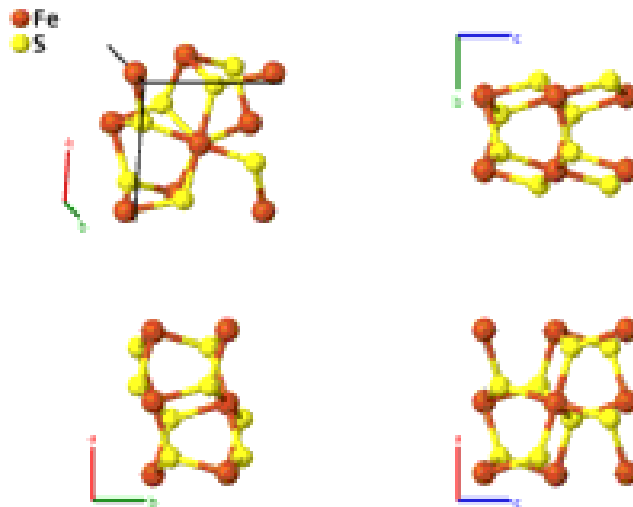
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. [820](#)
- POSCAR: pp. [820](#)

# Pyrite (FeS<sub>2</sub>, Low-temperature) Structure: AB2\_oP12\_29\_a\_2a



<b>Prototype</b>	:	FeS <sub>2</sub>
<b>AFLOW prototype label</b>	:	AB2_oP12_29_a_2a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP12
<b>Space group number</b>	:	29
<b>Space group symbol</b>	:	<i>Pca</i> 2 <sub>1</sub>
<b>AFLOW prototype command</b>	:	aflow --proto=AB2_oP12_29_a_2a --params= <i>a, b/a, c/a, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub></i>

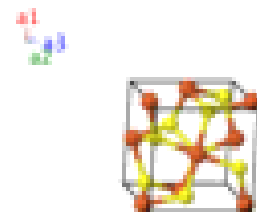
- ZrO<sub>2</sub> (pp. 106) and Pyrite (pp. 108) have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

## Simple Orthorhombic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	= $x_1 a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4a)	Fe
<b>B<sub>2</sub></b>	= $-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	= $-x_1 a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4a)	Fe

$$\begin{aligned}
\mathbf{B}_3 &= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3 &= \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}} & (4a) & \text{Fe} \\
\mathbf{B}_4 &= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}} & (4a) & \text{Fe} \\
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (4a) & \text{S I} \\
\mathbf{B}_6 &= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4a) & \text{S I} \\
\mathbf{B}_7 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (4a) & \text{S I} \\
\mathbf{B}_8 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4a) & \text{S I} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4a) & \text{S II} \\
\mathbf{B}_{10} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4a) & \text{S II} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4a) & \text{S II} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4a) & \text{S II}
\end{aligned}$$

---

### References:

- P. Bayliss, *Crystal chemistry and crystallography of some minerals within the pyrite group*, Am. Mineral. **74**, 1168–1176 (1989).

### Found in:

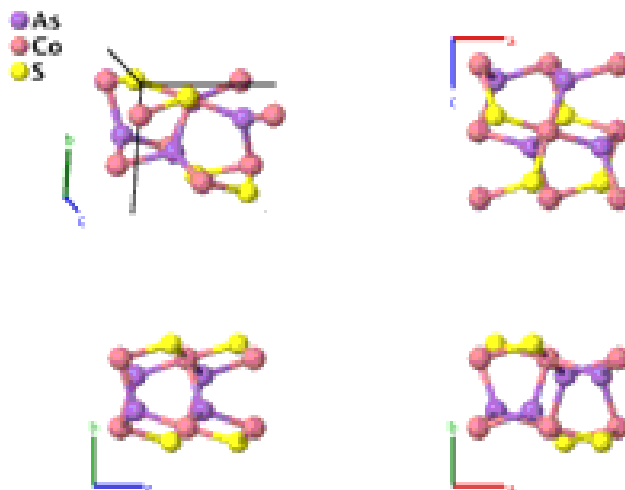
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. [820](#)  
- POSCAR: pp. [821](#)

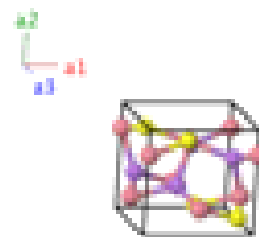
# Cobaltite (CoAsS) Structure: ABC\_oP12\_29\_a\_a\_a



**Prototype** : CoAsS  
**AFLOW prototype label** : ABC\_oP12\_29\_a\_a\_a  
**Strukturbericht designation** : None  
**Pearson symbol** : oP12  
**Space group number** : 29  
**Space group symbol** :  $Pca2_1$   
**AFLOW prototype command** : `aflow --proto=ABC_oP12_29_a_a_a`  
`--params=a, b/a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3`

## Simple Orthorhombic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4a)	As
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4a)	As
$\mathbf{B}_3$	$\left(\frac{1}{2} + x_1\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$\left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4a)	As
$\mathbf{B}_4$	$\left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4a)	As
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4a)	Co
$\mathbf{B}_6$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$-x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4a)	Co
$\mathbf{B}_7$	$\left(\frac{1}{2} + x_2\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$\left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4a)	Co

$$\begin{aligned}
\mathbf{B}_8 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4a) & \text{Co} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4a) & \text{S} \\
\mathbf{B}_{10} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4a) & \text{S} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4a) & \text{S} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4a) & \text{S}
\end{aligned}$$

**References:**

- M. E. Fleet and P. C. Burns, *Structure and twinning of cobaltite*, Can. Mineral. **28**, 719–723 (1990).

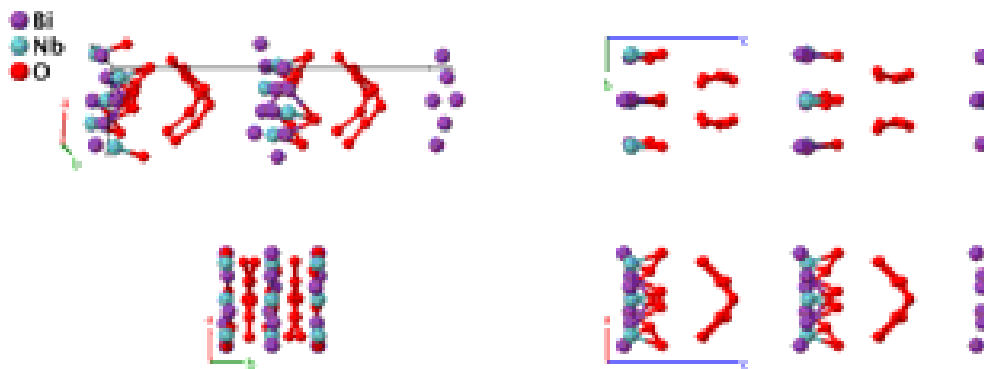
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [821](#)
- POSCAR: pp. [821](#)

# Bi<sub>5</sub>Nb<sub>3</sub>O<sub>15</sub> Structure: A5B3C15\_oP46\_30\_a2c\_bc\_a7c



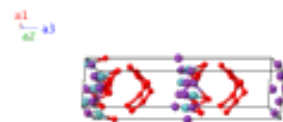
<b>Prototype</b>	:	Bi <sub>5</sub> Nb <sub>3</sub> O <sub>15</sub>
<b>AFLOW prototype label</b>	:	A5B3C15_oP46_30_a2c_bc_a7c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP46
<b>Space group number</b>	:	30
<b>Space group symbol</b>	:	<i>Pnc2</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A5B3C15_oP46_30_a2c_bc_a7c --params= <i>a, b/a, c/a, z<sub>1</sub>, z<sub>2</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>, y<sub>9</sub>, z<sub>9</sub>, x<sub>10</sub>, y<sub>10</sub>, z<sub>10</sub>, x<sub>11</sub>, y<sub>11</sub>, z<sub>11</sub>, x<sub>12</sub>, y<sub>12</sub>, z<sub>12</sub>, x<sub>13</sub>, y<sub>13</sub>, z<sub>13</sub></i>

## Simple Orthorhombic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $z_1 \mathbf{a}_3$	= $z_1 c \hat{\mathbf{z}}$	(2a)	Bi I
<b>B<sub>2</sub></b>	= $\frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	= $\frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Bi I
<b>B<sub>3</sub></b>	= $z_2 \mathbf{a}_3$	= $z_2 c \hat{\mathbf{z}}$	(2a)	O I
<b>B<sub>4</sub></b>	= $\frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	= $\frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(2a)	O I
<b>B<sub>5</sub></b>	= $\frac{1}{2} \mathbf{a}_1 + z_3 \mathbf{a}_3$	= $\frac{1}{2} a \hat{\mathbf{x}} + z_3 c \hat{\mathbf{z}}$	(2b)	Nb I
<b>B<sub>6</sub></b>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	= $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(2b)	Nb I
<b>B<sub>7</sub></b>	= $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	= $x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4c)	Bi II
<b>B<sub>8</sub></b>	= $-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	= $-x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4c)	Bi II
<b>B<sub>9</sub></b>	= $x_4 \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	= $x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(4c)	Bi II
<b>B<sub>10</sub></b>	= $-x_4 \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	= $-x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(4c)	Bi II
<b>B<sub>11</sub></b>	= $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	= $x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4c)	Bi III





$$\mathbf{B}_{46} = -x_{13} \mathbf{a}_1 + \left(\frac{1}{2} + y_{13}\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_{13}\right) \mathbf{a}_3 = -x_{13}a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_{13}\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{13}\right)c \hat{\mathbf{z}} \quad (4c) \quad \text{O VIII}$$

---

**References:**

- S. Tahara, A. Shimada, N. Kumada, and Y. Sugahara, *Characterization of  $\text{Bi}_5\text{Nb}_3\text{O}_{15}$  by refinement of neutron diffraction pattern, acid treatment and reaction of the acid-treated product with n-alkylamines*, J. Solid State Chem. **180**, 2517–2524 (2007), doi:[10.1016/j.jssc.2007.05.017](https://doi.org/10.1016/j.jssc.2007.05.017).

**Found in:**

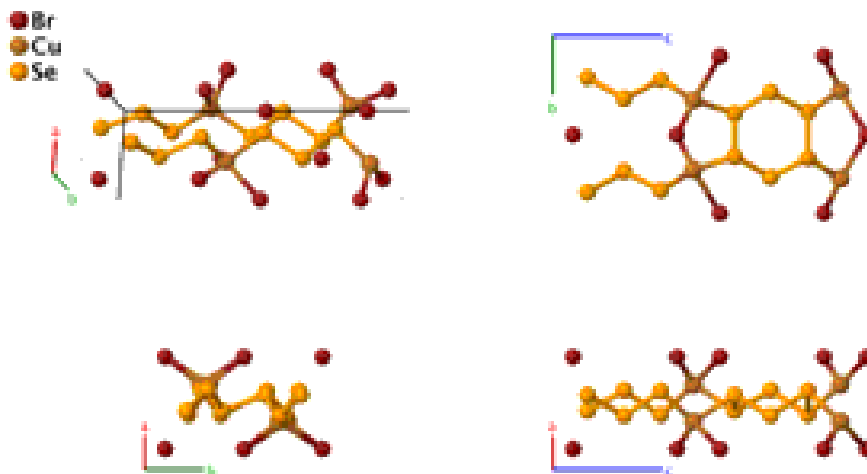
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [821](#)
- POSCAR: pp. [822](#)

# CuBrSe<sub>3</sub> Structure: ABC3\_oP20\_30\_2a\_c\_3c



<b>Prototype</b>	:	CuBrSe <sub>3</sub>
<b>AFLOW prototype label</b>	:	ABC3_oP20_30_2a_c_3c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP20
<b>Space group number</b>	:	30
<b>Space group symbol</b>	:	<i>Pnc2</i>
<b>AFLOW prototype command</b>	:	aflow --proto=ABC3_oP20_30_2a_c_3c --params= <i>a, b/a, c/a, z1, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6</i>

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $z_1 \mathbf{a}_3$	= $z_1 c \hat{\mathbf{z}}$	(2a)	Br I
<b>B<sub>2</sub></b>	= $\frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	= $\frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Br I
<b>B<sub>3</sub></b>	= $z_2 \mathbf{a}_3$	= $z_2 c \hat{\mathbf{z}}$	(2a)	Br II
<b>B<sub>4</sub></b>	= $\frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	= $\frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(2a)	Br II
<b>B<sub>5</sub></b>	= $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	= $x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4c)	Cu
<b>B<sub>6</sub></b>	= $-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	= $-x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4c)	Cu
<b>B<sub>7</sub></b>	= $x_3 \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	= $x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4c)	Cu
<b>B<sub>8</sub></b>	= $-x_3 \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	= $-x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4c)	Cu

$$\begin{aligned}
\mathbf{B}_9 &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (4c) & \text{Se I} \\
\mathbf{B}_{10} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (4c) & \text{Se I} \\
\mathbf{B}_{11} &= x_4 \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (4c) & \text{Se I} \\
\mathbf{B}_{12} &= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (4c) & \text{Se I} \\
\mathbf{B}_{13} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (4c) & \text{Se II} \\
\mathbf{B}_{14} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (4c) & \text{Se II} \\
\mathbf{B}_{15} &= x_5 \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (4c) & \text{Se II} \\
\mathbf{B}_{16} &= -x_5 \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (4c) & \text{Se II} \\
\mathbf{B}_{17} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (4c) & \text{Se III} \\
\mathbf{B}_{18} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= -x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (4c) & \text{Se III} \\
\mathbf{B}_{19} &= x_6 \mathbf{a}_1 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} & (4c) & \text{Se III} \\
\mathbf{B}_{20} &= -x_6 \mathbf{a}_1 + \left(\frac{1}{2} + y_6\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 &= -x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} & (4c) & \text{Se III}
\end{aligned}$$

### References:

- T. Sakuma, T. Kaneko, T. Kurita, and H. Takahashi, *Crystal structure of CuBrSe<sub>3</sub>*, J. Phys. Soc. Jpn. **60**, 1608–1611 (1991), doi:[10.1143/JPSJ.60.1608](https://doi.org/10.1143/JPSJ.60.1608).

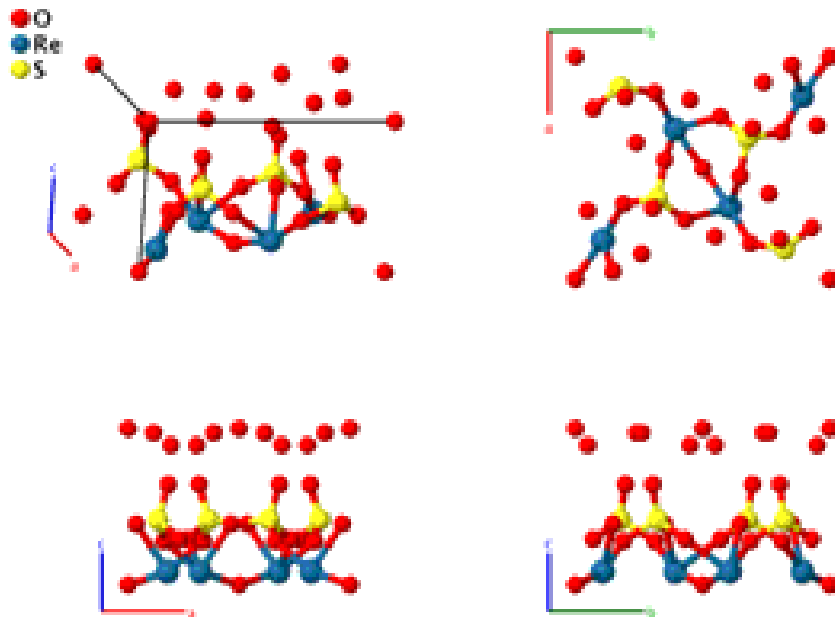
### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

### Geometry files:

- CIF: pp. [822](#)  
- POSCAR: pp. [822](#)

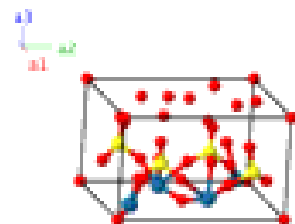
# Re<sub>2</sub>O<sub>5</sub>[SO<sub>4</sub>]<sub>2</sub> Structure: A13B2C2\_oP34\_32\_a6c\_c\_c



**Prototype** : Re<sub>2</sub>O<sub>5</sub>[SO<sub>4</sub>]<sub>2</sub>  
**AFLOW prototype label** : A13B2C2\_oP34\_32\_a6c\_c\_c  
**Strukturbericht designation** : None  
**Pearson symbol** : oP34  
**Space group number** : 32  
**Space group symbol** : *Pba*2  
**AFLOW prototype command** : aflow --proto=A13B2C2\_oP34\_32\_a6c\_c\_c  
 --params=*a, b/a, c/a, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>, y<sub>9</sub>, z<sub>9</sub>*

**Simple Orthorhombic primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(2a)	O I
<b>B<sub>2</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(2a)	O I
<b>B<sub>3</sub></b> =	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4c)	O II
<b>B<sub>4</sub></b> =	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$-x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4c)	O II

$\mathbf{B}_5$	$=$	$\left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_6$	$=$	$\left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_7$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_8$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_9$	$=$	$\left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{10}$	$=$	$\left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{11}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{12}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{13}$	$=$	$\left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{14}$	$=$	$\left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{15}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{16}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{17}$	$=$	$\left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{18}$	$=$	$\left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{19}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4c)	O VI
$\mathbf{B}_{20}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4c)	O VI
$\mathbf{B}_{21}$	$=$	$\left(\frac{1}{2} + x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4c)	O VI
$\mathbf{B}_{22}$	$=$	$\left(\frac{1}{2} - x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_6\right) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4c)	O VI
$\mathbf{B}_{23}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4c)	O VII
$\mathbf{B}_{24}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4c)	O VII
$\mathbf{B}_{25}$	$=$	$\left(\frac{1}{2} + x_7\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_7\right) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_7\right) b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4c)	O VII
$\mathbf{B}_{26}$	$=$	$\left(\frac{1}{2} - x_7\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_7\right) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_7\right) b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4c)	O VII
$\mathbf{B}_{27}$	$=$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$x_8 a \hat{\mathbf{x}} + y_8 b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4c)	Re
$\mathbf{B}_{28}$	$=$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-x_8 a \hat{\mathbf{x}} - y_8 b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4c)	Re
$\mathbf{B}_{29}$	$=$	$\left(\frac{1}{2} + x_8\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_8\right) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_8\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_8\right) b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4c)	Re
$\mathbf{B}_{30}$	$=$	$\left(\frac{1}{2} - x_8\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_8\right) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_8\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_8\right) b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4c)	Re
$\mathbf{B}_{31}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$x_9 a \hat{\mathbf{x}} + y_9 b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4c)	S
$\mathbf{B}_{32}$	$=$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-x_9 a \hat{\mathbf{x}} - y_9 b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4c)	S
$\mathbf{B}_{33}$	$=$	$\left(\frac{1}{2} + x_9\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_9\right) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_9\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_9\right) b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4c)	S
$\mathbf{B}_{34}$	$=$	$\left(\frac{1}{2} - x_9\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_9\right) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_9\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_9\right) b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4c)	S

## References:

- U. Betke and M. S. Wickleder, *Sulfates of the Refractory Metals: Crystal Structure and Thermal Behavior of  $Nb_2O_2(SO_4)_3$ ,  $MoO_2(SO_4)$ ,  $WO(SO_4)_2$ , and Two Modifications of  $Re_2O_5(SO_4)_2$* , *Inorg. Chem.* **50**, 858–872 (2011), [doi:10.1021/ic101455z](https://doi.org/10.1021/ic101455z).

## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

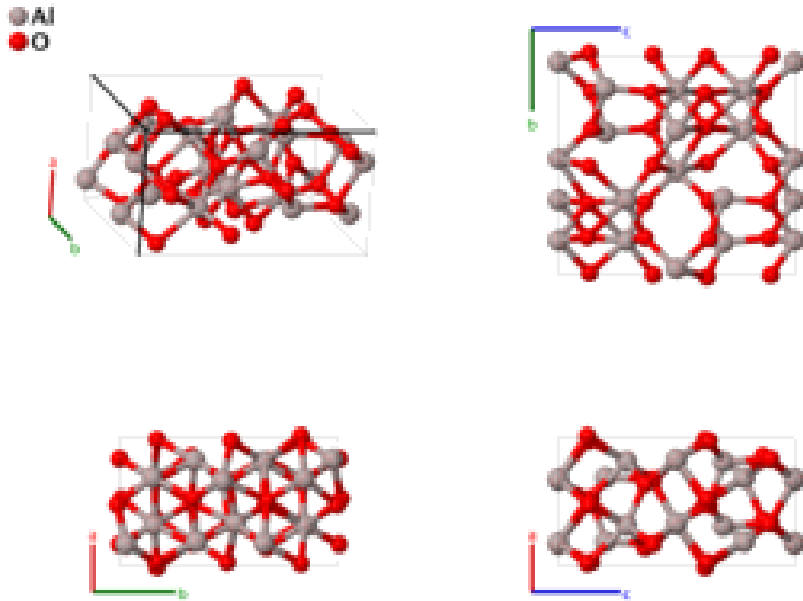
---

**Geometry files:**

- CIF: pp. [823](#)

- POSCAR: pp. [823](#)

# $\kappa$ -alumina ( $\text{Al}_2\text{O}_3$ ) Structure: A2B3\_oP40\_33\_4a\_6a



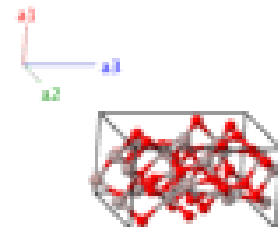
<b>Prototype</b>	:	$\kappa$ - $\text{Al}_2\text{O}_3$
<b>AFLOW prototype label</b>	:	A2B3_oP40_33_4a_6a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP40
<b>Space group number</b>	:	33
<b>Space group symbol</b>	:	$Pna2_1$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3_oP40_33_4a_6a --params= $a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

## Other compounds with this structure:

- $(1-x)\text{Fe}_2\text{O}_3 \cdot x\text{Al}_2\text{O}_3$ ,  $(1-x)\text{Fe}_2\text{O}_3 \cdot x\text{Ga}_2\text{O}_3$ . An approximation to the true crystal structure of  $\epsilon$ - $\text{Ga}_2\text{O}_3$  (Yoshioka, 2007).

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= b \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$



## Basis vectors:

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type





$$\begin{aligned}
\mathbf{B}_{32} &= \begin{pmatrix} \frac{1}{2} - x_8 \\ \frac{1}{2} + y_8 \\ \frac{1}{2} + z_8 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_8 \\ \frac{1}{2} + z_8 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} - x_8 \\ \frac{1}{2} + z_8 \end{pmatrix} \mathbf{a}_3 &= \begin{pmatrix} \frac{1}{2} - x_8 \\ \frac{1}{2} + y_8 \\ \frac{1}{2} + z_8 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_8 \\ \frac{1}{2} + z_8 \end{pmatrix} b \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} - x_8 \\ \frac{1}{2} + z_8 \end{pmatrix} c \hat{\mathbf{z}} & (4a) & \text{O IV} \\
\mathbf{B}_{33} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= x_9 a \hat{\mathbf{x}} + y_9 b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{34} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3 &= -x_9 a \hat{\mathbf{x}} - y_9 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{35} &= \left(\frac{1}{2} + x_9\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_9\right) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= \left(\frac{1}{2} + x_9\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_9\right) b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{36} &= \begin{pmatrix} \frac{1}{2} - x_9 \\ \frac{1}{2} + y_9 \\ \frac{1}{2} + z_9 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_9 \\ \frac{1}{2} + z_9 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} - x_9 \\ \frac{1}{2} + z_9 \end{pmatrix} \mathbf{a}_3 &= \begin{pmatrix} \frac{1}{2} - x_9 \\ \frac{1}{2} + y_9 \\ \frac{1}{2} + z_9 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_9 \\ \frac{1}{2} + z_9 \end{pmatrix} b \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} - x_9 \\ \frac{1}{2} + z_9 \end{pmatrix} c \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{37} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= x_{10} a \hat{\mathbf{x}} + y_{10} b \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{38} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3 &= -x_{10} a \hat{\mathbf{x}} - y_{10} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{39} &= \left(\frac{1}{2} + x_{10}\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_{10}\right) \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= \left(\frac{1}{2} + x_{10}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_{10}\right) b \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{40} &= \begin{pmatrix} \frac{1}{2} - x_{10} \\ \frac{1}{2} + y_{10} \\ \frac{1}{2} + z_{10} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_{10} \\ \frac{1}{2} + z_{10} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} - x_{10} \\ \frac{1}{2} + z_{10} \end{pmatrix} \mathbf{a}_3 &= \begin{pmatrix} \frac{1}{2} - x_{10} \\ \frac{1}{2} + y_{10} \\ \frac{1}{2} + z_{10} \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_{10} \\ \frac{1}{2} + z_{10} \end{pmatrix} b \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} - x_{10} \\ \frac{1}{2} + z_{10} \end{pmatrix} c \hat{\mathbf{z}} & (4a) & \text{O VI}
\end{aligned}$$

---

### References:

- B. Ollivier, R. Retoux, P. Lacorre, D. Massiot, and G. Férey, *Crystal structure of  $\kappa$ -alumina: an X-ray powder diffraction, TEM and NMR study*, J. Mater. Chem. **7**, 1049–1056 (1997), doi:10.1039/A700054E.

### Found in:

- K. Matsuzaki, H. Yanagi, T. Kamiya, H. Hiramatsu, K. Nomura, M. Hirano, and H. Hosono, *Field-induced current modulation in epitaxial film of deep-ultraviolet transparent oxide semiconductor  $Ga_2O_3$* , Appl. Phys. Lett. **88**, 092106 (2006), doi:10.1063/1.2179373.

- S. Yoshioka, H. Hayashi, A. Kuwabara, F. Oba, K. Matsunaga, and I. Tanaka, *Structures and energetics of  $Ga_2O_3$  polymorphs*, J. Phys.: Condens. Matter **19**, 346211 (2007), doi:10.1088/0953-8984/19/34/346211.

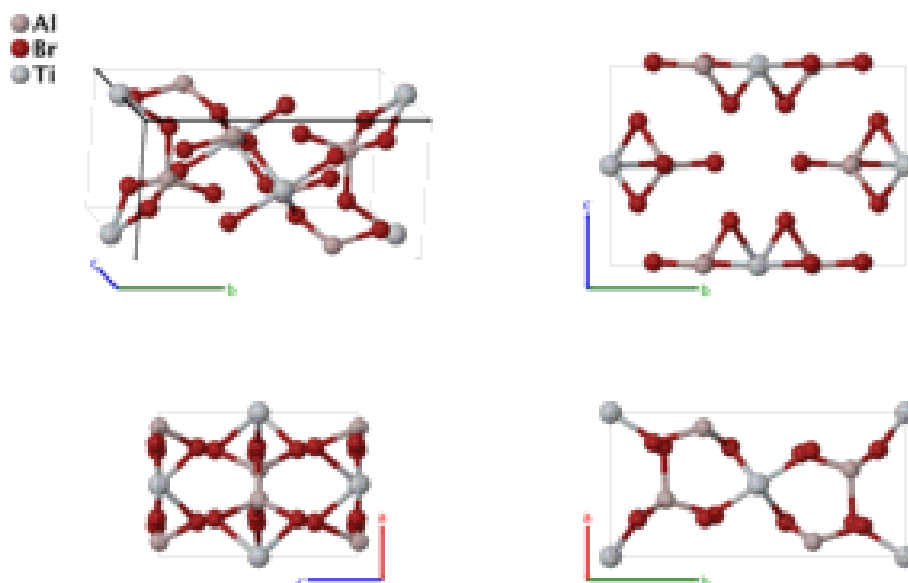
---

### Geometry files:

- CIF: pp. 823

- POSCAR: pp. 824

# TiAl<sub>2</sub>Br<sub>8</sub> Structure: A2B8C\_oP22\_34\_c\_4c\_a



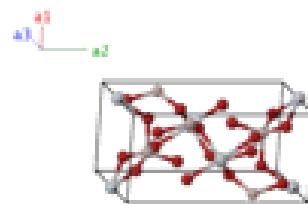
<b>Prototype</b>	:	TiAl <sub>2</sub> Br <sub>8</sub>
<b>AFLOW prototype label</b>	:	A2B8C_oP22_34_c_4c_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP22
<b>Space group number</b>	:	34
<b>Space group symbol</b>	:	<i>Pnn2</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B8C_oP22_34_c_4c_a --params= <i>a, b/a, c/a, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub></i>

**Simple Orthorhombic primitive vectors:**

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$z_1 \mathbf{a}_3$	$z_1 c \hat{\mathbf{z}}$	(2a)	Ti
<b>B<sub>2</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Ti
<b>B<sub>3</sub></b> =	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4c)	Al
<b>B<sub>4</sub></b> =	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$-x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4c)	Al
<b>B<sub>5</sub></b> =	$\left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$\left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4c)	Al

$$\begin{aligned}
\mathbf{B}_6 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4c) & \text{Al} \\
\mathbf{B}_7 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4c) & \text{Br I} \\
\mathbf{B}_8 &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4c) & \text{Br I} \\
\mathbf{B}_9 &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4c) & \text{Br I} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4c) & \text{Br I} \\
\mathbf{B}_{11} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (4c) & \text{Br II} \\
\mathbf{B}_{12} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (4c) & \text{Br II} \\
\mathbf{B}_{13} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (4c) & \text{Br II} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (4c) & \text{Br II} \\
\mathbf{B}_{15} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (4c) & \text{Br III} \\
\mathbf{B}_{16} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (4c) & \text{Br III} \\
\mathbf{B}_{17} &= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (4c) & \text{Br III} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (4c) & \text{Br III} \\
\mathbf{B}_{19} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (4c) & \text{Br IV} \\
\mathbf{B}_{20} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= -x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (4c) & \text{Br IV} \\
\mathbf{B}_{21} &= \left(\frac{1}{2} + x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} & (4c) & \text{Br IV} \\
\mathbf{B}_{22} &= \left(\frac{1}{2} - x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_6\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} & (4c) & \text{Br IV}
\end{aligned}$$

---

### References:

- S. I. Troyanov, V. B. Rybakov, and V. M. Ionov, *Synthesis and Crystal Structure of TiBr<sub>4</sub>, TiBr<sub>3</sub> and Ti(AlBr<sub>4</sub>)<sub>2</sub>*, Russ. J. Inorg. Chem. **35**, 882–887 (1990).

### Found in:

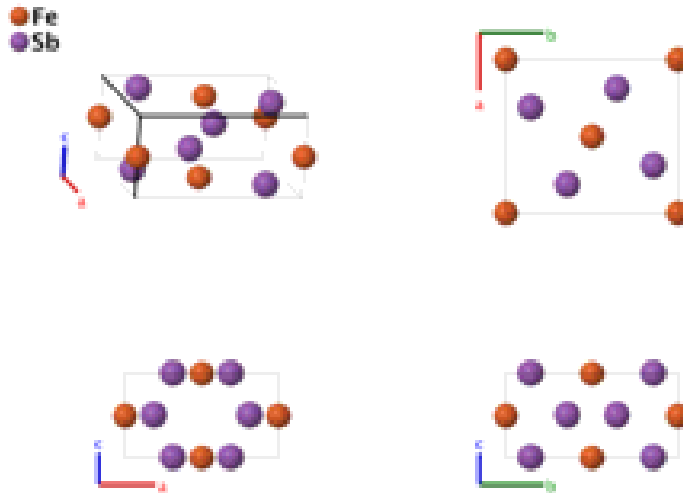
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. [824](#)  
- POSCAR: pp. [824](#)

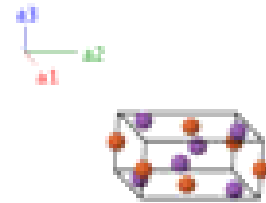
# FeSb<sub>2</sub> Structure: AB2\_oP6\_34\_a\_c



<b>Prototype</b>	:	FeSb <sub>2</sub>
<b>AFLOW prototype label</b>	:	AB2_oP6_34_a_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP6
<b>Space group number</b>	:	34
<b>Space group symbol</b>	:	<i>Pnn2</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB2_oP6_34_a_c --params=a, b/a, c/a, z <sub>1</sub> , x <sub>2</sub> , y <sub>2</sub> , z <sub>2</sub>

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= z <sub>1</sub> <b>a</b> <sub>3</sub>	=	z <sub>1</sub> c <b>z</b> <sup>^</sup>	(2a)	Fe
<b>B<sub>2</sub></b>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right)c \hat{\mathbf{z}}$	(2a)	Fe
<b>B<sub>3</sub></b>	= x <sub>2</sub> <b>a</b> <sub>1</sub> + y <sub>2</sub> <b>a</b> <sub>2</sub> + z <sub>2</sub> <b>a</b> <sub>3</sub>	=	x <sub>2</sub> a <b>x</b> <sup>^</sup> + y <sub>2</sub> b <b>y</b> <sup>^</sup> + z <sub>2</sub> c <b>z</b> <sup>^</sup>	(4c)	Sb
<b>B<sub>4</sub></b>	= -x <sub>2</sub> <b>a</b> <sub>1</sub> - y <sub>2</sub> <b>a</b> <sub>2</sub> + z <sub>2</sub> <b>a</b> <sub>3</sub>	=	-x <sub>2</sub> a <b>x</b> <sup>^</sup> - y <sub>2</sub> b <b>y</b> <sup>^</sup> + z <sub>2</sub> c <b>z</b> <sup>^</sup>	(4c)	Sb
<b>B<sub>5</sub></b>	= $\left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	=	$\left(\frac{1}{2} + x_2\right)a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right)b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right)c \hat{\mathbf{z}}$	(4c)	Sb

$$\mathbf{B}_6 = \begin{pmatrix} \frac{1}{2} - x_2 \\ \frac{1}{2} + y_2 \\ \frac{1}{2} + z_2 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_2 \\ \frac{1}{2} + z_2 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} - x_2 \\ \frac{1}{2} + z_2 \end{pmatrix} \mathbf{a}_3 = \begin{pmatrix} \frac{1}{2} - x_2 \\ \frac{1}{2} + y_2 \\ \frac{1}{2} + z_2 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_2 \\ \frac{1}{2} + z_2 \end{pmatrix} b \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} - x_2 \\ \frac{1}{2} + z_2 \end{pmatrix} c \hat{\mathbf{z}} \quad (4c) \quad \text{Sb}$$

---

**References:**

- H. Holseth and A. Kjekshus, *Compounds with the Marcasite Type Crystal Structure. IV. The Crystal Structure of FeSb<sub>2</sub>*, Acta Chem. Scand. **23**, 3043–3050 (1969), [doi:10.3891/acta.chem.scand.23-3043](https://doi.org/10.3891/acta.chem.scand.23-3043).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

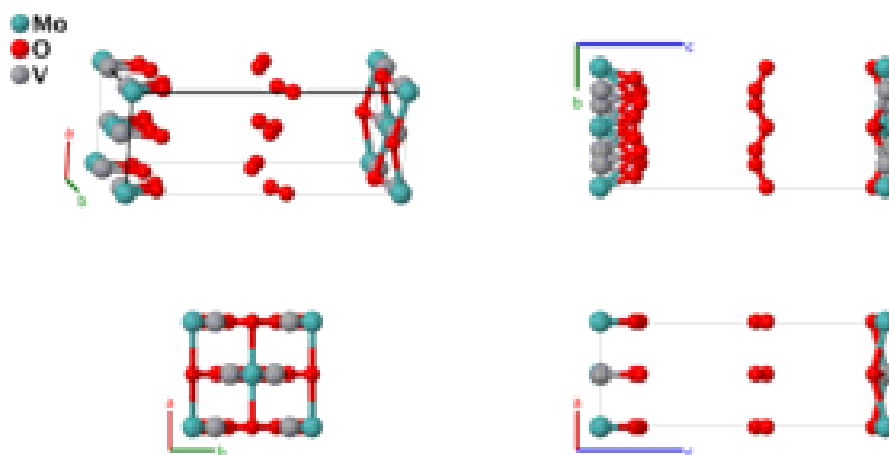
---

**Geometry files:**

- CIF: pp. [825](#)

- POSCAR: pp. [825](#)

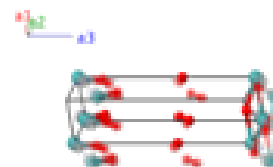
# V<sub>2</sub>MoO<sub>8</sub> Structure: AB8C2\_oC22\_35\_a\_ab3e\_e



<b>Prototype</b>	:	V <sub>2</sub> MoO <sub>8</sub>
<b>AFLOW prototype label</b>	:	AB8C2_oC22_35_a_ab3e_e
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC22
<b>Space group number</b>	:	35
<b>Space group symbol</b>	:	<i>Cmm2</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB8C2_oC22_35_a_ab3e_e --params=a, b/a, c/a, z <sub>1</sub> , z <sub>2</sub> , z <sub>3</sub> , y <sub>4</sub> , z <sub>4</sub> , y <sub>5</sub> , z <sub>5</sub> , y <sub>6</sub> , z <sub>6</sub> , y <sub>7</sub> , z <sub>7</sub>

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= z <sub>1</sub> <b>a</b> <sub>3</sub>	= z <sub>1</sub> c <b>z</b> <b>̂</b>	(2a)	Mo
<b>B<sub>2</sub></b>	= z <sub>2</sub> <b>a</b> <sub>3</sub>	= z <sub>2</sub> c <b>z</b> <b>̂</b>	(2a)	O I
<b>B<sub>3</sub></b>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	= $\frac{1}{2} a \hat{\mathbf{x}} + z_3 c \hat{\mathbf{z}}$	(2b)	O II
<b>B<sub>4</sub></b>	= -y <sub>4</sub> <b>a</b> <sub>1</sub> + y <sub>4</sub> <b>a</b> <sub>2</sub> + z <sub>4</sub> <b>a</b> <sub>3</sub>	= y <sub>4</sub> b <b>y</b> <b>̂</b> + z <sub>4</sub> c <b>z</b> <b>̂</b>	(4e)	O III
<b>B<sub>5</sub></b>	= y <sub>4</sub> <b>a</b> <sub>1</sub> - y <sub>4</sub> <b>a</b> <sub>2</sub> + z <sub>4</sub> <b>a</b> <sub>3</sub>	= -y <sub>4</sub> b <b>y</b> <b>̂</b> + z <sub>4</sub> c <b>z</b> <b>̂</b>	(4e)	O III
<b>B<sub>6</sub></b>	= -y <sub>5</sub> <b>a</b> <sub>1</sub> + y <sub>5</sub> <b>a</b> <sub>2</sub> + z <sub>5</sub> <b>a</b> <sub>3</sub>	= y <sub>5</sub> b <b>y</b> <b>̂</b> + z <sub>5</sub> c <b>z</b> <b>̂</b>	(4e)	O IV
<b>B<sub>7</sub></b>	= y <sub>5</sub> <b>a</b> <sub>1</sub> - y <sub>5</sub> <b>a</b> <sub>2</sub> + z <sub>5</sub> <b>a</b> <sub>3</sub>	= -y <sub>5</sub> b <b>y</b> <b>̂</b> + z <sub>5</sub> c <b>z</b> <b>̂</b>	(4e)	O IV
<b>B<sub>8</sub></b>	= -y <sub>6</sub> <b>a</b> <sub>1</sub> + y <sub>6</sub> <b>a</b> <sub>2</sub> + z <sub>6</sub> <b>a</b> <sub>3</sub>	= y <sub>6</sub> b <b>y</b> <b>̂</b> + z <sub>6</sub> c <b>z</b> <b>̂</b>	(4e)	O V
<b>B<sub>9</sub></b>	= y <sub>6</sub> <b>a</b> <sub>1</sub> - y <sub>6</sub> <b>a</b> <sub>2</sub> + z <sub>6</sub> <b>a</b> <sub>3</sub>	= -y <sub>6</sub> b <b>y</b> <b>̂</b> + z <sub>6</sub> c <b>z</b> <b>̂</b>	(4e)	O V

$$\mathbf{B}_{10} = -y_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} \quad (4e) \quad \mathbf{V}$$

$$\mathbf{B}_{11} = y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = -y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} \quad (4e) \quad \mathbf{V}$$

---

**References:**

- P. Mahé-Pailleret, *Contribution à l'étude chimique et structurale des composés AB<sub>2</sub>O rencontrés dans les systèmes Mo-VO, UVO et U-Mo-O*, Ph.D. thesis, Faculté des sciences de Paris (1970).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

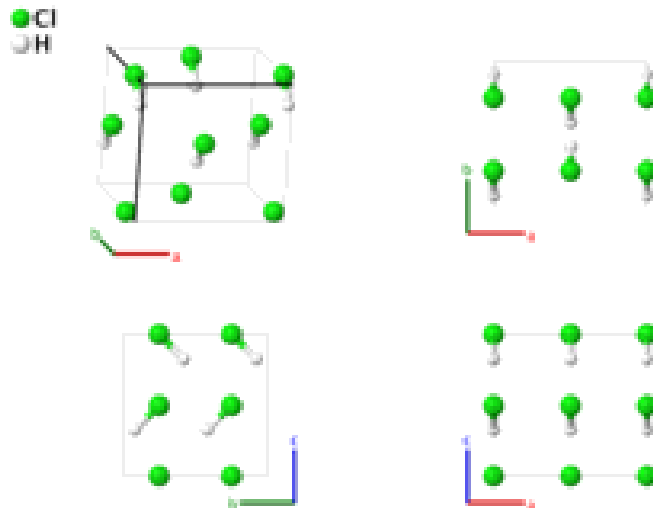
**Geometry files:**

- CIF: pp. [825](#)

- POSCAR: pp. [825](#)



# HCl Structure: AB\_oC8\_36\_a\_a

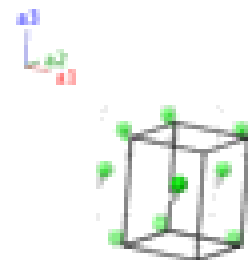


<b>Prototype</b>	:	HCl
<b>AFLOW prototype label</b>	:	AB_oC8_36_a_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC8
<b>Space group number</b>	:	36
<b>Space group symbol</b>	:	$Cmc2_1$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB_oC8_36_a_a --params=a, b/a, c/a, y1, z1, y2, z2</code>

- The original reference gives the positions of the atoms in the  $Bb2_1m$  setting of space group #36. We have transformed this into the standard  $Cmc2_1$  setting.

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4a)	Cl
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= -y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4a)	Cl
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4a)	H
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= -y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4a)	H

---

**References:**

- E. Sándor and R. F. C. Farrow, *Crystal Structure of Solid Hydrogen Chloride and Deuterium Chloride*, *Nature* **213**, 171–172 (1967), doi:[10.1038/213171a0](https://doi.org/10.1038/213171a0).

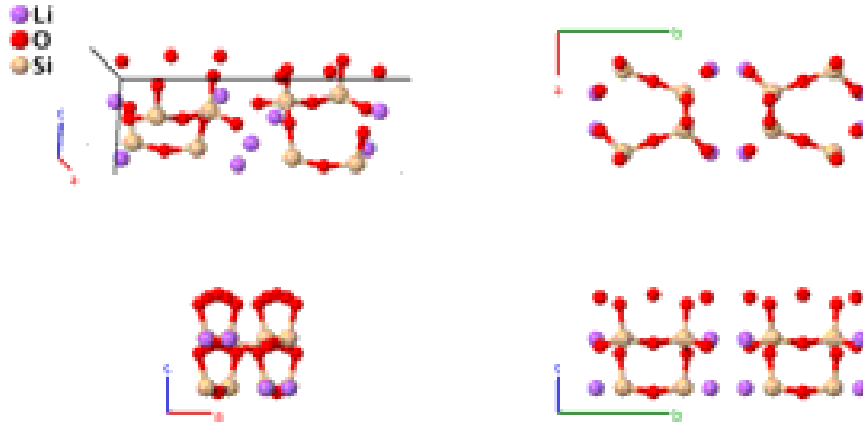
---

**Geometry files:**

- CIF: pp. [825](#)

- POSCAR: pp. [826](#)

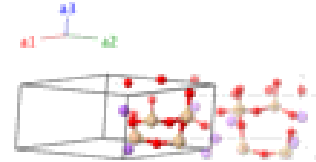
# Li<sub>2</sub>Si<sub>2</sub>O<sub>5</sub> Structure: A2B5C2\_oC36\_37\_d\_c2d\_d



<b>Prototype</b>	:	Li <sub>2</sub> Si <sub>2</sub> O <sub>5</sub>
<b>AFLOW prototype label</b>	:	A2B5C2_oC36_37_d_c2d_d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC36
<b>Space group number</b>	:	37
<b>Space group symbol</b>	:	<i>Ccc2</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B5C2_oC36_37_d_c2d_d --params=a, b/a, c/a, z <sub>1</sub> , x <sub>2</sub> , y <sub>2</sub> , z <sub>2</sub> , x <sub>3</sub> , y <sub>3</sub> , z <sub>3</sub> , x <sub>4</sub> , y <sub>4</sub> , z <sub>4</sub> , x <sub>5</sub> , y <sub>5</sub> , z <sub>5</sub>

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}b\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= \frac{1}{2}\mathbf{a}_2 + z_1\mathbf{a}_3$	$= \frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} + z_1c\hat{\mathbf{z}}$	(4c)	O I
<b>B<sub>2</sub></b>	$= \frac{1}{2}\mathbf{a}_1 + \left(\frac{1}{2} + z_1\right)\mathbf{a}_3$	$= \frac{1}{4}a\hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right)c\hat{\mathbf{z}}$	(4c)	O I
<b>B<sub>3</sub></b>	$= (x_2 - y_2)\mathbf{a}_1 + (x_2 + y_2)\mathbf{a}_2 + z_2\mathbf{a}_3$	$= x_2a\hat{\mathbf{x}} + y_2b\hat{\mathbf{y}} + z_2c\hat{\mathbf{z}}$	(8d)	Li
<b>B<sub>4</sub></b>	$= (-x_2 + y_2)\mathbf{a}_1 + (-x_2 - y_2)\mathbf{a}_2 + z_2\mathbf{a}_3$	$= -x_2a\hat{\mathbf{x}} - y_2b\hat{\mathbf{y}} + z_2c\hat{\mathbf{z}}$	(8d)	Li
<b>B<sub>5</sub></b>	$= (x_2 + y_2)\mathbf{a}_1 + (x_2 - y_2)\mathbf{a}_2 + \left(\frac{1}{2} + z_2\right)\mathbf{a}_3$	$= x_2a\hat{\mathbf{x}} - y_2b\hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right)c\hat{\mathbf{z}}$	(8d)	Li
<b>B<sub>6</sub></b>	$= (-x_2 - y_2)\mathbf{a}_1 + (-x_2 + y_2)\mathbf{a}_2 + \left(\frac{1}{2} + z_2\right)\mathbf{a}_3$	$= -x_2a\hat{\mathbf{x}} + y_2b\hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right)c\hat{\mathbf{z}}$	(8d)	Li
<b>B<sub>7</sub></b>	$= (x_3 - y_3)\mathbf{a}_1 + (x_3 + y_3)\mathbf{a}_2 + z_3\mathbf{a}_3$	$= x_3a\hat{\mathbf{x}} + y_3b\hat{\mathbf{y}} + z_3c\hat{\mathbf{z}}$	(8d)	O II
<b>B<sub>8</sub></b>	$= (-x_3 + y_3)\mathbf{a}_1 + (-x_3 - y_3)\mathbf{a}_2 + z_3\mathbf{a}_3$	$= -x_3a\hat{\mathbf{x}} - y_3b\hat{\mathbf{y}} + z_3c\hat{\mathbf{z}}$	(8d)	O II
<b>B<sub>9</sub></b>	$= (x_3 + y_3)\mathbf{a}_1 + (x_3 - y_3)\mathbf{a}_2 + \left(\frac{1}{2} + z_3\right)\mathbf{a}_3$	$= x_3a\hat{\mathbf{x}} - y_3b\hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right)c\hat{\mathbf{z}}$	(8d)	O II

$$\begin{aligned}
\mathbf{B}_{10} &= (-x_3 - y_3) \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{11} &= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{12} &= (-x_4 + y_4) \mathbf{a}_1 + (-x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{13} &= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{14} &= (-x_4 - y_4) \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{15} &= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8d) & \text{Si} \\
\mathbf{B}_{16} &= (-x_5 + y_5) \mathbf{a}_1 + (-x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8d) & \text{Si} \\
\mathbf{B}_{17} &= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (8d) & \text{Si} \\
\mathbf{B}_{18} &= (-x_5 - y_5) \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (8d) & \text{Si}
\end{aligned}$$

---

### References:

- B. H. W. S. de Jong, P. G. G. Slaats, H. T. J. Supèr, N. Veldman, and A. L. Spek, *Extended structures in crystalline phyllosilicates: silica ring systems in lithium, rubidium, cesium, and cesium/lithium phyllosilicate*, *J. Non Cryst. Solids* **176**, 164–171 (1994), doi:10.1016/0022-3093(94)90074-4.

### Found in:

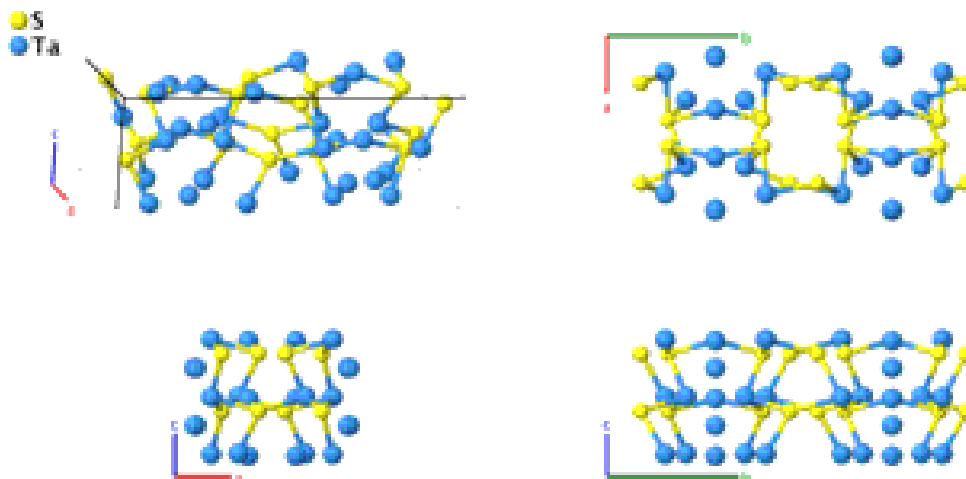
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. 826  
- POSCAR: pp. 826

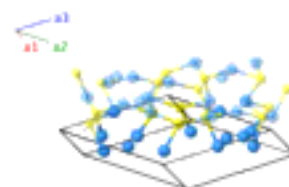
# Ta<sub>3</sub>S<sub>2</sub> Structure: A2B3\_oC40\_39\_2d\_2c2d



<b>Prototype</b>	:	Ta <sub>3</sub> S <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B3_oC40_39_2d_2c2d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC40
<b>Space group number</b>	:	39
<b>Space group symbol</b>	:	<i>Abm</i> 2
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3_oC40_39_2d_2c2d --params=a, b/a, c/a, x <sub>1</sub> , z <sub>1</sub> , x <sub>2</sub> , z <sub>2</sub> , x <sub>3</sub> , y <sub>3</sub> , z <sub>3</sub> , x <sub>4</sub> , y <sub>4</sub> , z <sub>4</sub> , x <sub>5</sub> , y <sub>5</sub> , z <sub>5</sub> , x <sub>6</sub> , y <sub>6</sub> , z <sub>6</sub>

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= \frac{1}{2} b \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$x_1 \mathbf{a}_1 + \left(\frac{1}{4} - z_1\right) \mathbf{a}_2 + \left(\frac{1}{4} + z_1\right) \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4c)	Ta I
<b>B<sub>2</sub></b>	$-x_1 \mathbf{a}_1 + \left(\frac{3}{4} - z_1\right) \mathbf{a}_2 + \left(\frac{3}{4} + z_1\right) \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4c)	Ta I
<b>B<sub>3</sub></b>	$x_2 \mathbf{a}_1 + \left(\frac{1}{4} - z_2\right) \mathbf{a}_2 + \left(\frac{1}{4} + z_2\right) \mathbf{a}_3$	$x_2 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4c)	Ta II
<b>B<sub>4</sub></b>	$-x_2 \mathbf{a}_1 + \left(\frac{3}{4} - z_2\right) \mathbf{a}_2 + \left(\frac{3}{4} + z_2\right) \mathbf{a}_3$	$-x_2 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4c)	Ta II
<b>B<sub>5</sub></b>	$x_3 \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8d)	S I
<b>B<sub>6</sub></b>	$-x_3 \mathbf{a}_1 + (-y_3 - z_3) \mathbf{a}_2 + (-y_3 + z_3) \mathbf{a}_3$	$-x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8d)	S I
<b>B<sub>7</sub></b>	$x_3 \mathbf{a}_1 + \left(\frac{1}{2} - y_3 - z_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_3 + z_3\right) \mathbf{a}_3$	$x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8d)	S I
<b>B<sub>8</sub></b>	$-x_3 \mathbf{a}_1 + \left(\frac{1}{2} + y_3 - z_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + y_3 + z_3\right) \mathbf{a}_3$	$-x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8d)	S I

$$\begin{aligned}
\mathbf{B}_9 &= x_4 \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8d) & \text{S II} \\
\mathbf{B}_{10} &= -x_4 \mathbf{a}_1 + (-y_4 - z_4) \mathbf{a}_2 + (-y_4 + z_4) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8d) & \text{S II} \\
\mathbf{B}_{11} &= x_4 \mathbf{a}_1 + \left(\frac{1}{2} - y_4 - z_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_4 + z_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8d) & \text{S II} \\
\mathbf{B}_{12} &= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} + y_4 - z_4\right) \mathbf{a}_2 + &= -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8d) & \text{S II} \\
&\quad \left(\frac{1}{2} + y_4 + z_4\right) \mathbf{a}_3 \\
\mathbf{B}_{13} &= x_5 \mathbf{a}_1 + (y_5 - z_5) \mathbf{a}_2 + (y_5 + z_5) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8d) & \text{Ta III} \\
\mathbf{B}_{14} &= -x_5 \mathbf{a}_1 + (-y_5 - z_5) \mathbf{a}_2 + (-y_5 + z_5) \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8d) & \text{Ta III} \\
\mathbf{B}_{15} &= x_5 \mathbf{a}_1 + \left(\frac{1}{2} - y_5 - z_5\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_5 + z_5\right) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8d) & \text{Ta III} \\
\mathbf{B}_{16} &= -x_5 \mathbf{a}_1 + \left(\frac{1}{2} + y_5 - z_5\right) \mathbf{a}_2 + &= -x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8d) & \text{Ta III} \\
&\quad \left(\frac{1}{2} + y_5 + z_5\right) \mathbf{a}_3 \\
\mathbf{B}_{17} &= x_6 \mathbf{a}_1 + (y_6 - z_6) \mathbf{a}_2 + (y_6 + z_6) \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (8d) & \text{Ta IV} \\
\mathbf{B}_{18} &= -x_6 \mathbf{a}_1 + (-y_6 - z_6) \mathbf{a}_2 + (-y_6 + z_6) \mathbf{a}_3 &= -x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (8d) & \text{Ta IV} \\
\mathbf{B}_{19} &= x_6 \mathbf{a}_1 + \left(\frac{1}{2} - y_6 - z_6\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_6 + z_6\right) \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (8d) & \text{Ta IV} \\
\mathbf{B}_{20} &= -x_6 \mathbf{a}_1 + \left(\frac{1}{2} + y_6 - z_6\right) \mathbf{a}_2 + &= -x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (8d) & \text{Ta IV} \\
&\quad \left(\frac{1}{2} + y_6 + z_6\right) \mathbf{a}_3
\end{aligned}$$

---

#### References:

- S. J. Kim, K. S. Nanjundaswamy, and T. Hughbanks, *Single-crystal structure of tantalum sulfide (Ta<sub>3</sub>S<sub>2</sub>). Structure and bonding in the Ta<sub>6</sub>Sn (n = 1, 3, 4, 5?) pentagonal-antiprismatic chain compounds*, *Inorg. Chem.* **30**, 159–164 (1991), [doi:10.1021/ic00002a004](https://doi.org/10.1021/ic00002a004).

#### Found in:

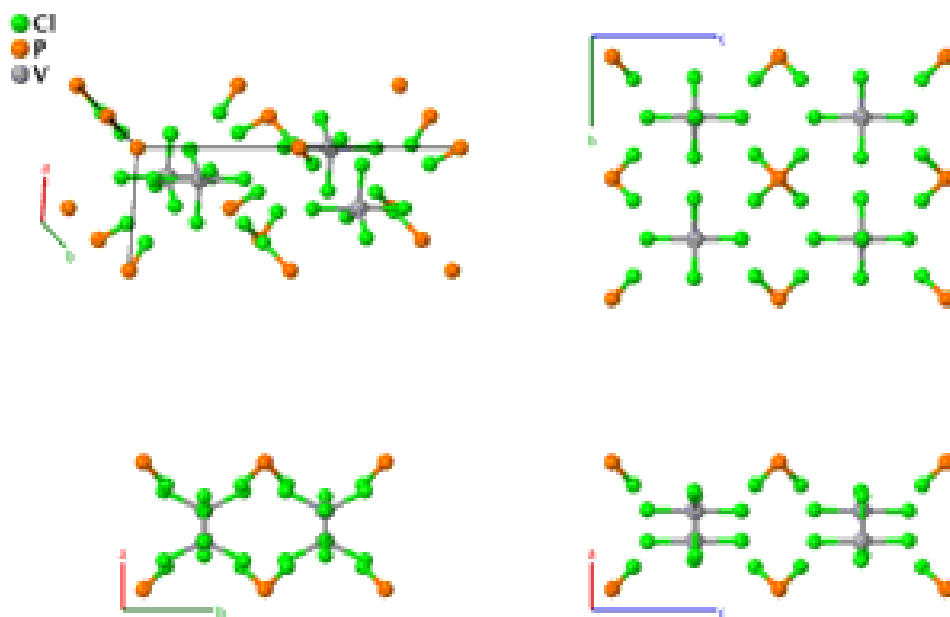
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [826](#)  
- POSCAR: pp. [827](#)

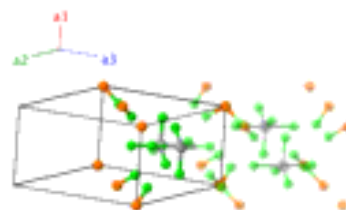
# VPCl<sub>9</sub> Structure: A9BC\_oC44\_39\_3c3d\_a\_c



<b>Prototype</b>	:	VPCl <sub>9</sub>
<b>AFLOW prototype label</b>	:	A9BC_oC44_39_3c3d_a_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC44
<b>Space group number</b>	:	39
<b>Space group symbol</b>	:	<i>Abm2</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A9BC_oC44_39_3c3d_a_c --params= <i>a, b/a, c/a, z1, x2, z2, x3, z3, x4, z4, x5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8</i>

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= \frac{1}{2} b \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $-z_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(4a)	P
<b>B<sub>2</sub></b>	= $\left(\frac{1}{2} - z_1\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$\frac{1}{2} b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4a)	P
<b>B<sub>3</sub></b>	= $x_2 \mathbf{a}_1 + \left(\frac{1}{4} - z_2\right) \mathbf{a}_2 + \left(\frac{1}{4} + z_2\right) \mathbf{a}_3$	=	$x_2 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4c)	Cl I
<b>B<sub>4</sub></b>	= $-x_2 \mathbf{a}_1 + \left(\frac{3}{4} - z_2\right) \mathbf{a}_2 + \left(\frac{3}{4} + z_2\right) \mathbf{a}_3$	=	$-x_2 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4c)	Cl I

$$\begin{aligned}
\mathbf{B}_5 &= x_3 \mathbf{a}_1 + \left(\frac{1}{4} - z_3\right) \mathbf{a}_2 + \left(\frac{1}{4} + z_3\right) \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} &(4c) & \text{CI II} \\
\mathbf{B}_6 &= -x_3 \mathbf{a}_1 + \left(\frac{3}{4} - z_3\right) \mathbf{a}_2 + \left(\frac{3}{4} + z_3\right) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} &(4c) & \text{CI II} \\
\mathbf{B}_7 &= x_4 \mathbf{a}_1 + \left(\frac{1}{4} - z_4\right) \mathbf{a}_2 + \left(\frac{1}{4} + z_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} &(4c) & \text{CI III} \\
\mathbf{B}_8 &= -x_4 \mathbf{a}_1 + \left(\frac{3}{4} - z_4\right) \mathbf{a}_2 + \left(\frac{3}{4} + z_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} &(4c) & \text{CI III} \\
\mathbf{B}_9 &= x_5 \mathbf{a}_1 + \left(\frac{1}{4} - z_5\right) \mathbf{a}_2 + \left(\frac{1}{4} + z_5\right) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} &(4c) & \text{V} \\
\mathbf{B}_{10} &= -x_5 \mathbf{a}_1 + \left(\frac{3}{4} - z_5\right) \mathbf{a}_2 + \left(\frac{3}{4} + z_5\right) \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} &(4c) & \text{V} \\
\mathbf{B}_{11} &= x_6 \mathbf{a}_1 + (y_6 - z_6) \mathbf{a}_2 + (y_6 + z_6) \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} &(8d) & \text{CI IV} \\
\mathbf{B}_{12} &= -x_6 \mathbf{a}_1 + (-y_6 - z_6) \mathbf{a}_2 + (-y_6 + z_6) \mathbf{a}_3 &= -x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} &(8d) & \text{CI IV} \\
\mathbf{B}_{13} &= x_6 \mathbf{a}_1 + \left(\frac{1}{2} - y_6 - z_6\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_6 + z_6\right) \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} &(8d) & \text{CI IV} \\
\mathbf{B}_{14} &= -x_6 \mathbf{a}_1 + \left(\frac{1}{2} + y_6 - z_6\right) \mathbf{a}_2 + &= -x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} &(8d) & \text{CI IV} \\
&\quad \left(\frac{1}{2} + y_6 + z_6\right) \mathbf{a}_3 \\
\mathbf{B}_{15} &= x_7 \mathbf{a}_1 + (y_7 - z_7) \mathbf{a}_2 + (y_7 + z_7) \mathbf{a}_3 &= x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} &(8d) & \text{CI V} \\
\mathbf{B}_{16} &= -x_7 \mathbf{a}_1 + (-y_7 - z_7) \mathbf{a}_2 + (-y_7 + z_7) \mathbf{a}_3 &= -x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} &(8d) & \text{CI V} \\
\mathbf{B}_{17} &= x_7 \mathbf{a}_1 + \left(\frac{1}{2} - y_7 - z_7\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_7 + z_7\right) \mathbf{a}_3 &= x_7 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_7\right) b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} &(8d) & \text{CI V} \\
\mathbf{B}_{18} &= -x_7 \mathbf{a}_1 + \left(\frac{1}{2} + y_7 - z_7\right) \mathbf{a}_2 + &= -x_7 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_7\right) b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} &(8d) & \text{CI V} \\
&\quad \left(\frac{1}{2} + y_7 + z_7\right) \mathbf{a}_3 \\
\mathbf{B}_{19} &= x_8 \mathbf{a}_1 + (y_8 - z_8) \mathbf{a}_2 + (y_8 + z_8) \mathbf{a}_3 &= x_8 a \hat{\mathbf{x}} + y_8 b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} &(8d) & \text{CI VI} \\
\mathbf{B}_{20} &= -x_8 \mathbf{a}_1 + (-y_8 - z_8) \mathbf{a}_2 + (-y_8 + z_8) \mathbf{a}_3 &= -x_8 a \hat{\mathbf{x}} - y_8 b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} &(8d) & \text{CI VI} \\
\mathbf{B}_{21} &= x_8 \mathbf{a}_1 + \left(\frac{1}{2} - y_8 - z_8\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_8 + z_8\right) \mathbf{a}_3 &= x_8 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_8\right) b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} &(8d) & \text{CI VI} \\
\mathbf{B}_{22} &= -x_8 \mathbf{a}_1 + \left(\frac{1}{2} + y_8 - z_8\right) \mathbf{a}_2 + &= -x_8 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_8\right) b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} &(8d) & \text{CI VI} \\
&\quad \left(\frac{1}{2} + y_8 + z_8\right) \mathbf{a}_3
\end{aligned}$$

---

### References:

- M. L. Ziegler, B. Nuber, K. Weidenhammer, and G. Hoch, *Die Molekül- und Kristallstruktur von Tetrachlorophosphoniumpentachlorovanadat (IV), [PCl<sub>4</sub>][VCl<sub>5</sub>]* / *The Molecular and Crystal Structure of Tetrachlorophosphoniumpentachlorovanadate (IV), [PCl<sub>4</sub>][VCl<sub>5</sub>]*, *Z. Naturforsch. B* **32**, 18–21 (1977), [doi:10.1515/znb-1977-0106](https://doi.org/10.1515/znb-1977-0106).

### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

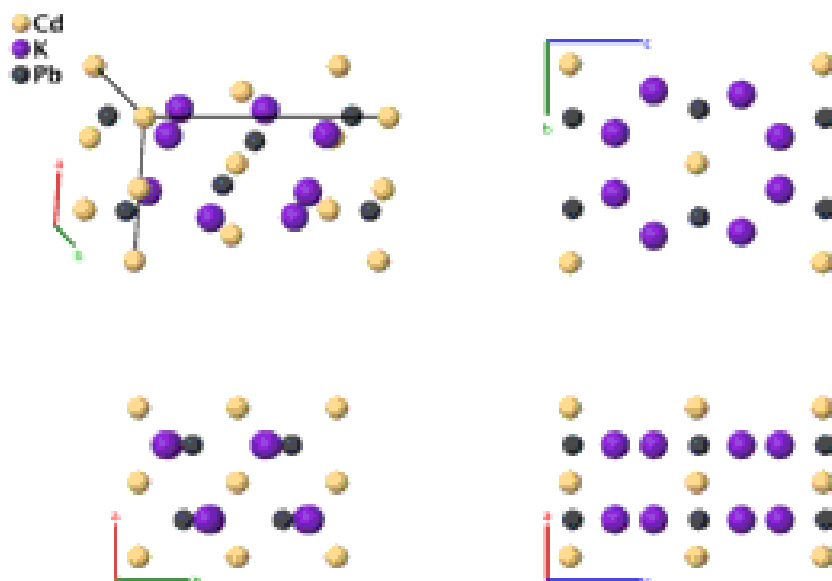
---

### Geometry files:

- CIF: pp. [827](#)  
- POSCAR: pp. [827](#)



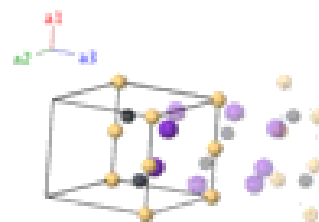
# K<sub>2</sub>CdPb Structure: AB2C\_oC16\_40\_a\_2b\_b



**Prototype** : K<sub>2</sub>CdPb  
**AFLOW prototype label** : AB2C\_oC16\_40\_a\_2b\_b  
**Strukturbericht designation** : None  
**Pearson symbol** : oC16  
**Space group number** : 40  
**Space group symbol** : *Ama*2  
**AFLOW prototype command** : aflow --proto=AB2C\_oC16\_40\_a\_2b\_b  
 --params=*a, b/a, c/a, z1, y2, z2, y3, z3, y4, z4*

**Base-centered Orthorhombic primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= \frac{1}{2} b \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \\
 \mathbf{a}_3 &= \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= -z_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= z_1 c \hat{\mathbf{z}}$	(4a)	Cd
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - z_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + z_1 c \hat{\mathbf{z}}$	(4a)	Cd
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4b)	K I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + (-y_2 - z_2) \mathbf{a}_2 + (-y_2 + z_2) \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4b)	K I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4b)	K II

$$\mathbf{B}_6 = \frac{3}{4} \mathbf{a}_1 + (-y_3 - z_3) \mathbf{a}_2 + (-y_3 + z_3) \mathbf{a}_3 = \frac{3}{4} a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} \quad (4b) \quad \text{K II}$$

$$\mathbf{B}_7 = \frac{1}{4} \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3 = \frac{1}{4} a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} \quad (4b) \quad \text{Pb}$$

$$\mathbf{B}_8 = \frac{3}{4} \mathbf{a}_1 + (-y_4 - z_4) \mathbf{a}_2 + (-y_4 + z_4) \mathbf{a}_3 = \frac{3}{4} a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} \quad (4b) \quad \text{Pb}$$

**References:**

- R. Matthes and H.-U. Schuster, *Synthese und Struktur der Phasen K<sub>2</sub>CdSn und K<sub>2</sub>CdPb/ Synthesis and Structure of the Phase K<sub>2</sub>CdSn and K<sub>2</sub>CdPb*, Z. Naturforsch. B **34**, 541–543 (1979), [doi:10.1515/znb-1979-0403](https://doi.org/10.1515/znb-1979-0403).

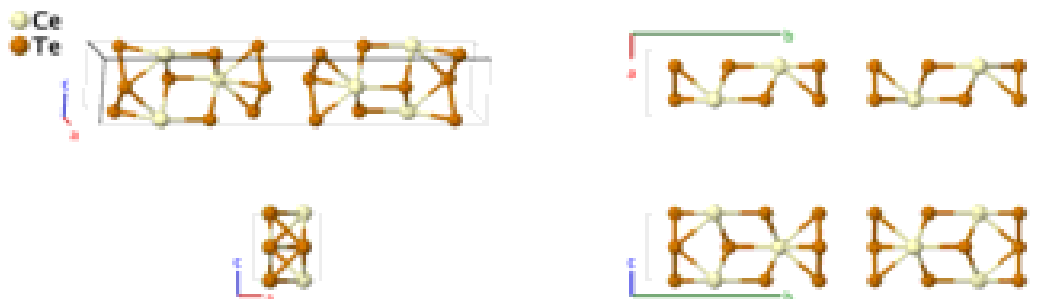
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [828](#)
- POSCAR: pp. [828](#)

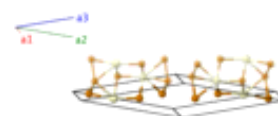
# CeTe<sub>3</sub> Structure: AB<sub>3</sub>\_oC16\_40\_b\_3b



<b>Prototype</b>	:	CeTe <sub>3</sub>
<b>AFLOW prototype label</b>	:	AB <sub>3</sub> _oC16_40_b_3b
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC16
<b>Space group number</b>	:	40
<b>Space group symbol</b>	:	<i>Ama</i> 2
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB<sub>3</sub>_oC16_40_b_3b --params=a, b/a, c/a, y<sub>1</sub>, z<sub>1</sub>, y<sub>2</sub>, z<sub>2</sub>, y<sub>3</sub>, z<sub>3</sub>, y<sub>4</sub>, z<sub>4</sub></code>

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= \frac{1}{2} b \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$\frac{1}{4} \mathbf{a}_1 + (y_1 - z_1) \mathbf{a}_2 + (y_1 + z_1) \mathbf{a}_3$	$\frac{1}{4} a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4b)	Ce
<b>B<sub>2</sub></b>	$\frac{3}{4} \mathbf{a}_1 + (-y_1 - z_1) \mathbf{a}_2 + (-y_1 + z_1) \mathbf{a}_3$	$\frac{3}{4} a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4b)	Ce
<b>B<sub>3</sub></b>	$\frac{1}{4} \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3$	$\frac{1}{4} a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4b)	Te I
<b>B<sub>4</sub></b>	$\frac{3}{4} \mathbf{a}_1 + (-y_2 - z_2) \mathbf{a}_2 + (-y_2 + z_2) \mathbf{a}_3$	$\frac{3}{4} a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4b)	Te I
<b>B<sub>5</sub></b>	$\frac{1}{4} \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$\frac{1}{4} a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4b)	Te II
<b>B<sub>6</sub></b>	$\frac{3}{4} \mathbf{a}_1 + (-y_3 - z_3) \mathbf{a}_2 + (-y_3 + z_3) \mathbf{a}_3$	$\frac{3}{4} a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4b)	Te II
<b>B<sub>7</sub></b>	$\frac{1}{4} \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3$	$\frac{1}{4} a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4b)	Te III
<b>B<sub>8</sub></b>	$\frac{3}{4} \mathbf{a}_1 + (-y_4 - z_4) \mathbf{a}_2 + (-y_4 + z_4) \mathbf{a}_3$	$\frac{3}{4} a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4b)	Te III

## References:

- C. Malliakas, S. J. L. Billinge, H. J. Kim, and M. G. Kanatzidis, *Square Nets of Tellurium: Rare-Earth Dependent Variation in the Charge-Density Wave of RETe<sub>3</sub> (RE = Rare-Earth Element)*, *J. Am. Chem. Soc.* **127**, 6510–6511 (2005), [doi:10.1021/ja0505292](https://doi.org/10.1021/ja0505292).

## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

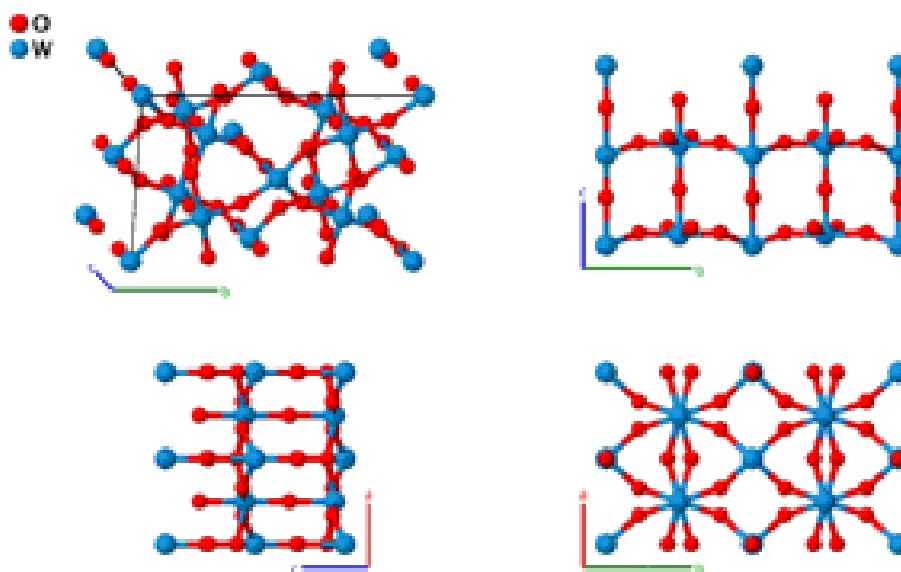
---

**Geometry files:**

- CIF: pp. [828](#)

- POSCAR: pp. [828](#)

# W<sub>3</sub>O<sub>10</sub> Structure: A10B3\_oF52\_42\_2abce\_ab



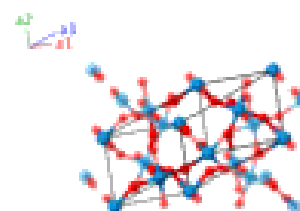
<b>Prototype</b>	:	W <sub>3</sub> O <sub>10</sub>
<b>AFLOW prototype label</b>	:	A10B3_oF52_42_2abce_ab
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oF52
<b>Space group number</b>	:	42
<b>Space group symbol</b>	:	<i>Fmm2</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A10B3_oF52_42_2abce_ab --params= <i>a, b/a, c/a, z1, z2, z3, z4, z5, y6, z6, x7, y7, z7</i>

## Face-centered Orthorhombic primitive vectors:

$$\mathbf{a}_1 = \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	= $z_1 c \hat{\mathbf{z}}$	(4 <i>a</i> )	O I
<b>B<sub>2</sub></b> =	$z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	= $z_2 c \hat{\mathbf{z}}$	(4 <i>a</i> )	O II
<b>B<sub>3</sub></b> =	$z_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	= $z_3 c \hat{\mathbf{z}}$	(4 <i>a</i> )	W I
<b>B<sub>4</sub></b> =	$z_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	= $\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8 <i>b</i> )	O III
<b>B<sub>5</sub></b> =	$\left(\frac{1}{2} + z_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	= $\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(8 <i>b</i> )	O III
<b>B<sub>6</sub></b> =	$z_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3$	= $\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8 <i>b</i> )	W II

$$\mathbf{B}_7 = \left(\frac{1}{2} + z_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_2 - z_5 \mathbf{a}_3 = \frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right)c \hat{\mathbf{z}} \quad (8b) \quad \text{W II}$$

$$\mathbf{B}_8 = (y_6 + z_6) \mathbf{a}_1 + (-y_6 + z_6) \mathbf{a}_2 + (y_6 - z_6) \mathbf{a}_3 = y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} \quad (8c) \quad \text{O IV}$$

$$\mathbf{B}_9 = (-y_6 + z_6) \mathbf{a}_1 + (y_6 + z_6) \mathbf{a}_2 + (-y_6 - z_6) \mathbf{a}_3 = -y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} \quad (8c) \quad \text{O IV}$$

$$\mathbf{B}_{10} = (-x_7 + y_7 + z_7) \mathbf{a}_1 + (x_7 - y_7 + z_7) \mathbf{a}_2 + (x_7 + y_7 - z_7) \mathbf{a}_3 = x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} \quad (16e) \quad \text{O V}$$

$$\mathbf{B}_{11} = (x_7 - y_7 + z_7) \mathbf{a}_1 + (-x_7 + y_7 + z_7) \mathbf{a}_2 + (-x_7 - y_7 - z_7) \mathbf{a}_3 = -x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} \quad (16e) \quad \text{O V}$$

$$\mathbf{B}_{12} = (-x_7 - y_7 + z_7) \mathbf{a}_1 + (x_7 + y_7 + z_7) \mathbf{a}_2 + (x_7 - y_7 - z_7) \mathbf{a}_3 = x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} \quad (16e) \quad \text{O V}$$

$$\mathbf{B}_{13} = (x_7 + y_7 + z_7) \mathbf{a}_1 + (-x_7 - y_7 + z_7) \mathbf{a}_2 + (-x_7 + y_7 - z_7) \mathbf{a}_3 = -x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} \quad (16e) \quad \text{O V}$$

### References:

- B. Gerand, G. Nowogrocki, and M. Figlarz, *A new tungsten trioxide hydrate, WO<sub>3</sub>·1/3H<sub>2</sub>O: Preparation, characterization, and crystallographic study*, J. Solid State Chem. **38**, 312–320 (1981), doi:10.1016/0022-4596(81)90062-1.

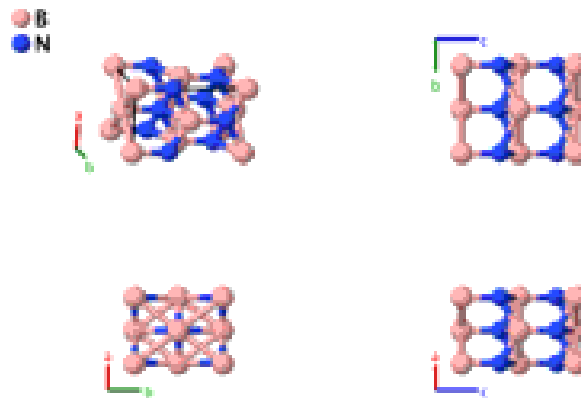
### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

### Geometry files:

- CIF: pp. [828](#)
- POSCAR: pp. [829](#)

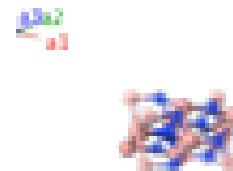
# BN (High-pressure, high-temperature) Structure: AB\_oF8\_42\_a\_a



<b>Prototype</b>	:	BN
<b>AFLOW prototype label</b>	:	AB_oF8_42_a_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oF8
<b>Space group number</b>	:	42
<b>Space group symbol</b>	:	<i>Fmm2</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB_oF8_42_a_a --params=a, b/a, c/a, z1, z2</code>

## Face-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$z_1 c \hat{\mathbf{z}}$	(4a)	B
$\mathbf{B}_2$	$= z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$z_2 c \hat{\mathbf{z}}$	(4a)	N

## References:

- A. V. Kurdyumov and G. S. Olejnik, *On metastable structures of graphite-like boron nitride*, *Kristallografiya* **29**, 792–793 (1984).

## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

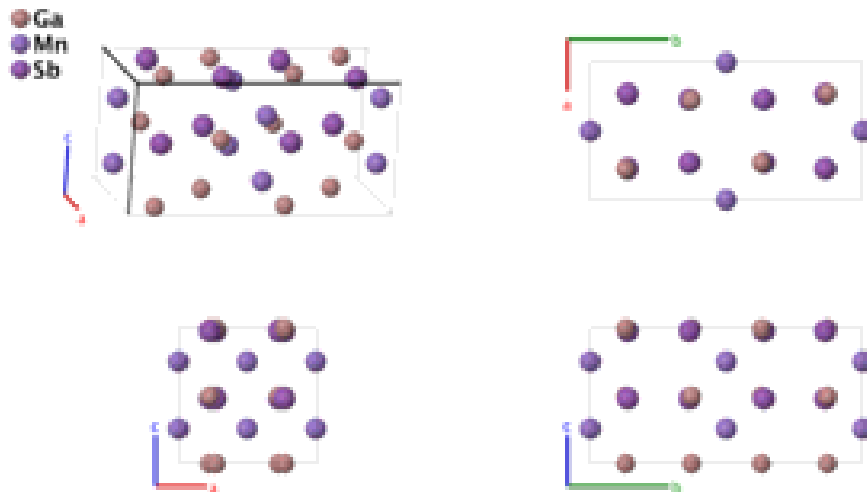
**Geometry files:**

- CIF: pp. [829](#)

- POSCAR: pp. [829](#)



# MnGa<sub>2</sub>Sb<sub>2</sub> Structure: A2BC2\_oI20\_45\_c\_b\_c

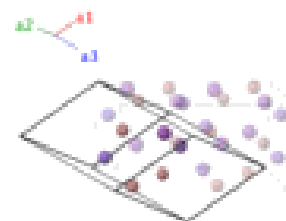


<b>Prototype</b>	:	MnGa <sub>2</sub> Sb <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2BC2_oI20_45_c_b_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oI20
<b>Space group number</b>	:	45
<b>Space group symbol</b>	:	<i>Iba</i> 2
<b>AFLOW prototype command</b>	:	aflow --proto=A2BC2_oI20_45_c_b_c --params=a, b/a, c/a, z <sub>1</sub> , x <sub>2</sub> , y <sub>2</sub> , z <sub>2</sub> , x <sub>3</sub> , y <sub>3</sub> , z <sub>3</sub>

- The Mn site (4b) is reported with an occupation of 0.94.

## Body-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{x} + \frac{1}{2}b\hat{y} + \frac{1}{2}c\hat{z} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{x} - \frac{1}{2}b\hat{y} + \frac{1}{2}c\hat{z} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{x} + \frac{1}{2}b\hat{y} - \frac{1}{2}c\hat{z} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$\left(\frac{1}{2} + z_1\right) \mathbf{a}_1 + z_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2}b\hat{y} + z_1c\hat{z}$	(4b)	Mn
<b>B<sub>2</sub></b>	$z_1 \mathbf{a}_1 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2}a\hat{x} + z_1c\hat{z}$	(4b)	Mn
<b>B<sub>3</sub></b>	$(y_2 + z_2) \mathbf{a}_1 + (x_2 + z_2) \mathbf{a}_2 + (x_2 + y_2) \mathbf{a}_3$	$x_2a\hat{x} + y_2b\hat{y} + z_2c\hat{z}$	(8c)	Ga
<b>B<sub>4</sub></b>	$(-y_2 + z_2) \mathbf{a}_1 + (-x_2 + z_2) \mathbf{a}_2 + (-x_2 - y_2) \mathbf{a}_3$	$-x_2a\hat{x} - y_2b\hat{y} + z_2c\hat{z}$	(8c)	Ga
<b>B<sub>5</sub></b>	$\left(\frac{1}{2} - y_2 + z_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_2 + z_2\right) \mathbf{a}_2 + (x_2 - y_2) \mathbf{a}_3$	$x_2a\hat{x} - y_2b\hat{y} + \left(\frac{1}{2} + z_2\right)c\hat{z}$	(8c)	Ga

$$\begin{aligned}
\mathbf{B}_6 &= \begin{pmatrix} \frac{1}{2} + y_2 + z_2 \\ (-x_2 + y_2) \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - x_2 + z_2 \\ (-x_2 + y_2) \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} -x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} \end{pmatrix} & (8c) & \text{Ga} \\
\mathbf{B}_7 &= (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3 = x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8c) & \text{Sb} \\
\mathbf{B}_8 &= \begin{pmatrix} -y_3 + z_3 \\ (-x_3 - y_3) \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} -x_3 + z_3 \\ (-x_3 - y_3) \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} \end{pmatrix} & (8c) & \text{Sb} \\
\mathbf{B}_9 &= \begin{pmatrix} \frac{1}{2} - y_3 + z_3 \\ (x_3 - y_3) \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + x_3 + z_3 \\ (x_3 - y_3) \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \end{pmatrix} & (8c) & \text{Sb} \\
\mathbf{B}_{10} &= \begin{pmatrix} \frac{1}{2} + y_3 + z_3 \\ (-x_3 + y_3) \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - x_3 + z_3 \\ (-x_3 + y_3) \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} -x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \end{pmatrix} & (8c) & \text{Sb}
\end{aligned}$$

**References:**

- W. Sakakibara, Y. Hayashi, and H. Takizawa, *MnGa<sub>2</sub>Sb<sub>2</sub>, a new ferromagnetic compound synthesized under high pressure*, J. Ceram. Soc. Jpn. **117**, 72–75 (2009), doi:10.2109/jcersj2.117.72.

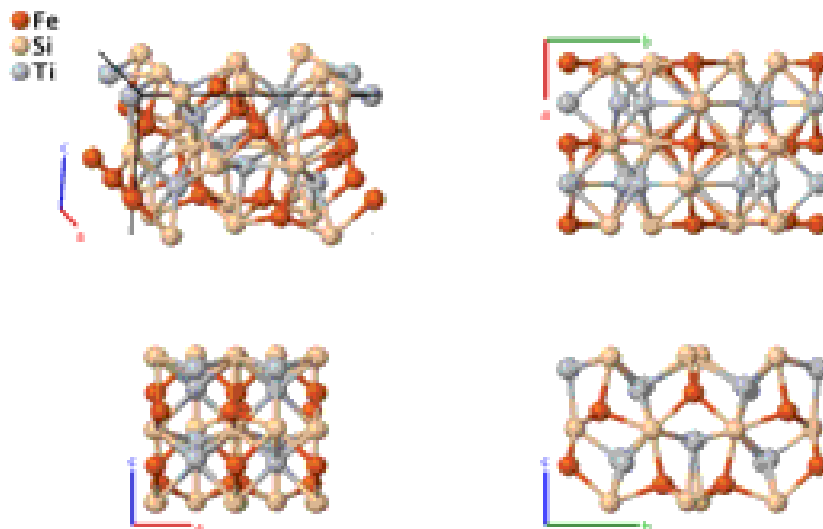
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [829](#)  
- POSCAR: pp. [830](#)

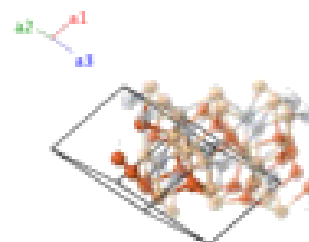
# TiFeSi Structure: ABC\_oI36\_46\_ac\_bc\_3b



**Prototype** : TiFeSi  
**AFLOW prototype label** : ABC\_oI36\_46\_ac\_bc\_3b  
**Strukturbericht designation** : None  
**Pearson symbol** : oI36  
**Space group number** : 46  
**Space group symbol** : *Ima2*  
**AFLOW prototype command** : aflow --proto=ABC\_oI36\_46\_ac\_bc\_3b  
 --params=*a, b/a, c/a, z1, y2, z2, y3, z3, y4, z4, y5, z5, x6, y6, z6, x7, y7, z7*

## Body-centered Orthorhombic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\
 \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2$	$=$	$z_1 c \hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B}_2$	$= z_1 \mathbf{a}_1 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + z_1 c \hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B}_3$	$= (y_2 + z_2) \mathbf{a}_1 + \left(\frac{1}{4} + z_2\right) \mathbf{a}_2 + \left(\frac{1}{4} + y_2\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4b)	Si I
$\mathbf{B}_4$	$= (-y_2 + z_2) \mathbf{a}_1 + \left(\frac{3}{4} + z_2\right) \mathbf{a}_2 + \left(\frac{3}{4} - y_2\right) \mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4b)	Si I
$\mathbf{B}_5$	$= (y_3 + z_3) \mathbf{a}_1 + \left(\frac{1}{4} + z_3\right) \mathbf{a}_2 + \left(\frac{1}{4} + y_3\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4b)	Ti I
$\mathbf{B}_6$	$= (-y_3 + z_3) \mathbf{a}_1 + \left(\frac{3}{4} + z_3\right) \mathbf{a}_2 + \left(\frac{3}{4} - y_3\right) \mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4b)	Ti I
$\mathbf{B}_7$	$= (y_4 + z_4) \mathbf{a}_1 + \left(\frac{1}{4} + z_4\right) \mathbf{a}_2 + \left(\frac{1}{4} + y_4\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4b)	Ti II

$$\begin{aligned}
\mathbf{B}_8 &= (-y_4 + z_4) \mathbf{a}_1 + \left(\frac{3}{4} + z_4\right) \mathbf{a}_2 + \left(\frac{3}{4} - y_4\right) \mathbf{a}_3 = \frac{3}{4}a \hat{\mathbf{x}} - y_4b \hat{\mathbf{y}} + z_4c \hat{\mathbf{z}} & (4b) & \text{Ti II} \\
\mathbf{B}_9 &= (y_5 + z_5) \mathbf{a}_1 + \left(\frac{1}{4} + z_5\right) \mathbf{a}_2 + \left(\frac{1}{4} + y_5\right) \mathbf{a}_3 = \frac{1}{4}a \hat{\mathbf{x}} + y_5b \hat{\mathbf{y}} + z_5c \hat{\mathbf{z}} & (4b) & \text{Ti III} \\
\mathbf{B}_{10} &= (-y_5 + z_5) \mathbf{a}_1 + \left(\frac{3}{4} + z_5\right) \mathbf{a}_2 + \left(\frac{3}{4} - y_5\right) \mathbf{a}_3 = \frac{3}{4}a \hat{\mathbf{x}} - y_5b \hat{\mathbf{y}} + z_5c \hat{\mathbf{z}} & (4b) & \text{Ti III} \\
\mathbf{B}_{11} &= (y_6 + z_6) \mathbf{a}_1 + (x_6 + z_6) \mathbf{a}_2 + (x_6 + y_6) \mathbf{a}_3 = x_6a \hat{\mathbf{x}} + y_6b \hat{\mathbf{y}} + z_6c \hat{\mathbf{z}} & (8c) & \text{Fe II} \\
\mathbf{B}_{12} &= (-y_6 + z_6) \mathbf{a}_1 + (-x_6 + z_6) \mathbf{a}_2 + (-x_6 - y_6) \mathbf{a}_3 = -x_6a \hat{\mathbf{x}} - y_6b \hat{\mathbf{y}} + z_6c \hat{\mathbf{z}} & (8c) & \text{Fe II} \\
\mathbf{B}_{13} &= (-y_6 + z_6) \mathbf{a}_1 + \left(\frac{1}{2} + x_6 + z_6\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_6 - y_6\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_6\right)a \hat{\mathbf{x}} - y_6b \hat{\mathbf{y}} + z_6c \hat{\mathbf{z}} & (8c) & \text{Fe II} \\
\mathbf{B}_{14} &= (y_6 + z_6) \mathbf{a}_1 + \left(\frac{1}{2} - x_6 + z_6\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_6 + y_6\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_6\right)a \hat{\mathbf{x}} + y_6b \hat{\mathbf{y}} + z_6c \hat{\mathbf{z}} & (8c) & \text{Fe II} \\
\mathbf{B}_{15} &= (y_7 + z_7) \mathbf{a}_1 + (x_7 + z_7) \mathbf{a}_2 + (x_7 + y_7) \mathbf{a}_3 = x_7a \hat{\mathbf{x}} + y_7b \hat{\mathbf{y}} + z_7c \hat{\mathbf{z}} & (8c) & \text{Si II} \\
\mathbf{B}_{16} &= (-y_7 + z_7) \mathbf{a}_1 + (-x_7 + z_7) \mathbf{a}_2 + (-x_7 - y_7) \mathbf{a}_3 = -x_7a \hat{\mathbf{x}} - y_7b \hat{\mathbf{y}} + z_7c \hat{\mathbf{z}} & (8c) & \text{Si II} \\
\mathbf{B}_{17} &= (-y_7 + z_7) \mathbf{a}_1 + \left(\frac{1}{2} + x_7 + z_7\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_7 - y_7\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_7\right)a \hat{\mathbf{x}} - y_7b \hat{\mathbf{y}} + z_7c \hat{\mathbf{z}} & (8c) & \text{Si II} \\
\mathbf{B}_{18} &= (y_7 + z_7) \mathbf{a}_1 + \left(\frac{1}{2} - x_7 + z_7\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_7 + y_7\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_7\right)a \hat{\mathbf{x}} + y_7b \hat{\mathbf{y}} + z_7c \hat{\mathbf{z}} & (8c) & \text{Si II}
\end{aligned}$$

---

#### References:

- W. Jeitschko, *The crystal structure of TiFeSi and related compounds*, Acta Crystallogr. Sect. B Struct. Sci. **26**, 815–822 (1970), doi:10.1107/S0567740870003163.

#### Found in:

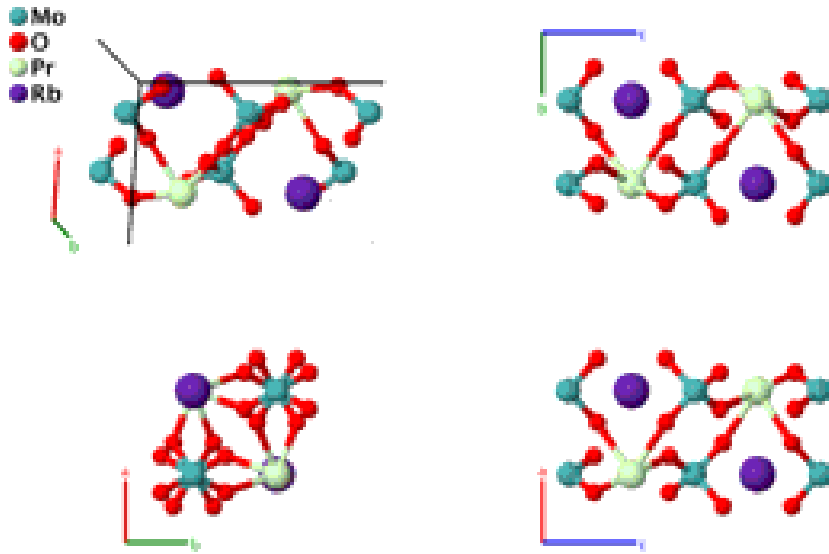
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 830  
- POSCAR: pp. 830

# $\alpha$ -RbPr[MoO<sub>4</sub>]<sub>2</sub> Structure: A2B8CD\_oP24\_48\_k\_2m\_d\_b



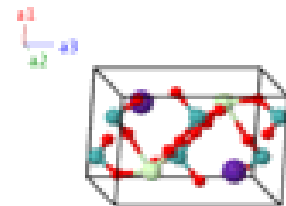
<b>Prototype</b>	:	$\alpha$ -RbPr[MoO <sub>4</sub> ] <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B8CD_oP24_48_k_2m_d_b
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP24
<b>Space group number</b>	:	48
<b>Space group symbol</b>	:	<i>Pnnn</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B8CD_oP24_48_k_2m_d_b --params= <i>a, b/a, c/a, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub></i>

## Simple Orthorhombic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2 <i>b</i> )	Rb
<b>B<sub>2</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2 <i>b</i> )	Rb
<b>B<sub>3</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2 <i>d</i> )	Pr
<b>B<sub>4</sub></b> =	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2 <i>d</i> )	Pr
<b>B<sub>5</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4 <i>k</i> )	Mo
<b>B<sub>6</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}}$	(4 <i>k</i> )	Mo
<b>B<sub>7</sub></b> =	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(4 <i>k</i> )	Mo

$$\begin{aligned}
\mathbf{B}_8 &= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} && (4k) && \text{Mo} \\
\mathbf{B}_9 &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (8m) && \text{O I} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (8m) && \text{O I} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} && (8m) && \text{O I} \\
\mathbf{B}_{12} &= x_4 \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} && (8m) && \text{O I} \\
\mathbf{B}_{13} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (8m) && \text{O I} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (8m) && \text{O I} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} && (8m) && \text{O I} \\
\mathbf{B}_{16} &= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} && (8m) && \text{O I} \\
\mathbf{B}_{17} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (8m) && \text{O II} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (8m) && \text{O II} \\
\mathbf{B}_{19} &= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} && (8m) && \text{O II} \\
\mathbf{B}_{20} &= x_5 \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} && (8m) && \text{O II} \\
\mathbf{B}_{21} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} && (8m) && \text{O II} \\
\mathbf{B}_{22} &= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 - z_5 \mathbf{a}_3 &= \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} && (8m) && \text{O II} \\
\mathbf{B}_{23} &= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} && (8m) && \text{O II} \\
\mathbf{B}_{24} &= -x_5 \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} && (8m) && \text{O II}
\end{aligned}$$

---

#### References:

- R. F. Klevtsova and P. V. Klevtsov, *Polymorphism of rubidium-praseodymium molybdate, RbPr(MoO<sub>4</sub>)<sub>2</sub>*, *Kristallografiya* **15**, 466–470 (1970).

#### Found in:

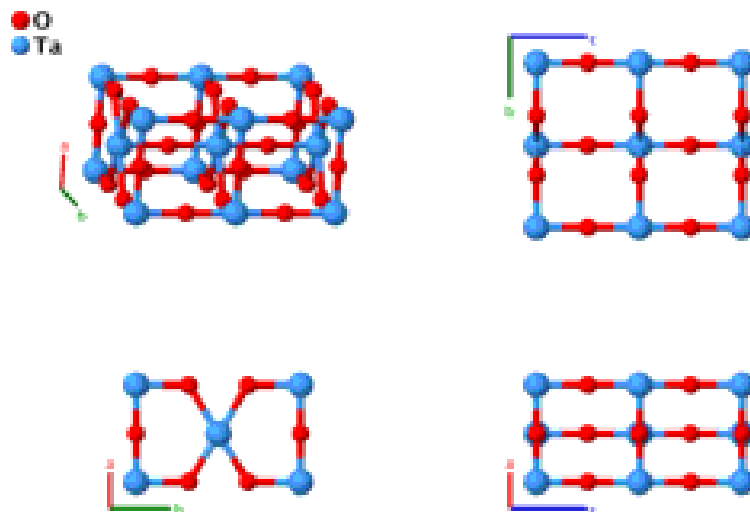
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [830](#)  
- POSCAR: pp. [831](#)

# $\beta$ -Ta<sub>2</sub>O<sub>5</sub> Structure: A5B2\_oP14\_49\_dehq\_ab

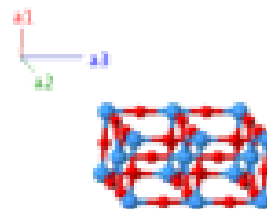


<b>Prototype</b>	:	$\beta$ -Ta <sub>2</sub> O <sub>5</sub>
<b>AFLOW prototype label</b>	:	A5B2_oP14_49_dehq_ab
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP14
<b>Space group number</b>	:	49
<b>Space group symbol</b>	:	<i>Pccm</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A5B2_oP14_49_dehq_ab --params=a, b/a, c/a, x<sub>6</sub>, y<sub>6</sub></code>

- While FINDSYM identifies space group #49 for this structure (consistent with the reference), AFLOW-SYM and Platon identify #47. Lowering the tolerance value for AFLOW-SYM resolves the expected space group #49. Space groups #47 and #49 are both reasonable classifications since they are commensurate with subgrain relations.

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	Ta I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Ta I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(2b)	Ta II

$$\begin{array}{llllll}
\mathbf{B}_4 & = & \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (2b) & \text{Ta II} \\
\mathbf{B}_5 & = & \frac{1}{2} \mathbf{a}_1 & = & \frac{1}{2} a \hat{\mathbf{x}} & (2d) & \text{O I} \\
\mathbf{B}_6 & = & \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}} & (2d) & \text{O I} \\
\mathbf{B}_7 & = & \frac{1}{4} \mathbf{a}_3 & = & \frac{1}{4} c \hat{\mathbf{z}} & (2e) & \text{O II} \\
\mathbf{B}_8 & = & \frac{3}{4} \mathbf{a}_3 & = & \frac{3}{4} c \hat{\mathbf{z}} & (2e) & \text{O II} \\
\mathbf{B}_9 & = & \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (2h) & \text{O III} \\
\mathbf{B}_{10} & = & \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (2h) & \text{O III} \\
\mathbf{B}_{11} & = & x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 & = & x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} & (4q) & \text{O IV} \\
\mathbf{B}_{12} & = & -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 & = & -x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} & (4q) & \text{O IV} \\
\mathbf{B}_{13} & = & -x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & -x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4q) & \text{O IV} \\
\mathbf{B}_{14} & = & x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4q) & \text{O IV}
\end{array}$$

---

### References:

- L. A. Aleshina and S. V. Loginova, *Rietveld analysis of X-ray diffraction pattern from  $\beta$ -Ta<sub>2</sub>O<sub>5</sub> oxide*, *Crystallogr. Rep.* **47**, 415–419 (2002), [doi:10.1134/1.1481927](https://doi.org/10.1134/1.1481927).
- H. T. Stokes and D. M. Hatch, *FINDSYM: Program for identifying the space group symmetry of a crystal*, *J. Appl. Crystallogr.* **38**, 237–238 (2005), [doi:10.1107/S0021889804031528](https://doi.org/10.1107/S0021889804031528).
- D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy, and S. Curtarolo, *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*, *Acta Crystallogr. Sect. A* **74**, 184–203 (2018), [doi:10.1107/S2053273318003066](https://doi.org/10.1107/S2053273318003066).
- A. L. Spek, *Single-crystal structure validation with the program PLATON*, *J. Appl. Crystallogr.* **36**, 7–13 (2003), [doi:10.1107/S0021889802022112](https://doi.org/10.1107/S0021889802022112).

### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

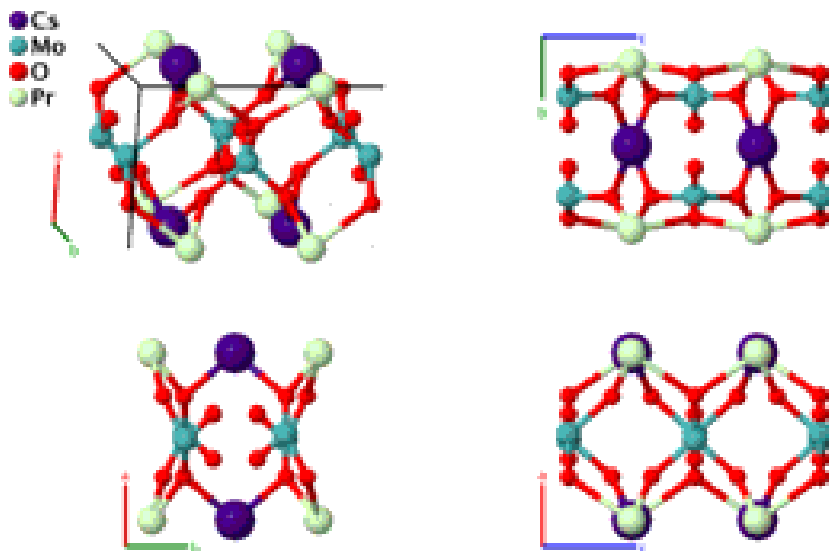
---

### Geometry files:

- CIF: pp. [831](#)
- POSCAR: pp. [831](#)



# CsPr[MoO<sub>4</sub>]<sub>2</sub> Structure: AB2C8D\_oP24\_49\_g\_q\_2qr\_e



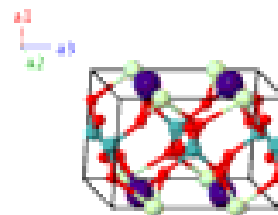
**Prototype** : CsPr[MoO<sub>4</sub>]<sub>2</sub>  
**AFLOW prototype label** : AB2C8D\_oP24\_49\_g\_q\_2qr\_e  
**Strukturbericht designation** : None  
**Pearson symbol** : oP24  
**Space group number** : 49  
**Space group symbol** : *Pccm*  
**AFLOW prototype command** : aflow --proto=AB2C8D\_oP24\_49\_g\_q\_2qr\_e  
 --params=*a, b/a, c/a, x<sub>3</sub>, y<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>*

Simple Orthorhombic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$\frac{1}{4} \mathbf{a}_3$	$\frac{1}{4} c \hat{\mathbf{z}}$	(2e)	Pr
<b>B<sub>2</sub></b> =	$\frac{3}{4} \mathbf{a}_3$	$\frac{3}{4} c \hat{\mathbf{z}}$	(2e)	Pr
<b>B<sub>3</sub></b> =	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2g)	Cs
<b>B<sub>4</sub></b> =	$\frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{1}{2} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2g)	Cs
<b>B<sub>5</sub></b> =	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}}$	(4q)	Mo
<b>B<sub>6</sub></b> =	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$-x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}}$	(4q)	Mo
<b>B<sub>7</sub></b> =	$-x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$-x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4q)	Mo

$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4q)	Mo
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}}$	(4q)	O I
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}}$	(4q)	O I
$\mathbf{B}_{11}$	$= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4q)	O I
$\mathbf{B}_{12}$	$= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4q)	O I
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}}$	(4q)	O II
$\mathbf{B}_{14}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$-x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}}$	(4q)	O II
$\mathbf{B}_{15}$	$= -x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4q)	O II
$\mathbf{B}_{16}$	$= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4q)	O II
$\mathbf{B}_{17}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B}_{18}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B}_{19}$	$= -x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \left(\frac{1}{2} - z_6\right) \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B}_{20}$	$= x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} - z_6\right) \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B}_{21}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B}_{22}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B}_{23}$	$= x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B}_{24}$	$= -x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(8r)	O III

---

#### References:

- V. A. Vinokurov and P. V. Klevtsov, *Polymorphism and crystallization of binary cesium-rare earth molybdates CsLn(MoO<sub>4</sub>)<sub>2</sub>*, Sov. Phys. Crystallogr. **17**, 102–106 (1972).

#### Found in:

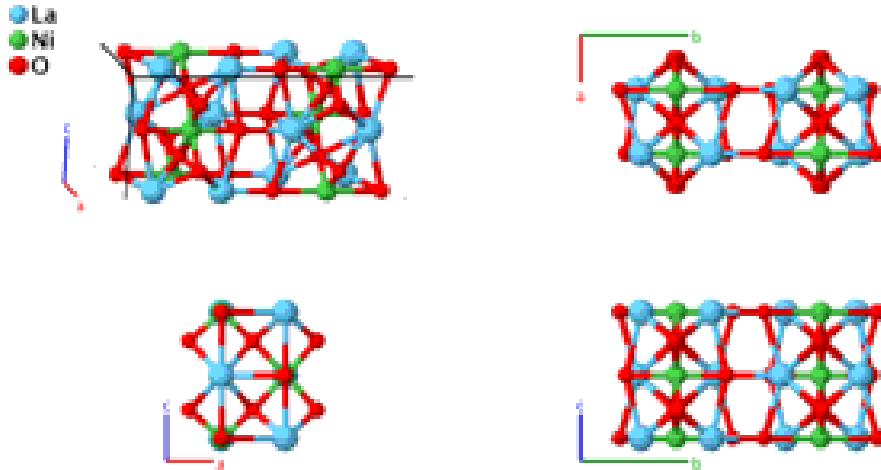
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [832](#)  
 - POSCAR: pp. [832](#)

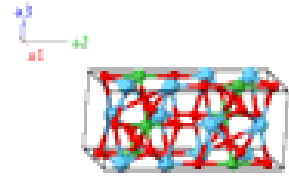
# La<sub>2</sub>NiO<sub>4</sub> Structure: A2BC4\_oP28\_50\_ij\_ac\_ijm



<b>Prototype</b>	:	La <sub>2</sub> NiO <sub>4</sub>
<b>AFLOW prototype label</b>	:	A2BC4_oP28_50_ij_ac_ijm
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP28
<b>Space group number</b>	:	50
<b>Space group symbol</b>	:	<i>Pban</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2BC4_oP28_50_ij_ac_ijm --params=a, b/a, c/a, y <sub>3</sub> , y <sub>4</sub> , y <sub>5</sub> , y <sub>6</sub> , x <sub>7</sub> , y <sub>7</sub> , z <sub>7</sub>

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}}$	(2a)	Ni I
<b>B<sub>2</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}}$	(2a)	Ni I
<b>B<sub>3</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2c)	Ni II
<b>B<sub>4</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2c)	Ni II
<b>B<sub>5</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + y_3 \mathbf{a}_2$	$= \frac{1}{4} a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}}$	(4i)	La I
<b>B<sub>6</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2$	$= \frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}}$	(4i)	La I
<b>B<sub>7</sub></b>	$= \frac{3}{4} \mathbf{a}_1 - y_3 \mathbf{a}_2$	$= \frac{3}{4} a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}}$	(4i)	La I
<b>B<sub>8</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2$	$= \frac{3}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}}$	(4i)	La I
<b>B<sub>9</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + y_4 \mathbf{a}_2$	$= \frac{1}{4} a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}}$	(4i)	O I

$$\begin{array}{llll}
\mathbf{B}_{10} & = & \frac{1}{4} \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 & = & \frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} & (4i) & \text{O I} \\
\mathbf{B}_{11} & = & \frac{3}{4} \mathbf{a}_1 - y_4 \mathbf{a}_2 & = & \frac{3}{4} a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} & (4i) & \text{O I} \\
\mathbf{B}_{12} & = & \frac{3}{4} \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 & = & \frac{3}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} & (4i) & \text{O I} \\
\mathbf{B}_{13} & = & \frac{1}{4} \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \frac{1}{4} a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4j) & \text{La II} \\
\mathbf{B}_{14} & = & \frac{1}{4} \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4j) & \text{La II} \\
\mathbf{B}_{15} & = & \frac{3}{4} \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \frac{3}{4} a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4j) & \text{La II} \\
\mathbf{B}_{16} & = & \frac{3}{4} \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \frac{3}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4j) & \text{La II} \\
\mathbf{B}_{17} & = & \frac{1}{4} \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \frac{1}{4} a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4j) & \text{O II} \\
\mathbf{B}_{18} & = & \frac{1}{4} \mathbf{a}_1 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4j) & \text{O II} \\
\mathbf{B}_{19} & = & \frac{3}{4} \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \frac{3}{4} a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4j) & \text{O II} \\
\mathbf{B}_{20} & = & \frac{3}{4} \mathbf{a}_1 + \left(\frac{1}{2} + y_6\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \frac{3}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4j) & \text{O II} \\
\mathbf{B}_{21} & = & x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 & = & x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (8m) & \text{O III} \\
\mathbf{B}_{22} & = & \left(\frac{1}{2} - x_7\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_7\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 & = & \left(\frac{1}{2} - x_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_7\right) b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (8m) & \text{O III} \\
\mathbf{B}_{23} & = & \left(\frac{1}{2} - x_7\right) \mathbf{a}_1 + y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 & = & \left(\frac{1}{2} - x_7\right) a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} & (8m) & \text{O III} \\
\mathbf{B}_{24} & = & x_7 \mathbf{a}_1 + \left(\frac{1}{2} - y_7\right) \mathbf{a}_2 - z_7 \mathbf{a}_3 & = & x_7 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_7\right) b \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} & (8m) & \text{O III} \\
\mathbf{B}_{25} & = & -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 & = & -x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} & (8m) & \text{O III} \\
\mathbf{B}_{26} & = & \left(\frac{1}{2} + x_7\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_7\right) \mathbf{a}_2 - z_7 \mathbf{a}_3 & = & \left(\frac{1}{2} + x_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_7\right) b \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} & (8m) & \text{O III} \\
\mathbf{B}_{27} & = & \left(\frac{1}{2} + x_7\right) \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 & = & \left(\frac{1}{2} + x_7\right) a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (8m) & \text{O III} \\
\mathbf{B}_{28} & = & -x_7 \mathbf{a}_1 + \left(\frac{1}{2} + y_7\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 & = & -x_7 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_7\right) b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (8m) & \text{O III}
\end{array}$$

---

#### References:

- P. Odier, M. Leblanc, and J. Choisnet, *Structural characterization of an orthorhombic form of La<sub>2</sub>NiO<sub>4</sub>*, Mater. Res. Bull. **21**, 787–796 (1986), doi:10.1016/0025-5408(86)90163-7.

#### Found in:

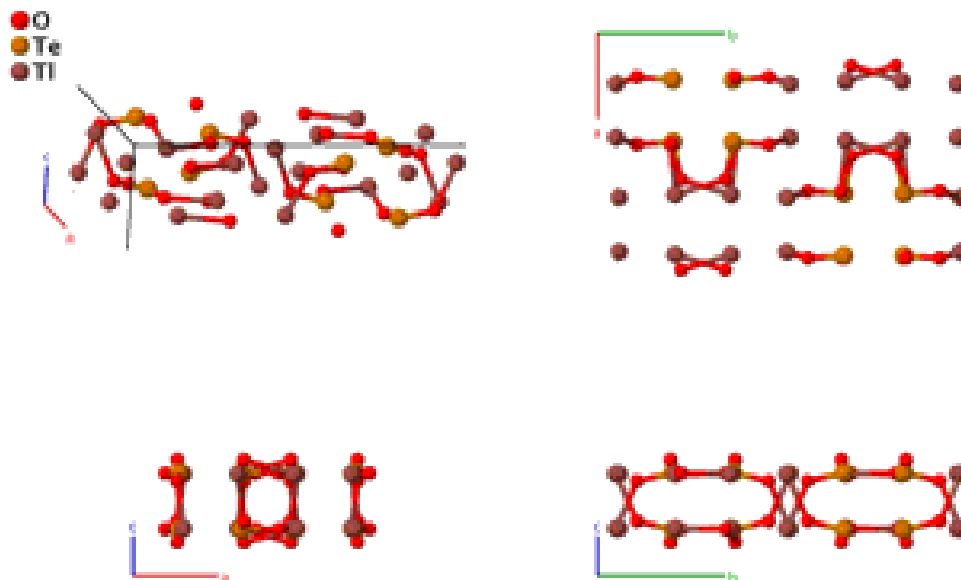
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 832  
- POSCAR: pp. 832

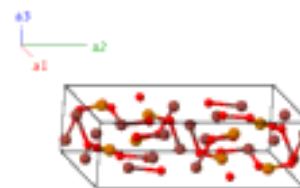
# $\alpha$ -Tl<sub>2</sub>TeO<sub>3</sub> Structure: A3BC2\_oP48\_50\_3m\_m\_2m



**Prototype** :  $\alpha$ -Tl<sub>2</sub>TeO<sub>3</sub>  
**AFLOW prototype label** : A3BC2\_oP48\_50\_3m\_m\_2m  
**Strukturbericht designation** : None  
**Pearson symbol** : oP48  
**Space group number** : 50  
**Space group symbol** : *Pban*  
**AFLOW prototype command** : `aflow --proto=A3BC2_oP48_50_3m_m_2m`  
`--params=a, b/a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6`

**Simple Orthorhombic primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8m)	O I
$\mathbf{B}_2$	$\left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8m)	O I
$\mathbf{B}_3$	$\left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(8m)	O I
$\mathbf{B}_4$	$x_1 \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(8m)	O I



$$\begin{aligned}
\mathbf{B}_{41} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (8m) & \text{Tl II} \\
\mathbf{B}_{42} &= \left(\frac{1}{2} - x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (8m) & \text{Tl II} \\
\mathbf{B}_{43} &= \left(\frac{1}{2} - x_6\right) \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} & (8m) & \text{Tl II} \\
\mathbf{B}_{44} &= x_6 \mathbf{a}_1 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} & (8m) & \text{Tl II} \\
\mathbf{B}_{45} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} & (8m) & \text{Tl II} \\
\mathbf{B}_{46} &= \left(\frac{1}{2} + x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_6\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} & (8m) & \text{Tl II} \\
\mathbf{B}_{47} &= \left(\frac{1}{2} + x_6\right) \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (8m) & \text{Tl II} \\
\mathbf{B}_{48} &= -x_6 \mathbf{a}_1 + \left(\frac{1}{2} + y_6\right) \mathbf{a}_2 + z_6 \mathbf{a}_3 &= -x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (8m) & \text{Tl II}
\end{aligned}$$

---

### References:

- F. Rieger and A.-V. Mudring, *Phase transition in  $\text{Tl}_2\text{TeO}_3$ : Influence and origin of the thallium lone pair distortion*, *Inorg. Chem.* **46**, 446–452 (2007), [doi:10.1021/ic061273j](https://doi.org/10.1021/ic061273j).

### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

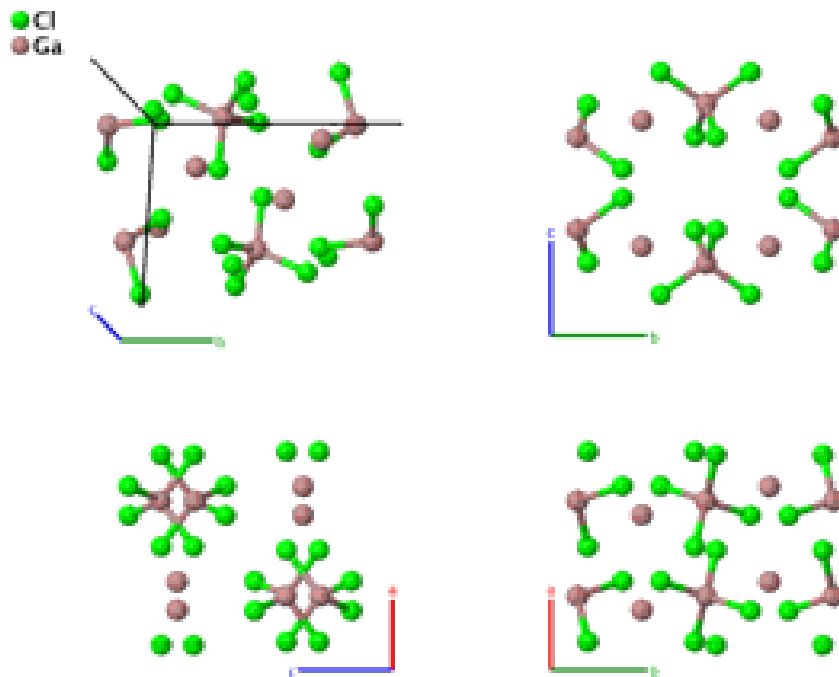
---

### Geometry files:

- CIF: pp. [833](#)  
- POSCAR: pp. [833](#)

# GaCl<sub>2</sub> (High-temperature) Structure:

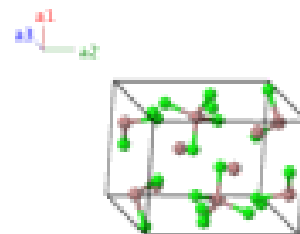
A2B\_oP24\_52\_2e\_cd



<b>Prototype</b>	:	GaCl <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_oP24_52_2e_cd
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP24
<b>Space group number</b>	:	52
<b>Space group symbol</b>	:	<i>Pnna</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_oP24_52_2e_cd --params= <i>a, b/a, c/a, z<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub></i>

**Simple Orthorhombic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + z_1 \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + z_1 c \hat{\mathbf{z}}$	(4c)	Ga I
<b>B<sub>2</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right)c \hat{\mathbf{z}}$	(4c)	Ga I



$$\begin{aligned}
\mathbf{B}_3 &= \frac{3}{4} \mathbf{a}_1 + -z_1 \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{x}} + -z_1 c \hat{\mathbf{z}} & (4c) & \text{Ga I} \\
\mathbf{B}_4 &= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}} & (4c) & \text{Ga I} \\
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (4d) & \text{Ga II} \\
\mathbf{B}_6 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (4d) & \text{Ga II} \\
\mathbf{B}_7 &= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (4d) & \text{Ga II} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (4d) & \text{Ga II} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8e) & \text{Cl I} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8e) & \text{Cl I} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + & (8e) & \text{Cl I} \\
&\quad \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{12} &= x_3 \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (8e) & \text{Cl I} \\
\mathbf{B}_{13} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8e) & \text{Cl I} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8e) & \text{Cl I} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + & (8e) & \text{Cl I} \\
&\quad \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{16} &= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (8e) & \text{Cl I} \\
\mathbf{B}_{17} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8e) & \text{Cl II} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8e) & \text{Cl II} \\
\mathbf{B}_{19} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + & (8e) & \text{Cl II} \\
&\quad \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{20} &= x_4 \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (8e) & \text{Cl II} \\
\mathbf{B}_{21} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8e) & \text{Cl II} \\
\mathbf{B}_{22} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8e) & \text{Cl II} \\
\mathbf{B}_{23} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + & (8e) & \text{Cl II} \\
&\quad \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{24} &= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (8e) & \text{Cl II}
\end{aligned}$$

## References:

- A. P. Wilkinson, A. K. Cheetham, and D. E. Cox, *Study of oxidation-state contrast in gallium dichloride by synchrotron X-ray anomalous scattering*, Acta Crystallogr. Sect. B Struct. Sci. **47**, 155–161 (1991), doi:10.1107/S0108768190010485.

## Found in:

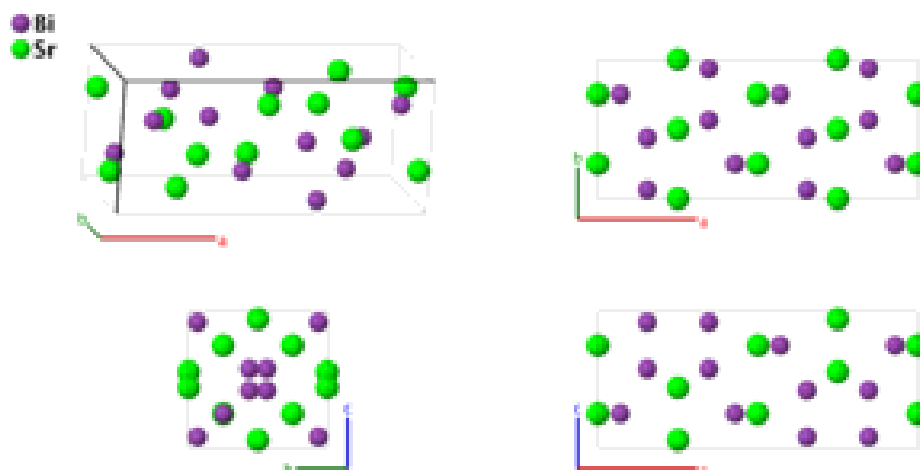
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

## Geometry files:

- CIF: pp. 833

- POSCAR: pp. 834

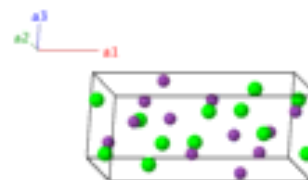
# Sr<sub>2</sub>Bi<sub>3</sub> Structure: A3B2\_oP20\_52\_de\_cd



**Prototype** : Sr<sub>2</sub>Bi<sub>3</sub>  
**AFLOW prototype label** : A3B2\_oP20\_52\_de\_cd  
**Strukturbericht designation** : None  
**Pearson symbol** : oP20  
**Space group number** : 52  
**Space group symbol** : *Pnma*  
**AFLOW prototype command** : `aflow --proto=A3B2_oP20_52_de_cd`  
`--params=a, b/a, c/a, z1, x2, x3, x4, y4, z4`

## Simple Orthorhombic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	$= \frac{1}{4} \mathbf{a}_1 + z_1 \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + z_1 c \hat{\mathbf{z}}$	(4c)	Sr I
<b>B</b> <sub>2</sub>	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	(4c)	Sr I
<b>B</b> <sub>3</sub>	$= \frac{3}{4} \mathbf{a}_1 + -z_1 \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + -z_1 c \hat{\mathbf{z}}$	(4c)	Sr I
<b>B</b> <sub>4</sub>	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4c)	Sr I
<b>B</b> <sub>5</sub>	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= x_2 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Bi I
<b>B</b> <sub>6</sub>	$= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Bi I
<b>B</b> <sub>7</sub>	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= -x_2 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Bi I
<b>B</b> <sub>8</sub>	$= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Bi I
<b>B</b> <sub>9</sub>	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Sr II

$$\begin{aligned}
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} &(4d) & \text{Sr II} \\
\mathbf{B}_{11} &= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} &(4d) & \text{Sr II} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} &(4d) & \text{Sr II} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} &(8e) & \text{Bi II} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} &(8e) & \text{Bi II} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + &(8e) & \text{Bi II} \\
&\quad \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{16} &= x_4 \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} &(8e) & \text{Bi II} \\
\mathbf{B}_{17} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} &(8e) & \text{Bi II} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} &(8e) & \text{Bi II} \\
\mathbf{B}_{19} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + &(8e) & \text{Bi II} \\
&\quad \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{20} &= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} &(8e) & \text{Bi II}
\end{aligned}$$

---

#### References:

- F. Merlo and M. L. Fornasini, *Crystal structure of some phases and alloying behaviour in alkaline earths, europium and ytterbium pnictides*, Mater. Res. Bull. **29**, 149–154 (1994), doi:10.1016/0025-5408(94)90135-X.

#### Found in:

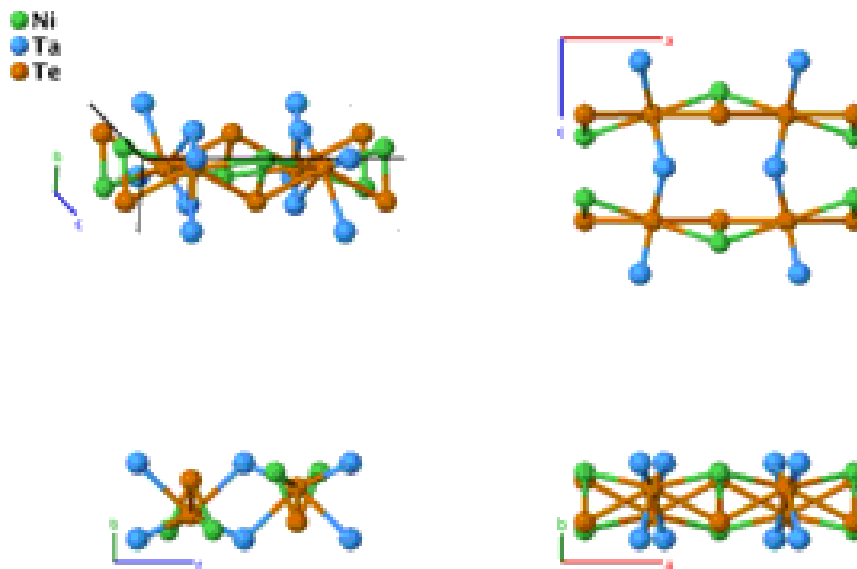
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 834  
- POSCAR: pp. 834

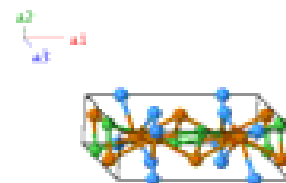
# TaNiTe<sub>2</sub> Structure: ABC2\_oP16\_53\_h\_e\_gh



**Prototype** : TaNiTe<sub>2</sub>  
**AFLOW prototype label** : ABC2\_oP16\_53\_h\_e\_gh  
**Strukturbericht designation** : None  
**Pearson symbol** : oP16  
**Space group number** : 53  
**Space group symbol** : *Pmna*  
**AFLOW prototype command** : aflow --proto=ABC2\_oP16\_53\_h\_e\_gh  
 --params=a, b/a, c/a, x<sub>1</sub>, y<sub>2</sub>, y<sub>3</sub>, z<sub>3</sub>, y<sub>4</sub>, z<sub>4</sub>

**Simple Orthorhombic primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$x_1 \mathbf{a}_1$	=	$x_1 a \hat{\mathbf{x}}$	(4e)	Ta
<b>B<sub>2</sub></b> =	$(\frac{1}{2} - x_1) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$(\frac{1}{2} - x_1) a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4e)	Ta
<b>B<sub>3</sub></b> =	$-x_1 \mathbf{a}_1$	=	$-x_1 a \hat{\mathbf{x}}$	(4e)	Ta
<b>B<sub>4</sub></b> =	$(\frac{1}{2} + x_1) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$(\frac{1}{2} + x_1) a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4e)	Ta
<b>B<sub>5</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4g)	Te I

$$\begin{array}{llllll}
\mathbf{B}_6 & = & \frac{1}{4} \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 & = & \frac{1}{4} a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (4g) & \text{Te I} \\
\mathbf{B}_7 & = & \frac{3}{4} \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 & = & \frac{3}{4} a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (4g) & \text{Te I} \\
\mathbf{B}_8 & = & \frac{3}{4} \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 & = & \frac{3}{4} a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (4g) & \text{Te I} \\
\mathbf{B}_9 & = & y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 & = & y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4h) & \text{Ni} \\
\mathbf{B}_{10} & = & \frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4h) & \text{Ni} \\
\mathbf{B}_{11} & = & \frac{1}{2} \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (4h) & \text{Ni} \\
\mathbf{B}_{12} & = & -y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 & = & -y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (4h) & \text{Ni} \\
\mathbf{B}_{13} & = & y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 & = & y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (4h) & \text{Te II} \\
\mathbf{B}_{14} & = & \frac{1}{2} \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (4h) & \text{Te II} \\
\mathbf{B}_{15} & = & \frac{1}{2} \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (4h) & \text{Te II} \\
\mathbf{B}_{16} & = & -y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 & = & -y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (4h) & \text{Te II}
\end{array}$$

---

#### References:

- W. Tremel, *Isolated and Condensed Ta<sub>2</sub>Ni<sub>2</sub> Clusters in the Layered Tellurides Ta<sub>2</sub>Ni<sub>2</sub>Te<sub>4</sub> and Ta<sub>2</sub>Ni<sub>3</sub>Te<sub>5</sub>*, *Angew. Chem. Int. Ed.* **30**, 840–843 (1991), [doi:10.1002/anie.199108401](https://doi.org/10.1002/anie.199108401).

#### Found in:

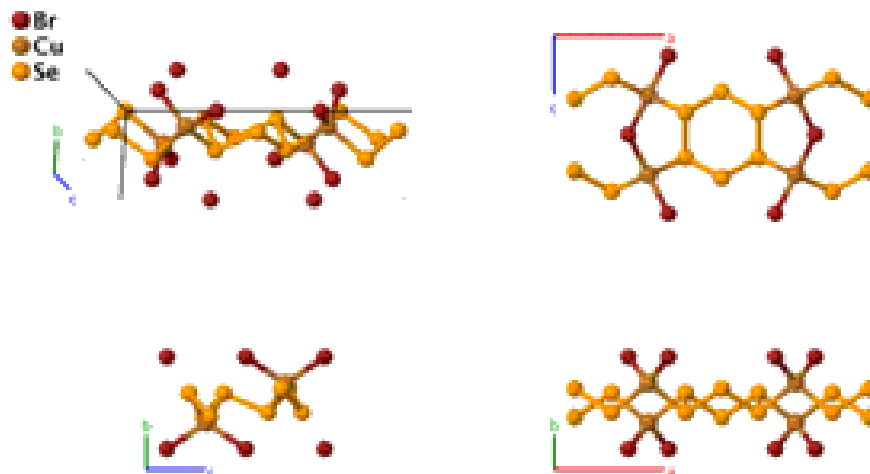
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [834](#)  
- POSCAR: pp. [835](#)

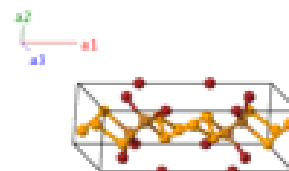
# CuBrSe<sub>3</sub> Structure: ABC3\_oP20\_53\_e\_g\_hi



<b>Prototype</b>	:	CuBrSe <sub>3</sub>
<b>AFLOW prototype label</b>	:	ABC3_oP20_53_e_g_hi
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP20
<b>Space group number</b>	:	53
<b>Space group symbol</b>	:	<i>Pmna</i>
<b>AFLOW prototype command</b>	:	aflow --proto=ABC3_oP20_53_e_g_hi --params= <i>a, b/a, c/a, x<sub>1</sub>, y<sub>2</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub></i>

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $x_1 \mathbf{a}_1$	=	$x_1 a \hat{\mathbf{x}}$	(4e)	Br
<b>B<sub>2</sub></b>	= $\left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4e)	Br
<b>B<sub>3</sub></b>	= $-x_1 \mathbf{a}_1$	=	$-x_1 a \hat{\mathbf{x}}$	(4e)	Br
<b>B<sub>4</sub></b>	= $\left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$\left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4e)	Br
<b>B<sub>5</sub></b>	= $\frac{1}{4} \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4g)	Cu
<b>B<sub>6</sub></b>	= $\frac{1}{4} \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4g)	Cu
<b>B<sub>7</sub></b>	= $\frac{3}{4} \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4g)	Cu
<b>B<sub>8</sub></b>	= $\frac{3}{4} \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4g)	Cu

$$\begin{aligned}
\mathbf{B}_9 &= y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4h) & \text{Se I} \\
\mathbf{B}_{10} &= \frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4h) & \text{Se I} \\
\mathbf{B}_{11} &= \frac{1}{2} \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (4h) & \text{Se I} \\
\mathbf{B}_{12} &= -y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (4h) & \text{Se I} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8i) & \text{Se II} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (8i) & \text{Se II} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (8i) & \text{Se II} \\
\mathbf{B}_{16} &= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8i) & \text{Se II} \\
\mathbf{B}_{17} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8i) & \text{Se II} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (8i) & \text{Se II} \\
\mathbf{B}_{19} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (8i) & \text{Se II} \\
\mathbf{B}_{20} &= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8i) & \text{Se II}
\end{aligned}$$

### References:

- H. M. Haendler and P. M. Carkner, *The crystal structure of copper bromide triselenide, CuBrSe<sub>3</sub>*, J. Solid State Chem. **29**, 35–39 (1979), doi:10.1016/0022-4596(79)90206-8.

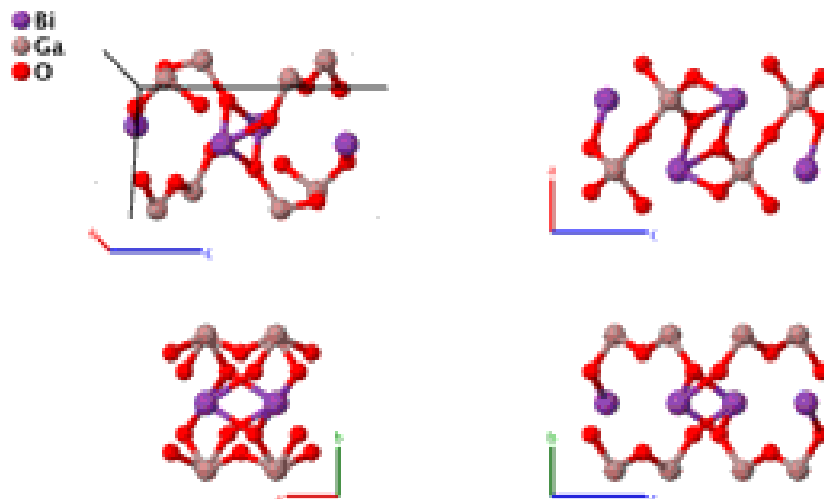
### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

### Geometry files:

- CIF: pp. 835  
- POSCAR: pp. 835

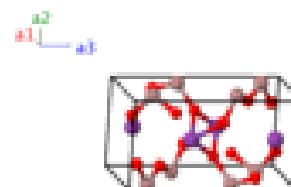
# BiGaO<sub>3</sub> Structure: ABC3\_oP20\_54\_e\_d\_cf



**Prototype** : BiGaO<sub>3</sub>  
**AFLOW prototype label** : ABC3\_oP20\_54\_e\_d\_cf  
**Strukturbericht designation** : None  
**Pearson symbol** : oP20  
**Space group number** : 54  
**Space group symbol** : *Pcca*  
**AFLOW prototype command** : aflow --proto=ABC3\_oP20\_54\_e\_d\_cf  
 --params=*a, b/a, c/a, y1, z2, z3, x4, y4, z4*

Simple Orthorhombic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$y_1 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	O I
<b>B<sub>2</sub></b> =	$\frac{1}{2} \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	O I
<b>B<sub>3</sub></b> =	$-y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-y_1 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	O I
<b>B<sub>4</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	O I
<b>B<sub>5</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + z_2 \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + z_2 c \hat{\mathbf{z}}$	(4d)	Ga
<b>B<sub>6</sub></b> =	$\frac{3}{4} \mathbf{a}_1 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(4d)	Ga
<b>B<sub>7</sub></b> =	$\frac{3}{4} \mathbf{a}_1 + -z_2 \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} + -z_2 c \hat{\mathbf{z}}$	(4d)	Ga
<b>B<sub>8</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4d)	Ga



$$\begin{aligned}
\mathbf{B}_9 &= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} &(4e) & \text{Bi} \\
\mathbf{B}_{10} &= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} &(4e) & \text{Bi} \\
\mathbf{B}_{11} &= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_3 \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} &(4e) & \text{Bi} \\
\mathbf{B}_{12} &= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} &(4e) & \text{Bi} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} &(8f) & \text{O II} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} &(8f) & \text{O II} \\
\mathbf{B}_{15} &= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} &(8f) & \text{O II} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} &(8f) & \text{O II} \\
\mathbf{B}_{17} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} &(8f) & \text{O II} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} &(8f) & \text{O II} \\
\mathbf{B}_{19} &= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} &(8f) & \text{O II} \\
\mathbf{B}_{20} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} &(8f) & \text{O II}
\end{aligned}$$

---

#### References:

- H. Yusa, A. A. Belik, E. Takayama-Muromachi, N. Hirao, and Y. Ohishi, *High-pressure phase transitions in BiMO<sub>3</sub> (M = Al, Ga, and In): In situ x-ray diffraction and Raman scattering experiments*, Phys. Rev. B **80**, 214103 (2009), [doi:10.1103/PhysRevB.80.214103](https://doi.org/10.1103/PhysRevB.80.214103).

#### Found in:

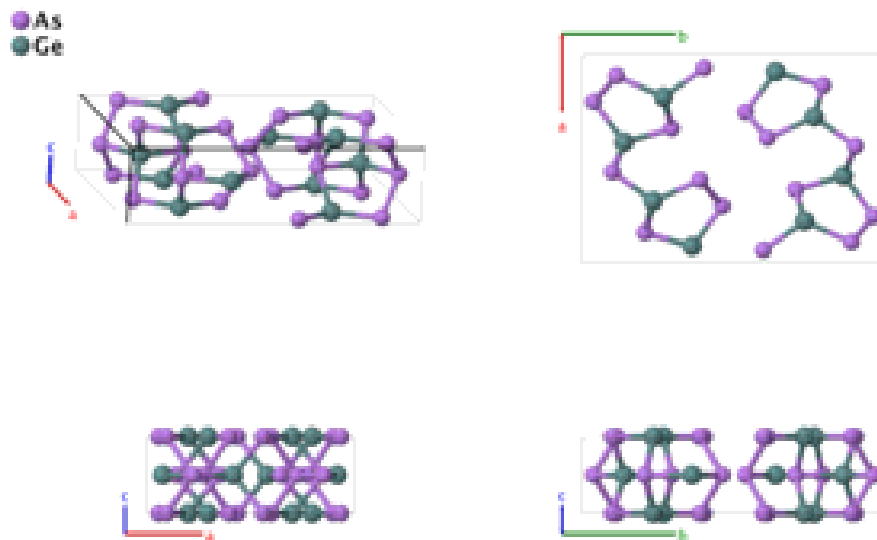
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [835](#)  
- POSCAR: pp. [836](#)

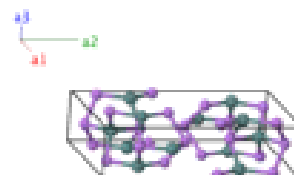
# GeAs<sub>2</sub> Structure: A2B\_oP24\_55\_2g2h\_gh



<b>Prototype</b>	:	GeAs <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_oP24_55_2g2h_gh
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP24
<b>Space group number</b>	:	55
<b>Space group symbol</b>	:	<i>Pbam</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_oP24_55_2g2h_gh --params= <i>a, b/a, c/a, x<sub>1</sub>, y<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub></i>

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	=	$x_1 a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}}$	(4g)	As I
<b>B<sub>2</sub></b>	= $-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	=	$-x_1 a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}}$	(4g)	As I
<b>B<sub>3</sub></b>	= $\left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_2$	=	$\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right) b \hat{\mathbf{y}}$	(4g)	As I
<b>B<sub>4</sub></b>	= $\left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2$	=	$\left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) b \hat{\mathbf{y}}$	(4g)	As I
<b>B<sub>5</sub></b>	= $x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	=	$x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}}$	(4g)	As II
<b>B<sub>6</sub></b>	= $-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	=	$-x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}}$	(4g)	As II

$$\begin{aligned}
\mathbf{B}_7 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 &= & \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} & (4g) & \text{As II} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 &= & \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) b \hat{\mathbf{y}} & (4g) & \text{As II} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 &= & x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} & (4g) & \text{Ge I} \\
\mathbf{B}_{10} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 &= & -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} & (4g) & \text{Ge I} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 &= & \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} & (4g) & \text{Ge I} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 &= & \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} & (4g) & \text{Ge I} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{As III} \\
\mathbf{B}_{14} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{As III} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{As III} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{As III} \\
\mathbf{B}_{17} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{As IV} \\
\mathbf{B}_{18} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{As IV} \\
\mathbf{B}_{19} &= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{As IV} \\
\mathbf{B}_{20} &= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{As IV} \\
\mathbf{B}_{21} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{Ge II} \\
\mathbf{B}_{22} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & -x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{Ge II} \\
\mathbf{B}_{23} &= \left(\frac{1}{2} - x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_6\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{Ge II} \\
\mathbf{B}_{24} &= \left(\frac{1}{2} + x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{Ge II}
\end{aligned}$$

---

### References:

- T. Wadsten, *Crystal structures of SiP<sub>2</sub>, SiAs<sub>2</sub>, and GeP*, Acta Chem. Scand. **21**, 593–594 (1967),  
[doi:10.3891/acta.chem.scand.21-0593](https://doi.org/10.3891/acta.chem.scand.21-0593).

### Found in:

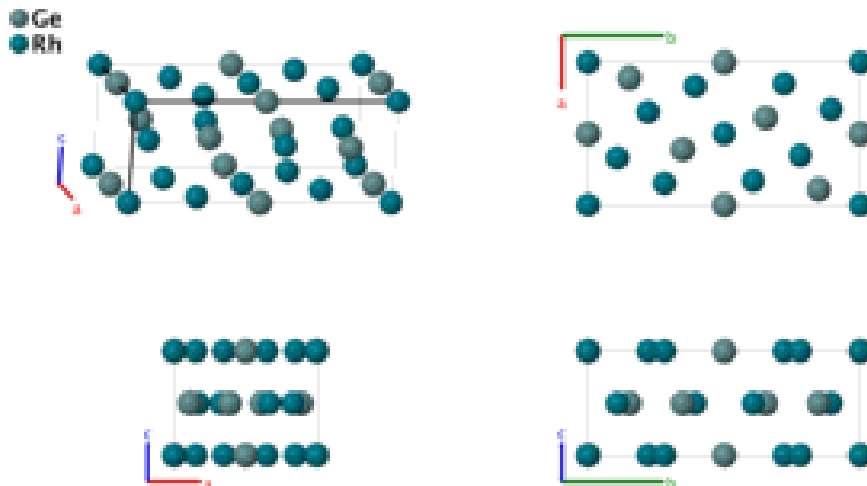
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. [836](#)  
- POSCAR: pp. [836](#)

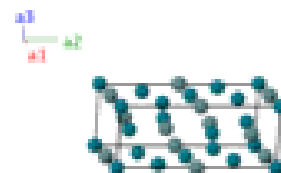
# Rh<sub>5</sub>Ge<sub>3</sub> Structure: A3B5\_oP16\_55\_ch\_agh



<b>Prototype</b>	:	Rh <sub>5</sub> Ge <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B5_oP16_55_ch_agh
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP16
<b>Space group number</b>	:	55
<b>Space group symbol</b>	:	<i>Pbam</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3B5_oP16_55_ch_agh --params= <i>a, b/a, c/a, x<sub>3</sub>, y<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub></i>

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	Rh I
<b>B<sub>2</sub></b>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(2a)	Rh I
<b>B<sub>3</sub></b>	= $\frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} b \hat{\mathbf{y}}$	(2c)	Ge I
<b>B<sub>4</sub></b>	= $\frac{1}{2} \mathbf{a}_1$	=	$\frac{1}{2} a \hat{\mathbf{x}}$	(2c)	Ge I
<b>B<sub>5</sub></b>	= $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	=	$x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}}$	(4g)	Rh II
<b>B<sub>6</sub></b>	= $-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	=	$-x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}}$	(4g)	Rh II
<b>B<sub>7</sub></b>	= $\left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2$	=	$\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}}$	(4g)	Rh II
<b>B<sub>8</sub></b>	= $\left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2$	=	$\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}}$	(4g)	Rh II

$$\begin{aligned}
\mathbf{B}_9 &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{Ge II} \\
\mathbf{B}_{10} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{Ge II} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{Ge II} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{Ge II} \\
\mathbf{B}_{13} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{Rh III} \\
\mathbf{B}_{14} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{Rh III} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{Rh III} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{Rh III}
\end{aligned}$$

---

### References:

- S. Geller, *The rhodium–germanium system. I. The crystal structures of Rh<sub>2</sub>Ge, Rh<sub>5</sub>Ge<sub>3</sub> and RhGe*, *Acta Cryst.* **8**, 15–21 (1955), [doi:10.1107/S0365110X55000030](https://doi.org/10.1107/S0365110X55000030).

### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. [836](#)  
- POSCAR: pp. [837](#)

# R-carbon Structure: A\_oP16\_55\_2g2h

● C



<b>Prototype</b>	:	C
<b>AFLOW prototype label</b>	:	A_oP16_55_2g2h
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP16
<b>Space group number</b>	:	55
<b>Space group symbol</b>	:	<i>Pbam</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A_oP16_55_2g2h --params= <i>a, b/a, c/a, x<sub>1</sub>, y<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub></i>

- This is a predicted “superhard” allotrope of carbon. Shortly after this paper was published, another paper predicted a similar phase, called “H-carbon” (He, 2012). The similarity between the two structures can be seen by shifting the origin by  $(1/2)\mathbf{a}_1$ . Other sources (Zhao, 2012) refer to this structure as “O-carbon.”

## Simple Orthorhombic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1 =$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$=$	$x_1 a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}}$	(4g)	C I
$\mathbf{B}_2 =$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	$=$	$-x_1 a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}}$	(4g)	C I
$\mathbf{B}_3 =$	$\left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_2$	$=$	$\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right) b \hat{\mathbf{y}}$	(4g)	C I
$\mathbf{B}_4 =$	$\left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2$	$=$	$\left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) b \hat{\mathbf{y}}$	(4g)	C I
$\mathbf{B}_5 =$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}}$	(4g)	C II

$$\begin{aligned}
\mathbf{B}_6 &= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 &= -x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} & (4g) & \text{C II} \\
\mathbf{B}_7 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} & (4g) & \text{C II} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) b \hat{\mathbf{y}} & (4g) & \text{C II} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{C III} \\
\mathbf{B}_{10} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{C III} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{C III} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{C III} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{C IV} \\
\mathbf{B}_{14} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{C IV} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{C IV} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{C IV}
\end{aligned}$$

---

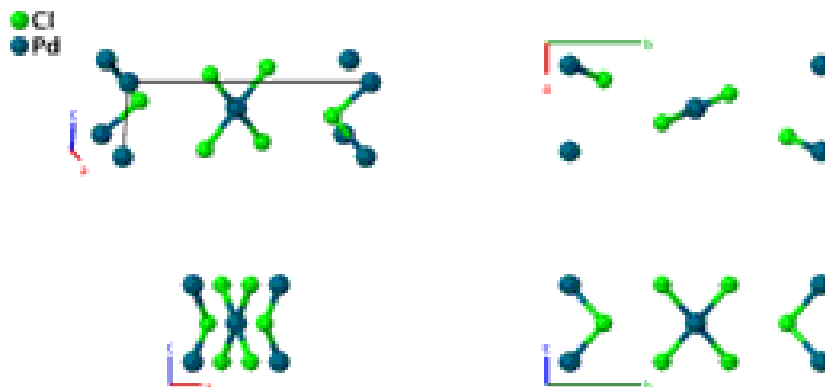
### References:

- H. Niu, X.-Q. Chen, S. Wang, D. Li, W. L. Mao, and Y. Li, *Families of Superhard Crystalline Carbon Allotropes Constructed via Cold Compression of Graphite and Nanotubes*, Phys. Rev. Lett. **108**, 135501 (2012), [doi:10.1103/PhysRevLett.108.135501](https://doi.org/10.1103/PhysRevLett.108.135501).
  - C. He, L. Sun, C. Zhang, X. Peng, K. Zhang, and J. Zhong, *New superhard carbon phases between graphite and diamond*, Solid State Commun. **152**, 1560–1563 (2012), [doi:10.1016/j.ssc.2012.05.022](https://doi.org/10.1016/j.ssc.2012.05.022).
  - C. He, L. Z. Sun, and J. Zhong, *Prediction of superhard carbon allotropes from the segment combination method*, J. Superhard Mater. **34**, 386–399 (2012), [doi:10.3103/S1063457612060123](https://doi.org/10.3103/S1063457612060123).
  - Z. Zhao, F. Tian, X. Dong, Q. Li, Q. Wang, H. Wang, X. Zhong, B. Xu, D. Yu, J. He, H.-T. Wang, Y. Ma, and Y. Tian, *Tetragonal Allotrope of Group 14 Elements*, J. Am. Chem. Soc. **134**, 12362–12365 (2012), [doi:10.1021/ja304380p](https://doi.org/10.1021/ja304380p).
- 

### Geometry files:

- CIF: pp. [837](#)
- POSCAR: pp. [837](#)

# $\alpha$ -PdCl<sub>2</sub> (C50) Structure: A2B\_oP6\_58\_g\_a

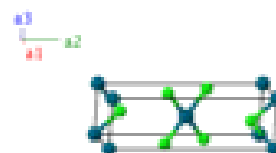


<b>Prototype</b>	:	$\alpha$ -PdCl <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_oP6_58_g_a
<b>Strukturbericht designation</b>	:	C50
<b>Pearson symbol</b>	:	oP6
<b>Space group number</b>	:	58
<b>Space group symbol</b>	:	<i>Pnmm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_oP6_58_g_a --params=a, b/a, c/a, x <sub>2</sub> , y <sub>2</sub>

- (Evers, 2010) implicitly places the Pd atoms at the (2b) Wyckoff position. We have shifted the Pd atoms to the (2a) site.

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	Pd
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Pd
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	=	$x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}}$	(4g)	Cl
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	=	$-x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}}$	(4g)	Cl
$\mathbf{B}_5$	$= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Cl
$\mathbf{B}_6$	$= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Cl

## References:



- J. Evers, W. Beck, M. Göbel, S. Jakob, P. Mayer, G. Oehlinger, M. Rotter, and T. M. Klapötke, *The Structures of  $\delta$ -PdCl<sub>2</sub> and  $\gamma$ -PdCl<sub>2</sub>: Phases with Negative Thermal Expansion in One Direction*, *Angew. Chem. Int. Ed.* **49**, 5677–5682 (2010), [doi:10.1002/anie.201000680](https://doi.org/10.1002/anie.201000680).

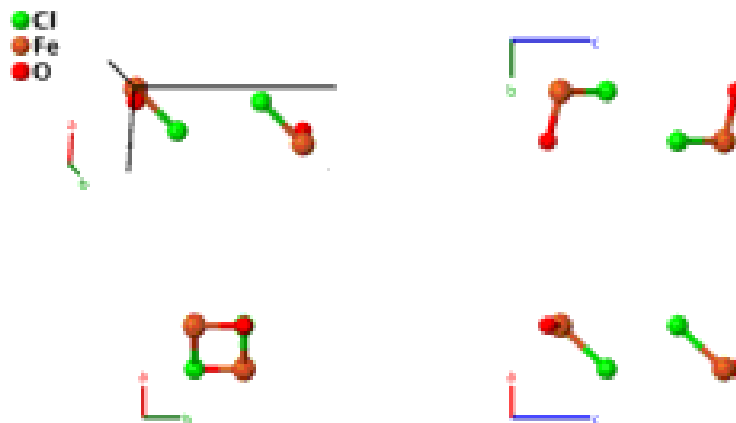
---

**Geometry files:**

- CIF: pp. [837](#)

- POSCAR: pp. [838](#)

# FeOCl Structure: ABC\_oP6\_59\_a\_b\_a



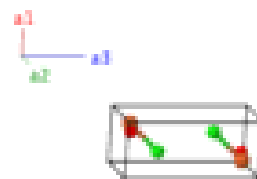
**Prototype** : FeOCl  
**AFLOW prototype label** : ABC\_oP6\_59\_a\_b\_a  
**Strukturbericht designation** : None  
**Pearson symbol** : oP6  
**Space group number** : 59  
**Space group symbol** : *Pmnn*  
**AFLOW prototype command** : aflow --proto=ABC\_oP6\_59\_a\_b\_a  
 --params=a, b/a, c/a, z<sub>1</sub>, z<sub>2</sub>, z<sub>3</sub>

## Other compounds with this structure:

- MOCl, (*M* = Ti, V, Cr, Fe), the superconducting alkali metal intercalates  $\alpha$ -MNX (*M* = Ti, Zr, Hf; *X* = Cl, Br, I).

## Simple Orthorhombic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(2a)	Cl
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(2a)	Cl
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2a)	O
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(2a)	O
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2b)	Fe
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(2b)	Fe

---

**References:**

- S. M. Kauzlarich, J. L. Stanton, J. Faber, and B. A. Averill, *Neutron profile refinement of the structure of FeOCl and FeOCl(TTF)<sub>1/8.5</sub>*, J. Am. Chem. Soc. **108**, 7946–7951 (1986), doi:[10.1021/ja00285a011](https://doi.org/10.1021/ja00285a011).

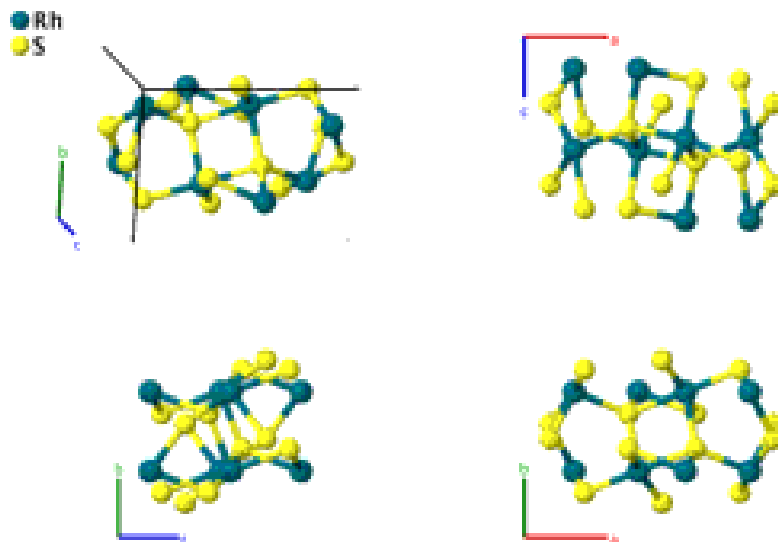
---

**Geometry files:**

- CIF: pp. [838](#)

- POSCAR: pp. [838](#)

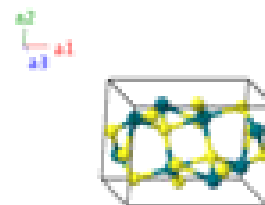
# Rh<sub>2</sub>S<sub>3</sub> Structure: A2B3\_oP20\_60\_d\_cd



**Prototype** : Rh<sub>2</sub>S<sub>3</sub>  
**AFLOW prototype label** : A2B3\_oP20\_60\_d\_cd  
**Strukturbericht designation** : None  
**Pearson symbol** : oP20  
**Space group number** : 60  
**Space group symbol** : *Pbcn*  
**AFLOW prototype command** : aflow --proto=A2B3\_oP20\_60\_d\_cd  
 --params=a, b/a, c/a, y<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>

Simple Orthorhombic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	= $y_1 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	S I
<b>B</b> <sub>2</sub>	= $\frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	= $\frac{1}{2} a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	S I
<b>B</b> <sub>3</sub>	= $-y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	= $-y_1 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	S I
<b>B</b> <sub>4</sub>	= $\frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	= $\frac{1}{2} a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right) b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	S I
<b>B</b> <sub>5</sub>	= $x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	= $x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8d)	Rh
<b>B</b> <sub>6</sub>	= $\left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	= $\left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(8d)	Rh

$$\begin{aligned}
\mathbf{B}_7 &= -x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} && (8d) && \text{Rh} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 - z_2 \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} && (8d) && \text{Rh} \\
\mathbf{B}_9 &= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} && (8d) && \text{Rh} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} + && (8d) && \text{Rh} \\
&\quad \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{11} &= x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} && (8d) && \text{Rh} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 + z_2 \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} && (8d) && \text{Rh} \\
\mathbf{B}_{13} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} && (8d) && \text{S II} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + && (8d) && \text{S II} \\
&\quad \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{15} &= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} && (8d) && \text{S II} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} && (8d) && \text{S II} \\
\mathbf{B}_{17} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} && (8d) && \text{S II} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + && (8d) && \text{S II} \\
&\quad \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{19} &= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} && (8d) && \text{S II} \\
\mathbf{B}_{20} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} && (8d) && \text{S II}
\end{aligned}$$

---

#### References:

- E. P. F. and Hulliger, *The crystal structure of Rh<sub>2</sub>S<sub>3</sub>*, in *Acta Cryst.* (Munksgaard Int Publ LTD 35 Norre Sogade, PO Box 2148, DK-1016 Copenhagen, Denmark, 1966), p. A66.

#### Found in:

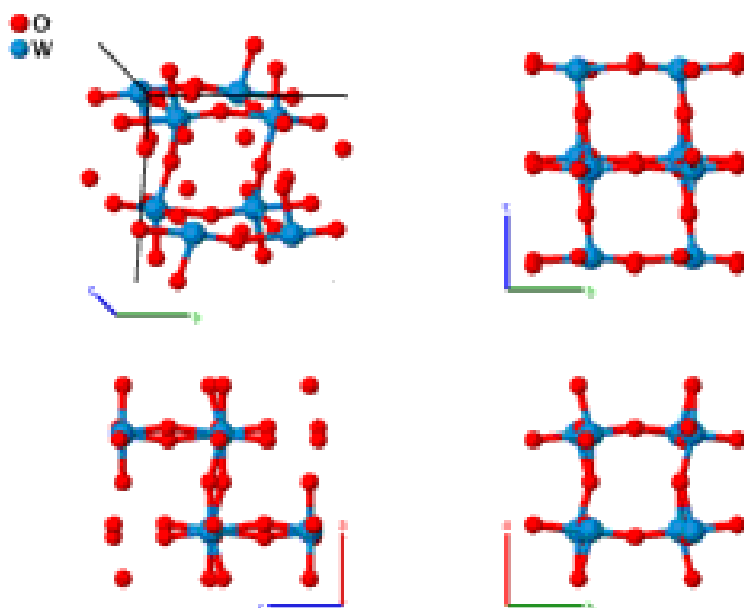
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [838](#)  
- POSCAR: pp. [839](#)

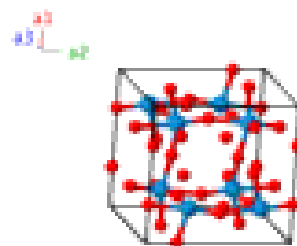
# WO<sub>3</sub> Structure: A3B\_oP32\_60\_3d\_d



<b>Prototype</b>	:	WO <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B_oP32_60_3d_d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP32
<b>Space group number</b>	:	60
<b>Space group symbol</b>	:	<i>Pbcn</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3B_oP32_60_3d_d --params= <i>a, b/a, c/a, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub></i>

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8 <i>d</i> )	O I
<b>B<sub>2</sub></b>	$\left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(8 <i>d</i> )	O I
<b>B<sub>3</sub></b>	$-x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	(8 <i>d</i> )	O I
<b>B<sub>4</sub></b>	$\left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$\left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(8 <i>d</i> )	O I

$\mathbf{B}_5$	$=$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-x_1 a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	$(8d)$	O I
$\mathbf{B}_6$	$=$	$\left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_2 +$ $\left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right) b \hat{\mathbf{y}} +$ $\left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	$(8d)$	O I
$\mathbf{B}_7$	$=$	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$=$	$x_1 a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	$(8d)$	O I
$\mathbf{B}_8$	$=$	$\left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right) b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	$(8d)$	O I
$\mathbf{B}_9$	$=$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	$(8d)$	O II
$\mathbf{B}_{10}$	$=$	$\left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 +$ $\left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) b \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	$(8d)$	O II
$\mathbf{B}_{11}$	$=$	$-x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	$=$	$-x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	$(8d)$	O II
$\mathbf{B}_{12}$	$=$	$\left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	$(8d)$	O II
$\mathbf{B}_{13}$	$=$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	$(8d)$	O II
$\mathbf{B}_{14}$	$=$	$\left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 +$ $\left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} +$ $\left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	$(8d)$	O II
$\mathbf{B}_{15}$	$=$	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	$(8d)$	O II
$\mathbf{B}_{16}$	$=$	$\left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	$(8d)$	O II
$\mathbf{B}_{17}$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{18}$	$=$	$\left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 +$ $\left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{19}$	$=$	$-x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{20}$	$=$	$\left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{21}$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{22}$	$=$	$\left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 +$ $\left(\frac{1}{2} - z_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} +$ $\left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{23}$	$=$	$x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{24}$	$=$	$\left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{25}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	$(8d)$	W
$\mathbf{B}_{26}$	$=$	$\left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 +$ $\left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	$(8d)$	W
$\mathbf{B}_{27}$	$=$	$-x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	$(8d)$	W
$\mathbf{B}_{28}$	$=$	$\left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	$(8d)$	W
$\mathbf{B}_{29}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	$(8d)$	W
$\mathbf{B}_{30}$	$=$	$\left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 +$ $\left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} +$ $\left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	$(8d)$	W
$\mathbf{B}_{31}$	$=$	$x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	$(8d)$	W
$\mathbf{B}_{32}$	$=$	$\left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	$(8d)$	W

## References:

- T. Vogt, P. M. Woodward, and B. A. Hunter, *The high-temperature phases of WO<sub>3</sub>*, J. Solid State Chem. **144**, 209–215 (1999), doi:10.1006/jssc.1999.8173.

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

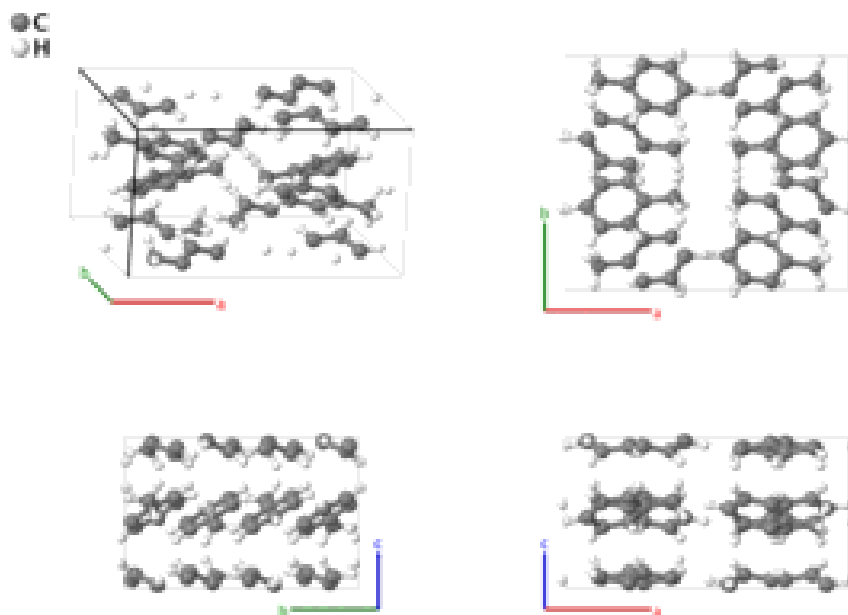
- CIF: pp. [839](#)

- POSCAR: pp. [839](#)



# $\beta$ -Toluene Structure: A7B8\_oP120\_60\_7d\_8d

---



<b>Prototype</b>	:	$\beta$ -C <sub>7</sub> H <sub>8</sub>
<b>AFLOW prototype label</b>	:	A7B8_oP120_60_7d_8d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP120
<b>Space group number</b>	:	60
<b>Space group symbol</b>	:	<i>Pbcn</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A7B8_oP120_60_7d_8d</code> <code>--params=a, b/a, c/a, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>, y<sub>9</sub>, z<sub>9</sub>, x<sub>10</sub>, y<sub>10</sub>, z<sub>10</sub>, x<sub>11</sub>, y<sub>11</sub>, z<sub>11</sub>, x<sub>12</sub>, y<sub>12</sub>, z<sub>12</sub>, x<sub>13</sub>, y<sub>13</sub>, z<sub>13</sub>, x<sub>14</sub>, y<sub>14</sub>, z<sub>14</sub>, x<sub>15</sub>, y<sub>15</sub>, z<sub>15</sub></code>

- 
- $\beta$ -Toluene is a metastable crystalline structure of the toluene molecule, C<sub>7</sub>H<sub>8</sub>, which crystallizes below 178 K. This data was constructed from experiments at 105 K.
  - The hydrogen atomic positions were approximated to agree with the chemistry of the toluene molecule.

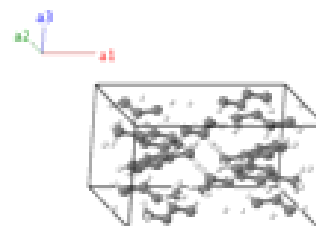
---

## Simple Orthorhombic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



---

## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	= $x_1 a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8d)	C I
<b>B</b> <sub>2</sub>	= $\left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	= $\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(8d)	C I
<b>B</b> <sub>3</sub>	= $-x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	= $-x_1 a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	(8d)	C I
<b>B</b> <sub>4</sub>	= $\left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	= $\left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(8d)	C I
<b>B</b> <sub>5</sub>	= $-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	= $-x_1 a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(8d)	C I
<b>B</b> <sub>6</sub>	= $\left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	= $\left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	(8d)	C I
<b>B</b> <sub>7</sub>	= $x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	= $x_1 a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(8d)	C I
<b>B</b> <sub>8</sub>	= $\left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	= $\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right) b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8d)	C I
<b>B</b> <sub>9</sub>	= $x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	= $x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8d)	C II
<b>B</b> <sub>10</sub>	= $\left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	= $\left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(8d)	C II
<b>B</b> <sub>11</sub>	= $-x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	= $-x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(8d)	C II
<b>B</b> <sub>12</sub>	= $\left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	= $\left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(8d)	C II
<b>B</b> <sub>13</sub>	= $-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	= $-x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(8d)	C II
<b>B</b> <sub>14</sub>	= $\left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	= $\left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(8d)	C II
<b>B</b> <sub>15</sub>	= $x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	= $x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(8d)	C II
<b>B</b> <sub>16</sub>	= $\left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	= $\left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8d)	C II
<b>B</b> <sub>17</sub>	= $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	= $x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8d)	C III
<b>B</b> <sub>18</sub>	= $\left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	= $\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(8d)	C III
<b>B</b> <sub>19</sub>	= $-x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3$	= $-x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}}$	(8d)	C III
<b>B</b> <sub>20</sub>	= $\left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	= $\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(8d)	C III
<b>B</b> <sub>21</sub>	= $-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	= $-x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(8d)	C III
<b>B</b> <sub>22</sub>	= $\left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3$	= $\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}}$	(8d)	C III
<b>B</b> <sub>23</sub>	= $x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	= $x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(8d)	C III
<b>B</b> <sub>24</sub>	= $\left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	= $\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8d)	C III
<b>B</b> <sub>25</sub>	= $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	= $x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8d)	C IV
<b>B</b> <sub>26</sub>	= $\left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	= $\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(8d)	C IV
<b>B</b> <sub>27</sub>	= $-x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	= $-x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	(8d)	C IV
<b>B</b> <sub>28</sub>	= $\left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	= $\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(8d)	C IV
<b>B</b> <sub>29</sub>	= $-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	= $-x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(8d)	C IV







$$\mathbf{B}_{120} = \left(\frac{1}{2} - x_{15}\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_{15}\right) \mathbf{a}_2 + z_{15} \mathbf{a}_3 = \left(\frac{1}{2} - x_{15}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_{15}\right) b \hat{\mathbf{y}} + z_{15} c \hat{\mathbf{z}} \quad (8d) \quad \text{H VIII}$$

---

**References:**

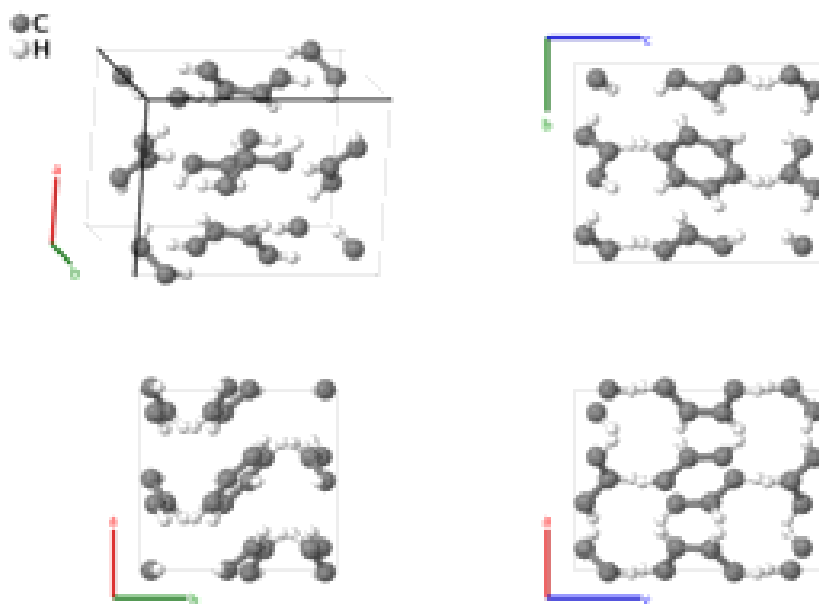
- D. Andre, R. Fourme, J. Bruneaux-Pouille, and L. Bosio, *Crystal structure of the metastable  $\beta$ -phase of toluene*, J. Mol. Struct. **81**, 253–259 (1982), doi:[10.1016/0022-2860\(82\)85338-6](https://doi.org/10.1016/0022-2860(82)85338-6).

---

**Geometry files:**

- CIF: pp. [839](#)
- POSCAR: pp. [840](#)

# Benzene Structure: AB\_oP48\_61\_3c\_3c



<b>Prototype</b>	:	Benzene
<b>AFLOW prototype label</b>	:	AB_oP48_61_3c_3c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oP48
<b>Space group number</b>	:	61
<b>Space group symbol</b>	:	<i>Pbca</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB_oP48_61_3c_3c --params= <i>a, b/a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6</i>

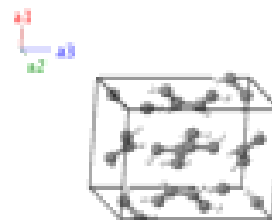
- Benzene is a liquid at temperatures above 6°C (279 K). This data was constructed from experiments at 150 K.
- The hydrogen atomic positions were approximated to agree with the chemistry of the benzene molecule.

**Simple Orthorhombic primitive vectors:**

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$x_1 a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8c)	C I





$$\begin{aligned}
\mathbf{B}_{38} &= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} & (8c) & \text{H II} \\
\mathbf{B}_{39} &= x_5 \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (8c) & \text{H II} \\
\mathbf{B}_{40} &= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3 = \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8c) & \text{H II} \\
\mathbf{B}_{41} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (8c) & \text{H III} \\
\mathbf{B}_{42} &= \left(\frac{1}{2} - x_6\right) \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} & (8c) & \text{H III} \\
\mathbf{B}_{43} &= -x_6 \mathbf{a}_1 + \left(\frac{1}{2} + y_6\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_6\right) \mathbf{a}_3 = -x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}} & (8c) & \text{H III} \\
\mathbf{B}_{44} &= \left(\frac{1}{2} + x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 = \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} & (8c) & \text{H III} \\
\mathbf{B}_{45} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = -x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} & (8c) & \text{H III} \\
\mathbf{B}_{46} &= \left(\frac{1}{2} + x_6\right) \mathbf{a}_1 + y_6 \mathbf{a}_2 + \left(\frac{1}{2} - z_6\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}} & (8c) & \text{H III} \\
\mathbf{B}_{47} &= x_6 \mathbf{a}_1 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} & (8c) & \text{H III} \\
\mathbf{B}_{48} &= \left(\frac{1}{2} - x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_6\right) \mathbf{a}_2 + z_6 \mathbf{a}_3 = \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (8c) & \text{H III}
\end{aligned}$$

---

### References:

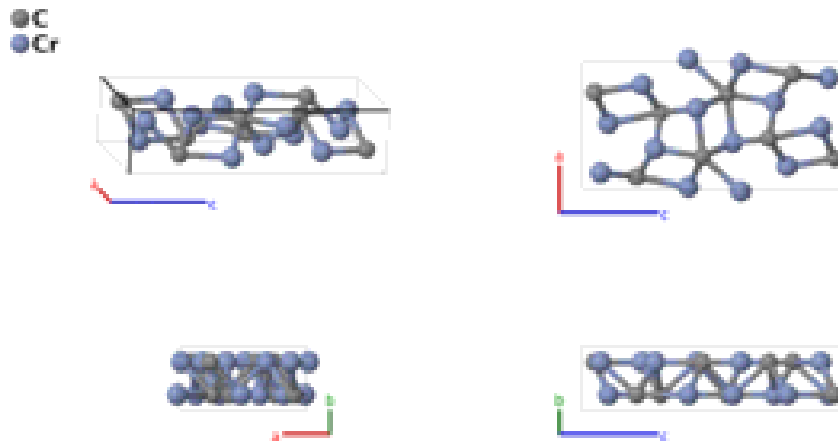
- S. K. Nayak, R. Sathishkumar, and T. N. Guru Row, *Directing role of functional groups in selective generation of C-H- $\pi$  interactions: In situ cryo-crystallographic studies on benzyl derivatives*, *CrystEngComm* **12**, 3112–3118 (2010), [doi:10.1039/C001190H](https://doi.org/10.1039/C001190H).

---

### Geometry files:

- CIF: pp. 841  
- POSCAR: pp. 841

# Tongbaite ( $\text{Cr}_3\text{C}_2$ , $D5_{10}$ ) Structure: A2B3\_oP20\_62\_2c\_3c



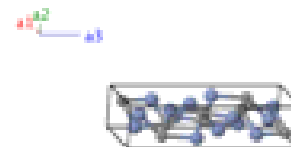
<b>Prototype</b>	:	$\text{Cr}_3\text{C}_2$
<b>AFLOW prototype label</b>	:	A2B3_oP20_62_2c_3c
<b>Strukturbericht designation</b>	:	$D5_{10}$
<b>Pearson symbol</b>	:	oP20
<b>Space group number</b>	:	62
<b>Space group symbol</b>	:	$Pnma$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3_oP20_62_2c_3c --params= $a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5$

## Other compounds with this structure:

- $\text{Hf}_3\text{P}_2$
- Several authors remark that this is the anti-type of [Stibnite](#) ( $\text{Sb}_2\text{S}_3$ ,  $D5_8$ , A3B2\_oP20\_62\_3c\_2c).

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4c)	CI
$\mathbf{B}_2$	$= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4c)	CI
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(4c)	CI

$$\begin{aligned}
\mathbf{B}_4 &= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}} & (4c) & \text{C I} \\
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3 = x_2 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (4c) & \text{C II} \\
\mathbf{B}_6 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4c) & \text{C II} \\
\mathbf{B}_7 &= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} & (4c) & \text{C II} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} & (4c) & \text{C II} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3 = x_3 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4c) & \text{Cr I} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4c) & \text{Cr I} \\
\mathbf{B}_{11} &= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3 = -x_3 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (4c) & \text{Cr I} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (4c) & \text{Cr I} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3 = x_4 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (4c) & \text{Cr II} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (4c) & \text{Cr II} \\
\mathbf{B}_{15} &= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3 = -x_4 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (4c) & \text{Cr II} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (4c) & \text{Cr II} \\
\mathbf{B}_{17} &= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3 = x_5 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (4c) & \text{Cr III} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (4c) & \text{Cr III} \\
\mathbf{B}_{19} &= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3 = -x_5 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (4c) & \text{Cr III} \\
\mathbf{B}_{20} &= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} & (4c) & \text{Cr III}
\end{aligned}$$

---

#### References:

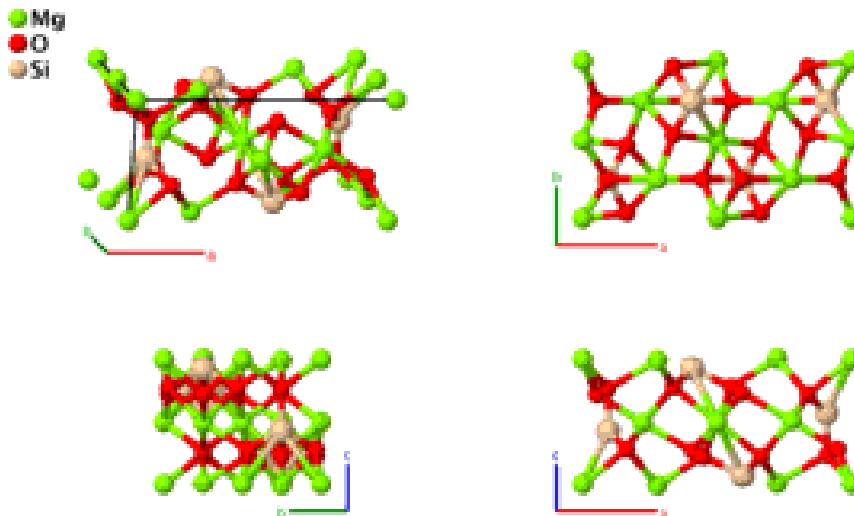
- S. Rundqvist and G. Runnsjö, *Crystal Structure Refinement of Cr<sub>3</sub>C<sub>2</sub>*, *Acta Chem. Scand.* **23**, 1191–1199 (1969), [doi:10.3891/acta.chem.scand.23-1191](https://doi.org/10.3891/acta.chem.scand.23-1191).

---

#### Geometry files:

- CIF: pp. [841](#)  
- POSCAR: pp. [842](#)

# Forsterite ( $\text{Mg}_2\text{SiO}_4$ , $S 1_2$ ) Structure: A2B4C\_oP28\_62\_ac\_2cd\_c



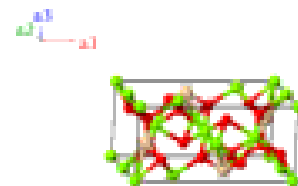
<b>Prototype</b>	:	$\text{Mg}_2\text{SiO}_4$
<b>AFLOW prototype label</b>	:	A2B4C_oP28_62_ac_2cd_c
<b>Strukturbericht designation</b>	:	$S 1_2$
<b>Pearson symbol</b>	:	oP28
<b>Space group number</b>	:	62
<b>Space group symbol</b>	:	$Pnma$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B4C_oP28_62_ac_2cd_c --params=a, b/a, c/a, $x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, y_6, z_6$

## Other compounds with this structure:

- $\text{Fe}_2\text{SiO}_4$  (fayalite),  $(\text{Mg,Fe})\text{CaSiO}_4$ ,  $(\text{Mg,Mn})\text{SiO}_4$ ,  $\text{Al}_2\text{BeO}_4$ ,  $\text{Fe}_2\text{SiS}_4$ ,  $\text{Mg}_2\text{GeS}_4$ ,  $\text{Mg}_2\text{GeS}_4$ ,  $\text{Mn}_2\text{GeS}_4$ ,  $\text{Tm}_2\text{ZnS}_4$
- This structure is the magnesium end-point of olivine,  $(\text{Mg,Fe})_2\text{SiO}_4$ . (Hazen, 1976) reports the structure in the  $Pbnm$  setting of space group #62. We have transformed this into the standard  $Pnma$  setting. We use the structural data at  $23^\circ\text{C}$ .

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
---------------------	-----------------------	------------------	-----------

$\mathbf{B}_1$	$=$	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	$(4a)$	Mg I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	$(4a)$	Mg I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} b \hat{\mathbf{y}}$	$(4a)$	Mg I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	$(4a)$	Mg I
$\mathbf{B}_5$	$=$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$x_2 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	$(4c)$	Mg II
$\mathbf{B}_6$	$=$	$(\frac{1}{2} - x_2) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (\frac{1}{2} + z_2) \mathbf{a}_3$	$=$	$(\frac{1}{2} - x_2) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + (\frac{1}{2} + z_2) c \hat{\mathbf{z}}$	$(4c)$	Mg II
$\mathbf{B}_7$	$=$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-x_2 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	$(4c)$	Mg II
$\mathbf{B}_8$	$=$	$(\frac{1}{2} + x_2) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (\frac{1}{2} - z_2) \mathbf{a}_3$	$=$	$(\frac{1}{2} + x_2) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + (\frac{1}{2} - z_2) c \hat{\mathbf{z}}$	$(4c)$	Mg II
$\mathbf{B}_9$	$=$	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	$(4c)$	O I
$\mathbf{B}_{10}$	$=$	$(\frac{1}{2} - x_3) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (\frac{1}{2} + z_3) \mathbf{a}_3$	$=$	$(\frac{1}{2} - x_3) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + (\frac{1}{2} + z_3) c \hat{\mathbf{z}}$	$(4c)$	O I
$\mathbf{B}_{11}$	$=$	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	$(4c)$	O I
$\mathbf{B}_{12}$	$=$	$(\frac{1}{2} + x_3) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (\frac{1}{2} - z_3) \mathbf{a}_3$	$=$	$(\frac{1}{2} + x_3) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + (\frac{1}{2} - z_3) c \hat{\mathbf{z}}$	$(4c)$	O I
$\mathbf{B}_{13}$	$=$	$x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	$(4c)$	O II
$\mathbf{B}_{14}$	$=$	$(\frac{1}{2} - x_4) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (\frac{1}{2} + z_4) \mathbf{a}_3$	$=$	$(\frac{1}{2} - x_4) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + (\frac{1}{2} + z_4) c \hat{\mathbf{z}}$	$(4c)$	O II
$\mathbf{B}_{15}$	$=$	$-x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	$(4c)$	O II
$\mathbf{B}_{16}$	$=$	$(\frac{1}{2} + x_4) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (\frac{1}{2} - z_4) \mathbf{a}_3$	$=$	$(\frac{1}{2} + x_4) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + (\frac{1}{2} - z_4) c \hat{\mathbf{z}}$	$(4c)$	O II
$\mathbf{B}_{17}$	$=$	$x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	$(4c)$	Si
$\mathbf{B}_{18}$	$=$	$(\frac{1}{2} - x_5) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (\frac{1}{2} + z_5) \mathbf{a}_3$	$=$	$(\frac{1}{2} - x_5) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + (\frac{1}{2} + z_5) c \hat{\mathbf{z}}$	$(4c)$	Si
$\mathbf{B}_{19}$	$=$	$-x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	$(4c)$	Si
$\mathbf{B}_{20}$	$=$	$(\frac{1}{2} + x_5) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (\frac{1}{2} - z_5) \mathbf{a}_3$	$=$	$(\frac{1}{2} + x_5) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + (\frac{1}{2} - z_5) c \hat{\mathbf{z}}$	$(4c)$	Si
$\mathbf{B}_{21}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{22}$	$=$	$(\frac{1}{2} - x_6) \mathbf{a}_1 - y_6 \mathbf{a}_2 + (\frac{1}{2} + z_6) \mathbf{a}_3$	$=$	$(\frac{1}{2} - x_6) a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + (\frac{1}{2} + z_6) c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{23}$	$=$	$-x_6 \mathbf{a}_1 + (\frac{1}{2} + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} + (\frac{1}{2} + y_6) b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{24}$	$=$	$(\frac{1}{2} + x_6) \mathbf{a}_1 + (\frac{1}{2} - y_6) \mathbf{a}_2 +$ $(\frac{1}{2} - z_6) \mathbf{a}_3$	$=$	$(\frac{1}{2} + x_6) a \hat{\mathbf{x}} + (\frac{1}{2} - y_6) b \hat{\mathbf{y}} +$ $(\frac{1}{2} - z_6) c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{25}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{26}$	$=$	$(\frac{1}{2} + x_6) \mathbf{a}_1 + y_6 \mathbf{a}_2 + (\frac{1}{2} - z_6) \mathbf{a}_3$	$=$	$(\frac{1}{2} + x_6) a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + (\frac{1}{2} - z_6) c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{27}$	$=$	$x_6 \mathbf{a}_1 + (\frac{1}{2} - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + (\frac{1}{2} - y_6) b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	$(8d)$	O III
$\mathbf{B}_{28}$	$=$	$(\frac{1}{2} - x_6) \mathbf{a}_1 + (\frac{1}{2} + y_6) \mathbf{a}_2 +$ $(\frac{1}{2} + z_6) \mathbf{a}_3$	$=$	$(\frac{1}{2} - x_6) a \hat{\mathbf{x}} + (\frac{1}{2} + y_6) b \hat{\mathbf{y}} +$ $(\frac{1}{2} + z_6) c \hat{\mathbf{z}}$	$(8d)$	O III

## References:

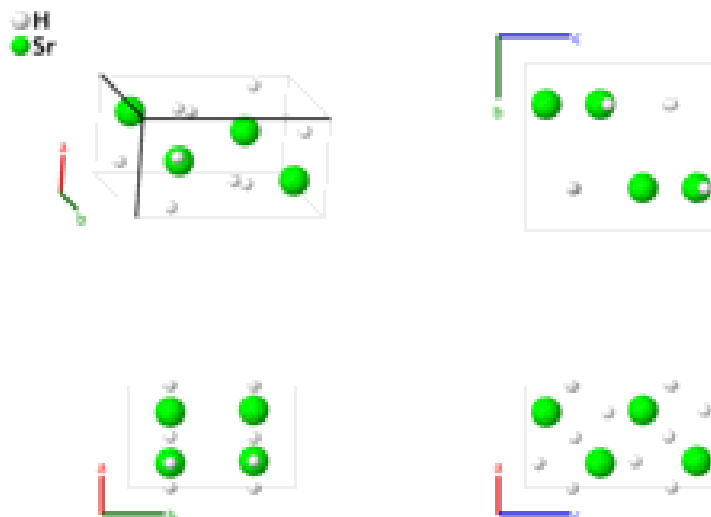
- R. M. Hazen, *Effects of temperature and pressure on the crystal structure of forsterite*, Am. Mineral. **61**, 1280–1293 (1976).

## Geometry files:

- CIF: pp. 842

- POSCAR: pp. 842

# SrH<sub>2</sub> (C29) Structure: A2B\_oP12\_62\_2c\_c



**Prototype** : SrH<sub>2</sub>  
**AFLOW prototype label** : A2B\_oP12\_62\_2c\_c  
**Strukturbericht designation** : C29  
**Pearson symbol** : oP12  
**Space group number** : 62  
**Space group symbol** : *Pnma*  
**AFLOW prototype command** : aflow --proto=A2B\_oP12\_62\_2c\_c  
 --params=*a, b/a, c/a, x<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, z<sub>3</sub>*

## Other compounds with this structure:

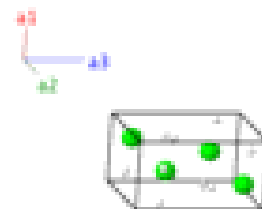
- CaH<sub>2</sub>

## Simple Orthorhombic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4c)	HI
<b>B<sub>2</sub></b> =	$(\frac{1}{2} - x_1) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (\frac{1}{2} + z_1) \mathbf{a}_3$	$(\frac{1}{2} - x_1) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + (\frac{1}{2} + z_1) c \hat{\mathbf{z}}$	(4c)	HI
<b>B<sub>3</sub></b> =	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(4c)	HI

$$\begin{aligned}
\mathbf{B}_4 &= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}} & (4c) & \text{H I} \\
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3 = x_2 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (4c) & \text{H II} \\
\mathbf{B}_6 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4c) & \text{H II} \\
\mathbf{B}_7 &= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} & (4c) & \text{H II} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} & (4c) & \text{H II} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3 = x_3 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4c) & \text{Sr} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4c) & \text{Sr} \\
\mathbf{B}_{11} &= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3 = -x_3 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (4c) & \text{Sr} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (4c) & \text{Sr}
\end{aligned}$$

---

### References:

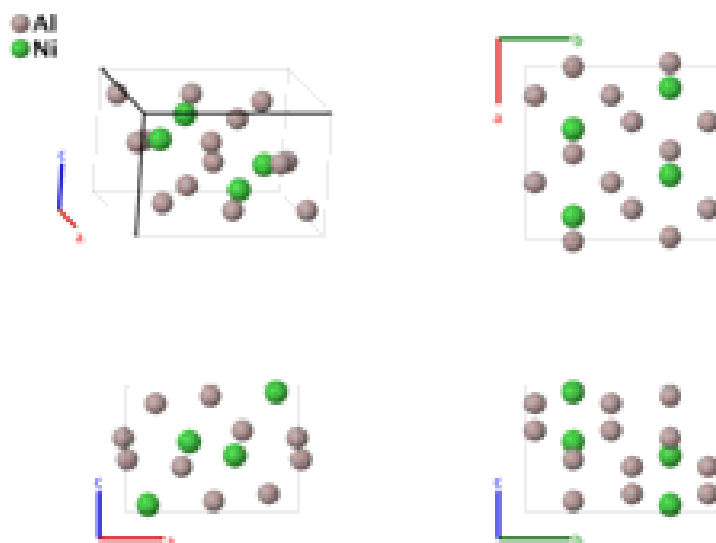
- R. C. Ropp, *Encyclopedia of the Alkaline Earth Compounds* (Elsevier, Oxford, 2013), chap. 2, pp. 30–31.

---

### Geometry files:

- CIF: pp. [842](#)  
- POSCAR: pp. [843](#)

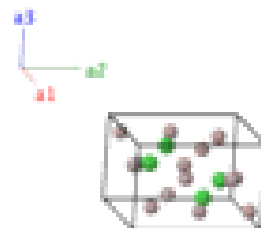
# $\epsilon$ -NiAl<sub>3</sub> (*D*0<sub>20</sub>) Structure: A3B\_oP16\_62\_cd\_c



<b>Prototype</b>	:	$\epsilon$ -NiAl <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B_oP16_62_cd_c
<b>Strukturbericht designation</b>	:	<i>D</i> 0 <sub>20</sub>
<b>Pearson symbol</b>	:	oP16
<b>Space group number</b>	:	62
<b>Space group symbol</b>	:	<i>Pnma</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3B_oP16_62_cd_c --params= <i>a, b/a, c/a, x<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub></i>

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4 <i>c</i> )	Al I
<b>B</b> <sub>2</sub>	$(\frac{1}{2} - x_1) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (\frac{1}{2} + z_1) \mathbf{a}_3$	$(\frac{1}{2} - x_1) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + (\frac{1}{2} + z_1) c \hat{\mathbf{z}}$	(4 <i>c</i> )	Al I
<b>B</b> <sub>3</sub>	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(4 <i>c</i> )	Al I
<b>B</b> <sub>4</sub>	$(\frac{1}{2} + x_1) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (\frac{1}{2} - z_1) \mathbf{a}_3$	$(\frac{1}{2} + x_1) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + (\frac{1}{2} - z_1) c \hat{\mathbf{z}}$	(4 <i>c</i> )	Al I
<b>B</b> <sub>5</sub>	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$x_2 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4 <i>c</i> )	Ni
<b>B</b> <sub>6</sub>	$(\frac{1}{2} - x_2) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (\frac{1}{2} + z_2) \mathbf{a}_3$	$(\frac{1}{2} - x_2) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + (\frac{1}{2} + z_2) c \hat{\mathbf{z}}$	(4 <i>c</i> )	Ni



$$\mathbf{B}_7 = -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} \quad (4c) \quad \text{Ni}$$

$$\mathbf{B}_8 = \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} \quad (4c) \quad \text{Ni}$$

$$\mathbf{B}_9 = x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} \quad (8d) \quad \text{Al II}$$

$$\mathbf{B}_{10} = \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \quad (8d) \quad \text{Al II}$$

$$\mathbf{B}_{11} = -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 = -x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} \quad (8d) \quad \text{Al II}$$

$$\mathbf{B}_{12} = \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} \quad (8d) \quad \text{Al II}$$

$$\mathbf{B}_{13} = -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} \quad (8d) \quad \text{Al II}$$

$$\mathbf{B}_{14} = \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} \quad (8d) \quad \text{Al II}$$

$$\mathbf{B}_{15} = x_3 \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 = x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} \quad (8d) \quad \text{Al II}$$

$$\mathbf{B}_{16} = \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \quad (8d) \quad \text{Al II}$$

### References:

- A. J. Bradley and A. Taylor, *The crystal structures of Ni<sub>2</sub>Al<sub>3</sub> and NiAl<sub>3</sub>*, *Philos. Mag.* **23**, 1049–1067 (1937), [doi:10.1080/14786443708561875](https://doi.org/10.1080/14786443708561875).

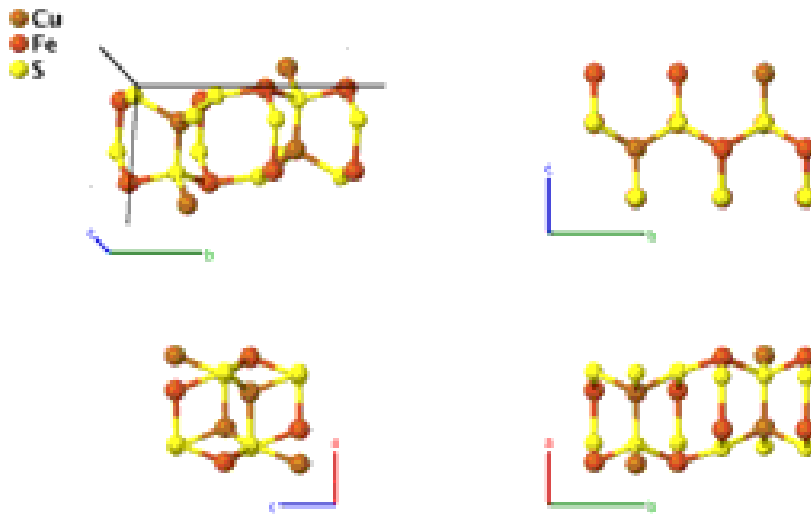
### Found in:

- W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

### Geometry files:

- CIF: pp. 843  
- POSCAR: pp. 843

# Cubanite ( $\text{CuFe}_2\text{S}_3$ , $E9_e$ ) Structure: AB2C3\_oP24\_62\_c\_d\_cd



<b>Prototype</b>	:	$\text{CuFe}_2\text{S}_3$
<b>AFLOW prototype label</b>	:	AB2C3_oP24_62_c_d_cd
<b>Strukturbericht designation</b>	:	$E9_e$
<b>Pearson symbol</b>	:	oP24
<b>Space group number</b>	:	62
<b>Space group symbol</b>	:	$Pnma$
<b>AFLOW prototype command</b>	:	aflow --proto=AB2C3_oP24_62_c_d_cd --params=a, b/a, c/a, $x_1, z_1, x_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

- (Szymański, 1974) uses the  $Pcmn$  orientation of space group #62 to describe this structure. We have swapped the  $\hat{x}$  and  $\hat{z}$  axis to transform this into the standard  $Pnma$  orientation.

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= b \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= x_1 a \hat{x} + \frac{1}{4} b \hat{y} + z_1 c \hat{z}$	(4c)	Cu
$\mathbf{B}_2$	$= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - x_1\right) a \hat{x} + \frac{3}{4} b \hat{y} + \left(\frac{1}{2} + z_1\right) c \hat{z}$	(4c)	Cu
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= -x_1 a \hat{x} + \frac{3}{4} b \hat{y} - z_1 c \hat{z}$	(4c)	Cu
$\mathbf{B}_4$	$= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} + x_1\right) a \hat{x} + \frac{1}{4} b \hat{y} + \left(\frac{1}{2} - z_1\right) c \hat{z}$	(4c)	Cu

$$\begin{aligned}
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (4c) & \text{S I} \\
\mathbf{B}_6 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4c) & \text{S I} \\
\mathbf{B}_7 &= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} & (4c) & \text{S I} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} & (4c) & \text{S I} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8d) & \text{Fe} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (8d) & \text{Fe} \\
\mathbf{B}_{11} &= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8d) & \text{Fe} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + & (8d) & \text{Fe} \\
&\quad \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{13} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8d) & \text{Fe} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (8d) & \text{Fe} \\
\mathbf{B}_{15} &= x_3 \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8d) & \text{Fe} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) b \hat{\mathbf{y}} + & (8d) & \text{Fe} \\
&\quad \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{17} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8d) & \text{S II} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (8d) & \text{S II} \\
\mathbf{B}_{19} &= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8d) & \text{S II} \\
\mathbf{B}_{20} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + & (8d) & \text{S II} \\
&\quad \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{21} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8d) & \text{S II} \\
\mathbf{B}_{22} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (8d) & \text{S II} \\
\mathbf{B}_{23} &= x_4 \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8d) & \text{S II} \\
\mathbf{B}_{24} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} + & (8d) & \text{S II} \\
&\quad \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}
\end{aligned}$$

---

#### References:

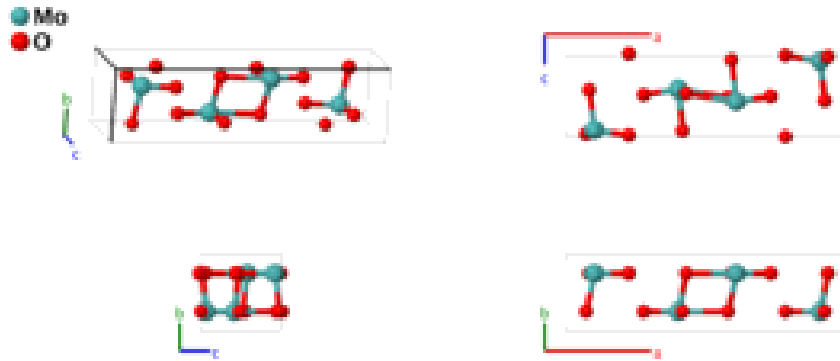
- T. Szymański, *A refinement of the structure of cubanite, CuFe<sub>2</sub>S<sub>3</sub>*, *Zeitschrift für Kristallographie - Crystalline Materials* **140**, 218–239 (1974), [doi:10.1524/zkri-1974-3-407](https://doi.org/10.1524/zkri-1974-3-407).

---

#### Geometry files:

- CIF: pp. [843](#)  
- POSCAR: pp. [844](#)

# Molybdate ( $\text{MoO}_3$ , $D0_8$ ) Structure: AB3\_oP16\_62\_c\_3c

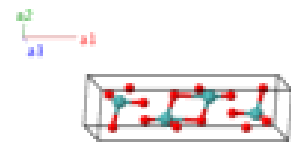


<b>Prototype</b>	:	$\text{MoO}_3$
<b>AFLOW prototype label</b>	:	AB3_oP16_62_c_3c
<b>Strukturbericht designation</b>	:	$D0_8$
<b>Pearson symbol</b>	:	oP16
<b>Space group number</b>	:	62
<b>Space group symbol</b>	:	$Pnma$
<b>AFLOW prototype command</b>	:	aflow --proto=AB3_oP16_62_c_3c --params= $a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4$

- The unit cell and atomic positions were originally given in the  $Pbnm$  orientation of space group #62. We have rotated the crystal axis so that  $\hat{y} \rightarrow \hat{x} \rightarrow \hat{z}$  to put the system in the standard  $Pnma$  representation.

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4c)	Mo
$\mathbf{B}_2$	$= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4c)	Mo
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(4c)	Mo
$\mathbf{B}_4$	$= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	(4c)	Mo
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= x_2 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_6$	$= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$= -x_2 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_8$	$= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	$= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(4c)	O I

$$\begin{aligned}
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4c) & \text{O II} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4c) & \text{O II} \\
\mathbf{B}_{11} &= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (4c) & \text{O II} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (4c) & \text{O II} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (4c) & \text{O III} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (4c) & \text{O III} \\
\mathbf{B}_{15} &= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (4c) & \text{O III} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (4c) & \text{O III}
\end{aligned}$$

---

### References:

- H. Sitepu, B. H. O'Connor, and D. Li, *Comparative evaluation of the March and generalized spherical harmonic preferred orientation models using X-ray diffraction data for molybdate and calcite powders*, J. Appl. Crystallogr. **38**, 158–167 (2005), [doi:10.1107/S0021889804031231](https://doi.org/10.1107/S0021889804031231).

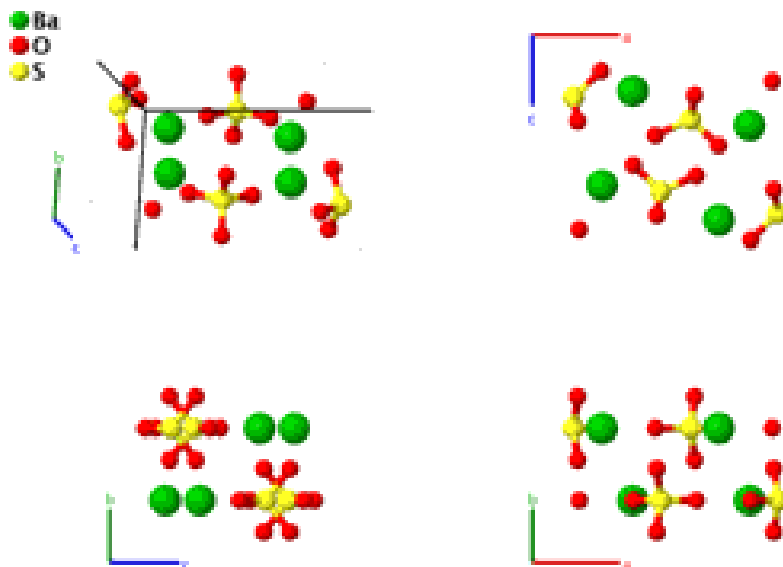
---

### Geometry files:

- CIF: pp. [844](#)  
- POSCAR: pp. [844](#)

# Barite ( $\text{BaSO}_4$ , $H0_2$ ) Structure:

AB4C\_oP24\_62\_c\_2cd\_c



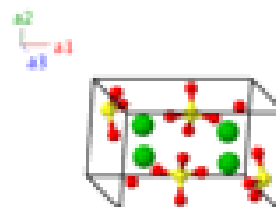
**Prototype** :  $\text{BaSO}_4$   
**AFLOW prototype label** : AB4C\_oP24\_62\_c\_2cd\_c  
**Strukturbericht designation** :  $H0_2$   
**Pearson symbol** : oP24  
**Space group number** : 62  
**Space group symbol** :  $Pnma$   
**AFLOW prototype command** : aflow --proto=AB4C\_oP24\_62\_c\_2cd\_c  
 --params= $a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, y_5, z_5$

## Other compounds with this structure:

- $\text{SrSO}_4$  (celestite),  $\text{PbSO}_4$  (anglesite),  $\text{KGaH}_4$

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$x_1 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4c)	Ba
$\mathbf{B}_2$	$= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4c)	Ba

$$\begin{aligned}
\mathbf{B}_3 &= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3 &= -x_1 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}} &(4c) & \text{Ba} \\
\mathbf{B}_4 &= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}} &(4c) & \text{Ba} \\
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} &(4c) & \text{O I} \\
\mathbf{B}_6 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} &(4c) & \text{O I} \\
\mathbf{B}_7 &= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} &(4c) & \text{O I} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} &(4c) & \text{O I} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} &(4c) & \text{O II} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} &(4c) & \text{O II} \\
\mathbf{B}_{11} &= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} &(4c) & \text{O II} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} &(4c) & \text{O II} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} &(4c) & \text{S} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} &(4c) & \text{S} \\
\mathbf{B}_{15} &= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} &(4c) & \text{S} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} &(4c) & \text{S} \\
\mathbf{B}_{17} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} &(8d) & \text{O III} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} &(8d) & \text{O III} \\
\mathbf{B}_{19} &= -x_5 \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} &(8d) & \text{O III} \\
\mathbf{B}_{20} &= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + &(8d) & \text{O III} \\
&\quad \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{21} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} &(8d) & \text{O III} \\
\mathbf{B}_{22} &= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} &(8d) & \text{O III} \\
\mathbf{B}_{23} &= x_5 \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} &(8d) & \text{O III} \\
\mathbf{B}_{24} &= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} + &(8d) & \text{O III} \\
&\quad \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}
\end{aligned}$$

---

#### References:

- A. A. Colville and K. Staudhammer, *A refinement of the structure of barite*, Am. Mineral. **52**, 1877–1880 (1967).

#### Found in:

- D. Barthelmy, *Mineralogy Database* (2012). Barite.

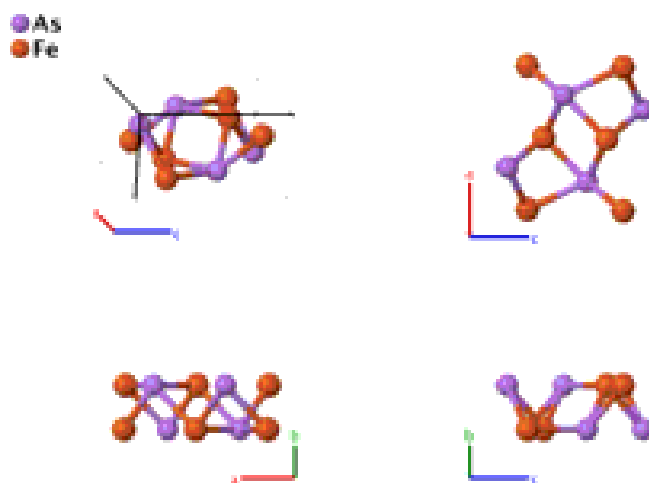
---

#### Geometry files:

- CIF: pp. [844](#)

- POSCAR: pp. [845](#)

# Westerveldite (FeAs, *B14*) Structure: AB\_oP8\_62\_c\_c



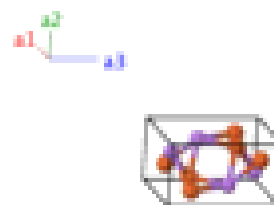
<b>Prototype</b>	:	FeAs
<b>AFLOW prototype label</b>	:	AB_oP8_62_c_c
<b>Strukturbericht designation</b>	:	<i>B14</i>
<b>Pearson symbol</b>	:	oP8
<b>Space group number</b>	:	62
<b>Space group symbol</b>	:	<i>Pnma</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB_oP8_62_c_c --params=a, b/a, c/a, x<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub></code>

## Other compounds with this structure:

- CoAs
- The *B31* ([MnP](#), [AB\\_oP8\\_62\\_c\\_c](#)) structure is similar to this one. (Brandes, 1992) lists *B31* as the primary structure, but we include FeAs here for completeness. We use the data (Selte, 1972) reported at 14 K.

## Simple Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
---------------------	-----------------------	------------------	-----------



$$\begin{aligned}
\mathbf{B}_1 &= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3 &= x_1 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}} & (4c) & \text{As} \\
\mathbf{B}_2 &= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}} & (4c) & \text{As} \\
\mathbf{B}_3 &= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3 &= -x_1 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}} & (4c) & \text{As} \\
\mathbf{B}_4 &= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}} & (4c) & \text{As} \\
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (4c) & \text{Fe} \\
\mathbf{B}_6 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4c) & \text{Fe} \\
\mathbf{B}_7 &= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} & (4c) & \text{Fe} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} & (4c) & \text{Fe}
\end{aligned}$$

---

### References:

- K. Selte, A. Kjekshus, and A. F. Andresen, *Magnetic Structure and Properties of FeAs*, *Acta Chem. Scand.* **26**, 3101–3113 (1972), [doi:10.3891/acta.chem.scand.26-3101](https://doi.org/10.3891/acta.chem.scand.26-3101).
- E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types*, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., [doi:10.1007/978-3-662-02909-1\\_3](https://doi.org/10.1007/978-3-662-02909-1_3).

### Found in:

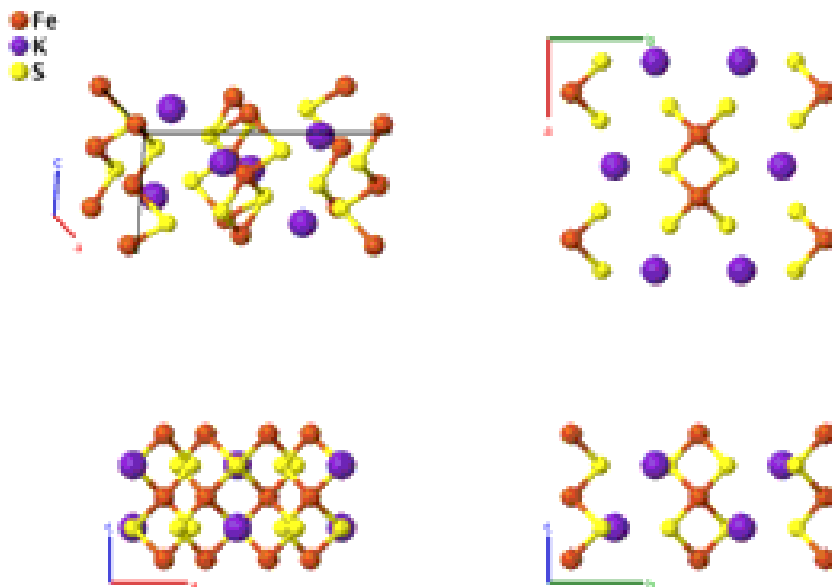
- J. R. Jeffries, N. P. Butch, H. Cynn, S. R. Saha, K. Kirshenbaum, S. T. Weir, Y. K. Vohra, and J. Paglione, *Interplay between magnetism, structure, and strong electron-phonon coupling in binary FeAs under pressure*, *Phys. Rev. B* **83**, 134520 (2011), [doi:10.1103/PhysRevB.83.134520](https://doi.org/10.1103/PhysRevB.83.134520).

---

### Geometry files:

- CIF: pp. [845](#)
- POSCAR: pp. [845](#)

# Rasvumite (KFe<sub>2</sub>S<sub>3</sub>) Structure: A2BC3\_oC24\_63\_e\_c\_cg



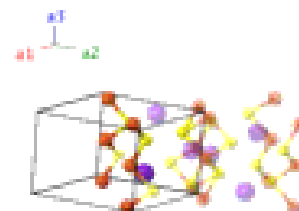
**Prototype** : KFe<sub>2</sub>S<sub>3</sub>  
**AFLOW prototype label** : A2BC3\_oC24\_63\_e\_c\_cg  
**Strukturbericht designation** : None  
**Pearson symbol** : oC24  
**Space group number** : 63  
**Space group symbol** : *Cmcm*  
**AFLOW prototype command** : aflow --proto=A2BC3\_oC24\_63\_e\_c\_cg  
 --params=a, b/a, c/a, y<sub>1</sub>, y<sub>2</sub>, x<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>

## Other compounds with this structure:

- BaFe<sub>2</sub>S<sub>3</sub>, RbFe<sub>2</sub>S<sub>3</sub>, CsFe<sub>2</sub>S<sub>3</sub>

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$-y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$y_1 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	K
<b>B<sub>2</sub></b> =	$y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-y_1 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	K

$$\begin{array}{llllll}
\mathbf{B}_3 & = & -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 & = & y_2 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (4c) & \text{S I} \\
\mathbf{B}_4 & = & y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 & = & -y_2 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (4c) & \text{S I} \\
\mathbf{B}_5 & = & x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 & = & x_3 a \hat{\mathbf{x}} & (8e) & \text{Fe} \\
\mathbf{B}_6 & = & -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & -x_3 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}} & (8e) & \text{Fe} \\
\mathbf{B}_7 & = & -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 & = & -x_3 a \hat{\mathbf{x}} & (8e) & \text{Fe} \\
\mathbf{B}_8 & = & x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & x_3 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}} & (8e) & \text{Fe} \\
\mathbf{B}_9 & = & (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 & = & x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{S II} \\
\mathbf{B}_{10} & = & (-x_4 + y_4) \mathbf{a}_1 + (-x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 & = & -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{S II} \\
\mathbf{B}_{11} & = & (-x_4 - y_4) \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 & = & -x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{S II} \\
\mathbf{B}_{12} & = & (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 & = & x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{S II}
\end{array}$$

---

**References:**

- J. R. Clark and G. E. Brown, Jr., *Crystal structure of rasvumite, KFe<sub>2</sub>S<sub>3</sub>*, Am. Mineral. **65**, 477–482 (1980).

**Found in:**

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

---

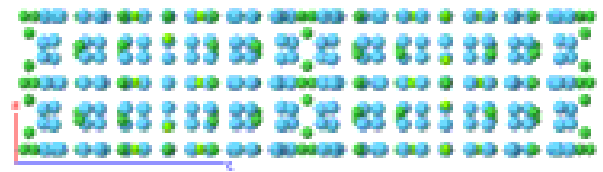
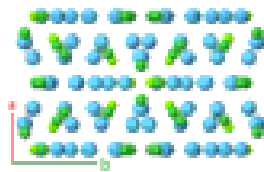
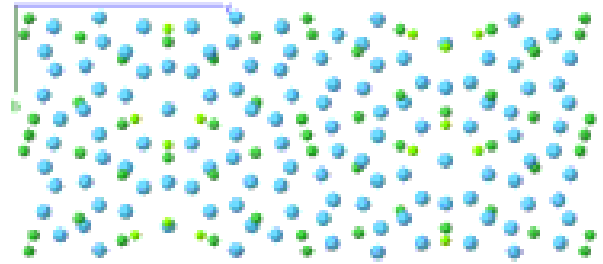
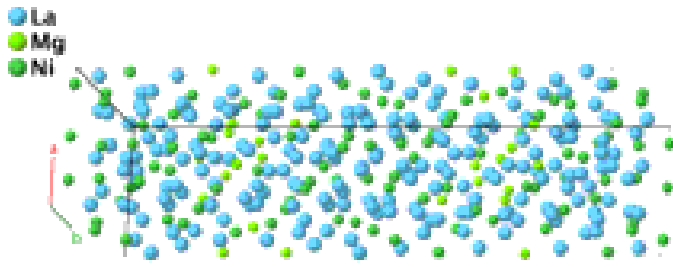
**Geometry files:**

- CIF: pp. [845](#)

- POSCAR: pp. [846](#)

# La<sub>43</sub>Ni<sub>17</sub>Mg<sub>5</sub> Structure:

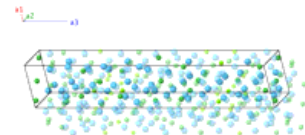
## A43B5C17\_oC260\_63\_c8fg6h\_cfg\_ce3f2h



<b>Prototype</b>	:	La <sub>43</sub> Ni <sub>17</sub> Mg <sub>5</sub>
<b>AFLOW prototype label</b>	:	A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC260
<b>Space group number</b>	:	63
<b>Space group symbol</b>	:	<i>Cmcm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h --params= <i>a, b/a, c/a, y<sub>1</sub>, y<sub>2</sub>, y<sub>3</sub>, x<sub>4</sub>, y<sub>5</sub>, z<sub>5</sub>, y<sub>6</sub>, z<sub>6</sub>, y<sub>7</sub>, z<sub>7</sub>, y<sub>8</sub>, z<sub>8</sub>, y<sub>9</sub>, z<sub>9</sub>, y<sub>10</sub>, z<sub>10</sub>, y<sub>11</sub>, z<sub>11</sub>, y<sub>12</sub>, z<sub>12</sub>, y<sub>13</sub>, z<sub>13</sub>, y<sub>14</sub>, z<sub>14</sub>, y<sub>15</sub>, z<sub>15</sub>, y<sub>16</sub>, z<sub>16</sub>, x<sub>17</sub>, y<sub>17</sub>, x<sub>18</sub>, y<sub>18</sub>, x<sub>19</sub>, y<sub>19</sub>, z<sub>19</sub>, x<sub>20</sub>, y<sub>20</sub>, z<sub>20</sub>, x<sub>21</sub>, y<sub>21</sub>, z<sub>21</sub>, x<sub>22</sub>, y<sub>22</sub>, z<sub>22</sub>, x<sub>23</sub>, y<sub>23</sub>, z<sub>23</sub>, x<sub>24</sub>, y<sub>24</sub>, z<sub>24</sub>, x<sub>25</sub>, y<sub>25</sub>, z<sub>25</sub>, x<sub>26</sub>, y<sub>26</sub>, z<sub>26</sub></i>

### Base-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



### Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$-y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$y_1 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	La I
<b>B<sub>2</sub></b> =	$y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-y_1 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	La I
<b>B<sub>3</sub></b> =	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$y_2 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Mg I
<b>B<sub>4</sub></b> =	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-y_2 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Mg I

$\mathbf{B}_5$	$=$	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$y_3 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Ni I
$\mathbf{B}_6$	$=$	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-y_3 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Ni I
$\mathbf{B}_7$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$x_4 a \hat{\mathbf{x}}$	(8e)	Ni II
$\mathbf{B}_8$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8e)	Ni II
$\mathbf{B}_9$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-x_4 a \hat{\mathbf{x}}$	(8e)	Ni II
$\mathbf{B}_{10}$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8e)	Ni II
$\mathbf{B}_{11}$	$=$	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8f)	La II
$\mathbf{B}_{12}$	$=$	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$-y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(8f)	La II
$\mathbf{B}_{13}$	$=$	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3$	$=$	$y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}}$	(8f)	La II
$\mathbf{B}_{14}$	$=$	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-y_5 b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(8f)	La II
$\mathbf{B}_{15}$	$=$	$-y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8f)	La III
$\mathbf{B}_{16}$	$=$	$y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	$=$	$-y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(8f)	La III
$\mathbf{B}_{17}$	$=$	$-y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \left(\frac{1}{2} - z_6\right) \mathbf{a}_3$	$=$	$y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}}$	(8f)	La III
$\mathbf{B}_{18}$	$=$	$y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-y_6 b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(8f)	La III
$\mathbf{B}_{19}$	$=$	$-y_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8f)	La IV
$\mathbf{B}_{20}$	$=$	$y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	$=$	$-y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(8f)	La IV
$\mathbf{B}_{21}$	$=$	$-y_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + \left(\frac{1}{2} - z_7\right) \mathbf{a}_3$	$=$	$y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_7\right) c \hat{\mathbf{z}}$	(8f)	La IV
$\mathbf{B}_{22}$	$=$	$y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-y_7 b \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}}$	(8f)	La IV
$\mathbf{B}_{23}$	$=$	$-y_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$y_8 b \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(8f)	La V
$\mathbf{B}_{24}$	$=$	$y_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3$	$=$	$-y_8 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \hat{\mathbf{z}}$	(8f)	La V
$\mathbf{B}_{25}$	$=$	$-y_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + \left(\frac{1}{2} - z_8\right) \mathbf{a}_3$	$=$	$y_8 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_8\right) c \hat{\mathbf{z}}$	(8f)	La V
$\mathbf{B}_{26}$	$=$	$y_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-y_8 b \hat{\mathbf{y}} - z_8 c \hat{\mathbf{z}}$	(8f)	La V
$\mathbf{B}_{27}$	$=$	$-y_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$y_9 b \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(8f)	La VI
$\mathbf{B}_{28}$	$=$	$y_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3$	$=$	$-y_9 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}}$	(8f)	La VI
$\mathbf{B}_{29}$	$=$	$-y_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + \left(\frac{1}{2} - z_9\right) \mathbf{a}_3$	$=$	$y_9 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_9\right) c \hat{\mathbf{z}}$	(8f)	La VI
$\mathbf{B}_{30}$	$=$	$y_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-y_9 b \hat{\mathbf{y}} - z_9 c \hat{\mathbf{z}}$	(8f)	La VI
$\mathbf{B}_{31}$	$=$	$-y_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$y_{10} b \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(8f)	La VII
$\mathbf{B}_{32}$	$=$	$y_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3$	$=$	$-y_{10} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}}$	(8f)	La VII
$\mathbf{B}_{33}$	$=$	$-y_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + \left(\frac{1}{2} - z_{10}\right) \mathbf{a}_3$	$=$	$y_{10} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{10}\right) c \hat{\mathbf{z}}$	(8f)	La VII
$\mathbf{B}_{34}$	$=$	$y_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-y_{10} b \hat{\mathbf{y}} - z_{10} c \hat{\mathbf{z}}$	(8f)	La VII
$\mathbf{B}_{35}$	$=$	$-y_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$y_{11} b \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}}$	(8f)	La VIII
$\mathbf{B}_{36}$	$=$	$y_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + \left(\frac{1}{2} + z_{11}\right) \mathbf{a}_3$	$=$	$-y_{11} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{11}\right) c \hat{\mathbf{z}}$	(8f)	La VIII
$\mathbf{B}_{37}$	$=$	$-y_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + \left(\frac{1}{2} - z_{11}\right) \mathbf{a}_3$	$=$	$y_{11} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{11}\right) c \hat{\mathbf{z}}$	(8f)	La VIII
$\mathbf{B}_{38}$	$=$	$y_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-y_{11} b \hat{\mathbf{y}} - z_{11} c \hat{\mathbf{z}}$	(8f)	La VIII
$\mathbf{B}_{39}$	$=$	$-y_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$y_{12} b \hat{\mathbf{y}} + z_{12} c \hat{\mathbf{z}}$	(8f)	La IX
$\mathbf{B}_{40}$	$=$	$y_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + \left(\frac{1}{2} + z_{12}\right) \mathbf{a}_3$	$=$	$-y_{12} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{12}\right) c \hat{\mathbf{z}}$	(8f)	La IX









$$\begin{aligned} \mathbf{B}_{124} &= (-x_{26} + y_{26}) \mathbf{a}_1 + (-x_{26} - y_{26}) \mathbf{a}_2 + \left(\frac{1}{2} + z_{26}\right) \mathbf{a}_3 = -x_{26}a \hat{\mathbf{x}} - y_{26}b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{26}\right)c \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\ \mathbf{B}_{125} &= (-x_{26} - y_{26}) \mathbf{a}_1 + (-x_{26} + y_{26}) \mathbf{a}_2 + \left(\frac{1}{2} - z_{26}\right) \mathbf{a}_3 = -x_{26}a \hat{\mathbf{x}} + y_{26}b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{26}\right)c \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\ \mathbf{B}_{126} &= (x_{26} + y_{26}) \mathbf{a}_1 + (x_{26} - y_{26}) \mathbf{a}_2 - z_{26} \mathbf{a}_3 = x_{26}a \hat{\mathbf{x}} - y_{26}b \hat{\mathbf{y}} - z_{26}c \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\ \mathbf{B}_{127} &= (-x_{26} + y_{26}) \mathbf{a}_1 + (-x_{26} - y_{26}) \mathbf{a}_2 - z_{26} \mathbf{a}_3 = -x_{26}a \hat{\mathbf{x}} - y_{26}b \hat{\mathbf{y}} - z_{26}c \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\ \mathbf{B}_{128} &= (x_{26} - y_{26}) \mathbf{a}_1 + (x_{26} + y_{26}) \mathbf{a}_2 + \left(\frac{1}{2} - z_{26}\right) \mathbf{a}_3 = x_{26}a \hat{\mathbf{x}} + y_{26}b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{26}\right)c \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\ \mathbf{B}_{129} &= (x_{26} + y_{26}) \mathbf{a}_1 + (x_{26} - y_{26}) \mathbf{a}_2 + \left(\frac{1}{2} + z_{26}\right) \mathbf{a}_3 = x_{26}a \hat{\mathbf{x}} - y_{26}b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{26}\right)c \hat{\mathbf{z}} & (16h) & \text{Ni VII} \\ \mathbf{B}_{130} &= (-x_{26} - y_{26}) \mathbf{a}_1 + (-x_{26} + y_{26}) \mathbf{a}_2 + z_{26} \mathbf{a}_3 = -x_{26}a \hat{\mathbf{x}} + y_{26}b \hat{\mathbf{y}} + z_{26}c \hat{\mathbf{z}} & (16h) & \text{Ni VII} \end{aligned}$$

---

### References:

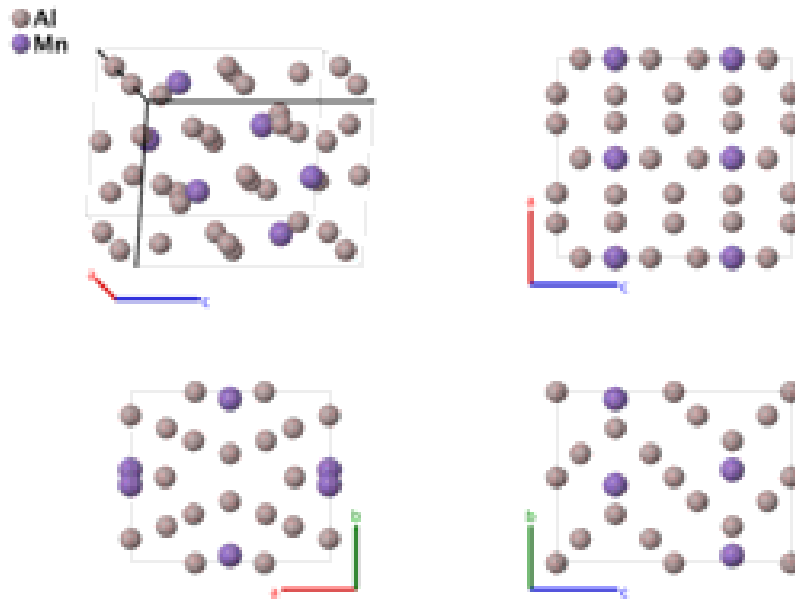
- P. Solokha, S. De Negri, V. Pavlyuk, and A. Saccone, *Anti-Mackay Polyicosahedral Clusters in La-Ni-Mg Ternary Compounds: Synthesis and Crystal Structure of the La<sub>43</sub>Ni<sub>17</sub>Mg<sub>5</sub> New Intermetallic Phase*, *Inorg. Chem.* **48**, 11586–11593 (2009), doi:[10.1021/jc901422v](https://doi.org/10.1021/jc901422v).

---

### Geometry files:

- CIF: pp. [846](#)  
- POSCAR: pp. [846](#)

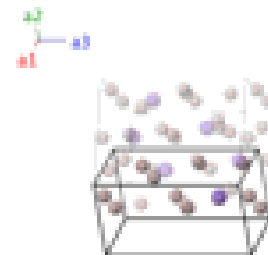
# MnAl<sub>6</sub> (*D*<sub>2h</sub>) Structure: A6B\_oC28\_63\_efg\_c



**Prototype** : MnAl<sub>6</sub>  
**AFLOW prototype label** : A6B\_oC28\_63\_efg\_c  
**Strukturbericht designation** : *D*<sub>2h</sub>  
**Pearson symbol** : oC28  
**Space group number** : 63  
**Space group symbol** : *Cmcm*  
**AFLOW prototype command** : aflow --proto=A6B\_oC28\_63\_efg\_c  
 --params=*a, b/a, c/a, y<sub>1</sub>, x<sub>2</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>*

**Base-centered Orthorhombic primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub> =	$-y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$y_1 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Mn
<b>B</b> <sub>2</sub> =	$y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-y_1 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Mn
<b>B</b> <sub>3</sub> =	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$x_2 a \hat{\mathbf{x}}$	(8e)	Al I
<b>B</b> <sub>4</sub> =	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$-x_2 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8e)	Al I
<b>B</b> <sub>5</sub> =	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$-x_2 a \hat{\mathbf{x}}$	(8e)	Al I

$$\begin{aligned}
\mathbf{B}_6 &= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}} & (8e) & \text{Al I} \\
\mathbf{B}_7 &= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8f) & \text{Al II} \\
\mathbf{B}_8 &= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= -y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (8f) & \text{Al II} \\
\mathbf{B}_9 &= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (8f) & \text{Al II} \\
\mathbf{B}_{10} &= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8f) & \text{Al II} \\
\mathbf{B}_{11} &= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{Al III} \\
\mathbf{B}_{12} &= (-x_4 + y_4) \mathbf{a}_1 + (-x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{Al III} \\
\mathbf{B}_{13} &= (-x_4 - y_4) \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{Al III} \\
\mathbf{B}_{14} &= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{Al III}
\end{aligned}$$

---

**References:**

- A. Kontio and P. Coppens, *New study of the structure of MnAl<sub>6</sub>*, Acta Crystallogr. Sect. B Struct. Sci. **37**, 433–435 (1981), doi:10.1107/S0567740881003191.

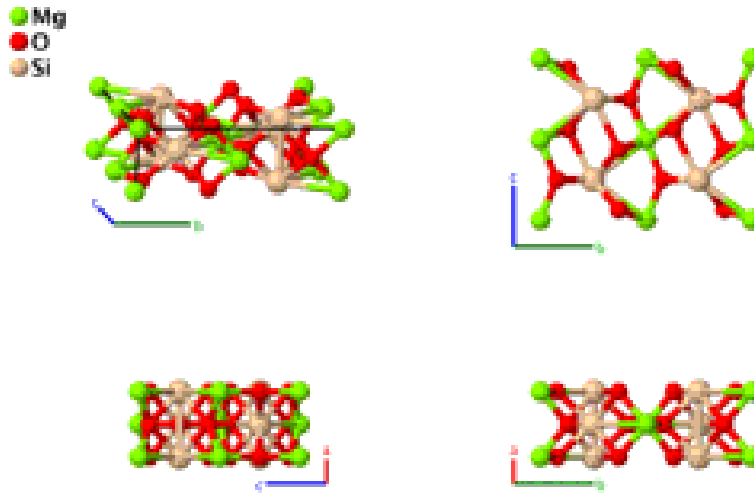
---

**Geometry files:**

- CIF: pp. 847  
- POSCAR: pp. 847

# Post-perovskite (MgSiO<sub>3</sub>) Structure: AB3C\_oC20\_63\_a\_cf\_c

---



<b>Prototype</b>	:	MgSiO <sub>3</sub>
<b>AFLOW prototype label</b>	:	AB3C_oC20_63_a_cf_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC20
<b>Space group number</b>	:	63
<b>Space group symbol</b>	:	<i>Cmcm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB3C_oC20_63_a_cf_c --params= <i>a, b/a, c/a, y<sub>2</sub>, y<sub>3</sub>, y<sub>4</sub>, z<sub>4</sub></i>

---

## Other compounds with this structure:

- CaIrO<sub>3</sub>, MgGeO<sub>3</sub>, NaMgF<sub>3</sub>
- 
- This structure was determined by a combination of x-ray diffraction measurements and atomistic simulations of MgSiO<sub>3</sub> at a pressure of 121 GPa and a temperature of 300 K. This approximates the conditions at the Earth's core-mantle boundary.

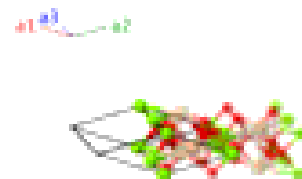
---

## Base-centered Orthorhombic primitive vectors:

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$




---

## Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(4a)	Mg
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} c \hat{\mathbf{z}}$	(4a)	Mg
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$y_2 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-y_2 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$y_3 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Si
$\mathbf{B}_6$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-y_3 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Si
$\mathbf{B}_7$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_8$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	=	$-y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_9$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	=	$y_4 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{10}$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(8f)	O II

---

#### References:

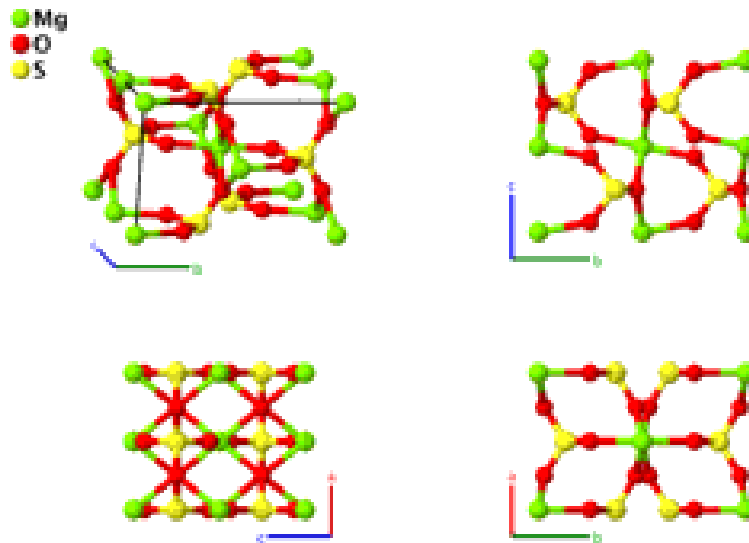
- M. Murakami, K. Hirose, K. Kawamura, N. Sata, and Y. Ohishi, *Post-Perovskite Phase Transition in MgSiO<sub>3</sub>*, *Science* **304**, 855–858 (2004), doi:[10.1126/science.1095932](https://doi.org/10.1126/science.1095932).

---

#### Geometry files:

- CIF: pp. [848](#)  
- POSCAR: pp. [848](#)

# MgSO<sub>4</sub> Structure: AB4C\_oC24\_63\_a\_fg\_c



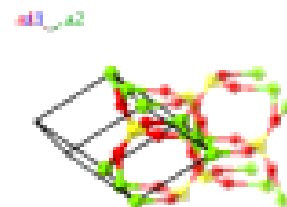
<b>Prototype</b>	:	MgO <sub>4</sub> S
<b>AFLOW prototype label</b>	:	AB4C_oC24_63_a_fg_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC24
<b>Space group number</b>	:	63
<b>Space group symbol</b>	:	<i>Cmcm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB4C_oC24_63_a_fg_c --params=a, b/a, c/a, y <sub>2</sub> , y <sub>3</sub> , z <sub>3</sub> , x <sub>4</sub> , y <sub>4</sub>

## Other compounds with this structure:

- CdCrO<sub>4</sub>, CoCrO<sub>4</sub>, MgCrO<sub>4</sub>, NiCrO<sub>4</sub>, NiSO<sub>4</sub>

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(4a)	Mg
<b>B<sub>2</sub></b> =	$\frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} c \hat{\mathbf{z}}$	(4a)	Mg
<b>B<sub>3</sub></b> =	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$y_2 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	S

$$\begin{aligned}
\mathbf{B}_4 &= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -y_2 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (4c) & \text{S} \\
\mathbf{B}_5 &= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8f) & \text{OI} \\
\mathbf{B}_6 &= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= -y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (8f) & \text{OI} \\
\mathbf{B}_7 &= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (8f) & \text{OI} \\
\mathbf{B}_8 &= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8f) & \text{OI} \\
\mathbf{B}_9 &= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{O II} \\
\mathbf{B}_{10} &= (-x_4 + y_4) \mathbf{a}_1 + (-x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{O II} \\
\mathbf{B}_{11} &= (-x_4 - y_4) \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{O II} \\
\mathbf{B}_{12} &= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{O II}
\end{aligned}$$

---

### References:

- P. J. Rentzeperis and C. T. Soldatos, *The crystal structure of the anhydrous magnesium sulphate*, Acta Cryst. **11**, 686–688 (1958), doi:[10.1107/S0365110X58001857](https://doi.org/10.1107/S0365110X58001857).

### Found in:

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

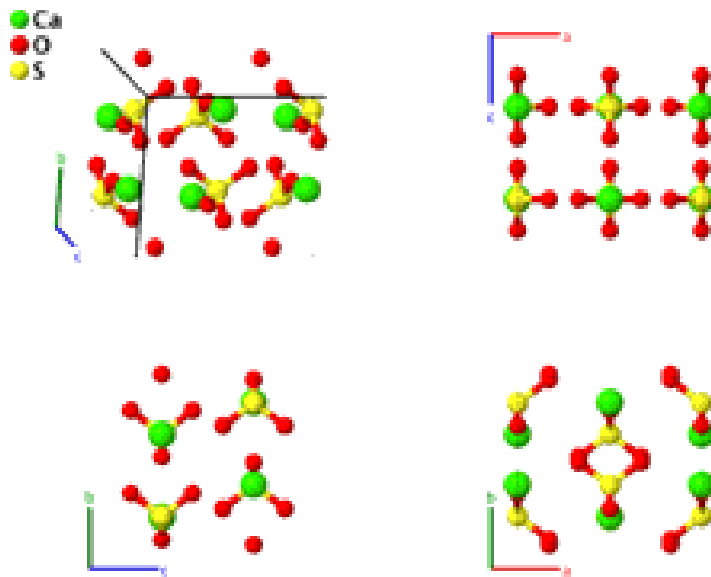
---

### Geometry files:

- CIF: pp. [848](#)  
- POSCAR: pp. [848](#)

# Anhydrite (CaSO<sub>4</sub>, *H0*<sub>1</sub>) Structure: AB4C\_oC24\_63\_c\_fg\_c

---



<b>Prototype</b>	:	CaSO <sub>4</sub>
<b>AFLOW prototype label</b>	:	AB4C_oC24_63_c_fg_c
<b>Strukturbericht designation</b>	:	<i>H0</i> <sub>1</sub>
<b>Pearson symbol</b>	:	oC24
<b>Space group number</b>	:	63
<b>Space group symbol</b>	:	<i>Cmcm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB4C_oC24_63_c_fg_c --params= <i>a, b/a, c/a, y</i> <sub>1</sub> , <i>y</i> <sub>2</sub> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub>

---

## Other compounds with this structure:

- CdCrO<sub>4</sub>, MgCrO<sub>4</sub>, MgSO<sub>4</sub>, NaBF<sub>4</sub>, NaCrO<sub>4</sub>, NiSO<sub>4</sub>

- (Hawthorne, 1975) give the structure in the *Amma* setting of space group #63. We have transformed this to the standard *Cmcm* setting. The addition of water into the anhydrite crystal transforms it into gypsum.

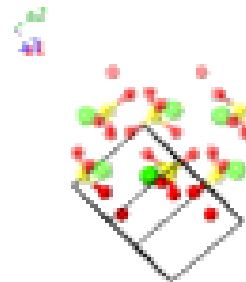
---

## Base-centered Orthorhombic primitive vectors:

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$




---

## Basis vectors:



	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$y_1 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Ca
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-y_1 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Ca
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$y_2 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	S
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-y_2 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	S
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$y_3 b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_6$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$-y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_7$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3$	$=$	$y_3 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_8$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-y_3 b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_9$	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{10}$	$= (-x_4 + y_4) \mathbf{a}_1 + (-x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{11}$	$= (-x_4 - y_4) \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{12}$	$= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8g)	O II

---

#### References:

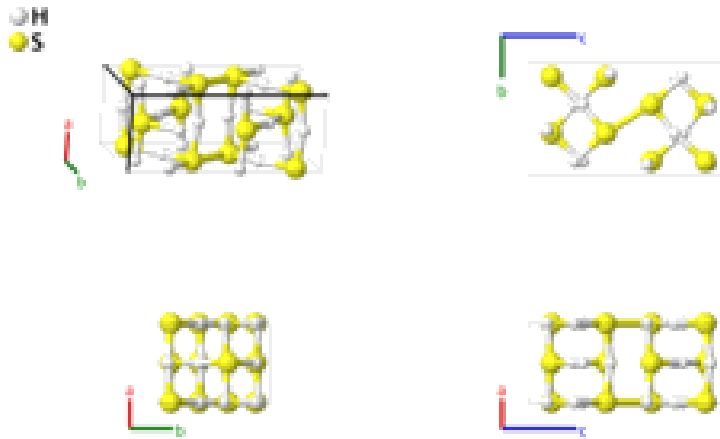
- F. C. Hawthorne and R. B. Ferguson, *Anhydrous sulphates. II. Refinement of the crystal structure of anhydrite*, Can. Mineral. **13**, 289–292 (1975).

---

#### Geometry files:

- CIF: pp. [849](#)  
- POSCAR: pp. [849](#)

# H<sub>2</sub>S (170 GPa) Structure: A2B\_oC24\_64\_2f\_f

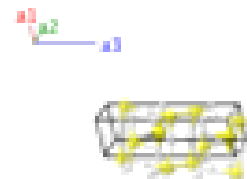


<b>Prototype</b>	:	H <sub>2</sub> S
<b>AFLOW prototype label</b>	:	A2B_oC24_64_2f_f
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC24
<b>Space group number</b>	:	64
<b>Space group symbol</b>	:	<i>Cmca</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A2B_oC24_64_2f_f --params=a, b/a, c/a, y1, z1, y2, z2, y3, z3</code>

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H<sub>2</sub>S for pressures > 140 GPa. At 160 GPa it is predicted to be a conventional superconductor with an approximate transition temperature of 80 K, however it is unlikely that this is the crystal structure of the 190 K superconductor, which is likely the [A3B\\_c18\\_229\\_b\\_a phase of H<sub>3</sub>S](#) (Bernstein, 2015). The data presented here was computed at 170 GPa.

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$-y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$y_1 b \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8f)	H I
<b>B<sub>2</sub></b> =	$\left(\frac{1}{2} + y_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} - y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(8f)	H I
<b>B<sub>3</sub></b> =	$\left(\frac{1}{2} - y_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	(8f)	H I
<b>B<sub>4</sub></b> =	$y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$-y_1 b \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(8f)	H I
<b>B<sub>5</sub></b> =	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8f)	H II

$$\begin{aligned}
\mathbf{B}_6 &= \left(\frac{1}{2} + y_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} - y_2b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right)c \hat{\mathbf{z}} & (8f) & \text{H II} \\
\mathbf{B}_7 &= \left(\frac{1}{2} - y_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} + y_2b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right)c \hat{\mathbf{z}} & (8f) & \text{H II} \\
\mathbf{B}_8 &= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3 = -y_2b \hat{\mathbf{y}} - z_2c \hat{\mathbf{z}} & (8f) & \text{H II} \\
\mathbf{B}_9 &= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = y_3b \hat{\mathbf{y}} + z_3c \hat{\mathbf{z}} & (8f) & \text{S} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} + y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} - y_3b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right)c \hat{\mathbf{z}} & (8f) & \text{S} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} - y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} + y_3b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right)c \hat{\mathbf{z}} & (8f) & \text{S} \\
\mathbf{B}_{12} &= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = -y_3b \hat{\mathbf{y}} - z_3c \hat{\mathbf{z}} & (8f) & \text{S}
\end{aligned}$$

---

### References:

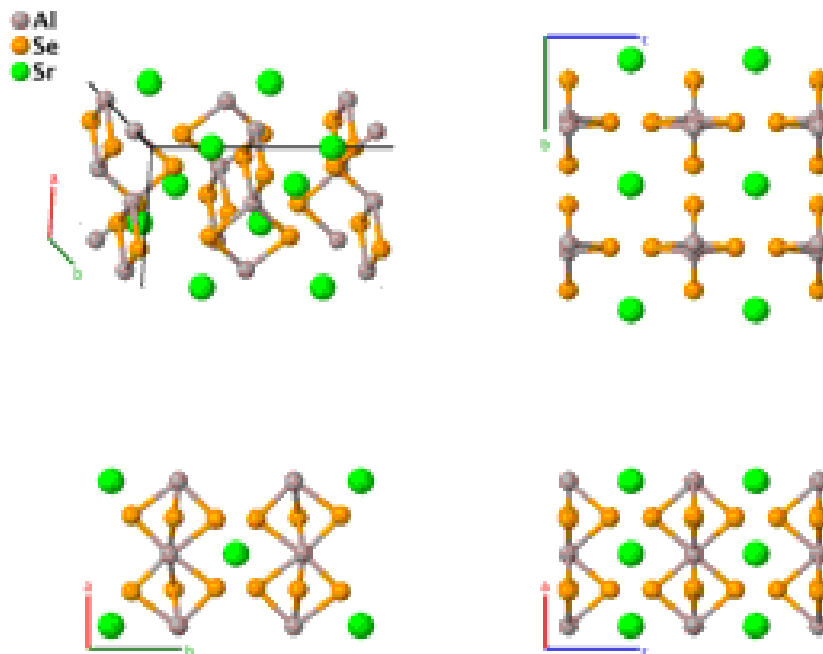
- Y. Li, J. Hao, H. Liu, Y. Li, and Y. Ma, *The metallization and superconductivity of dense hydrogen sulfide*, J. Chem. Phys. **140**, 174712 (2014), doi:10.1063/1.4874158.

---

### Geometry files:

- CIF: pp. 849  
- POSCAR: pp. 849

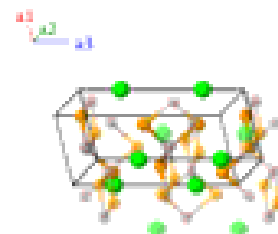
# SrAl<sub>2</sub>Se<sub>4</sub> Structure: A2B4C\_oC28\_66\_1\_kl\_a



<b>Prototype</b>	:	SrAl <sub>2</sub> Se <sub>4</sub>
<b>AFLOW prototype label</b>	:	A2B4C_oC28_66_1_kl_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC28
<b>Space group number</b>	:	66
<b>Space group symbol</b>	:	<i>Cccm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B4C_oC28_66_1_kl_a --params=a, b/a, c/a, z <sub>2</sub> , x <sub>3</sub> , y <sub>3</sub> , x <sub>4</sub> , y <sub>4</sub>

**Base-centered Orthorhombic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$\frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4} c \hat{\mathbf{z}}$	(4a)	Sr
<b>B<sub>2</sub></b> =	$\frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4} c \hat{\mathbf{z}}$	(4a)	Sr
<b>B<sub>3</sub></b> =	$\frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8k)	Se I

$$\begin{aligned}
\mathbf{B}_4 &= \frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} - \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} & (8k) & \text{Se I} \\
\mathbf{B}_5 &= \frac{1}{2} \mathbf{a}_2 - z_2 \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} & (8k) & \text{Se I} \\
\mathbf{B}_6 &= \frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (8k) & \text{Se I} \\
\mathbf{B}_7 &= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 &= x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} & (8l) & \text{Al} \\
\mathbf{B}_8 &= (-x_3 + y_3) \mathbf{a}_1 + (-x_3 - y_3) \mathbf{a}_2 &= -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} & (8l) & \text{Al} \\
\mathbf{B}_9 &= (-x_3 - y_3) \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8l) & \text{Al} \\
\mathbf{B}_{10} &= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8l) & \text{Al} \\
\mathbf{B}_{11} &= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} & (8l) & \text{Se II} \\
\mathbf{B}_{12} &= (-x_4 + y_4) \mathbf{a}_1 + (-x_4 - y_4) \mathbf{a}_2 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} & (8l) & \text{Se II} \\
\mathbf{B}_{13} &= (-x_4 - y_4) \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8l) & \text{Se II} \\
\mathbf{B}_{14} &= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8l) & \text{Se II}
\end{aligned}$$

---

### References:

- W. Klee and H. Schäfer, *CaAl<sub>2</sub>Se<sub>4</sub> und SrAl<sub>2</sub>Se<sub>4</sub>-Strukturvarianten des TlSe-Typs / CaAl<sub>2</sub>Se<sub>4</sub> and SrAl<sub>2</sub>Se<sub>4</sub>-Variants of the TlSe-Structure*, Z. Naturforsch. B **33**, 829–833 (1978), [doi:10.1515/znb-1978-0803](https://doi.org/10.1515/znb-1978-0803).

### Found in:

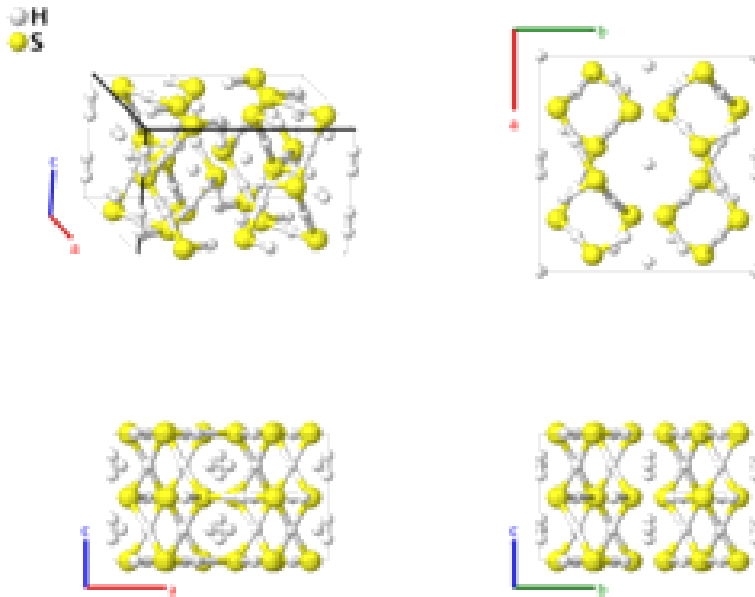
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. [850](#)  
- POSCAR: pp. [850](#)

# H<sub>3</sub>S (60 GPa) Structure: A3B\_oC64\_66\_gi2lm\_2l

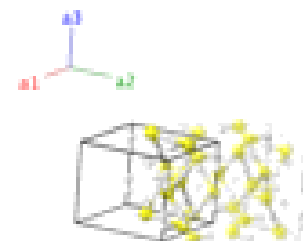


**Prototype** : H<sub>3</sub>S  
**AFLOW prototype label** : A3B\_oC64\_66\_gi2lm\_2l  
**Strukturbericht designation** : None  
**Pearson symbol** : oC64  
**Space group number** : 66  
**Space group symbol** : *Cccm*  
**AFLOW prototype command** : `aflow --proto=A3B_oC64_66_gi2lm_2l`  
`--params=a, b/a, c/a, x1, z2, x3, y3, x4, y4, x5, y5, x6, y6, x7, y7, z7`

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H<sub>3</sub>S for pressures between 40 and 90 GPa.
- The data presented here was computed at 60 GPa.

**Base-centered Orthorhombic primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type

$$\begin{aligned}
\mathbf{B}_1 &= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= x_1 a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}} &(8g) & \text{H I} \\
\mathbf{B}_2 &= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -x_1 a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}} &(8g) & \text{H I} \\
\mathbf{B}_3 &= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -x_1 a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}} &(8g) & \text{H I} \\
\mathbf{B}_4 &= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= x_1 a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}} &(8g) & \text{H I} \\
\mathbf{B}_5 &= z_2 \mathbf{a}_3 &= z_2 c \hat{\mathbf{z}} &(8i) & \text{H II} \\
\mathbf{B}_6 &= \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} &(8i) & \text{H II} \\
\mathbf{B}_7 &= -z_2 \mathbf{a}_3 &= -z_2 c \hat{\mathbf{z}} &(8i) & \text{H II} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} &(8i) & \text{H II} \\
\mathbf{B}_9 &= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 &= x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} &(8l) & \text{H III} \\
\mathbf{B}_{10} &= (-x_3 + y_3) \mathbf{a}_1 + (-x_3 - y_3) \mathbf{a}_2 &= -x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} &(8l) & \text{H III} \\
\mathbf{B}_{11} &= (-x_3 - y_3) \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + y_3 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} &(8l) & \text{H III} \\
\mathbf{B}_{12} &= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} - y_3 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} &(8l) & \text{H III} \\
\mathbf{B}_{13} &= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 &= x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} &(8l) & \text{H IV} \\
\mathbf{B}_{14} &= (-x_4 + y_4) \mathbf{a}_1 + (-x_4 - y_4) \mathbf{a}_2 &= -x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} &(8l) & \text{H IV} \\
\mathbf{B}_{15} &= (-x_4 - y_4) \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} &(8l) & \text{H IV} \\
\mathbf{B}_{16} &= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} &(8l) & \text{H IV} \\
\mathbf{B}_{17} &= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 &= x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} &(8l) & \text{S I} \\
\mathbf{B}_{18} &= (-x_5 + y_5) \mathbf{a}_1 + (-x_5 - y_5) \mathbf{a}_2 &= -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} &(8l) & \text{S I} \\
\mathbf{B}_{19} &= (-x_5 - y_5) \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} &(8l) & \text{S I} \\
\mathbf{B}_{20} &= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} &(8l) & \text{S I} \\
\mathbf{B}_{21} &= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 &= x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} &(8l) & \text{S II} \\
\mathbf{B}_{22} &= (-x_6 + y_6) \mathbf{a}_1 + (-x_6 - y_6) \mathbf{a}_2 &= -x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} &(8l) & \text{S II} \\
\mathbf{B}_{23} &= (-x_6 - y_6) \mathbf{a}_1 + (-x_6 + y_6) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} &(8l) & \text{S II} \\
\mathbf{B}_{24} &= (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} &(8l) & \text{S II} \\
\mathbf{B}_{25} &= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} &(16m) & \text{H V} \\
\mathbf{B}_{26} &= (-x_7 + y_7) \mathbf{a}_1 + (-x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= -x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} &(16m) & \text{H V} \\
\mathbf{B}_{27} &= (-x_7 - y_7) \mathbf{a}_1 + (-x_7 + y_7) \mathbf{a}_2 + \left(\frac{1}{2} - z_7\right) \mathbf{a}_3 &= -x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_7\right) c \hat{\mathbf{z}} &(16m) & \text{H V} \\
\mathbf{B}_{28} &= (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \left(\frac{1}{2} - z_7\right) \mathbf{a}_3 &= x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_7\right) c \hat{\mathbf{z}} &(16m) & \text{H V} \\
\mathbf{B}_{29} &= (-x_7 + y_7) \mathbf{a}_1 + (-x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} &(16m) & \text{H V} \\
\mathbf{B}_{30} &= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3 &= x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} &(16m) & \text{H V} \\
\mathbf{B}_{31} &= (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3 &= x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}} &(16m) & \text{H V} \\
\mathbf{B}_{32} &= (-x_7 - y_7) \mathbf{a}_1 + (-x_7 + y_7) \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3 &= -x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}} &(16m) & \text{H V}
\end{aligned}$$

## References:

- D. Duan, Y. Liu, F. Tian, D. Li, X. Huang, Z. Zhao, H. Yu, B. Liu, W. Tian, and T. Cui, *Pressure-induced metallization of dense  $(\text{H}_2\text{S})_2\text{H}_2$  with high- $T_c$  superconductivity*, *Sci. Rep.* **4**, 6968 (2014), [doi:10.1038/srep06968](https://doi.org/10.1038/srep06968).

---

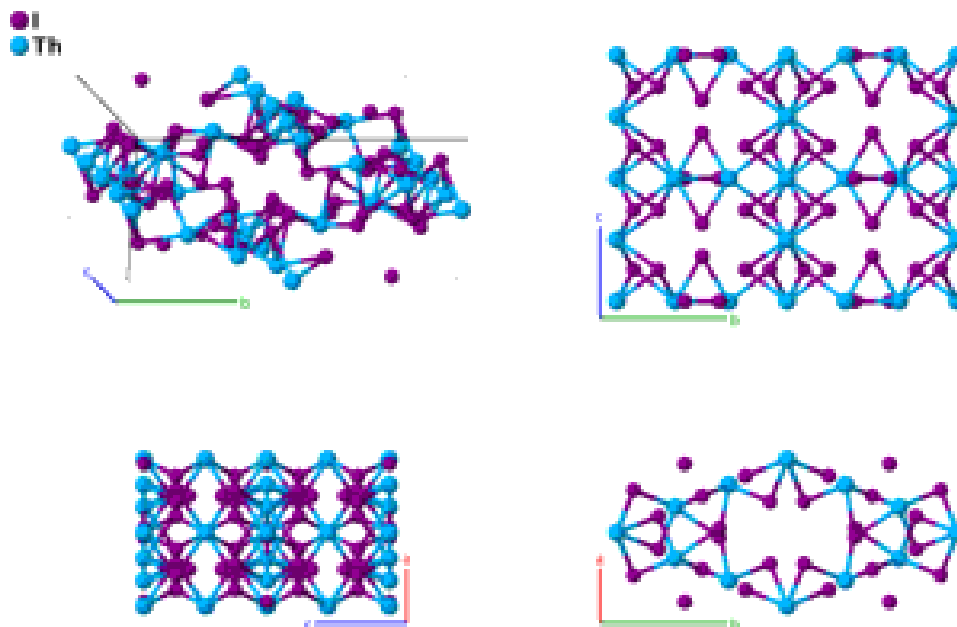
**Geometry files:**

- CIF: pp. [850](#)

- POSCAR: pp. [850](#)



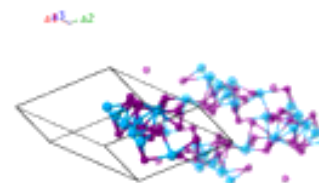
# $\beta$ -ThI<sub>3</sub> Structure: A3B\_oC64\_66\_kl2m\_bdl



<b>Prototype</b>	:	$\beta$ -ThI <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B_oC64_66_kl2m_bdl
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC64
<b>Space group number</b>	:	66
<b>Space group symbol</b>	:	<i>Ccm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3B_oC64_66_kl2m_bdl --params= <i>a, b/a, c/a, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub></i>

**Base-centered Orthorhombic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4b)	Th I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4b)	Th I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}}$	(4d)	Th II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4d)	Th II

$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8k)	I I
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}}$	(8k)	I I
$\mathbf{B}_7$	$=$	$\frac{1}{2} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(8k)	I I
$\mathbf{B}_8$	$=$	$\frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(8k)	I I
$\mathbf{B}_9$	$=$	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}}$	(8l)	I II
$\mathbf{B}_{10}$	$=$	$(-x_4 + y_4) \mathbf{a}_1 + (-x_4 - y_4) \mathbf{a}_2$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}}$	(8l)	I II
$\mathbf{B}_{11}$	$=$	$(-x_4 - y_4) \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8l)	I II
$\mathbf{B}_{12}$	$=$	$(x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} - y_4 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8l)	I II
$\mathbf{B}_{13}$	$=$	$(x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}}$	(8l)	Th III
$\mathbf{B}_{14}$	$=$	$(-x_5 + y_5) \mathbf{a}_1 + (-x_5 - y_5) \mathbf{a}_2$	$=$	$-x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}}$	(8l)	Th III
$\mathbf{B}_{15}$	$=$	$(-x_5 - y_5) \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8l)	Th III
$\mathbf{B}_{16}$	$=$	$(x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8l)	Th III
$\mathbf{B}_{17}$	$=$	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{18}$	$=$	$(-x_6 + y_6) \mathbf{a}_1 + (-x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{19}$	$=$	$(-x_6 - y_6) \mathbf{a}_1 + (-x_6 + y_6) \mathbf{a}_2 +$ $\left(\frac{1}{2} - z_6\right) \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{20}$	$=$	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \left(\frac{1}{2} - z_6\right) \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{21}$	$=$	$(-x_6 + y_6) \mathbf{a}_1 + (-x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{22}$	$=$	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{23}$	$=$	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} - y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{24}$	$=$	$(-x_6 - y_6) \mathbf{a}_1 + (-x_6 + y_6) \mathbf{a}_2 +$ $\left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} + y_6 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{25}$	$=$	$(x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(16m)	I IV
$\mathbf{B}_{26}$	$=$	$(-x_7 + y_7) \mathbf{a}_1 + (-x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(16m)	I IV
$\mathbf{B}_{27}$	$=$	$(-x_7 - y_7) \mathbf{a}_1 + (-x_7 + y_7) \mathbf{a}_2 +$ $\left(\frac{1}{2} - z_7\right) \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_7\right) c \hat{\mathbf{z}}$	(16m)	I IV
$\mathbf{B}_{28}$	$=$	$(x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \left(\frac{1}{2} - z_7\right) \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_7\right) c \hat{\mathbf{z}}$	(16m)	I IV
$\mathbf{B}_{29}$	$=$	$(-x_7 + y_7) \mathbf{a}_1 + (-x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}}$	(16m)	I IV
$\mathbf{B}_{30}$	$=$	$(x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}}$	(16m)	I IV
$\mathbf{B}_{31}$	$=$	$(x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} - y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(16m)	I IV
$\mathbf{B}_{32}$	$=$	$(-x_7 - y_7) \mathbf{a}_1 + (-x_7 + y_7) \mathbf{a}_2 +$ $\left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} + y_7 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(16m)	I IV

## References:

- H. P. Beck and C. Strobel, *ThI<sub>3</sub>, ein Janus unter den Verbindungen mit Metall-Metall-Wechselwirkungen*, *Angew. Chem.* **94**, 558–559 (1982), [doi:10.1002/ange.19820940731](https://doi.org/10.1002/ange.19820940731).

## Found in:

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, *Am. Mineral.* **88**, 247–250 (2003).

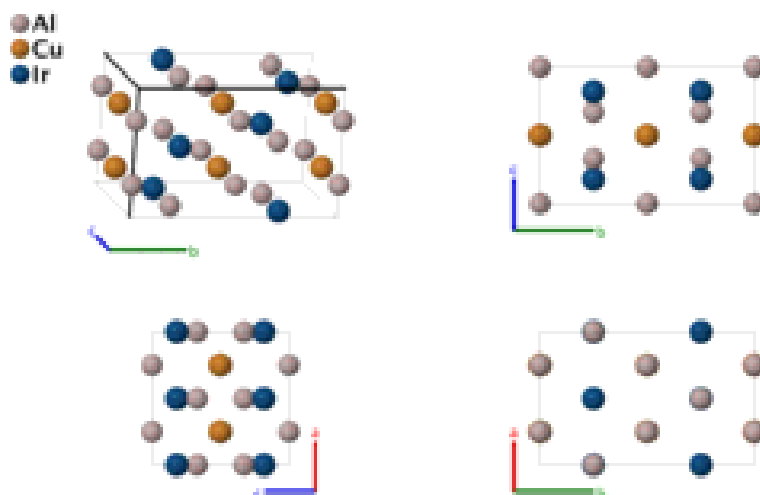
---

**Geometry files:**

- CIF: pp. [851](#)

- POSCAR: pp. [851](#)

# Al<sub>2</sub>CuIr Structure: A2BC\_oC16\_67\_ag\_b\_g

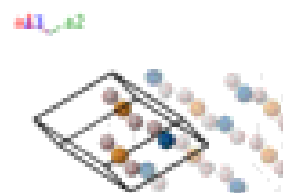


<b>Prototype</b>	:	Al <sub>2</sub> CuIr
<b>AFLOW prototype label</b>	:	A2BC_oC16_67_ag_b_g
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC16
<b>Space group number</b>	:	67
<b>Space group symbol</b>	:	<i>Cmma</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2BC_oC16_67_ag_b_g --params=a, b/a, c/a, z <sub>3</sub> , z <sub>4</sub>

- Al<sub>2</sub>CuIr (pp. 236) and CuHoP<sub>2</sub> (pp. 238) have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	= $\frac{1}{4} a \hat{\mathbf{x}}$	(4a)	Al I
<b>B<sub>2</sub></b>	= $\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	= $\frac{3}{4} a \hat{\mathbf{x}}$	(4a)	Al I
<b>B<sub>3</sub></b>	= $\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	= $\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4b)	Cu
<b>B<sub>4</sub></b>	= $\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	= $\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4b)	Cu

$$\begin{aligned}
 \mathbf{B}_5 &= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4g) & \text{Al II} \\
 \mathbf{B}_6 &= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (4g) & \text{Al II} \\
 \mathbf{B}_7 &= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (4g) & \text{Ir} \\
 \mathbf{B}_8 &= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (4g) & \text{Ir}
 \end{aligned}$$

**References:**

- L. Meshi, V. Ezersky, D. Kapush, and B. Grushko, *Crystal structure of the Al<sub>2</sub>CuIr phase*, J. Alloys Compd. **496**, 208–211 (2010), doi:[10.1016/j.jallcom.2010.02.129](https://doi.org/10.1016/j.jallcom.2010.02.129).

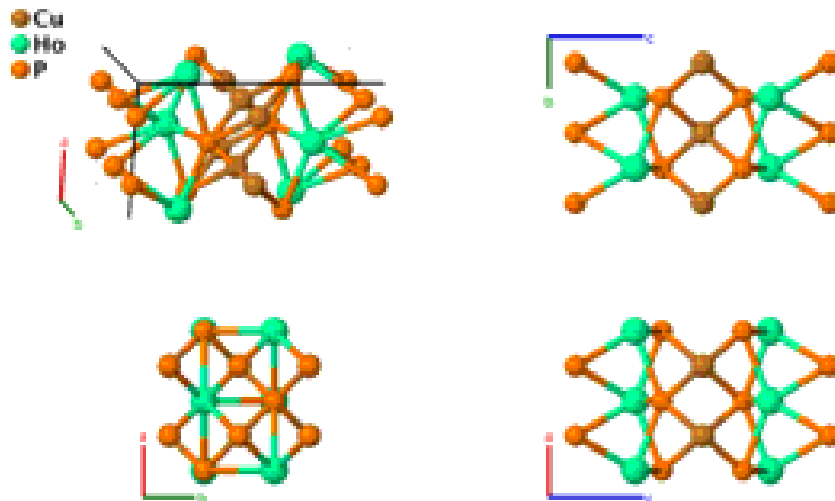
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [851](#)  
 - POSCAR: pp. [852](#)

# HoCuP<sub>2</sub> Structure: ABC2\_oC16\_67\_b\_g\_ag

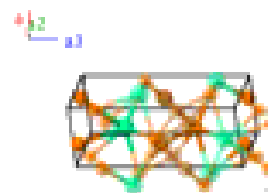


<b>Prototype</b>	:	HoCuP <sub>2</sub>
<b>AFLOW prototype label</b>	:	ABC2_oC16_67_b_g_ag
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC16
<b>Space group number</b>	:	67
<b>Space group symbol</b>	:	<i>Cmma</i>
<b>AFLOW prototype command</b>	:	aflow --proto=ABC2_oC16_67_b_g_ag --params=a, b/a, c/a, z <sub>3</sub> , z <sub>4</sub>

- Al<sub>2</sub>CuIr (pp. 236) and CuHoP<sub>2</sub> (pp. 238) have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$= \frac{1}{4} a \hat{\mathbf{x}}$	(4a)	P I
<b>B<sub>2</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$= \frac{3}{4} a \hat{\mathbf{x}}$	(4a)	P I
<b>B<sub>3</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4b)	Cu
<b>B<sub>4</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4b)	Cu

$$\begin{aligned} \mathbf{B}_5 &= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} && (4g) && \text{Ho} \\ \mathbf{B}_6 &= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} && (4g) && \text{Ho} \\ \mathbf{B}_7 &= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (4g) && \text{P II} \\ \mathbf{B}_8 &= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (4g) && \text{P II} \end{aligned}$$

**References:**

- Y. Mozharivsky, D. Kaczorowski, and H. F. Franzen, *Symmetry-Breaking Transitions in HoCuAs<sub>2-x</sub>P<sub>x</sub> and ErCuAs<sub>2-x</sub>P<sub>x</sub> (x = 0 – 2): Crystal Structure, Application of Landau Theory, Magnetic and Electrical Properties*, Z. Anorg. Allg. Chem. **627**, 2163–2172 (2001), doi:10.1002/1521-3749(200109)627:9<2163::AID-ZAAC2163>3.0.CO;2-N.

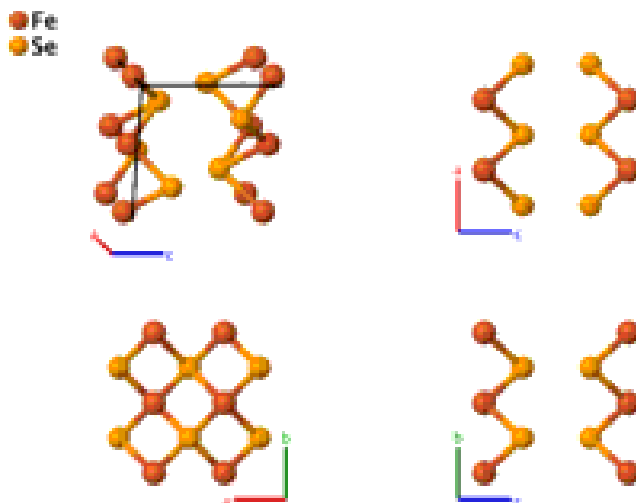
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [852](#)  
 - POSCAR: pp. [852](#)

# $\alpha$ -FeSe Structure: AB\_oC8\_67\_a\_g



<b>Prototype</b>	:	$\alpha$ -FeSe
<b>AFLOW prototype label</b>	:	AB_oC8_67_a_g
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC8
<b>Space group number</b>	:	67
<b>Space group symbol</b>	:	<i>Cmma</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB_oC8_67_a_g --params=a, b/a, c/a, z2</code>

- We follow the reference in calling this  $\alpha$ -FeSe. Some other authorities refer to the *B10 (PbO)*-like phase of FeSe as  $\alpha$ -FeSe, calling this phase  $\beta$ -FeSe. The authors note that “the Se ion concentration is close to 1.” The data is presented for the structure at 7 K.  $\alpha$ -FeSe (pp. 240) and  $\alpha$ -PbO (pp. 242)) have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$= \frac{1}{4} a \hat{\mathbf{x}}$	(4a)	Fe
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$= \frac{3}{4} a \hat{\mathbf{x}}$	(4a)	Fe



$$\mathbf{B}_3 = \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} \quad (4g) \quad \text{Se}$$

$$\mathbf{B}_4 = \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} \quad (4g) \quad \text{Se}$$

---

**References:**

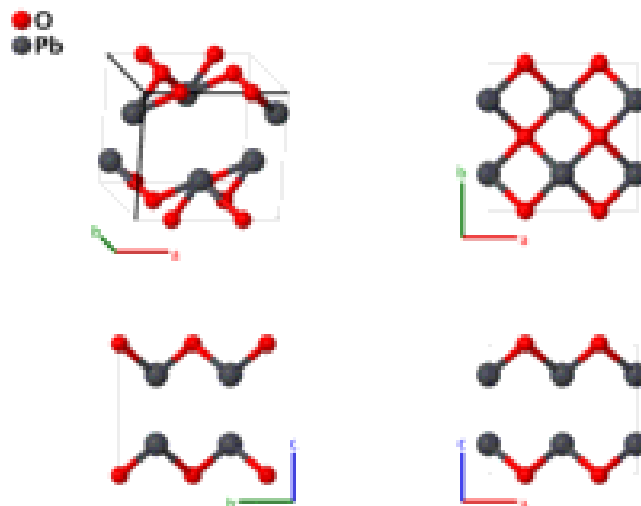
- D. Louca, K. Horigane, A. Llobet, R. Arita, S. Ji, N. Katayama, S. Konbu, K. Nakamura, T.-Y. Koo, P. Tong, and K. Yamada, *Local atomic structure of superconducting FeSe<sub>1-x</sub>Te<sub>x</sub>*, Phys. Rev. B **81**, 134524 (2010), [doi:10.1103/PhysRevB.81.134524](https://doi.org/10.1103/PhysRevB.81.134524).

---

**Geometry files:**

- CIF: pp. [852](#)  
- POSCAR: pp. [853](#)

# $\alpha$ -PbO Structure: AB\_oC8\_67\_a\_g

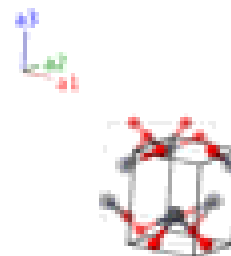


<b>Prototype</b>	:	$\alpha$ -PbO
<b>AFLOW prototype label</b>	:	AB_oC8_67_a_g
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC8
<b>Space group number</b>	:	67
<b>Space group symbol</b>	:	<i>Cmma</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB_oC8_67_a_g --params=a, b/a, c/a, z <sub>2</sub>

- FINDSYM identifies space group #67 for this structure (consistent with the reference); however, since  $b/a \approx 1$ , AFLOW-SYM and Platon identify #129. Lowering the tolerance value for AFLOW-SYM resolves the expected space group #67. Space groups #67 and #129 are both reasonable classifications since they are commensurate with subgroup relations.  $\alpha$ -FeSe (pp. 240) and  $\alpha$ -PbO (pp. 242) have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters (--params) specified in their corresponding CIF files.

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}}$	(4a)	O
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}}$	(4a)	O

$$\mathbf{B}_3 = \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + z_2c \hat{\mathbf{z}} \quad (4g) \quad \text{Pb}$$

$$\mathbf{B}_4 = \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - z_2c \hat{\mathbf{z}} \quad (4g) \quad \text{Pb}$$

#### References:

- P. Boher, P. Garnier, J. R. Gavarri, and A. W. Hewat, *Monoxyde quadratique PbO $\alpha$  (I): Description de la transition structurale ferroélastique*, J. Solid State Chem. **57**, 343–350 (1985), doi:10.1016/0022-4596(85)90197-5.
- H. T. Stokes and D. M. Hatch, *FINDSYM: Program for identifying the space group symmetry of a crystal*, J. Appl. Crystallogr. **38**, 237–238 (2005), doi:10.1107/S0021889804031528.
- D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy, and S. Curtarolo, *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*, Acta Crystallogr. Sect. A **74**, 184–203 (2018), doi:10.1107/S2053273318003066.
- A. L. Spek, *Single-crystal structure validation with the program PLATON*, J. Appl. Crystallogr. **36**, 7–13 (2003), doi:10.1107/S0021889802022112.

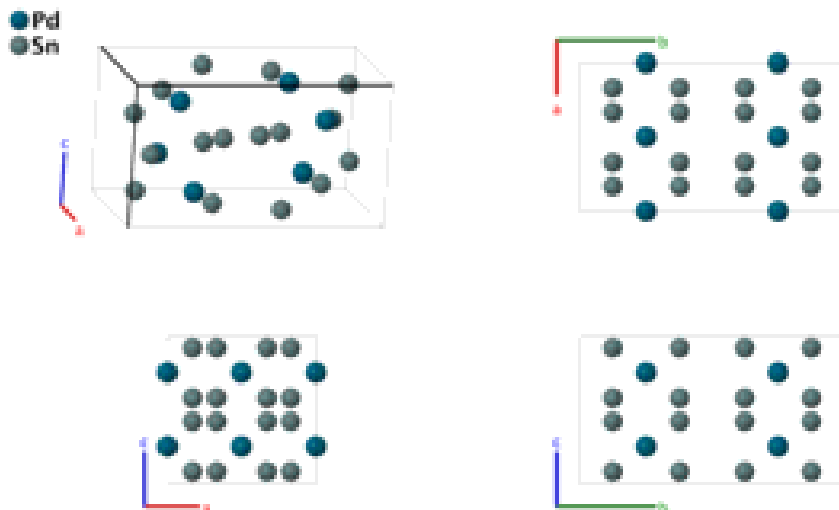
#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. 853
- POSCAR: pp. 853

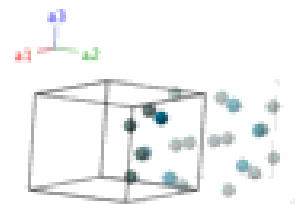
# PdSn<sub>4</sub> Structure: AB<sub>4</sub>\_oC20\_68\_a\_i



<b>Prototype</b>	:	PdSn <sub>4</sub>
<b>AFLOW prototype label</b>	:	AB <sub>4</sub> _oC20_68_a_i
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oC20
<b>Space group number</b>	:	68
<b>Space group symbol</b>	:	<i>Ccca</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB <sub>4</sub> _oC20_68_a_i --params= <i>a, b/a, c/a, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub></i>

## Base-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4 <i>a</i> )	Pd
<b>B<sub>2</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4 <i>a</i> )	Pd
<b>B<sub>3</sub></b>	$= (x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(16 <i>i</i> )	Sn
<b>B<sub>4</sub></b>	$= \left(\frac{1}{2} - x_2 + y_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_2 - y_2\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(16 <i>i</i> )	Sn
<b>B<sub>5</sub></b>	$= (-x_2 - y_2) \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	$= -x_2 a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(16 <i>i</i> )	Sn
<b>B<sub>6</sub></b>	$= \left(\frac{1}{2} + x_2 + y_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_2 - y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	$= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(16 <i>i</i> )	Sn

$$\mathbf{B}_7 = (-x_2 + y_2) \mathbf{a}_1 + (-x_2 - y_2) \mathbf{a}_2 - z_2 \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} \quad (16i) \quad \text{Sn}$$

$$\mathbf{B}_8 = \left(\frac{1}{2} + x_2 - y_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_2 + y_2\right) \mathbf{a}_2 - z_2 \mathbf{a}_3 = \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} \quad (16i) \quad \text{Sn}$$

$$\mathbf{B}_9 = (x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = x_2 a \hat{\mathbf{x}} - y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} \quad (16i) \quad \text{Sn}$$

$$\mathbf{B}_{10} = \left(\frac{1}{2} - x_2 - y_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_2 + y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + y_2 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} \quad (16i) \quad \text{Sn}$$

### References:

- J. Nylén, F. J. García García, B. D. Mosel, R. Pöttgen, and U. Häussermann, *Structural relationships, phase stability and bonding of compounds PdSn<sub>n</sub> (n = 2, 3, 4)*, *Solid State Sci.* **6**, 147–155 (2004), [doi:10.1016/j.solidstatesciences.2003.09.011](https://doi.org/10.1016/j.solidstatesciences.2003.09.011).

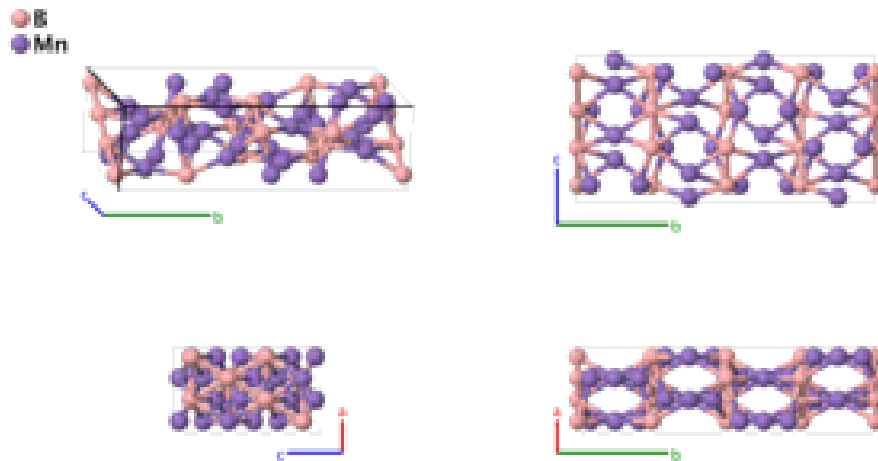
### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

### Geometry files:

- CIF: pp. [853](#)  
 - POSCAR: pp. [854](#)

# Mn<sub>2</sub>B (*D*1<sub>*f*</sub>) Structure: AB2\_oF48\_70\_f\_fg



<b>Prototype</b>	:	Mn <sub>2</sub> B
<b>AFLOW prototype label</b>	:	AB2_oF48_70_f_fg
<b>Strukturbericht designation</b>	:	<i>D</i> 1 <sub><i>f</i></sub>
<b>Pearson symbol</b>	:	oF48
<b>Space group number</b>	:	70
<b>Space group symbol</b>	:	<i>Fddd</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB2_oF48_70_f_fg --params=a, b/a, c/a, y1, y2, z3</code>

## Other compounds with this structure:

- Cr<sub>2</sub>B

- Early works, *e.g.* (Pearson, 1958) referred to this structure as Mn<sub>4</sub>B, with the same space group and Wyckoff positions. The stoichiometry was fixed by assuming that the (16e) Boron positions were only half-occupied. Tergenius's 1981 refinement of the structure showed that the (16e) sites were totally filled, fixing the stoichiometry to Mn<sub>2</sub>B. A similar reanalysis showed that the similar structure known has Cr<sub>4</sub>B also had composition Cr<sub>2</sub>B. Tergenius gives the atomic positions using the first setting of space group *Fddd* #70. We have translated this into the second setting, where the origin is on an inversion site. As a part of this process the primitive axes were also rotated compared to Tergenius.

## Face-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= y_1 \mathbf{a}_1 + \left(\frac{1}{4} - y_1\right) \mathbf{a}_2 + y_1 \mathbf{a}_3$	$= \frac{1}{8} a \hat{\mathbf{x}} + y_1 b \hat{\mathbf{y}} + \frac{1}{8} c \hat{\mathbf{z}}$	(16 <i>f</i> )	B

$$\begin{aligned}
\mathbf{B}_2 &= \left(\frac{1}{4} - y_1\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 + \left(\frac{1}{4} - y_1\right) \mathbf{a}_3 = \frac{1}{8}a \hat{\mathbf{x}} + \left(\frac{1}{4} - y_1\right)b \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}} & (16f) & \quad \text{B} \\
\mathbf{B}_3 &= -y_1 \mathbf{a}_1 + \left(\frac{3}{4} + y_1\right) \mathbf{a}_2 - y_1 \mathbf{a}_3 = \frac{3}{8}a \hat{\mathbf{x}} - y_1b \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}} & (16f) & \quad \text{B} \\
\mathbf{B}_4 &= \left(\frac{3}{4} + y_1\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{3}{4} + y_1\right) \mathbf{a}_3 = \frac{3}{8}a \hat{\mathbf{x}} + \left(\frac{3}{4} + y_1\right)b \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}} & (16f) & \quad \text{B} \\
\mathbf{B}_5 &= y_2 \mathbf{a}_1 + \left(\frac{1}{4} - y_2\right) \mathbf{a}_2 + y_2 \mathbf{a}_3 = \frac{1}{8}a \hat{\mathbf{x}} + y_2b \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}} & (16f) & \quad \text{Mn I} \\
\mathbf{B}_6 &= \left(\frac{1}{4} - y_2\right) \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(\frac{1}{4} - y_2\right) \mathbf{a}_3 = \frac{1}{8}a \hat{\mathbf{x}} + \left(\frac{1}{4} - y_2\right)b \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}} & (16f) & \quad \text{Mn I} \\
\mathbf{B}_7 &= -y_2 \mathbf{a}_1 + \left(\frac{3}{4} + y_2\right) \mathbf{a}_2 - y_2 \mathbf{a}_3 = \frac{3}{8}a \hat{\mathbf{x}} - y_2b \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}} & (16f) & \quad \text{Mn I} \\
\mathbf{B}_8 &= \left(\frac{3}{4} + y_2\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{3}{4} + y_2\right) \mathbf{a}_3 = \frac{3}{8}a \hat{\mathbf{x}} + \left(\frac{3}{4} + y_2\right)b \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}} & (16f) & \quad \text{Mn I} \\
\mathbf{B}_9 &= z_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + \left(\frac{1}{4} - z_3\right) \mathbf{a}_3 = \frac{1}{8}a \hat{\mathbf{x}} + \frac{1}{8}b \hat{\mathbf{y}} + z_3c \hat{\mathbf{z}} & (16g) & \quad \text{Mn II} \\
\mathbf{B}_{10} &= \left(\frac{1}{4} - z_3\right) \mathbf{a}_1 + \left(\frac{1}{4} - z_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 = \frac{1}{8}a \hat{\mathbf{x}} + \frac{1}{8}b \hat{\mathbf{y}} + \left(\frac{1}{4} - z_3\right)c \hat{\mathbf{z}} & (16g) & \quad \text{Mn II} \\
\mathbf{B}_{11} &= -z_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 + \left(\frac{3}{4} + z_3\right) \mathbf{a}_3 = \frac{3}{8}a \hat{\mathbf{x}} + \frac{3}{8}b \hat{\mathbf{y}} - z_3c \hat{\mathbf{z}} & (16g) & \quad \text{Mn II} \\
\mathbf{B}_{12} &= \left(\frac{3}{4} + z_3\right) \mathbf{a}_1 + \left(\frac{3}{4} + z_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 = \frac{3}{8}a \hat{\mathbf{x}} + \frac{3}{8}b \hat{\mathbf{y}} + \left(\frac{3}{4} + z_3\right)c \hat{\mathbf{z}} & (16g) & \quad \text{Mn II}
\end{aligned}$$

---

### References:

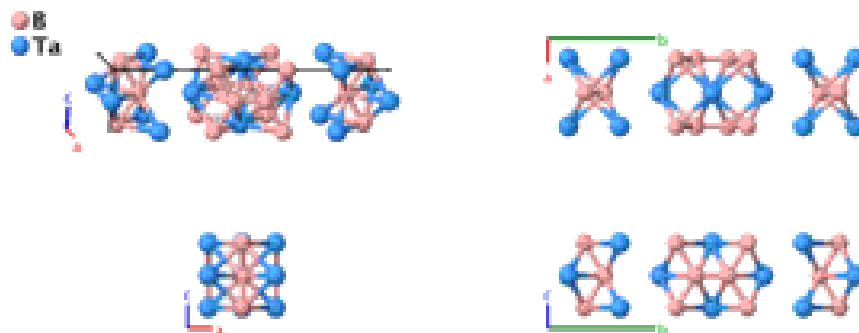
- L.-E. Tergenius, *Refinement of the crystal structure of orthorhombic Mn<sub>2</sub>B (formerly denoted Mn<sub>4</sub>B)*, J. Less-Common Met. **82**, 335–340 (1981), doi:10.1016/0022-5088(81)90236-8.
- W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

---

### Geometry files:

- CIF: pp. 854
- POSCAR: pp. 854

# Ta<sub>3</sub>B<sub>4</sub> (*D7<sub>b</sub>*) Structure: A4B3\_oI14\_71\_gh\_cg



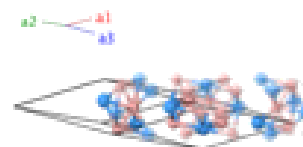
<b>Prototype</b>	:	Ta <sub>3</sub> B <sub>4</sub>
<b>AFLOW prototype label</b>	:	A4B3_oI14_71_gh_cg
<b>Strukturbericht designation</b>	:	<i>D7<sub>b</sub></i>
<b>Pearson symbol</b>	:	oI14
<b>Space group number</b>	:	71
<b>Space group symbol</b>	:	<i>Immm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A4B3_oI14_71_gh_cg --params=a, b/a, c/a, y <sub>2</sub> , y <sub>3</sub> , y <sub>4</sub>

## Other compounds with this structure:

- B<sub>4</sub>CoMo<sub>2</sub>, B<sub>4</sub>Cr<sub>3</sub>, B<sub>4</sub>FeMo<sub>2</sub>, B<sub>4</sub>Mn<sub>3</sub>, B<sub>4</sub>Mo<sub>2</sub>Ni, B<sub>4</sub>Nb<sub>3</sub>, B<sub>4</sub>Ta<sub>3</sub>, B<sub>4</sub>V<sub>3</sub>

## Body-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	=	$\frac{1}{2}c\hat{\mathbf{z}}$	(2c) Ta I
<b>B<sub>2</sub></b>	=	$y_2\mathbf{a}_1 + y_2\mathbf{a}_3$	=	$y_2b\hat{\mathbf{y}}$	(4g) B I
<b>B<sub>3</sub></b>	=	$-y_2\mathbf{a}_1 + -y_2\mathbf{a}_3$	=	$-y_2b\hat{\mathbf{y}}$	(4g) B I
<b>B<sub>4</sub></b>	=	$y_3\mathbf{a}_1 + y_3\mathbf{a}_3$	=	$y_3b\hat{\mathbf{y}}$	(4g) Ta II
<b>B<sub>5</sub></b>	=	$-y_3\mathbf{a}_1 + -y_3\mathbf{a}_3$	=	$-y_3b\hat{\mathbf{y}}$	(4g) Ta II
<b>B<sub>6</sub></b>	=	$(\frac{1}{2} + y_4)\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + y_4\mathbf{a}_3$	=	$y_4b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(4h) B II
<b>B<sub>7</sub></b>	=	$(\frac{1}{2} - y_4)\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 - y_4\mathbf{a}_3$	=	$-y_4b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(4h) B II

## References:

- R. Kiessling, *The Borides of Tantalum*, Acta Chem. Scand. **3**, 603–615 (1949), doi:10.3891/acta.chem.scand.03-0603.



**Found in:**

- R. M. Minyaev and R. Hoffmann, *Transition-metal borides with the tantalum boride ( $Ta_3B_4$ ) crystal structure: their electronic and bonding properties*, Chem. Mater. **3**, 547–557 (1991), [doi:10.1021/cm00015a035](https://doi.org/10.1021/cm00015a035).

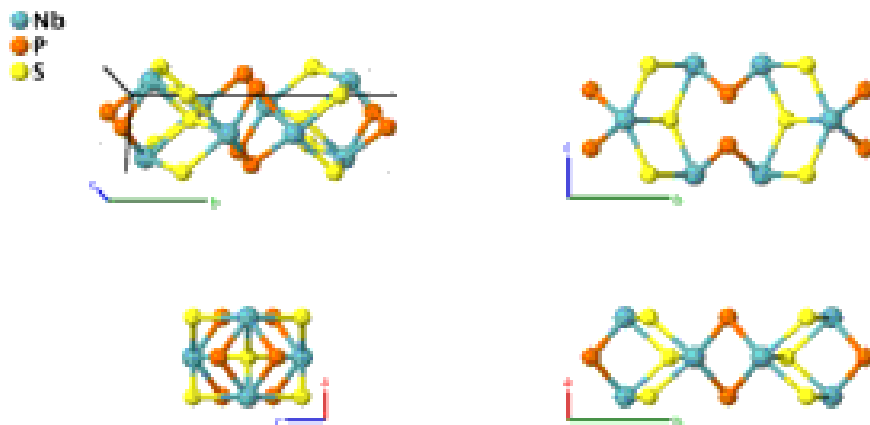
---

**Geometry files:**

- CIF: pp. [854](#)

- POSCAR: pp. [855](#)

# NbPS Structure: ABC\_oI12\_71\_h\_j\_g



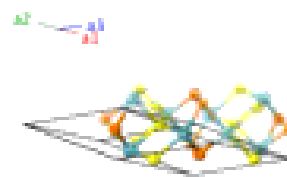
<b>Prototype</b>	:	NbPS
<b>AFLOW prototype label</b>	:	ABC_oI12_71_h_j_g
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oI12
<b>Space group number</b>	:	71
<b>Space group symbol</b>	:	<i>Immm</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=ABC_oI12_71_h_j_g --params=a,b/a,c/a,y1,y2,z3</code>

## Other compounds with this structure:

- TaPS, NbPSe, HfSbTe, ZrSbTe

## Body-centered Orthorhombic primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_1 + y_1 \mathbf{a}_3$	$= y_1 b \hat{\mathbf{y}}$	(4g)	S
$\mathbf{B}_2$	$= -y_1 \mathbf{a}_1 + -y_1 \mathbf{a}_3$	$= -y_1 b \hat{\mathbf{y}}$	(4g)	S
$\mathbf{B}_3$	$= \left(\frac{1}{2} + y_2\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_2 \mathbf{a}_3$	$= y_2 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb
$\mathbf{B}_4$	$= \left(\frac{1}{2} - y_2\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_2 \mathbf{a}_3$	$= -y_2 b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb
$\mathbf{B}_5$	$= z_3 \mathbf{a}_1 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + z_3 c \hat{\mathbf{z}}$	(4j)	P
$\mathbf{B}_6$	$= -z_3 \mathbf{a}_1 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + -z_3 c \hat{\mathbf{z}}$	(4j)	P

---

**References:**

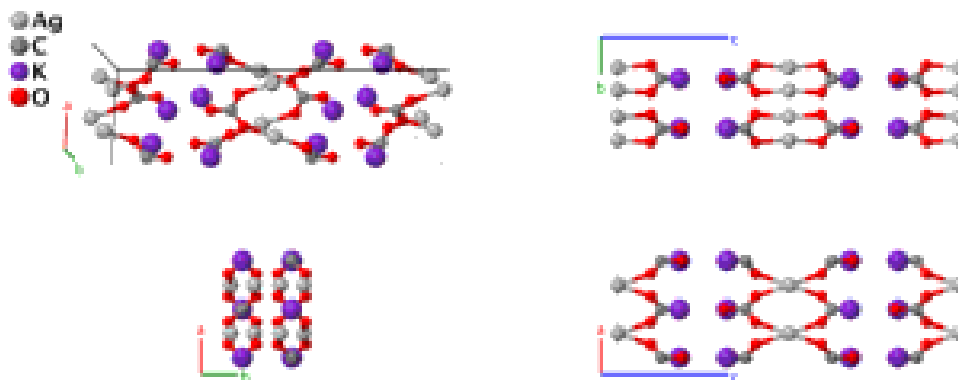
- P. C. Donohue and P. E. Bierstedt, *Synthesis, crystal structure, and superconducting properties of niobium phosphorus sulfide, niobium phosphorus selenide and tantalum phosphorus sulfide*, *Inorg. Chem.* **8**, 2690–2694 (1969), [doi:10.1021/ic50082a031](https://doi.org/10.1021/ic50082a031).

---

**Geometry files:**

- CIF: pp. [855](#)
- POSCAR: pp. [855](#)

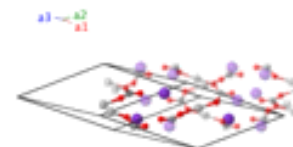
# KAg[CO<sub>3</sub>] Structure: ABCD3\_oI48\_73\_d\_e\_e\_ef



**Prototype** : KAg[CO<sub>3</sub>]  
**AFLOW prototype label** : ABCD3\_oI48\_73\_d\_e\_e\_ef  
**Strukturbericht designation** : None  
**Pearson symbol** : oI48  
**Space group number** : 73  
**Space group symbol** : *Ibca*  
**AFLOW prototype command** : aflow --proto=ABCD3\_oI48\_73\_d\_e\_e\_ef  
 --params=*a, b/a, c/a, y<sub>1</sub>, z<sub>2</sub>, z<sub>3</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>*

**Body-centered Orthorhombic primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\
 \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$y_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{4} + y_1\right) \mathbf{a}_3$	$\frac{1}{4}a\hat{\mathbf{x}} + y_1b\hat{\mathbf{y}}$	(8 <i>d</i> )	Ag
<b>B<sub>2</sub></b>	$\left(\frac{1}{2} - y_1\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{4} - y_1\right) \mathbf{a}_3$	$\frac{1}{4}a\hat{\mathbf{x}} - y_1b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(8 <i>d</i> )	Ag
<b>B<sub>3</sub></b>	$-y_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{3}{4} - y_1\right) \mathbf{a}_3$	$\frac{3}{4}a\hat{\mathbf{x}} - y_1b\hat{\mathbf{y}}$	(8 <i>d</i> )	Ag
<b>B<sub>4</sub></b>	$\left(\frac{1}{2} + y_1\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{3}{4} + y_1\right) \mathbf{a}_3$	$\frac{1}{4}a\hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right)b\hat{\mathbf{y}}$	(8 <i>d</i> )	Ag
<b>B<sub>5</sub></b>	$\left(\frac{1}{4} + z_2\right) \mathbf{a}_1 + z_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{1}{4}b\hat{\mathbf{y}} + z_2c\hat{\mathbf{z}}$	(8 <i>e</i> )	C
<b>B<sub>6</sub></b>	$\left(\frac{1}{4} - z_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} - z_2c\hat{\mathbf{z}}$	(8 <i>e</i> )	C
<b>B<sub>7</sub></b>	$\left(\frac{3}{4} - z_2\right) \mathbf{a}_1 - z_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{3}{4}b\hat{\mathbf{y}} - z_2c\hat{\mathbf{z}}$	(8 <i>e</i> )	C
<b>B<sub>8</sub></b>	$\left(\frac{3}{4} + z_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{1}{4}b\hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right)c\hat{\mathbf{z}}$	(8 <i>e</i> )	C
<b>B<sub>9</sub></b>	$\left(\frac{1}{4} + z_3\right) \mathbf{a}_1 + z_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{1}{4}b\hat{\mathbf{y}} + z_3c\hat{\mathbf{z}}$	(8 <i>e</i> )	K
<b>B<sub>10</sub></b>	$\left(\frac{1}{4} - z_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} - z_3c\hat{\mathbf{z}}$	(8 <i>e</i> )	K
<b>B<sub>11</sub></b>	$\left(\frac{3}{4} - z_3\right) \mathbf{a}_1 - z_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{3}{4}b\hat{\mathbf{y}} - z_3c\hat{\mathbf{z}}$	(8 <i>e</i> )	K

$$\begin{aligned}
\mathbf{B}_{12} &= \left(\frac{3}{4} + z_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} && (8e) && \text{K} \\
\mathbf{B}_{13} &= \left(\frac{1}{4} + z_4\right) \mathbf{a}_1 + z_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{4} b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (8e) && \text{O I} \\
\mathbf{B}_{14} &= \left(\frac{1}{4} - z_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (8e) && \text{O I} \\
\mathbf{B}_{15} &= \left(\frac{3}{4} - z_4\right) \mathbf{a}_1 - z_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{3}{4} b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (8e) && \text{O I} \\
\mathbf{B}_{16} &= \left(\frac{3}{4} + z_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{4} b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} && (8e) && \text{O I} \\
\mathbf{B}_{17} &= (y_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + (x_5 + y_5) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (16f) && \text{O II} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} - y_5 + z_5\right) \mathbf{a}_1 + (-x_5 + z_5) \mathbf{a}_2 + &= -x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (16f) && \text{O II} \\
&\quad \left(\frac{1}{2} - x_5 - y_5\right) \mathbf{a}_3 \\
\mathbf{B}_{19} &= (y_5 - z_5) \mathbf{a}_1 + \left(\frac{1}{2} - x_5 - z_5\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} && (16f) && \text{O II} \\
&\quad \left(\frac{1}{2} - x_5 + y_5\right) \mathbf{a}_3 \\
\mathbf{B}_{20} &= \left(\frac{1}{2} - y_5 - z_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_5 - z_5\right) \mathbf{a}_2 + &= x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} && (16f) && \text{O II} \\
&\quad (x_5 - y_5) \mathbf{a}_3 \\
\mathbf{B}_{21} &= (-y_5 - z_5) \mathbf{a}_1 + (-x_5 - z_5) \mathbf{a}_2 + &= -x_5 a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} && (16f) && \text{O II} \\
&\quad (-x_5 - y_5) \mathbf{a}_3 \\
\mathbf{B}_{22} &= \left(\frac{1}{2} + y_5 - z_5\right) \mathbf{a}_1 + (x_5 - z_5) \mathbf{a}_2 + &= x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) b \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} && (16f) && \text{O II} \\
&\quad \left(\frac{1}{2} + x_5 + y_5\right) \mathbf{a}_3 \\
\mathbf{B}_{23} &= (-y_5 + z_5) \mathbf{a}_1 + \left(\frac{1}{2} + x_5 + z_5\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} - y_5 b \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (16f) && \text{O II} \\
&\quad \left(\frac{1}{2} + x_5 - y_5\right) \mathbf{a}_3 \\
\mathbf{B}_{24} &= \left(\frac{1}{2} + y_5 + z_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_5 + z_5\right) \mathbf{a}_2 + &= -x_5 a \hat{\mathbf{x}} + y_5 b \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} && (16f) && \text{O II} \\
&\quad (-x_5 + y_5) \mathbf{a}_3
\end{aligned}$$

---

#### References:

- Y.-Q. Zheng, L.-X. Zhou, J.-L. Lin, and S.-W. Zhang, *Refinement of the crystal structure of potassium catena-carbonato-argentate(I), K[Ag(CO<sub>3</sub>)], Zeitschrift für Kristallographie - New Crystal Structures* **215**, 467–468 (2000), doi:10.1515/ncrs-2000-0405.

#### Found in:

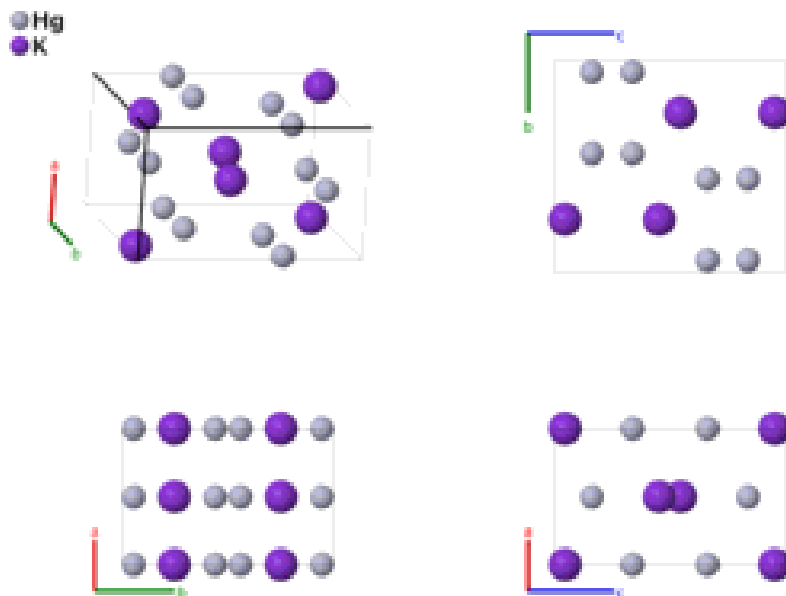
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 855  
- POSCAR: pp. 856

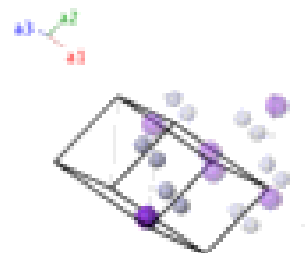
# KHg<sub>2</sub> Structure: A2B\_oI12\_74\_h\_e



<b>Prototype</b>	:	KHg <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_oI12_74_h_e
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	oI12
<b>Space group number</b>	:	74
<b>Space group symbol</b>	:	<i>Imma</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_oI12_74_h_e --params=a, b/a, c/a, z <sub>1</sub> , y <sub>2</sub> , z <sub>2</sub>

**Body-centered Orthorhombic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \left(\frac{1}{4} + z_1\right) \mathbf{a}_1 + z_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{4}b\hat{\mathbf{y}} + z_1c\hat{\mathbf{z}}$	(4e)	K
$\mathbf{B}_2$	$= \left(\frac{3}{4} - z_1\right) \mathbf{a}_1 - z_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{3}{4}b\hat{\mathbf{y}} - z_1c\hat{\mathbf{z}}$	(4e)	K
$\mathbf{B}_3$	$= (y_2 + z_2) \mathbf{a}_1 + z_2 \mathbf{a}_2 + y_2 \mathbf{a}_3$	$= y_2b\hat{\mathbf{y}} + z_2c\hat{\mathbf{z}}$	(8h)	Hg
$\mathbf{B}_4$	$= \left(\frac{1}{2} - y_2 + z_2\right) \mathbf{a}_1 + z_2 \mathbf{a}_2 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - y_2\right)b\hat{\mathbf{y}} + z_2c\hat{\mathbf{z}}$	(8h)	Hg

$$\mathbf{B}_5 = \left(\frac{1}{2} + y_2 - z_2\right) \mathbf{a}_1 - z_2 \mathbf{a}_2 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_2\right) b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} \quad (8h) \quad \text{Hg}$$

$$\mathbf{B}_6 = (-y_2 - z_2) \mathbf{a}_1 - z_2 \mathbf{a}_2 - y_2 \mathbf{a}_3 = -y_2 b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} \quad (8h) \quad \text{Hg}$$

---

**References:**

- E. J. Duwell and N. C. Baenziger, *The crystal structures of KHg and KHg<sub>2</sub>*, *Acta Cryst.* **8**, 705–710 (1955), [doi:10.1107/S0365110X55002168](https://doi.org/10.1107/S0365110X55002168).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

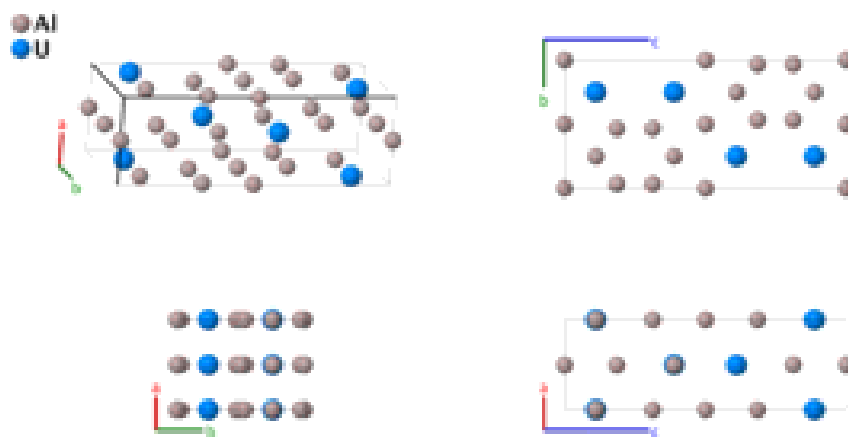
---

**Geometry files:**

- CIF: pp. [856](#)

- POSCAR: pp. [856](#)

# Al<sub>4</sub>U (*D*1<sub>b</sub>) Structure: A4B\_oI20\_74\_beh\_e



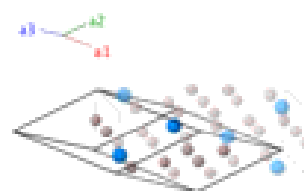
<b>Prototype</b>	:	Al <sub>4</sub> U
<b>AFLOW prototype label</b>	:	A4B_oI20_74_beh_e
<b>Strukturbericht designation</b>	:	<i>D</i> 1 <sub>b</sub>
<b>Pearson symbol</b>	:	oI20
<b>Space group number</b>	:	74
<b>Space group symbol</b>	:	<i>Imma</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A4B_oI20_74_beh_e --params= <i>a, b/a, c/a, z<sub>2</sub>, z<sub>3</sub>, y<sub>4</sub>, z<sub>4</sub></i>

## Other compounds with this structure:

- Al<sub>4</sub>Gd, Al<sub>4</sub>Np, Al<sub>4</sub>Pu

## Body-centered Orthorhombic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} c \hat{\mathbf{z}}$	(4 <i>b</i> )	Al I
<b>B<sub>2</sub></b>	= $\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}}$	(4 <i>b</i> )	Al I
<b>B<sub>3</sub></b>	= $\left(\frac{1}{4} + z_2\right) \mathbf{a}_1 + z_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4} b \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4 <i>e</i> )	Al II
<b>B<sub>4</sub></b>	= $\left(\frac{3}{4} - z_2\right) \mathbf{a}_1 - z_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4} b \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(4 <i>e</i> )	Al II
<b>B<sub>5</sub></b>	= $\left(\frac{1}{4} + z_3\right) \mathbf{a}_1 + z_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4} b \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4 <i>e</i> )	U
<b>B<sub>6</sub></b>	= $\left(\frac{3}{4} - z_3\right) \mathbf{a}_1 - z_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4} b \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(4 <i>e</i> )	U
<b>B<sub>7</sub></b>	= $(y_4 + z_4) \mathbf{a}_1 + z_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	=	$y_4 b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8 <i>h</i> )	Al III



$$\mathbf{B}_8 = \left(\frac{1}{2} - y_4 + z_4\right) \mathbf{a}_1 + z_4 \mathbf{a}_2 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_3 = \left(\frac{1}{2} - y_4\right) b \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} \quad (8h) \quad \text{Al III}$$

$$\mathbf{B}_9 = \left(\frac{1}{2} + y_4 - z_4\right) \mathbf{a}_1 - z_4 \mathbf{a}_2 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_4\right) b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} \quad (8h) \quad \text{Al III}$$

$$\mathbf{B}_{10} = (-y_4 - z_4) \mathbf{a}_1 - z_4 \mathbf{a}_2 - y_4 \mathbf{a}_3 = -y_4 b \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} \quad (8h) \quad \text{Al III}$$

---

**References:**

- H. U. Borgstedt and H. Wedemeyer, *Gmelin Handbook of Inorganic Chemistry* (Springer-Verlag, Berlin Heidelberg, 1989), vol. Supplement B 2, chap. 3, p. 144.

---

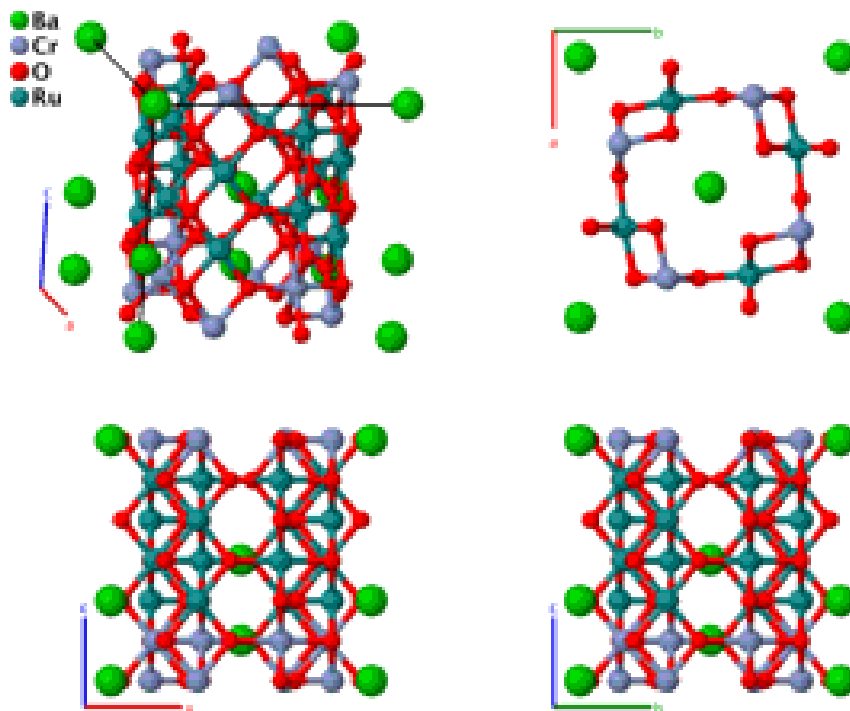
**Geometry files:**

- CIF: pp. [856](#)

- POSCAR: pp. [857](#)

# BaCr<sub>2</sub>Ru<sub>4</sub>O<sub>12</sub> Structure:

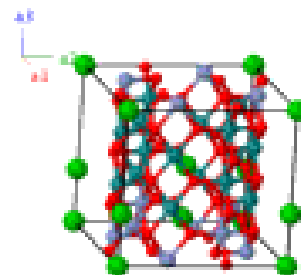
## AB2C12D4\_tP76\_75\_2a2b\_2d\_12d\_4d



<b>Prototype</b>	:	BaCr <sub>2</sub> Ru <sub>4</sub> O <sub>12</sub>
<b>AFLOW prototype label</b>	:	AB2C12D4_tP76_75_2a2b_2d_12d_4d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP76
<b>Space group number</b>	:	75
<b>Space group symbol</b>	:	<i>P</i> 4
<b>AFLOW prototype command</b>	:	aflow --proto=AB2C12D4_tP76_75_2a2b_2d_12d_4d --params= <i>a</i> , <i>c/a</i> , <i>z</i> <sub>1</sub> , <i>z</i> <sub>2</sub> , <i>z</i> <sub>3</sub> , <i>z</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>x</i> <sub>6</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub> , <i>x</i> <sub>7</sub> , <i>y</i> <sub>7</sub> , <i>z</i> <sub>7</sub> , <i>x</i> <sub>8</sub> , <i>y</i> <sub>8</sub> , <i>z</i> <sub>8</sub> , <i>x</i> <sub>9</sub> , <i>y</i> <sub>9</sub> , <i>z</i> <sub>9</sub> , <i>x</i> <sub>10</sub> , <i>y</i> <sub>10</sub> , <i>z</i> <sub>10</sub> , <i>x</i> <sub>11</sub> , <i>y</i> <sub>11</sub> , <i>z</i> <sub>11</sub> , <i>x</i> <sub>12</sub> , <i>y</i> <sub>12</sub> , <i>z</i> <sub>12</sub> , <i>x</i> <sub>13</sub> , <i>y</i> <sub>13</sub> , <i>z</i> <sub>13</sub> , <i>x</i> <sub>14</sub> , <i>y</i> <sub>14</sub> , <i>z</i> <sub>14</sub> , <i>x</i> <sub>15</sub> , <i>y</i> <sub>15</sub> , <i>z</i> <sub>15</sub> , <i>x</i> <sub>16</sub> , <i>y</i> <sub>16</sub> , <i>z</i> <sub>16</sub> , <i>x</i> <sub>17</sub> , <i>y</i> <sub>17</sub> , <i>z</i> <sub>17</sub> , <i>x</i> <sub>18</sub> , <i>y</i> <sub>18</sub> , <i>z</i> <sub>18</sub> , <i>x</i> <sub>19</sub> , <i>y</i> <sub>19</sub> , <i>z</i> <sub>19</sub> , <i>x</i> <sub>20</sub> , <i>y</i> <sub>20</sub> , <i>z</i> <sub>20</sub> , <i>x</i> <sub>21</sub> , <i>y</i> <sub>21</sub> , <i>z</i> <sub>21</sub> , <i>x</i> <sub>22</sub> , <i>y</i> <sub>22</sub> , <i>z</i> <sub>22</sub>

### Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= a \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$



### Basis vectors:

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type

$\mathbf{B}_1$	$=$	$z_1 \mathbf{a}_3$	$=$	$z_1 c \hat{\mathbf{z}}$	(1a)	Ba I
$\mathbf{B}_2$	$=$	$z_2 \mathbf{a}_3$	$=$	$z_2 c \hat{\mathbf{z}}$	(1a)	Ba II
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(1b)	Ba III
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(1b)	Ba IV
$\mathbf{B}_5$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4d)	Cr I
$\mathbf{B}_6$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4d)	Cr I
$\mathbf{B}_7$	$=$	$-y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4d)	Cr I
$\mathbf{B}_8$	$=$	$y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4d)	Cr I
$\mathbf{B}_9$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4d)	Cr II
$\mathbf{B}_{10}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4d)	Cr II
$\mathbf{B}_{11}$	$=$	$-y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4d)	Cr II
$\mathbf{B}_{12}$	$=$	$y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4d)	Cr II
$\mathbf{B}_{13}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B}_{14}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B}_{15}$	$=$	$-y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B}_{16}$	$=$	$y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B}_{17}$	$=$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$x_8 a \hat{\mathbf{x}} + y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B}_{18}$	$=$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-x_8 a \hat{\mathbf{x}} - y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B}_{19}$	$=$	$-y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-y_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B}_{20}$	$=$	$y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$y_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B}_{21}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$x_9 a \hat{\mathbf{x}} + y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B}_{22}$	$=$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-x_9 a \hat{\mathbf{x}} - y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B}_{23}$	$=$	$-y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-y_9 a \hat{\mathbf{x}} + x_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B}_{24}$	$=$	$y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$y_9 a \hat{\mathbf{x}} - x_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B}_{25}$	$=$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$x_{10} a \hat{\mathbf{x}} + y_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B}_{26}$	$=$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-x_{10} a \hat{\mathbf{x}} - y_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B}_{27}$	$=$	$-y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-y_{10} a \hat{\mathbf{x}} + x_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B}_{28}$	$=$	$y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$y_{10} a \hat{\mathbf{x}} - x_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B}_{29}$	$=$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$x_{11} a \hat{\mathbf{x}} + y_{11} a \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}}$	(4d)	O V
$\mathbf{B}_{30}$	$=$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$-x_{11} a \hat{\mathbf{x}} - y_{11} a \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}}$	(4d)	O V
$\mathbf{B}_{31}$	$=$	$-y_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$-y_{11} a \hat{\mathbf{x}} + x_{11} a \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}}$	(4d)	O V
$\mathbf{B}_{32}$	$=$	$y_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$y_{11} a \hat{\mathbf{x}} - x_{11} a \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}}$	(4d)	O V
$\mathbf{B}_{33}$	$=$	$x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$x_{12} a \hat{\mathbf{x}} + y_{12} a \hat{\mathbf{y}} + z_{12} c \hat{\mathbf{z}}$	(4d)	O VI
$\mathbf{B}_{34}$	$=$	$-x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$-x_{12} a \hat{\mathbf{x}} - y_{12} a \hat{\mathbf{y}} + z_{12} c \hat{\mathbf{z}}$	(4d)	O VI
$\mathbf{B}_{35}$	$=$	$-y_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$-y_{12} a \hat{\mathbf{x}} + x_{12} a \hat{\mathbf{y}} + z_{12} c \hat{\mathbf{z}}$	(4d)	O VI
$\mathbf{B}_{36}$	$=$	$y_{12} \mathbf{a}_1 - x_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$y_{12} a \hat{\mathbf{x}} - x_{12} a \hat{\mathbf{y}} + z_{12} c \hat{\mathbf{z}}$	(4d)	O VI



$$\begin{aligned}
 \mathbf{B}_{73} &= x_{22} \mathbf{a}_1 + y_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3 &= x_{22}a \hat{\mathbf{x}} + y_{22}a \hat{\mathbf{y}} + z_{22}c \hat{\mathbf{z}} & (4d) & \text{Ru IV} \\
 \mathbf{B}_{74} &= -x_{22} \mathbf{a}_1 - y_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3 &= -x_{22}a \hat{\mathbf{x}} - y_{22}a \hat{\mathbf{y}} + z_{22}c \hat{\mathbf{z}} & (4d) & \text{Ru IV} \\
 \mathbf{B}_{75} &= -y_{22} \mathbf{a}_1 + x_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3 &= -y_{22}a \hat{\mathbf{x}} + x_{22}a \hat{\mathbf{y}} + z_{22}c \hat{\mathbf{z}} & (4d) & \text{Ru IV} \\
 \mathbf{B}_{76} &= y_{22} \mathbf{a}_1 - x_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3 &= y_{22}a \hat{\mathbf{x}} - x_{22}a \hat{\mathbf{y}} + z_{22}c \hat{\mathbf{z}} & (4d) & \text{Ru IV}
 \end{aligned}$$

**References:**

- M. C. Cadée and A. Prodan, *Tripling of the short axis in the hollandite structure*, Mater. Res. Bull. **14**, 613–618 (1979), [doi:10.1016/0025-5408\(79\)90043-6](https://doi.org/10.1016/0025-5408(79)90043-6).

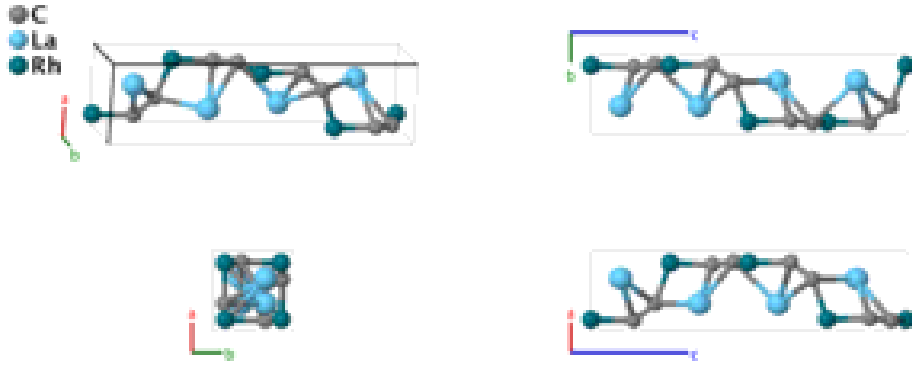
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [857](#)  
 - POSCAR: pp. [857](#)

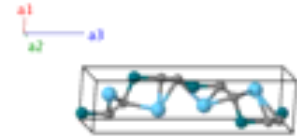
# LaRhC<sub>2</sub> Structure: A2BC\_tP16\_76\_2a\_a\_a



**Prototype** : LaRhC<sub>2</sub>  
**AFLOW prototype label** : A2BC\_tP16\_76\_2a\_a\_a  
**Strukturbericht designation** : None  
**Pearson symbol** : tP16  
**Space group number** : 76  
**Space group symbol** :  $P4_1$   
**AFLOW prototype command** : `aflow --proto=A2BC_tP16_76_2a_a_a`  
`--params=a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4`

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4a)	C I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4a)	C I
$\mathbf{B}_3$	$-y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{1}{4} + z_1\right) \mathbf{a}_3$	$-y_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_1\right) c \hat{\mathbf{z}}$	(4a)	C I
$\mathbf{B}_4$	$y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{3}{4} + z_1\right) \mathbf{a}_3$	$y_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_1\right) c \hat{\mathbf{z}}$	(4a)	C I
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4a)	C II
$\mathbf{B}_6$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$-x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4a)	C II
$\mathbf{B}_7$	$-y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{4} + z_2\right) \mathbf{a}_3$	$-y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_2\right) c \hat{\mathbf{z}}$	(4a)	C II
$\mathbf{B}_8$	$y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{3}{4} + z_2\right) \mathbf{a}_3$	$y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_2\right) c \hat{\mathbf{z}}$	(4a)	C II
$\mathbf{B}_9$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4a)	La
$\mathbf{B}_{10}$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$-x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4a)	La
$\mathbf{B}_{11}$	$-y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{4} + z_3\right) \mathbf{a}_3$	$-y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_3\right) c \hat{\mathbf{z}}$	(4a)	La
$\mathbf{B}_{12}$	$y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{3}{4} + z_3\right) \mathbf{a}_3$	$y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_3\right) c \hat{\mathbf{z}}$	(4a)	La

$$\mathbf{B}_{13} = x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} \quad (4a) \quad \text{Rh}$$

$$\mathbf{B}_{14} = -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} \quad (4a) \quad \text{Rh}$$

$$\mathbf{B}_{15} = -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{4} + z_4\right) \mathbf{a}_3 = -y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_4\right) c \hat{\mathbf{z}} \quad (4a) \quad \text{Rh}$$

$$\mathbf{B}_{16} = y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{3}{4} + z_4\right) \mathbf{a}_3 = y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_4\right) c \hat{\mathbf{z}} \quad (4a) \quad \text{Rh}$$

**References:**

- A. O. Tsokol', O. I. Bodak, E. P. Marusin, and V. E. Zavodnik, *X-ray diffraction studies of ternary RRhC<sub>2</sub> (R = La, Ce, Pr, Nd, Sm) compounds*, *Kristallografiya* **33**, 345–348 (1988).

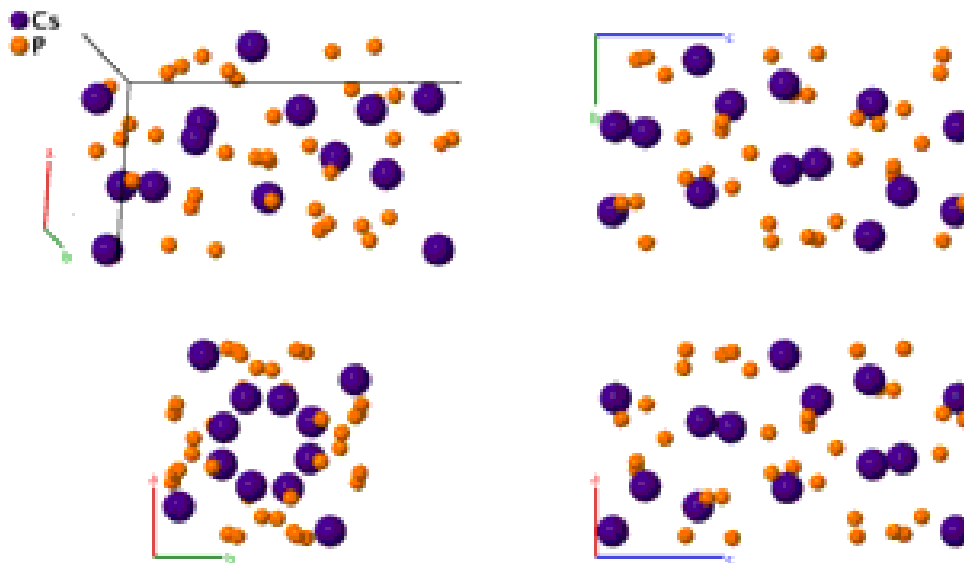
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [858](#)
- POSCAR: pp. [858](#)

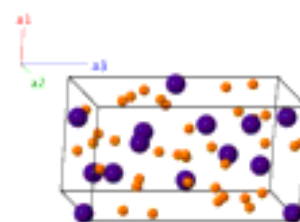
# Cs<sub>3</sub>P<sub>7</sub> Structure: A3B7\_tP40\_76\_3a\_7a



**Prototype** : Cs<sub>3</sub>P<sub>7</sub>  
**AFLOW prototype label** : A3B7\_tP40\_76\_3a\_7a  
**Strukturbericht designation** : None  
**Pearson symbol** : tP40  
**Space group number** : 76  
**Space group symbol** : *P4*<sub>1</sub>  
**AFLOW prototype command** : `aflow --proto=A3B7_tP40_76_3a_7a`  
`--params=a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7,`  
`y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10`

## Simple Tetragonal primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4a)	Cs I
<b>B</b> <sub>2</sub>	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4a)	Cs I
<b>B</b> <sub>3</sub>	$-y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{1}{4} + z_1\right) \mathbf{a}_3$	$-y_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_1\right) c \hat{\mathbf{z}}$	(4a)	Cs I
<b>B</b> <sub>4</sub>	$y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{3}{4} + z_1\right) \mathbf{a}_3$	$y_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_1\right) c \hat{\mathbf{z}}$	(4a)	Cs I
<b>B</b> <sub>5</sub>	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4a)	Cs II
<b>B</b> <sub>6</sub>	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$-x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4a)	Cs II



$\mathbf{B}_7$	$=$	$-y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{4} + z_2\right) \mathbf{a}_3$	$=$	$-y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_2\right) c \hat{\mathbf{z}}$	(4a)	Cs II
$\mathbf{B}_8$	$=$	$y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{3}{4} + z_2\right) \mathbf{a}_3$	$=$	$y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_2\right) c \hat{\mathbf{z}}$	(4a)	Cs II
$\mathbf{B}_9$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4a)	Cs III
$\mathbf{B}_{10}$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4a)	Cs III
$\mathbf{B}_{11}$	$=$	$-y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{4} + z_3\right) \mathbf{a}_3$	$=$	$-y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_3\right) c \hat{\mathbf{z}}$	(4a)	Cs III
$\mathbf{B}_{12}$	$=$	$y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{3}{4} + z_3\right) \mathbf{a}_3$	$=$	$y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_3\right) c \hat{\mathbf{z}}$	(4a)	Cs III
$\mathbf{B}_{13}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B}_{14}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B}_{15}$	$=$	$-y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{4} + z_4\right) \mathbf{a}_3$	$=$	$-y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_4\right) c \hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B}_{16}$	$=$	$y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{3}{4} + z_4\right) \mathbf{a}_3$	$=$	$y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_4\right) c \hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B}_{17}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4a)	P II
$\mathbf{B}_{18}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(4a)	P II
$\mathbf{B}_{19}$	$=$	$-y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{4} + z_5\right) \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_5\right) c \hat{\mathbf{z}}$	(4a)	P II
$\mathbf{B}_{20}$	$=$	$y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{3}{4} + z_5\right) \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_5\right) c \hat{\mathbf{z}}$	(4a)	P II
$\mathbf{B}_{21}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4a)	P III
$\mathbf{B}_{22}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(4a)	P III
$\mathbf{B}_{23}$	$=$	$-y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(\frac{1}{4} + z_6\right) \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_6\right) c \hat{\mathbf{z}}$	(4a)	P III
$\mathbf{B}_{24}$	$=$	$y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(\frac{3}{4} + z_6\right) \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_6\right) c \hat{\mathbf{z}}$	(4a)	P III
$\mathbf{B}_{25}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4a)	P IV
$\mathbf{B}_{26}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(4a)	P IV
$\mathbf{B}_{27}$	$=$	$-y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(\frac{1}{4} + z_7\right) \mathbf{a}_3$	$=$	$-y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_7\right) c \hat{\mathbf{z}}$	(4a)	P IV
$\mathbf{B}_{28}$	$=$	$y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(\frac{3}{4} + z_7\right) \mathbf{a}_3$	$=$	$y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_7\right) c \hat{\mathbf{z}}$	(4a)	P IV
$\mathbf{B}_{29}$	$=$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$x_8 a \hat{\mathbf{x}} + y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4a)	P V
$\mathbf{B}_{30}$	$=$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3$	$=$	$-x_8 a \hat{\mathbf{x}} - y_8 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \hat{\mathbf{z}}$	(4a)	P V
$\mathbf{B}_{31}$	$=$	$-y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + \left(\frac{1}{4} + z_8\right) \mathbf{a}_3$	$=$	$-y_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_8\right) c \hat{\mathbf{z}}$	(4a)	P V
$\mathbf{B}_{32}$	$=$	$y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + \left(\frac{3}{4} + z_8\right) \mathbf{a}_3$	$=$	$y_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_8\right) c \hat{\mathbf{z}}$	(4a)	P V
$\mathbf{B}_{33}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$x_9 a \hat{\mathbf{x}} + y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4a)	P VI
$\mathbf{B}_{34}$	$=$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3$	$=$	$-x_9 a \hat{\mathbf{x}} - y_9 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}}$	(4a)	P VI
$\mathbf{B}_{35}$	$=$	$-y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + \left(\frac{1}{4} + z_9\right) \mathbf{a}_3$	$=$	$-y_9 a \hat{\mathbf{x}} + x_9 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_9\right) c \hat{\mathbf{z}}$	(4a)	P VI
$\mathbf{B}_{36}$	$=$	$y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + \left(\frac{3}{4} + z_9\right) \mathbf{a}_3$	$=$	$y_9 a \hat{\mathbf{x}} - x_9 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_9\right) c \hat{\mathbf{z}}$	(4a)	P VI
$\mathbf{B}_{37}$	$=$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$x_{10} a \hat{\mathbf{x}} + y_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(4a)	P VII
$\mathbf{B}_{38}$	$=$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3$	$=$	$-x_{10} a \hat{\mathbf{x}} - y_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}}$	(4a)	P VII
$\mathbf{B}_{39}$	$=$	$-y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + \left(\frac{1}{4} + z_{10}\right) \mathbf{a}_3$	$=$	$-y_{10} a \hat{\mathbf{x}} + x_{10} a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_{10}\right) c \hat{\mathbf{z}}$	(4a)	P VII
$\mathbf{B}_{40}$	$=$	$y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + \left(\frac{3}{4} + z_{10}\right) \mathbf{a}_3$	$=$	$y_{10} a \hat{\mathbf{x}} - x_{10} a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_{10}\right) c \hat{\mathbf{z}}$	(4a)	P VII

## References:

- T. Meyer, W. Hönlle, and H. G. von Schnering, *Zur Chemie und Strukturchemie von Phosphiden und Polyphosphiden*. 44.

*Tricäsiumheptaphosphid Cs<sub>3</sub>P<sub>7</sub>: Darstellung, Struktur und Eigenschaften*, Z. Anorg. Allg. Chem. **552**, 69–80 (1987), [doi:10.1002/zaac.19875520907](https://doi.org/10.1002/zaac.19875520907).

**Found in:**

- R. J. D. Tilley, *Crystals and Crystal Structures* (Wiley, Chichester, England, 2006), chap. 5, p. 102.

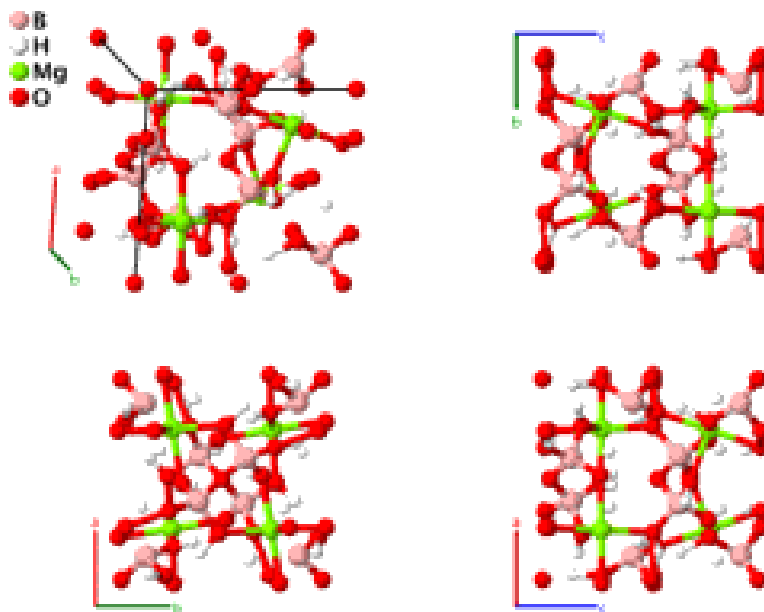
---

**Geometry files:**

- CIF: pp. [858](#)

- POSCAR: pp. [859](#)

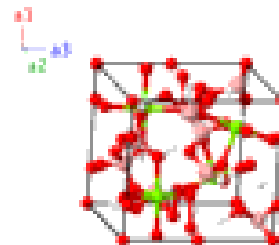
# Pinnoite ( $\text{MgB}_2\text{O}(\text{OH})_6$ ) Structure: A2B6CD7\_tP64\_77\_2d\_6d\_d\_ab6d



<b>Prototype</b>	:	$\text{MgB}_2\text{O}(\text{OH})_6$
<b>AFLOW prototype label</b>	:	A2B6CD7_tP64_77_2d_6d_d_ab6d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP64
<b>Space group number</b>	:	77
<b>Space group symbol</b>	:	$P4_2$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B6CD7_tP64_77_2d_6d_d_ab6d --params= $a, c/a, z_1, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}$

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$z_1 c \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_2$	$= \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	O I

$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B}_5$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4d)	B I
$\mathbf{B}_6$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4d)	B I
$\mathbf{B}_7$	$=$	$-y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$-y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4d)	B I
$\mathbf{B}_8$	$=$	$y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4d)	B I
$\mathbf{B}_9$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4d)	B II
$\mathbf{B}_{10}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4d)	B II
$\mathbf{B}_{11}$	$=$	$-y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$-y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(4d)	B II
$\mathbf{B}_{12}$	$=$	$y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(4d)	B II
$\mathbf{B}_{13}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B}_{14}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B}_{15}$	$=$	$-y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B}_{16}$	$=$	$y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B}_{17}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B}_{18}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B}_{19}$	$=$	$-y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B}_{20}$	$=$	$y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B}_{21}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4d)	H III
$\mathbf{B}_{22}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4d)	H III
$\mathbf{B}_{23}$	$=$	$-y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	$=$	$-y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(4d)	H III
$\mathbf{B}_{24}$	$=$	$y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	$=$	$y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(4d)	H III
$\mathbf{B}_{25}$	$=$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$x_8 a \hat{\mathbf{x}} + y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4d)	H IV
$\mathbf{B}_{26}$	$=$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-x_8 a \hat{\mathbf{x}} - y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4d)	H IV
$\mathbf{B}_{27}$	$=$	$-y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3$	$=$	$-y_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \hat{\mathbf{z}}$	(4d)	H IV
$\mathbf{B}_{28}$	$=$	$y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3$	$=$	$y_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \hat{\mathbf{z}}$	(4d)	H IV
$\mathbf{B}_{29}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$x_9 a \hat{\mathbf{x}} + y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4d)	H V
$\mathbf{B}_{30}$	$=$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-x_9 a \hat{\mathbf{x}} - y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4d)	H V
$\mathbf{B}_{31}$	$=$	$-y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3$	$=$	$-y_9 a \hat{\mathbf{x}} + x_9 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}}$	(4d)	H V
$\mathbf{B}_{32}$	$=$	$y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3$	$=$	$y_9 a \hat{\mathbf{x}} - x_9 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}}$	(4d)	H V
$\mathbf{B}_{33}$	$=$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$x_{10} a \hat{\mathbf{x}} + y_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(4d)	H VI
$\mathbf{B}_{34}$	$=$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-x_{10} a \hat{\mathbf{x}} - y_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	(4d)	H VI
$\mathbf{B}_{35}$	$=$	$-y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3$	$=$	$-y_{10} a \hat{\mathbf{x}} + x_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}}$	(4d)	H VI
$\mathbf{B}_{36}$	$=$	$y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3$	$=$	$y_{10} a \hat{\mathbf{x}} - x_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}}$	(4d)	H VI
$\mathbf{B}_{37}$	$=$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$x_{11} a \hat{\mathbf{x}} + y_{11} a \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}}$	(4d)	Mg
$\mathbf{B}_{38}$	$=$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$-x_{11} a \hat{\mathbf{x}} - y_{11} a \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}}$	(4d)	Mg

<b>B</b> <sub>39</sub>	=	$-y_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + \left(\frac{1}{2} + z_{11}\right) \mathbf{a}_3$	=	$-y_{11}a \hat{\mathbf{x}} + x_{11}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{11}\right)c \hat{\mathbf{z}}$	(4d)	Mg
<b>B</b> <sub>40</sub>	=	$y_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 + \left(\frac{1}{2} + z_{11}\right) \mathbf{a}_3$	=	$y_{11}a \hat{\mathbf{x}} - x_{11}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{11}\right)c \hat{\mathbf{z}}$	(4d)	Mg
<b>B</b> <sub>41</sub>	=	$x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	=	$x_{12}a \hat{\mathbf{x}} + y_{12}a \hat{\mathbf{y}} + z_{12}c \hat{\mathbf{z}}$	(4d)	O III
<b>B</b> <sub>42</sub>	=	$-x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	=	$-x_{12}a \hat{\mathbf{x}} - y_{12}a \hat{\mathbf{y}} + z_{12}c \hat{\mathbf{z}}$	(4d)	O III
<b>B</b> <sub>43</sub>	=	$-y_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 + \left(\frac{1}{2} + z_{12}\right) \mathbf{a}_3$	=	$-y_{12}a \hat{\mathbf{x}} + x_{12}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{12}\right)c \hat{\mathbf{z}}$	(4d)	O III
<b>B</b> <sub>44</sub>	=	$y_{12} \mathbf{a}_1 - x_{12} \mathbf{a}_2 + \left(\frac{1}{2} + z_{12}\right) \mathbf{a}_3$	=	$y_{12}a \hat{\mathbf{x}} - x_{12}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{12}\right)c \hat{\mathbf{z}}$	(4d)	O III
<b>B</b> <sub>45</sub>	=	$x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	=	$x_{13}a \hat{\mathbf{x}} + y_{13}a \hat{\mathbf{y}} + z_{13}c \hat{\mathbf{z}}$	(4d)	O IV
<b>B</b> <sub>46</sub>	=	$-x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	=	$-x_{13}a \hat{\mathbf{x}} - y_{13}a \hat{\mathbf{y}} + z_{13}c \hat{\mathbf{z}}$	(4d)	O IV
<b>B</b> <sub>47</sub>	=	$-y_{13} \mathbf{a}_1 + x_{13} \mathbf{a}_2 + \left(\frac{1}{2} + z_{13}\right) \mathbf{a}_3$	=	$-y_{13}a \hat{\mathbf{x}} + x_{13}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{13}\right)c \hat{\mathbf{z}}$	(4d)	O IV
<b>B</b> <sub>48</sub>	=	$y_{13} \mathbf{a}_1 - x_{13} \mathbf{a}_2 + \left(\frac{1}{2} + z_{13}\right) \mathbf{a}_3$	=	$y_{13}a \hat{\mathbf{x}} - x_{13}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{13}\right)c \hat{\mathbf{z}}$	(4d)	O IV
<b>B</b> <sub>49</sub>	=	$x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	=	$x_{14}a \hat{\mathbf{x}} + y_{14}a \hat{\mathbf{y}} + z_{14}c \hat{\mathbf{z}}$	(4d)	O V
<b>B</b> <sub>50</sub>	=	$-x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	=	$-x_{14}a \hat{\mathbf{x}} - y_{14}a \hat{\mathbf{y}} + z_{14}c \hat{\mathbf{z}}$	(4d)	O V
<b>B</b> <sub>51</sub>	=	$-y_{14} \mathbf{a}_1 + x_{14} \mathbf{a}_2 + \left(\frac{1}{2} + z_{14}\right) \mathbf{a}_3$	=	$-y_{14}a \hat{\mathbf{x}} + x_{14}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{14}\right)c \hat{\mathbf{z}}$	(4d)	O V
<b>B</b> <sub>52</sub>	=	$y_{14} \mathbf{a}_1 - x_{14} \mathbf{a}_2 + \left(\frac{1}{2} + z_{14}\right) \mathbf{a}_3$	=	$y_{14}a \hat{\mathbf{x}} - x_{14}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{14}\right)c \hat{\mathbf{z}}$	(4d)	O V
<b>B</b> <sub>53</sub>	=	$x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3$	=	$x_{15}a \hat{\mathbf{x}} + y_{15}a \hat{\mathbf{y}} + z_{15}c \hat{\mathbf{z}}$	(4d)	O VI
<b>B</b> <sub>54</sub>	=	$-x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3$	=	$-x_{15}a \hat{\mathbf{x}} - y_{15}a \hat{\mathbf{y}} + z_{15}c \hat{\mathbf{z}}$	(4d)	O VI
<b>B</b> <sub>55</sub>	=	$-y_{15} \mathbf{a}_1 + x_{15} \mathbf{a}_2 + \left(\frac{1}{2} + z_{15}\right) \mathbf{a}_3$	=	$-y_{15}a \hat{\mathbf{x}} + x_{15}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{15}\right)c \hat{\mathbf{z}}$	(4d)	O VI
<b>B</b> <sub>56</sub>	=	$y_{15} \mathbf{a}_1 - x_{15} \mathbf{a}_2 + \left(\frac{1}{2} + z_{15}\right) \mathbf{a}_3$	=	$y_{15}a \hat{\mathbf{x}} - x_{15}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{15}\right)c \hat{\mathbf{z}}$	(4d)	O VI
<b>B</b> <sub>57</sub>	=	$x_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3$	=	$x_{16}a \hat{\mathbf{x}} + y_{16}a \hat{\mathbf{y}} + z_{16}c \hat{\mathbf{z}}$	(4d)	O VII
<b>B</b> <sub>58</sub>	=	$-x_{16} \mathbf{a}_1 - y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3$	=	$-x_{16}a \hat{\mathbf{x}} - y_{16}a \hat{\mathbf{y}} + z_{16}c \hat{\mathbf{z}}$	(4d)	O VII
<b>B</b> <sub>59</sub>	=	$-y_{16} \mathbf{a}_1 + x_{16} \mathbf{a}_2 + \left(\frac{1}{2} + z_{16}\right) \mathbf{a}_3$	=	$-y_{16}a \hat{\mathbf{x}} + x_{16}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{16}\right)c \hat{\mathbf{z}}$	(4d)	O VII
<b>B</b> <sub>60</sub>	=	$y_{16} \mathbf{a}_1 - x_{16} \mathbf{a}_2 + \left(\frac{1}{2} + z_{16}\right) \mathbf{a}_3$	=	$y_{16}a \hat{\mathbf{x}} - x_{16}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{16}\right)c \hat{\mathbf{z}}$	(4d)	O VII
<b>B</b> <sub>61</sub>	=	$x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	=	$x_{17}a \hat{\mathbf{x}} + y_{17}a \hat{\mathbf{y}} + z_{17}c \hat{\mathbf{z}}$	(4d)	O VIII
<b>B</b> <sub>62</sub>	=	$-x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	=	$-x_{17}a \hat{\mathbf{x}} - y_{17}a \hat{\mathbf{y}} + z_{17}c \hat{\mathbf{z}}$	(4d)	O VIII
<b>B</b> <sub>63</sub>	=	$-y_{17} \mathbf{a}_1 + x_{17} \mathbf{a}_2 + \left(\frac{1}{2} + z_{17}\right) \mathbf{a}_3$	=	$-y_{17}a \hat{\mathbf{x}} + x_{17}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{17}\right)c \hat{\mathbf{z}}$	(4d)	O VIII
<b>B</b> <sub>64</sub>	=	$y_{17} \mathbf{a}_1 - x_{17} \mathbf{a}_2 + \left(\frac{1}{2} + z_{17}\right) \mathbf{a}_3$	=	$y_{17}a \hat{\mathbf{x}} - x_{17}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{17}\right)c \hat{\mathbf{z}}$	(4d)	O VIII

---

#### References:

- E. A. Genkina and Y. A. Malinovskii, *Refinement of the structure of pinnoite: Location of hydrogen atoms*, Sov. Phys. Crystallogr. **28**, 475–477 (1983).

#### Found in:

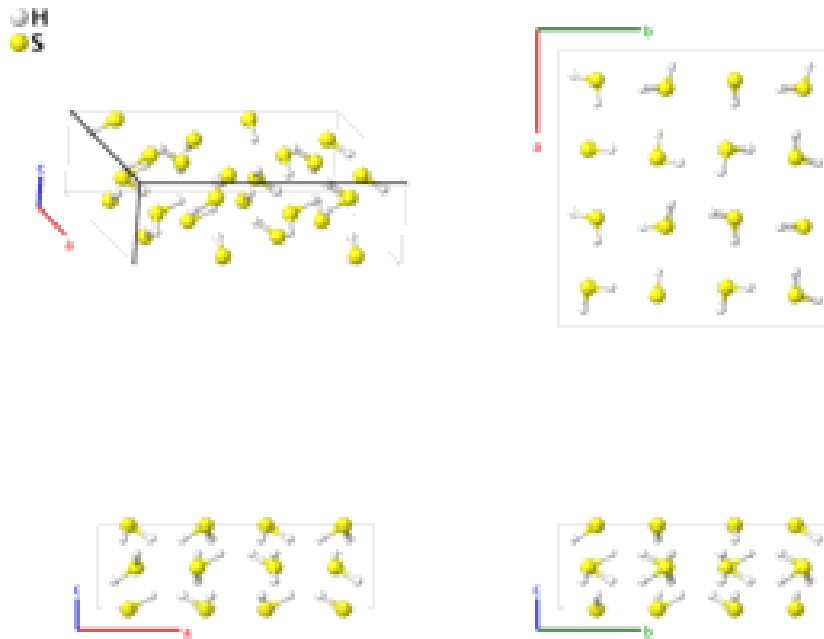
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [859](#)  
- POSCAR: pp. [859](#)

# H<sub>2</sub>S III Structure: A2B\_tP48\_77\_8d\_4d

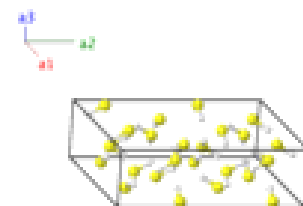


<b>Prototype</b>	:	H <sub>2</sub> S
<b>AFLOW prototype label</b>	:	A2B_tP48_77_8d_4d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP48
<b>Space group number</b>	:	77
<b>Space group symbol</b>	:	<i>P</i> 4 <sub>2</sub>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_tP48_77_8d_4d --params= <i>a, c/a, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>, y<sub>9</sub>, z<sub>9</sub>, x<sub>10</sub>, y<sub>10</sub>, z<sub>10</sub>, x<sub>11</sub>, y<sub>11</sub>, z<sub>11</sub>, x<sub>12</sub>, y<sub>12</sub>, z<sub>12</sub></i>

- This is one candidate structure for the H<sub>2</sub>S III structure, which is stable at pressures under 4 GPa and temperatures less than  $\approx 100$  K (Shimizu, 1995). The data presented here was for D<sub>2</sub>S at 102 K and ambient pressure.

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4d)	H I
<b>B<sub>2</sub></b>	= $-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$-x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4d)	H I
<b>B<sub>3</sub></b>	= $-y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$-y_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4d)	H I
<b>B<sub>4</sub></b>	= $y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$y_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4d)	H I
<b>B<sub>5</sub></b>	= $x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4d)	H II
<b>B<sub>6</sub></b>	= $-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$-x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4d)	H II
<b>B<sub>7</sub></b>	= $-y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	=	$-y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4d)	H II
<b>B<sub>8</sub></b>	= $y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	=	$y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4d)	H II
<b>B<sub>9</sub></b>	= $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4d)	H III
<b>B<sub>10</sub></b>	= $-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$-x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4d)	H III
<b>B<sub>11</sub></b>	= $-y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	=	$-y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4d)	H III
<b>B<sub>12</sub></b>	= $y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	=	$y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4d)	H III
<b>B<sub>13</sub></b>	= $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4d)	H IV
<b>B<sub>14</sub></b>	= $-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$-x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4d)	H IV
<b>B<sub>15</sub></b>	= $-y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	=	$-y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(4d)	H IV
<b>B<sub>16</sub></b>	= $y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	=	$y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(4d)	H IV
<b>B<sub>17</sub></b>	= $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4d)	H V
<b>B<sub>18</sub></b>	= $-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$-x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4d)	H V
<b>B<sub>19</sub></b>	= $-y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	=	$-y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(4d)	H V
<b>B<sub>20</sub></b>	= $y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	=	$y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(4d)	H V
<b>B<sub>21</sub></b>	= $x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4d)	H VI
<b>B<sub>22</sub></b>	= $-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$-x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4d)	H VI
<b>B<sub>23</sub></b>	= $-y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	=	$-y_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(4d)	H VI
<b>B<sub>24</sub></b>	= $y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	=	$y_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(4d)	H VI
<b>B<sub>25</sub></b>	= $x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4d)	H VII
<b>B<sub>26</sub></b>	= $-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(4d)	H VII
<b>B<sub>27</sub></b>	= $-y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	=	$-y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(4d)	H VII
<b>B<sub>28</sub></b>	= $y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	=	$y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(4d)	H VII
<b>B<sub>29</sub></b>	= $x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$x_8 a \hat{\mathbf{x}} + y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4d)	H VIII
<b>B<sub>30</sub></b>	= $-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$-x_8 a \hat{\mathbf{x}} - y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(4d)	H VIII
<b>B<sub>31</sub></b>	= $-y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3$	=	$-y_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \hat{\mathbf{z}}$	(4d)	H VIII
<b>B<sub>32</sub></b>	= $y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3$	=	$y_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \hat{\mathbf{z}}$	(4d)	H VIII
<b>B<sub>33</sub></b>	= $x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$x_9 a \hat{\mathbf{x}} + y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4d)	S I
<b>B<sub>34</sub></b>	= $-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$-x_9 a \hat{\mathbf{x}} - y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(4d)	S I
<b>B<sub>35</sub></b>	= $-y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3$	=	$-y_9 a \hat{\mathbf{x}} + x_9 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}}$	(4d)	S I

$$\begin{aligned}
\mathbf{B}_{36} &= y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3 &= y_9 a \hat{\mathbf{x}} - x_9 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}} & (4d) & \text{S I} \\
\mathbf{B}_{37} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= x_{10} a \hat{\mathbf{x}} + y_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}} & (4d) & \text{S II} \\
\mathbf{B}_{38} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= -x_{10} a \hat{\mathbf{x}} - y_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}} & (4d) & \text{S II} \\
\mathbf{B}_{39} &= -y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3 &= -y_{10} a \hat{\mathbf{x}} + x_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}} & (4d) & \text{S II} \\
\mathbf{B}_{40} &= y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3 &= y_{10} a \hat{\mathbf{x}} - x_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}} & (4d) & \text{S II} \\
\mathbf{B}_{41} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= x_{11} a \hat{\mathbf{x}} + y_{11} a \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}} & (4d) & \text{S III} \\
\mathbf{B}_{42} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= -x_{11} a \hat{\mathbf{x}} - y_{11} a \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}} & (4d) & \text{S III} \\
\mathbf{B}_{43} &= -y_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + \left(\frac{1}{2} + z_{11}\right) \mathbf{a}_3 &= -y_{11} a \hat{\mathbf{x}} + x_{11} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{11}\right) c \hat{\mathbf{z}} & (4d) & \text{S III} \\
\mathbf{B}_{44} &= y_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 + \left(\frac{1}{2} + z_{11}\right) \mathbf{a}_3 &= y_{11} a \hat{\mathbf{x}} - x_{11} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{11}\right) c \hat{\mathbf{z}} & (4d) & \text{S III} \\
\mathbf{B}_{45} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= x_{12} a \hat{\mathbf{x}} + y_{12} a \hat{\mathbf{y}} + z_{12} c \hat{\mathbf{z}} & (4d) & \text{S IV} \\
\mathbf{B}_{46} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= -x_{12} a \hat{\mathbf{x}} - y_{12} a \hat{\mathbf{y}} + z_{12} c \hat{\mathbf{z}} & (4d) & \text{S IV} \\
\mathbf{B}_{47} &= -y_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 + \left(\frac{1}{2} + z_{12}\right) \mathbf{a}_3 &= -y_{12} a \hat{\mathbf{x}} + x_{12} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{12}\right) c \hat{\mathbf{z}} & (4d) & \text{S IV} \\
\mathbf{B}_{48} &= y_{12} \mathbf{a}_1 - x_{12} \mathbf{a}_2 + \left(\frac{1}{2} + z_{12}\right) \mathbf{a}_3 &= y_{12} a \hat{\mathbf{x}} - x_{12} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{12}\right) c \hat{\mathbf{z}} & (4d) & \text{S IV}
\end{aligned}$$

---

#### References:

- E. Sándor and S. O. Ogunade, *Structure and Phase Transition in Solid Hydrogen and Deuterium Sulphides*, Nature **224**, 905–907 (1969), [doi:10.1038/224905b0](https://doi.org/10.1038/224905b0).

#### Found in:

- H. Shimizu, H. Yamaguchi, S. Sasaki, A. Honda, S. Endo, and M. Kobayashi, *Pressure-temperature phase diagram of solid hydrogen sulfide determined by Raman spectroscopy*, Phys. Rev. B **51**, 9391–9394 (1995), [doi:10.1103/PhysRevB.51.9391](https://doi.org/10.1103/PhysRevB.51.9391).

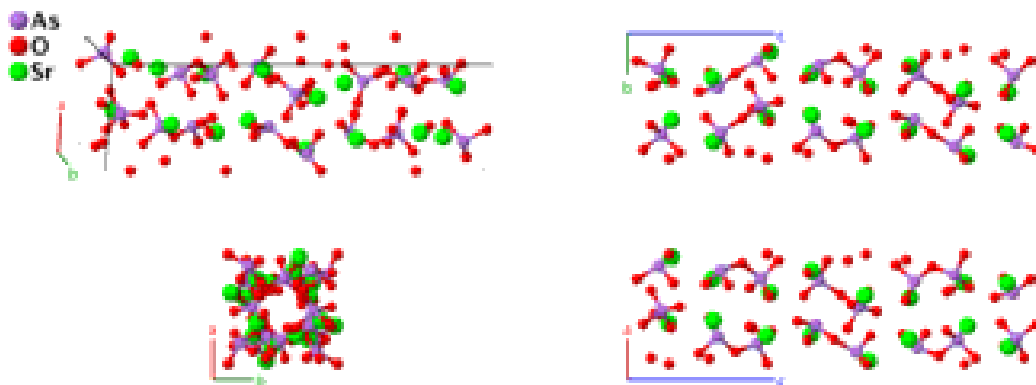
---

#### Geometry files:

- CIF: pp. 860  
- POSCAR: pp. 860



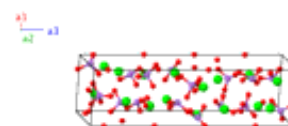
# Sr<sub>2</sub>As<sub>2</sub>O<sub>7</sub> Structure: A2B7C2\_tP88\_78\_4a\_14a\_4a



<b>Prototype</b>	:	Sr <sub>2</sub> As <sub>2</sub> O <sub>7</sub>
<b>AFLOW prototype label</b>	:	A2B7C2_tP88_78_4a_14a_4a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP88
<b>Space group number</b>	:	78
<b>Space group symbol</b>	:	<i>P</i> 4 <sub>3</sub>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B7C2_tP88_78_4a_14a_4a --params= <i>a</i> , <i>c/a</i> , <i>x</i> <sub>1</sub> , <i>y</i> <sub>1</sub> , <i>z</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>y</i> <sub>2</sub> , <i>z</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>x</i> <sub>6</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub> , <i>x</i> <sub>7</sub> , <i>y</i> <sub>7</sub> , <i>z</i> <sub>7</sub> , <i>x</i> <sub>8</sub> , <i>y</i> <sub>8</sub> , <i>z</i> <sub>8</sub> , <i>x</i> <sub>9</sub> , <i>y</i> <sub>9</sub> , <i>z</i> <sub>9</sub> , <i>x</i> <sub>10</sub> , <i>y</i> <sub>10</sub> , <i>z</i> <sub>10</sub> , <i>x</i> <sub>11</sub> , <i>y</i> <sub>11</sub> , <i>z</i> <sub>11</sub> , <i>x</i> <sub>12</sub> , <i>y</i> <sub>12</sub> , <i>z</i> <sub>12</sub> , <i>x</i> <sub>13</sub> , <i>y</i> <sub>13</sub> , <i>z</i> <sub>13</sub> , <i>x</i> <sub>14</sub> , <i>y</i> <sub>14</sub> , <i>z</i> <sub>14</sub> , <i>x</i> <sub>15</sub> , <i>y</i> <sub>15</sub> , <i>z</i> <sub>15</sub> , <i>x</i> <sub>16</sub> , <i>y</i> <sub>16</sub> , <i>z</i> <sub>16</sub> , <i>x</i> <sub>17</sub> , <i>y</i> <sub>17</sub> , <i>z</i> <sub>17</sub> , <i>x</i> <sub>18</sub> , <i>y</i> <sub>18</sub> , <i>z</i> <sub>18</sub> , <i>x</i> <sub>19</sub> , <i>y</i> <sub>19</sub> , <i>z</i> <sub>19</sub> , <i>x</i> <sub>20</sub> , <i>y</i> <sub>20</sub> , <i>z</i> <sub>20</sub> , <i>x</i> <sub>21</sub> , <i>y</i> <sub>21</sub> , <i>z</i> <sub>21</sub> , <i>x</i> <sub>22</sub> , <i>y</i> <sub>22</sub> , <i>z</i> <sub>22</sub>

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	= $x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4a)	As I
<b>B</b> <sub>2</sub>	= $-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	= $-x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4a)	As I
<b>B</b> <sub>3</sub>	= $-y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{3}{4} + z_1\right) \mathbf{a}_3$	= $-y_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_1\right) c \hat{\mathbf{z}}$	(4a)	As I
<b>B</b> <sub>4</sub>	= $y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{1}{4} + z_1\right) \mathbf{a}_3$	= $y_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_1\right) c \hat{\mathbf{z}}$	(4a)	As I
<b>B</b> <sub>5</sub>	= $x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	= $x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4a)	As II
<b>B</b> <sub>6</sub>	= $-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	= $-x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4a)	As II
<b>B</b> <sub>7</sub>	= $-y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{3}{4} + z_2\right) \mathbf{a}_3$	= $-y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_2\right) c \hat{\mathbf{z}}$	(4a)	As II
<b>B</b> <sub>8</sub>	= $y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{4} + z_2\right) \mathbf{a}_3$	= $y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_2\right) c \hat{\mathbf{z}}$	(4a)	As II
<b>B</b> <sub>9</sub>	= $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	= $x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4a)	As III
<b>B</b> <sub>10</sub>	= $-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	= $-x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4a)	As III

$\mathbf{B}_{11}$	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{3}{4} + z_3\right) \mathbf{a}_3$	$=$	$-y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_3\right) c \hat{\mathbf{z}}$	$(4a)$	As III
$\mathbf{B}_{12}$	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{4} + z_3\right) \mathbf{a}_3$	$=$	$y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_3\right) c \hat{\mathbf{z}}$	$(4a)$	As III
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	$(4a)$	As IV
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	$(4a)$	As IV
$\mathbf{B}_{15}$	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{3}{4} + z_4\right) \mathbf{a}_3$	$=$	$-y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_4\right) c \hat{\mathbf{z}}$	$(4a)$	As IV
$\mathbf{B}_{16}$	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{4} + z_4\right) \mathbf{a}_3$	$=$	$y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_4\right) c \hat{\mathbf{z}}$	$(4a)$	As IV
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	$(4a)$	O I
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	$(4a)$	O I
$\mathbf{B}_{19}$	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{3}{4} + z_5\right) \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_5\right) c \hat{\mathbf{z}}$	$(4a)$	O I
$\mathbf{B}_{20}$	$= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{4} + z_5\right) \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_5\right) c \hat{\mathbf{z}}$	$(4a)$	O I
$\mathbf{B}_{21}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	$(4a)$	O II
$\mathbf{B}_{22}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	$(4a)$	O II
$\mathbf{B}_{23}$	$= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(\frac{3}{4} + z_6\right) \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_6\right) c \hat{\mathbf{z}}$	$(4a)$	O II
$\mathbf{B}_{24}$	$= y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(\frac{1}{4} + z_6\right) \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_6\right) c \hat{\mathbf{z}}$	$(4a)$	O II
$\mathbf{B}_{25}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	$(4a)$	O III
$\mathbf{B}_{26}$	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	$(4a)$	O III
$\mathbf{B}_{27}$	$= -y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(\frac{3}{4} + z_7\right) \mathbf{a}_3$	$=$	$-y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_7\right) c \hat{\mathbf{z}}$	$(4a)$	O III
$\mathbf{B}_{28}$	$= y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(\frac{1}{4} + z_7\right) \mathbf{a}_3$	$=$	$y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_7\right) c \hat{\mathbf{z}}$	$(4a)$	O III
$\mathbf{B}_{29}$	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$x_8 a \hat{\mathbf{x}} + y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	$(4a)$	O IV
$\mathbf{B}_{30}$	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(\frac{1}{2} + z_8\right) \mathbf{a}_3$	$=$	$-x_8 a \hat{\mathbf{x}} - y_8 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_8\right) c \hat{\mathbf{z}}$	$(4a)$	O IV
$\mathbf{B}_{31}$	$= -y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + \left(\frac{3}{4} + z_8\right) \mathbf{a}_3$	$=$	$-y_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_8\right) c \hat{\mathbf{z}}$	$(4a)$	O IV
$\mathbf{B}_{32}$	$= y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + \left(\frac{1}{4} + z_8\right) \mathbf{a}_3$	$=$	$y_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_8\right) c \hat{\mathbf{z}}$	$(4a)$	O IV
$\mathbf{B}_{33}$	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$x_9 a \hat{\mathbf{x}} + y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	$(4a)$	O V
$\mathbf{B}_{34}$	$= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_3$	$=$	$-x_9 a \hat{\mathbf{x}} - y_9 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}}$	$(4a)$	O V
$\mathbf{B}_{35}$	$= -y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + \left(\frac{3}{4} + z_9\right) \mathbf{a}_3$	$=$	$-y_9 a \hat{\mathbf{x}} + x_9 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_9\right) c \hat{\mathbf{z}}$	$(4a)$	O V
$\mathbf{B}_{36}$	$= y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + \left(\frac{1}{4} + z_9\right) \mathbf{a}_3$	$=$	$y_9 a \hat{\mathbf{x}} - x_9 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_9\right) c \hat{\mathbf{z}}$	$(4a)$	O V
$\mathbf{B}_{37}$	$= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$x_{10} a \hat{\mathbf{x}} + y_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}}$	$(4a)$	O VI
$\mathbf{B}_{38}$	$= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3$	$=$	$-x_{10} a \hat{\mathbf{x}} - y_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}}$	$(4a)$	O VI
$\mathbf{B}_{39}$	$= -y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + \left(\frac{3}{4} + z_{10}\right) \mathbf{a}_3$	$=$	$-y_{10} a \hat{\mathbf{x}} + x_{10} a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_{10}\right) c \hat{\mathbf{z}}$	$(4a)$	O VI
$\mathbf{B}_{40}$	$= y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + \left(\frac{1}{4} + z_{10}\right) \mathbf{a}_3$	$=$	$y_{10} a \hat{\mathbf{x}} - x_{10} a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_{10}\right) c \hat{\mathbf{z}}$	$(4a)$	O VI
$\mathbf{B}_{41}$	$= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$x_{11} a \hat{\mathbf{x}} + y_{11} a \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}}$	$(4a)$	O VII
$\mathbf{B}_{42}$	$= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + \left(\frac{1}{2} + z_{11}\right) \mathbf{a}_3$	$=$	$-x_{11} a \hat{\mathbf{x}} - y_{11} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{11}\right) c \hat{\mathbf{z}}$	$(4a)$	O VII
$\mathbf{B}_{43}$	$= -y_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + \left(\frac{3}{4} + z_{11}\right) \mathbf{a}_3$	$=$	$-y_{11} a \hat{\mathbf{x}} + x_{11} a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_{11}\right) c \hat{\mathbf{z}}$	$(4a)$	O VII
$\mathbf{B}_{44}$	$= y_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 + \left(\frac{1}{4} + z_{11}\right) \mathbf{a}_3$	$=$	$y_{11} a \hat{\mathbf{x}} - x_{11} a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_{11}\right) c \hat{\mathbf{z}}$	$(4a)$	O VII
$\mathbf{B}_{45}$	$= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$x_{12} a \hat{\mathbf{x}} + y_{12} a \hat{\mathbf{y}} + z_{12} c \hat{\mathbf{z}}$	$(4a)$	O VIII
$\mathbf{B}_{46}$	$= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + \left(\frac{1}{2} + z_{12}\right) \mathbf{a}_3$	$=$	$-x_{12} a \hat{\mathbf{x}} - y_{12} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{12}\right) c \hat{\mathbf{z}}$	$(4a)$	O VIII



$$\begin{aligned}
\mathbf{B}_{83} &= -y_{21} \mathbf{a}_1 + x_{21} \mathbf{a}_2 + \left(\frac{3}{4} + z_{21}\right) \mathbf{a}_3 &= -y_{21}a \hat{\mathbf{x}} + x_{21}a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_{21}\right)c \hat{\mathbf{z}} && (4a) && \text{Sr III} \\
\mathbf{B}_{84} &= y_{21} \mathbf{a}_1 - x_{21} \mathbf{a}_2 + \left(\frac{1}{4} + z_{21}\right) \mathbf{a}_3 &= y_{21}a \hat{\mathbf{x}} - x_{21}a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_{21}\right)c \hat{\mathbf{z}} && (4a) && \text{Sr III} \\
\mathbf{B}_{85} &= x_{22} \mathbf{a}_1 + y_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3 &= x_{22}a \hat{\mathbf{x}} + y_{22}a \hat{\mathbf{y}} + z_{22}c \hat{\mathbf{z}} && (4a) && \text{Sr IV} \\
\mathbf{B}_{86} &= -x_{22} \mathbf{a}_1 - y_{22} \mathbf{a}_2 + \left(\frac{1}{2} + z_{22}\right) \mathbf{a}_3 &= -x_{22}a \hat{\mathbf{x}} - y_{22}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{22}\right)c \hat{\mathbf{z}} && (4a) && \text{Sr IV} \\
\mathbf{B}_{87} &= -y_{22} \mathbf{a}_1 + x_{22} \mathbf{a}_2 + \left(\frac{3}{4} + z_{22}\right) \mathbf{a}_3 &= -y_{22}a \hat{\mathbf{x}} + x_{22}a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_{22}\right)c \hat{\mathbf{z}} && (4a) && \text{Sr IV} \\
\mathbf{B}_{88} &= y_{22} \mathbf{a}_1 - x_{22} \mathbf{a}_2 + \left(\frac{1}{4} + z_{22}\right) \mathbf{a}_3 &= y_{22}a \hat{\mathbf{x}} - x_{22}a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_{22}\right)c \hat{\mathbf{z}} && (4a) && \text{Sr IV}
\end{aligned}$$

**References:**

- A. Mbarek and F. Edhokkar, *The P4<sub>3</sub> enantiomorph of Sr<sub>2</sub>As<sub>2</sub>O<sub>7</sub>*, Acta Crystallogr. E **69**, i84–i84 (2013), [doi:10.1107/S1600536813031619](https://doi.org/10.1107/S1600536813031619).

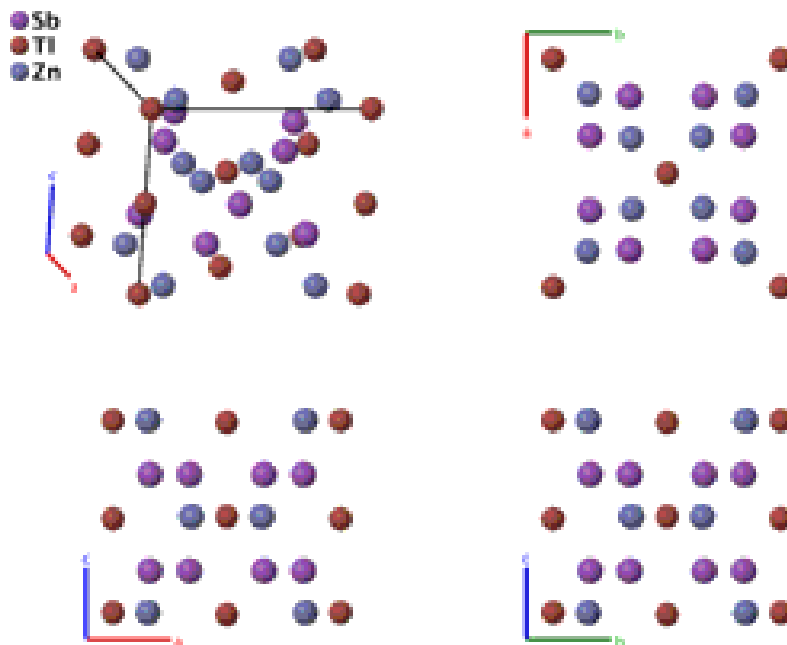
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [860](#)
- POSCAR: pp. [861](#)

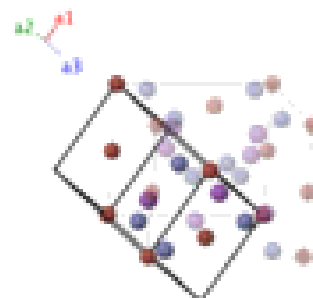
# TlZn<sub>2</sub>Sb<sub>2</sub> Structure: A2BC2\_tI20\_79\_c\_2a\_c



<b>Prototype</b>	:	TlZn <sub>2</sub> Sb <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2BC2_tI20_79_c_2a_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI20
<b>Space group number</b>	:	79
<b>Space group symbol</b>	:	I4
<b>AFLOW prototype command</b>	:	aflow --proto=A2BC2_tI20_79_c_2a_c --params=a, c/a, z <sub>1</sub> , z <sub>2</sub> , x <sub>3</sub> , y <sub>3</sub> , z <sub>3</sub> , x <sub>4</sub> , y <sub>4</sub> , z <sub>4</sub>

**Body-centered Tetragonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= z <sub>1</sub> <b>a</b> <sub>1</sub> + z <sub>1</sub> <b>a</b> <sub>2</sub>	= z <sub>1</sub> c <b>z</b> <sub>hat</sub>	(2a)	Tl I
<b>B<sub>2</sub></b>	= z <sub>2</sub> <b>a</b> <sub>1</sub> + z <sub>2</sub> <b>a</b> <sub>2</sub>	= z <sub>2</sub> c <b>z</b> <sub>hat</sub>	(2a)	Tl II
<b>B<sub>3</sub></b>	= (y <sub>3</sub> + z <sub>3</sub> ) <b>a</b> <sub>1</sub> + (x <sub>3</sub> + z <sub>3</sub> ) <b>a</b> <sub>2</sub> + (x <sub>3</sub> + y <sub>3</sub> ) <b>a</b> <sub>3</sub>	= x <sub>3</sub> a <b>x</b> <sub>hat</sub> + y <sub>3</sub> a <b>y</b> <sub>hat</sub> + z <sub>3</sub> c <b>z</b> <sub>hat</sub>	(8c)	Sb
<b>B<sub>4</sub></b>	= (-y <sub>3</sub> + z <sub>3</sub> ) <b>a</b> <sub>1</sub> + (-x <sub>3</sub> + z <sub>3</sub> ) <b>a</b> <sub>2</sub> + (-x <sub>3</sub> - y <sub>3</sub> ) <b>a</b> <sub>3</sub>	= -x <sub>3</sub> a <b>x</b> <sub>hat</sub> - y <sub>3</sub> a <b>y</b> <sub>hat</sub> + z <sub>3</sub> c <b>z</b> <sub>hat</sub>	(8c)	Sb

$$\begin{aligned}
\mathbf{B}_5 &= (x_3 + z_3) \mathbf{a}_1 + (-y_3 + z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3 = -y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8c) & \text{Sb} \\
\mathbf{B}_6 &= (-x_3 + z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 + (-x_3 + y_3) \mathbf{a}_3 = y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8c) & \text{Sb} \\
\mathbf{B}_7 &= (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3 = x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8c) & \text{Zn} \\
\mathbf{B}_8 &= (-y_4 + z_4) \mathbf{a}_1 + (-x_4 + z_4) \mathbf{a}_2 + (-x_4 - y_4) \mathbf{a}_3 = -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8c) & \text{Zn} \\
\mathbf{B}_9 &= (x_4 + z_4) \mathbf{a}_1 + (-y_4 + z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3 = -y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8c) & \text{Zn} \\
\mathbf{B}_{10} &= (-x_4 + z_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + (-x_4 + y_4) \mathbf{a}_3 = y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8c) & \text{Zn}
\end{aligned}$$

---

#### References:

- A. Czybulka, B. Krenkel, and H.-U. Schuster, *Ternäre zintl-Verbindungen mit thallium als elektronendonator*, J. Less-Common Met. **137**, 311–322 (1988), doi:10.1016/0022-5088(88)90096-3.

#### Found in:

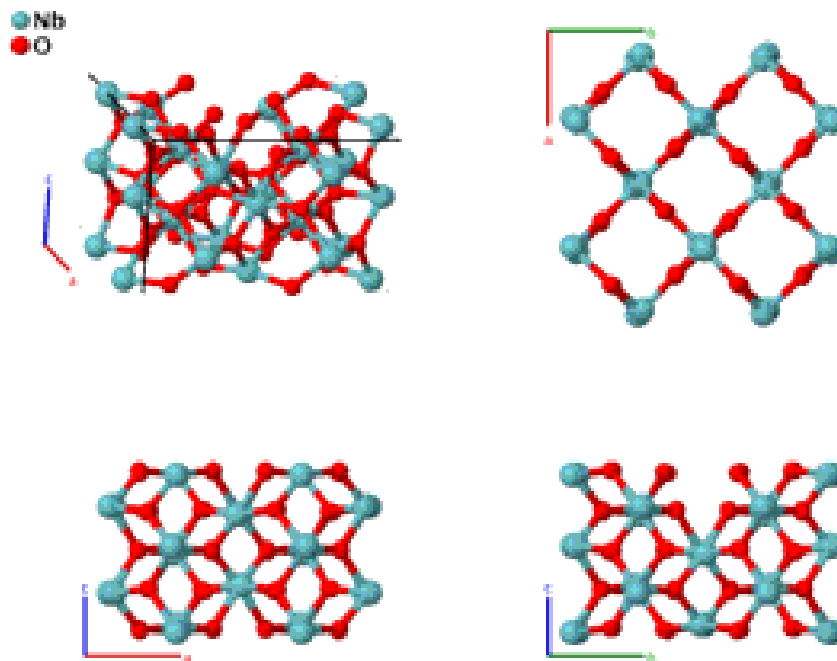
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [861](#)  
- POSCAR: pp. [862](#)

# $\beta$ -NbO<sub>2</sub> Structure: AB2\_tI48\_80\_2b\_4b

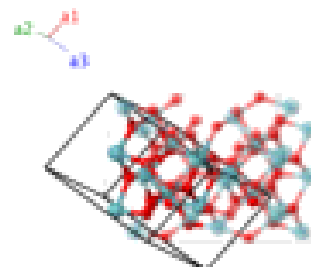


<b>Prototype</b>	:	$\beta$ -NbO <sub>2</sub>
<b>AFLOW prototype label</b>	:	AB2_tI48_80_2b_4b
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI48
<b>Space group number</b>	:	80
<b>Space group symbol</b>	:	$I4_1$
<b>AFLOW prototype command</b>	:	aflow --proto=AB2_tI48_80_2b_4b --params= $a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- This crystal is not quite stoichiometric. The actual composition was found to be NbO<sub>2-x</sub>, where  $0.002 \leq x \leq 0.01$ .

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= (y_1 + z_1) \mathbf{a}_1 + (x_1 + z_1) \mathbf{a}_2 + (x_1 + y_1) \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8b)	Nb I





$$\mathbf{B}_{24} = \begin{pmatrix} \frac{3}{4} - x_6 + z_6 \\ \frac{1}{4} + y_6 + z_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - x_6 + y_6 \\ \frac{1}{2} - x_6 + y_6 \end{pmatrix} \mathbf{a}_3 = y_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_6\right) c \hat{\mathbf{z}} \quad (8b) \quad \text{O IV}$$

**References:**

- H.-J. Schweizer and R. Gruehn, *Zur Darstellung und Kristallstruktur von  $\beta\text{-NbO}_2$  / Synthesis and Crystal Structure of  $\beta\text{-NbO}_2$* , Z. Naturforsch. B **37**, 1361–1368 (1982), [doi:10.1515/znb-1982-1101](https://doi.org/10.1515/znb-1982-1101).

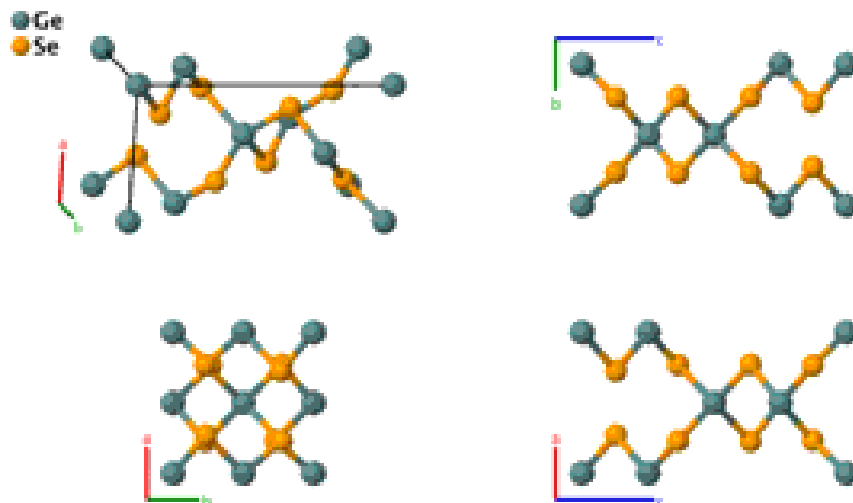
**Found in:**

- P. Villars and L. D. Calvert, eds., *Pearson's Handbook of Crystallographic Data* (ASM International, Materials Park OH, 1991), vol. IV, chap. , p. 4535.

**Geometry files:**

- CIF: pp. [862](#)
- POSCAR: pp. [862](#)

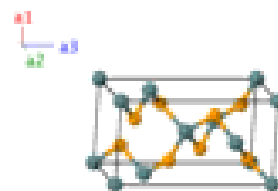
# GeSe<sub>2</sub> (High-pressure) Structure: AB2\_tP12\_81\_adg\_2h



<b>Prototype</b>	:	GeSe <sub>2</sub>
<b>AFLOW prototype label</b>	:	AB2_tP12_81_adg_2h
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP12
<b>Space group number</b>	:	81
<b>Space group symbol</b>	:	$P\bar{4}$
<b>AFLOW prototype command</b>	:	aflow --proto=AB2_tP12_81_adg_2h --params=a, c/a, z <sub>3</sub> , x <sub>4</sub> , y <sub>4</sub> , z <sub>4</sub> , x <sub>5</sub> , y <sub>5</sub> , z <sub>5</sub>

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Ge I
<b>B<sub>2</sub></b>	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(1d)	Ge II
<b>B<sub>3</sub></b>	$= \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2g)	Ge III
<b>B<sub>4</sub></b>	$= \frac{1}{2} \mathbf{a}_1 + -z_3 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + -z_3 c \hat{\mathbf{z}}$	(2g)	Ge III
<b>B<sub>5</sub></b>	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4h)	Se I
<b>B<sub>6</sub></b>	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4h)	Se I
<b>B<sub>7</sub></b>	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$= y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(4h)	Se I
<b>B<sub>8</sub></b>	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$= -y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(4h)	Se I

$$\mathbf{B}_9 = x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} \quad (4h) \quad \text{Se II}$$

$$\mathbf{B}_{10} = -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = -x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} \quad (4h) \quad \text{Se II}$$

$$\mathbf{B}_{11} = y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} \quad (4h) \quad \text{Se II}$$

$$\mathbf{B}_{12} = -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = -y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} \quad (4h) \quad \text{Se II}$$

---

**References:**

- A. Grzechnik, S. Stølen, E. Bakken, T. Grande, and M. Mezouar, *Structural transformations in three-dimensional crystalline GeSe<sub>2</sub> at high pressures and high temperatures*, J. Solid State Chem. **150**, 121–127 (2000), [doi:10.1006/jssc.1999.8557](https://doi.org/10.1006/jssc.1999.8557).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

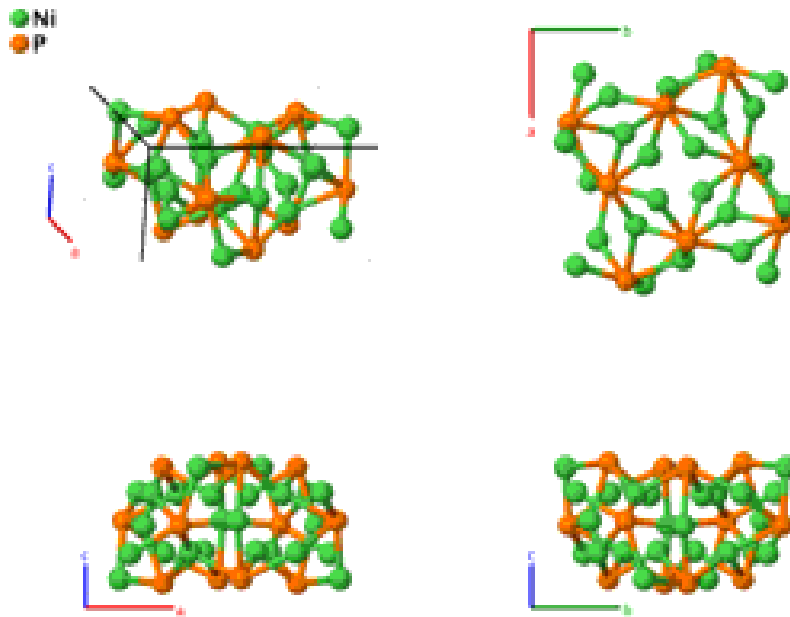
---

**Geometry files:**

- CIF: pp. [862](#)

- POSCAR: pp. [863](#)

# Ni<sub>3</sub>P (*D*0<sub>e</sub>) Structure: A3B\_tI32\_82\_3g\_g



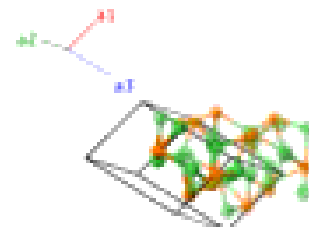
<b>Prototype</b>	:	Ni <sub>3</sub> P
<b>AFLOW prototype label</b>	:	A3B_tI32_82_3g_g
<b>Strukturbericht designation</b>	:	<i>D</i> 0 <sub>e</sub>
<b>Pearson symbol</b>	:	tI32
<b>Space group number</b>	:	82
<b>Space group symbol</b>	:	<i>I</i> $\bar{4}$
<b>AFLOW prototype command</b>	:	aflow --proto=A3B_tI32_82_3g_g --params= <i>a</i> , <i>c/a</i> , <i>x</i> <sub>1</sub> , <i>y</i> <sub>1</sub> , <i>z</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>y</i> <sub>2</sub> , <i>z</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub>

## Other compounds with this structure:

- Cr<sub>3</sub>P, Fe<sub>3</sub>P, Mn<sub>3</sub>P, Mo<sub>3</sub>P, Ti<sub>3</sub>P, V<sub>3</sub>P, BFe<sub>3</sub>

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$(y_1 + z_1) \mathbf{a}_1 + (x_1 + z_1) \mathbf{a}_2 + (x_1 + y_1) \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8g)	Ni I

$\mathbf{B}_2$	$=$	$(-y_1 + z_1) \mathbf{a}_1 + (-x_1 + z_1) \mathbf{a}_2 + (-x_1 - y_1) \mathbf{a}_3$	$=$	$-x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	$(8g)$	Ni I
$\mathbf{B}_3$	$=$	$(-x_1 - z_1) \mathbf{a}_1 + (y_1 - z_1) \mathbf{a}_2 + (-x_1 + y_1) \mathbf{a}_3$	$=$	$y_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	$(8g)$	Ni I
$\mathbf{B}_4$	$=$	$(x_1 - z_1) \mathbf{a}_1 + (-y_1 - z_1) \mathbf{a}_2 + (x_1 - y_1) \mathbf{a}_3$	$=$	$-y_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	$(8g)$	Ni I
$\mathbf{B}_5$	$=$	$(y_2 + z_2) \mathbf{a}_1 + (x_2 + z_2) \mathbf{a}_2 + (x_2 + y_2) \mathbf{a}_3$	$=$	$x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	$(8g)$	Ni II
$\mathbf{B}_6$	$=$	$(-y_2 + z_2) \mathbf{a}_1 + (-x_2 + z_2) \mathbf{a}_2 + (-x_2 - y_2) \mathbf{a}_3$	$=$	$-x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	$(8g)$	Ni II
$\mathbf{B}_7$	$=$	$(-x_2 - z_2) \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (-x_2 + y_2) \mathbf{a}_3$	$=$	$y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	$(8g)$	Ni II
$\mathbf{B}_8$	$=$	$(x_2 - z_2) \mathbf{a}_1 + (-y_2 - z_2) \mathbf{a}_2 + (x_2 - y_2) \mathbf{a}_3$	$=$	$-y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	$(8g)$	Ni II
$\mathbf{B}_9$	$=$	$(y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	$(8g)$	Ni III
$\mathbf{B}_{10}$	$=$	$(-y_3 + z_3) \mathbf{a}_1 + (-x_3 + z_3) \mathbf{a}_2 + (-x_3 - y_3) \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	$(8g)$	Ni III
$\mathbf{B}_{11}$	$=$	$(-x_3 - z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (-x_3 + y_3) \mathbf{a}_3$	$=$	$y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	$(8g)$	Ni III
$\mathbf{B}_{12}$	$=$	$(x_3 - z_3) \mathbf{a}_1 + (-y_3 - z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$-y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	$(8g)$	Ni III
$\mathbf{B}_{13}$	$=$	$(y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	$(8g)$	P
$\mathbf{B}_{14}$	$=$	$(-y_4 + z_4) \mathbf{a}_1 + (-x_4 + z_4) \mathbf{a}_2 + (-x_4 - y_4) \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	$(8g)$	P
$\mathbf{B}_{15}$	$=$	$(-x_4 - z_4) \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (-x_4 + y_4) \mathbf{a}_3$	$=$	$y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	$(8g)$	P
$\mathbf{B}_{16}$	$=$	$(x_4 - z_4) \mathbf{a}_1 + (-y_4 - z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	$=$	$-y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	$(8g)$	P

---

#### References:

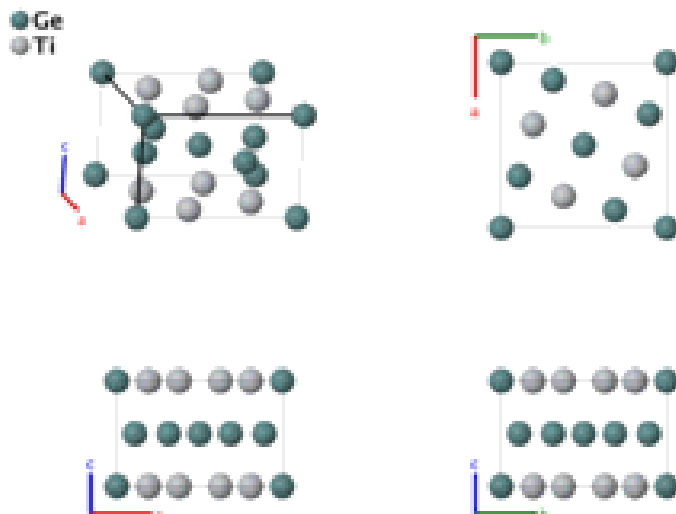
- S. Rundqvist, E. Hassler, and L. Lundvik, *Refinement of the Ni<sub>3</sub>P Structure*, Acta Chem. Scand. **16**, 242–243 (1962), [doi:10.3891/acta.chem.scand.16-0242](https://doi.org/10.3891/acta.chem.scand.16-0242).

---

#### Geometry files:

- CIF: pp. [863](#)  
- POSCAR: pp. [863](#)

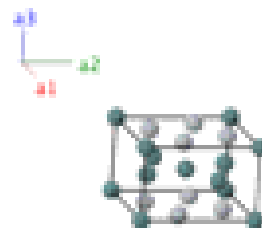
# Ti<sub>2</sub>Ge<sub>3</sub> Structure: A3B2\_tP10\_83\_adk\_j



<b>Prototype</b>	:	Ti <sub>2</sub> Ge <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B2_tP10_83_adk_j
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP10
<b>Space group number</b>	:	83
<b>Space group symbol</b>	:	<i>P4/m</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3B2_tP10_83_adk_j --params= <i>a, c/a, x<sub>3</sub>, y<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub></i>

**Simple Tetragonal primitive vectors:**

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= 0 <b>a</b> <sub>1</sub> + 0 <b>a</b> <sub>2</sub> + 0 <b>a</b> <sub>3</sub>	= 0 <b>x̂</b> + 0 <b>ŷ</b> + 0 <b>ẑ</b>	(1 <i>a</i> )	Ge I
<b>B<sub>2</sub></b>	= $\frac{1}{2}$ <b>a</b> <sub>1</sub> + $\frac{1}{2}$ <b>a</b> <sub>2</sub> + $\frac{1}{2}$ <b>a</b> <sub>3</sub>	= $\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(1 <i>d</i> )	Ge II
<b>B<sub>3</sub></b>	= $x_3$ <b>a</b> <sub>1</sub> + $y_3$ <b>a</b> <sub>2</sub>	= $x_3a \hat{\mathbf{x}} + y_3a \hat{\mathbf{y}}$	(4 <i>j</i> )	Ti
<b>B<sub>4</sub></b>	= $-x_3$ <b>a</b> <sub>1</sub> - $y_3$ <b>a</b> <sub>2</sub>	= $-x_3a \hat{\mathbf{x}} - y_3a \hat{\mathbf{y}}$	(4 <i>j</i> )	Ti
<b>B<sub>5</sub></b>	= $-y_3$ <b>a</b> <sub>1</sub> + $x_3$ <b>a</b> <sub>2</sub>	= $-y_3a \hat{\mathbf{x}} + x_3a \hat{\mathbf{y}}$	(4 <i>j</i> )	Ti
<b>B<sub>6</sub></b>	= $y_3$ <b>a</b> <sub>1</sub> - $x_3$ <b>a</b> <sub>2</sub>	= $y_3a \hat{\mathbf{x}} - x_3a \hat{\mathbf{y}}$	(4 <i>j</i> )	Ti

$$\mathbf{B}_7 = x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \quad (4k) \quad \text{Ge III}$$

$$\mathbf{B}_8 = -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \quad (4k) \quad \text{Ge III}$$

$$\mathbf{B}_9 = -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \quad (4k) \quad \text{Ge III}$$

$$\mathbf{B}_{10} = y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \quad (4k) \quad \text{Ge III}$$

---

**References:**

- K. Schubert, H. G. Meissner, M. Pötzschke, W. Rossteutscher, and E. Stolz, *Einige Strukturdaten metallischer Phasen (7)*, *Naturwissenschaften* **49**, 57–57 (1962), [doi:10.1007/BF00595382](https://doi.org/10.1007/BF00595382).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

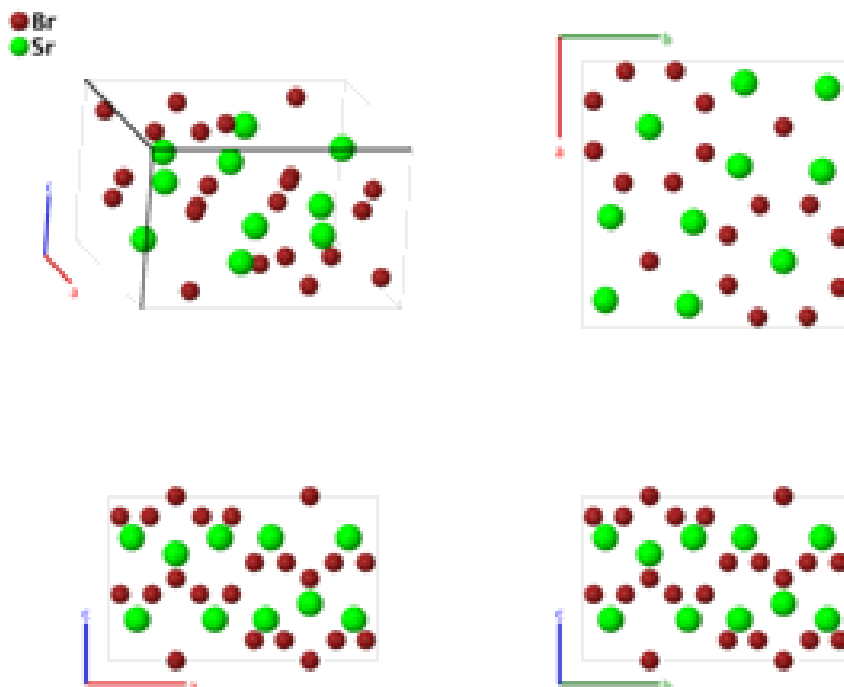
---

**Geometry files:**

- CIF: pp. [863](#)

- POSCAR: pp. [864](#)

# SrBr<sub>2</sub> Structure: A2B\_tP30\_85\_ab2g\_cg

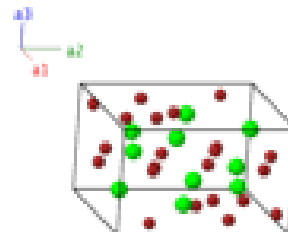


<b>Prototype</b>	:	SrBr <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_tP30_85_ab2g_cg
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP30
<b>Space group number</b>	:	85
<b>Space group symbol</b>	:	<i>P4/n</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A2B_tP30_85_ab2g_cg --params=a, c/a, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6</code>

- Using the work of (Kamermans, 1939), (Herrmann, 1943) designated the structure SrBr<sub>2</sub> as *Strukturbericht C53*, and placed it in space group *Pnma* #62. (Sass, 1963) pointed out that the structure proposed by Kamermans did not agree with powder diffraction data, and proposed this structure, also found by (Frit, 1969). (Parthé, 1993) gives the current structure the *C53* designation. We will follow the original *Strukturbericht*, and give the *C53* designation to the *Pnma* structure.

## Simple Tetragonal primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= a \hat{y} \\ \mathbf{a}_3 &= c \hat{z}\end{aligned}$$



## Basis vectors:



	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(2a)	Br I
<b>B</b> <sub>2</sub>	= $\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	=	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(2a)	Br I
<b>B</b> <sub>3</sub>	= $\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2b)	Br II
<b>B</b> <sub>4</sub>	= $\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2b)	Br II
<b>B</b> <sub>5</sub>	= $\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2c)	Sr I
<b>B</b> <sub>6</sub>	= $\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(2c)	Sr I
<b>B</b> <sub>7</sub>	= $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8g)	Br III
<b>B</b> <sub>8</sub>	= $(\frac{1}{2} - x_4) \mathbf{a}_1 + (\frac{1}{2} - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(\frac{1}{2} - x_4) a \hat{\mathbf{x}} + (\frac{1}{2} - y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8g)	Br III
<b>B</b> <sub>9</sub>	= $(\frac{1}{2} - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(\frac{1}{2} - y_4) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8g)	Br III
<b>B</b> <sub>10</sub>	= $y_4 \mathbf{a}_1 + (\frac{1}{2} - x_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$y_4 a \hat{\mathbf{x}} + (\frac{1}{2} - x_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8g)	Br III
<b>B</b> <sub>11</sub>	= $-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(8g)	Br III
<b>B</b> <sub>12</sub>	= $(\frac{1}{2} + x_4) \mathbf{a}_1 + (\frac{1}{2} + y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$(\frac{1}{2} + x_4) a \hat{\mathbf{x}} + (\frac{1}{2} + y_4) a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(8g)	Br III
<b>B</b> <sub>13</sub>	= $(\frac{1}{2} + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$(\frac{1}{2} + y_4) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(8g)	Br III
<b>B</b> <sub>14</sub>	= $-y_4 \mathbf{a}_1 + (\frac{1}{2} + x_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-y_4 a \hat{\mathbf{x}} + (\frac{1}{2} + x_4) a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(8g)	Br III
<b>B</b> <sub>15</sub>	= $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8g)	Br IV
<b>B</b> <sub>16</sub>	= $(\frac{1}{2} - x_5) \mathbf{a}_1 + (\frac{1}{2} - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(\frac{1}{2} - x_5) a \hat{\mathbf{x}} + (\frac{1}{2} - y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8g)	Br IV
<b>B</b> <sub>17</sub>	= $(\frac{1}{2} - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(\frac{1}{2} - y_5) a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8g)	Br IV
<b>B</b> <sub>18</sub>	= $y_5 \mathbf{a}_1 + (\frac{1}{2} - x_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$y_5 a \hat{\mathbf{x}} + (\frac{1}{2} - x_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8g)	Br IV
<b>B</b> <sub>19</sub>	= $-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(8g)	Br IV
<b>B</b> <sub>20</sub>	= $(\frac{1}{2} + x_5) \mathbf{a}_1 + (\frac{1}{2} + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$(\frac{1}{2} + x_5) a \hat{\mathbf{x}} + (\frac{1}{2} + y_5) a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(8g)	Br IV
<b>B</b> <sub>21</sub>	= $(\frac{1}{2} + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$(\frac{1}{2} + y_5) a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(8g)	Br IV
<b>B</b> <sub>22</sub>	= $-y_5 \mathbf{a}_1 + (\frac{1}{2} + x_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-y_5 a \hat{\mathbf{x}} + (\frac{1}{2} + x_5) a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(8g)	Br IV
<b>B</b> <sub>23</sub>	= $x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8g)	Sr II
<b>B</b> <sub>24</sub>	= $(\frac{1}{2} - x_6) \mathbf{a}_1 + (\frac{1}{2} - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(\frac{1}{2} - x_6) a \hat{\mathbf{x}} + (\frac{1}{2} - y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8g)	Sr II
<b>B</b> <sub>25</sub>	= $(\frac{1}{2} - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(\frac{1}{2} - y_6) a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8g)	Sr II
<b>B</b> <sub>26</sub>	= $y_6 \mathbf{a}_1 + (\frac{1}{2} - x_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$y_6 a \hat{\mathbf{x}} + (\frac{1}{2} - x_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8g)	Sr II
<b>B</b> <sub>27</sub>	= $-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(8g)	Sr II
<b>B</b> <sub>28</sub>	= $(\frac{1}{2} + x_6) \mathbf{a}_1 + (\frac{1}{2} + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$(\frac{1}{2} + x_6) a \hat{\mathbf{x}} + (\frac{1}{2} + y_6) a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(8g)	Sr II
<b>B</b> <sub>29</sub>	= $(\frac{1}{2} + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$(\frac{1}{2} + y_6) a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(8g)	Sr II
<b>B</b> <sub>30</sub>	= $-y_6 \mathbf{a}_1 + (\frac{1}{2} + x_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-y_6 a \hat{\mathbf{x}} + (\frac{1}{2} + x_6) a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(8g)	Sr II

## References:

- B. Frit and M. M. Chbany, *Les halogeno-carbonates de strontium*, J. Inorg. Nucl. Chem. **31**, 2685–2693 (1969), [doi:10.1016/0022-1902\(69\)80182-X](https://doi.org/10.1016/0022-1902(69)80182-X).
- K. Herrmann, ed., *Strukturbericht Band VII 1939* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1943).
- M. A. Kamermans, *The Crystal Structure of SrBr<sub>2</sub>*, Zeitschrift für Kristallographie - Crystalline Materials **101**, 406–411 (1939), [doi:10.1524/zkri.1939.101.1.406](https://doi.org/10.1524/zkri.1939.101.1.406).

- R. L. Sass, T. Brackett, and E. Brackett, *The Crystal Structure of Strontium Bromide*, J. Phys. Chem. **67**, 2862–2863 (1963), [doi:10.1021/j100806a516](https://doi.org/10.1021/j100806a516).
- E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types*, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., [doi:10.1007/978-3-662-02909-1\\_3](https://doi.org/10.1007/978-3-662-02909-1_3).

**Found in:**

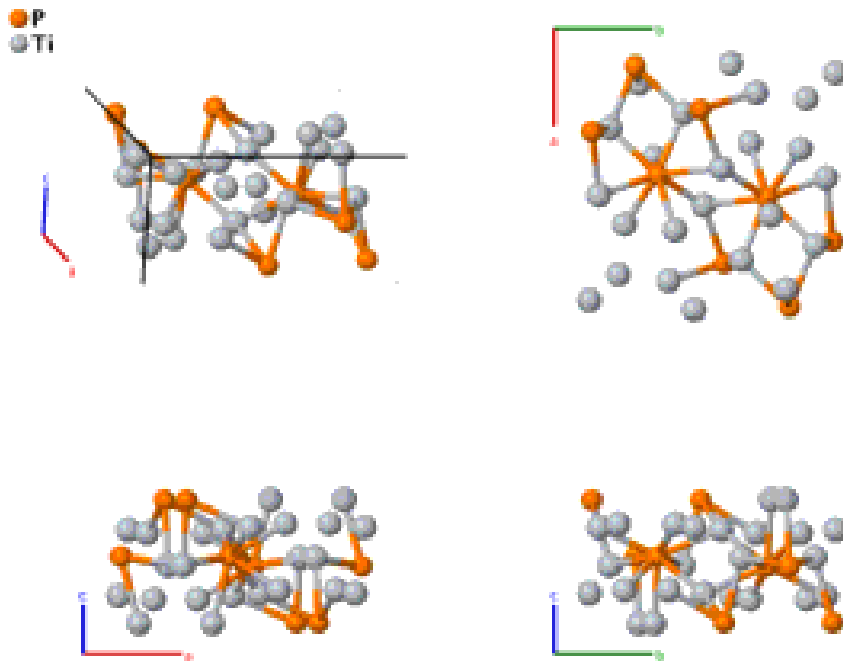
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [864](#)
- POSCAR: pp. [864](#)

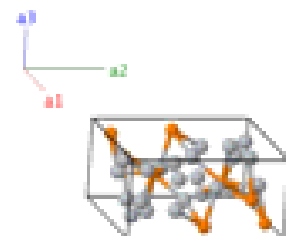
# Ti<sub>3</sub>P Structure: AB3\_tP32\_86\_g\_3g



**Prototype** : Ti<sub>3</sub>P  
**AFLOW prototype label** : AB3\_tP32\_86\_g\_3g  
**Strukturbericht designation** : None  
**Pearson symbol** : tP32  
**Space group number** : 86  
**Space group symbol** :  $P4_2/n$   
**AFLOW prototype command** : aflow --proto=AB3\_tP32\_86\_g\_3g  
 --params= $a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

Simple Tetragonal primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8g)	P
$\mathbf{B}_2$	$= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8g)	P

$$\begin{aligned}
\mathbf{B}_3 &= -y_1 \mathbf{a}_1 + \left(\frac{1}{2} + x_1\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3 = -y_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}} & (8g) & \text{P} \\
\mathbf{B}_4 &= \left(\frac{1}{2} + y_1\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_1\right) a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}} & (8g) & \text{P} \\
\mathbf{B}_5 &= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3 = -x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}} & (8g) & \text{P} \\
\mathbf{B}_6 &= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_2 - z_1 \mathbf{a}_3 = \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right) a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}} & (8g) & \text{P} \\
\mathbf{B}_7 &= y_1 \mathbf{a}_1 + \left(\frac{1}{2} - x_1\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3 = y_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}} & (8g) & \text{P} \\
\mathbf{B}_8 &= \left(\frac{1}{2} - y_1\right) \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3 = \left(\frac{1}{2} - y_1\right) a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}} & (8g) & \text{P} \\
\mathbf{B}_9 &= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 = x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (8g) & \text{Ti I} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 + z_2 \mathbf{a}_3 = \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (8g) & \text{Ti I} \\
\mathbf{B}_{11} &= -y_2 \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = -y_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (8g) & \text{Ti I} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + y_2\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (8g) & \text{Ti I} \\
\mathbf{B}_{13} &= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} & (8g) & \text{Ti I} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 - z_2 \mathbf{a}_3 = \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} & (8g) & \text{Ti I} \\
\mathbf{B}_{15} &= y_2 \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 = y_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} & (8g) & \text{Ti I} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} - y_2\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 = \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} & (8g) & \text{Ti I} \\
\mathbf{B}_{17} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8g) & \text{Ti II} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 = \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8g) & \text{Ti II} \\
\mathbf{B}_{19} &= -y_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = -y_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (8g) & \text{Ti II} \\
\mathbf{B}_{20} &= \left(\frac{1}{2} + y_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (8g) & \text{Ti II} \\
\mathbf{B}_{21} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = -x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8g) & \text{Ti II} \\
\mathbf{B}_{22} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 = \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8g) & \text{Ti II} \\
\mathbf{B}_{23} &= y_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = y_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (8g) & \text{Ti II} \\
\mathbf{B}_{24} &= \left(\frac{1}{2} - y_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (8g) & \text{Ti II} \\
\mathbf{B}_{25} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8g) & \text{Ti III} \\
\mathbf{B}_{26} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3 = \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8g) & \text{Ti III} \\
\mathbf{B}_{27} &= -y_4 \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = -y_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (8g) & \text{Ti III} \\
\mathbf{B}_{28} &= \left(\frac{1}{2} + y_4\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (8g) & \text{Ti III} \\
\mathbf{B}_{29} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8g) & \text{Ti III} \\
\mathbf{B}_{30} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 - z_4 \mathbf{a}_3 = \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8g) & \text{Ti III} \\
\mathbf{B}_{31} &= y_4 \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 = y_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (8g) & \text{Ti III} \\
\mathbf{B}_{32} &= \left(\frac{1}{2} - y_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (8g) & \text{Ti III}
\end{aligned}$$

## References:

- V. N. Eremenko and V. E. Listovnichii, *State diagram of the Ti-P system*, Dopov. Akad. Nauk Ukr. RSR pp. 1176–1179 (1965).

## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

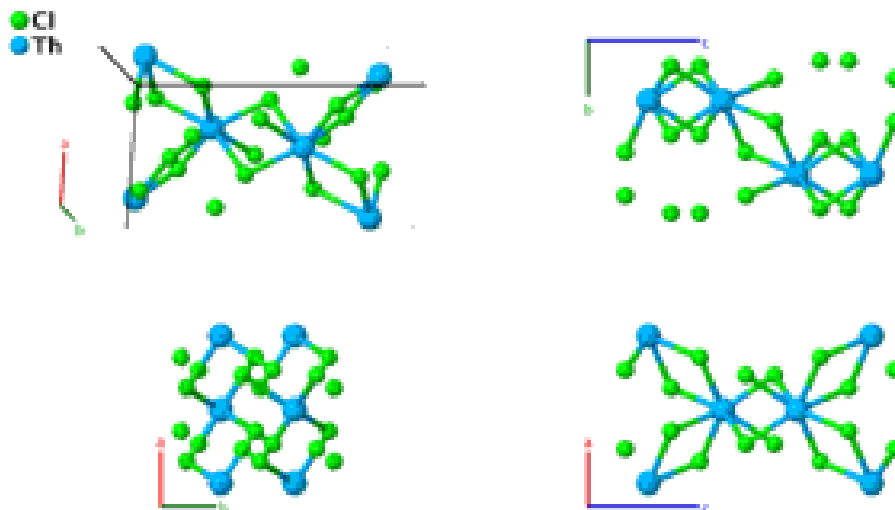
---

**Geometry files:**

- CIF: pp. [865](#)

- POSCAR: pp. [865](#)

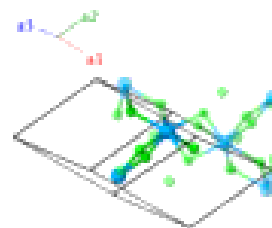
# ThCl<sub>4</sub> Structure: A4B\_tI20\_88\_f\_a



**Prototype** : ThCl<sub>4</sub>  
**AFLOW prototype label** : A4B\_tI20\_88\_f\_a  
**Strukturbericht designation** : None  
**Pearson symbol** : tI20  
**Space group number** : 88  
**Space group symbol** : *I4*<sub>1</sub>/*a*  
**AFLOW prototype command** : aflow --proto=A4B\_tI20\_88\_f\_a  
 --params=*a, c/a, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>*

**Body-centered Tetragonal primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\
 \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= \frac{3}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$= \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{8}c\hat{\mathbf{z}}$	(4 <i>a</i> )	Th
<b>B<sub>2</sub></b>	$= \frac{5}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}c\hat{\mathbf{z}}$	(4 <i>a</i> )	Th
<b>B<sub>3</sub></b>	$= (y_2 + z_2)\mathbf{a}_1 + (x_2 + z_2)\mathbf{a}_2 + (x_2 + y_2)\mathbf{a}_3$	$= x_2a\hat{\mathbf{x}} + y_2a\hat{\mathbf{y}} + z_2c\hat{\mathbf{z}}$	(16 <i>f</i> )	Cl
<b>B<sub>4</sub></b>	$= \left(\frac{1}{2} - y_2 + z_2\right)\mathbf{a}_1 + (-x_2 + z_2)\mathbf{a}_2 + \left(\frac{1}{2} - x_2 - y_2\right)\mathbf{a}_3$	$= -x_2a\hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right)a\hat{\mathbf{y}} + z_2c\hat{\mathbf{z}}$	(16 <i>f</i> )	Cl
<b>B<sub>5</sub></b>	$= \left(\frac{1}{2} + x_2 + z_2\right)\mathbf{a}_1 + (-y_2 + z_2)\mathbf{a}_2 + (x_2 - y_2)\mathbf{a}_3$	$= \left(\frac{3}{4} - y_2\right)a\hat{\mathbf{x}} + \left(\frac{1}{4} + x_2\right)a\hat{\mathbf{y}} + \left(\frac{1}{4} + z_2\right)c\hat{\mathbf{z}}$	(16 <i>f</i> )	Cl

$$\mathbf{B}_6 = \begin{pmatrix} \frac{1}{2} - x_2 + z_2 \\ \frac{1}{2} + y_2 + z_2 \\ \frac{1}{2} - x_2 + y_2 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \\ \\ \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \\ \\ \end{pmatrix} \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} + y_2 \\ \frac{1}{4} + z_2 \\ \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} - x_2 \\ \\ \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (16f) \quad \text{Cl}$$

$$\mathbf{B}_7 = \begin{pmatrix} -y_2 - z_2 \\ -x_2 - z_2 \\ -x_2 - y_2 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} -x_2 - z_2 \\ \\ \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \\ \\ \end{pmatrix} \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} \quad (16f) \quad \text{Cl}$$

$$\mathbf{B}_8 = \begin{pmatrix} \frac{1}{2} + y_2 - z_2 \\ \frac{1}{2} + x_2 + y_2 \\ \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_2 - z_2 \\ \\ \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \\ \\ \end{pmatrix} \mathbf{a}_3 = x_2 a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_2 \\ \\ \end{pmatrix} a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} \quad (16f) \quad \text{Cl}$$

$$\mathbf{B}_9 = \begin{pmatrix} \frac{1}{2} - x_2 - z_2 \\ -x_2 + y_2 \\ \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_2 - z_2 \\ \\ \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \\ \\ \end{pmatrix} \mathbf{a}_3 = \begin{pmatrix} -\frac{1}{4} + y_2 \\ \frac{1}{4} - z_2 \\ \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} - x_2 \\ \\ \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (16f) \quad \text{Cl}$$

$$\mathbf{B}_{10} = \begin{pmatrix} \frac{1}{2} + x_2 - z_2 \\ \frac{1}{2} - y_2 - z_2 \\ \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \\ \\ \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} + x_2 - y_2 \\ \\ \end{pmatrix} \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} - y_2 \\ \frac{1}{4} - z_2 \\ \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + x_2 \\ \\ \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (16f) \quad \text{Cl}$$

### References:

- J. T. Mason, M. C. Jha, and P. Chiotti, *Crystal structures of ThCl<sub>4</sub> polymorphs*, J. Less-Common Met. **34**, 143–151 (1974), doi:10.1016/0022-5088(74)90224-0.

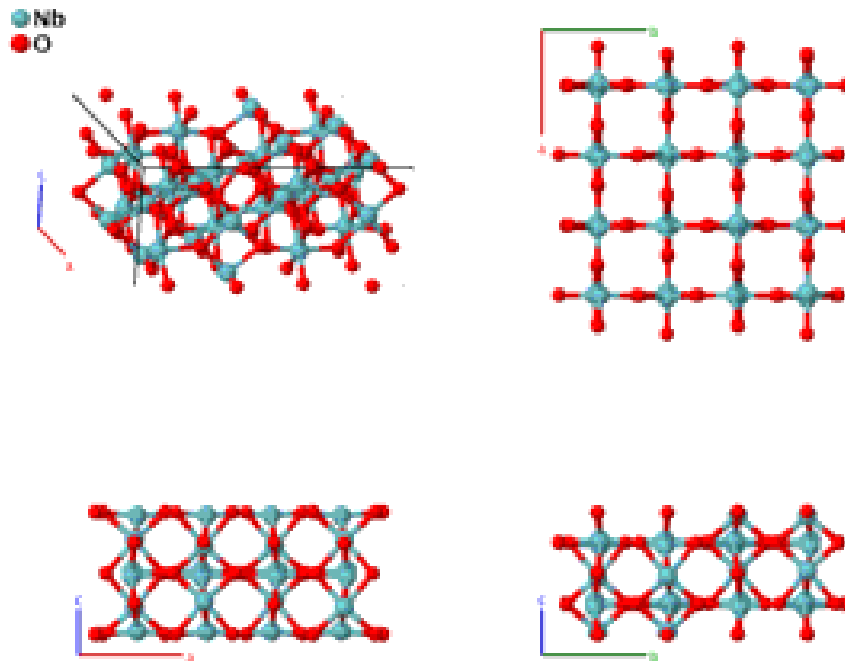
### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

### Geometry files:

- CIF: pp. 865
- POSCAR: pp. 865

# $\alpha$ -NbO<sub>2</sub> Structure: AB2\_tI96\_88\_2f\_4f

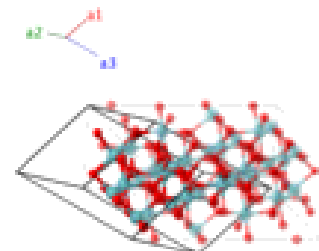


<b>Prototype</b>	:	$\alpha$ -NbO <sub>2</sub>
<b>AFLOW prototype label</b>	:	AB2_tI96_88_2f_4f
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI96
<b>Space group number</b>	:	88
<b>Space group symbol</b>	:	$I4_1/a$
<b>AFLOW prototype command</b>	:	aflow --proto=AB2_tI96_88_2f_4f --params= $a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- Although Bolzan *et al.* (Bolzan, 1994) also gives structural information  $\alpha$ -NbO<sub>2</sub>, Pynn *et al.* (Pynn, 1996) is the only reference we found which unambiguously states that this structure is reported in setting 2 of space group #88.

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:



	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= (y_1 + z_1) \mathbf{a}_1 + (x_1 + z_1) \mathbf{a}_2 + (x_1 + y_1) \mathbf{a}_3$	$=$	$x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(16f)	Nb I
<b>B<sub>2</sub></b>	$= \left(\frac{1}{2} - y_1 + z_1\right) \mathbf{a}_1 + (-x_1 + z_1) \mathbf{a}_2 + \left(\frac{1}{2} - x_1 - y_1\right) \mathbf{a}_3$	$=$	$-x_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(16f)	Nb I
<b>B<sub>3</sub></b>	$= \left(\frac{1}{2} + x_1 + z_1\right) \mathbf{a}_1 + (-y_1 + z_1) \mathbf{a}_2 + (x_1 - y_1) \mathbf{a}_3$	$=$	$\left(\frac{3}{4} - y_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_1\right) c \hat{\mathbf{z}}$	(16f)	Nb I
<b>B<sub>4</sub></b>	$= \left(\frac{1}{2} - x_1 + z_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_1 + z_1\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_1 + y_1\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} + y_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_1\right) c \hat{\mathbf{z}}$	(16f)	Nb I
<b>B<sub>5</sub></b>	$= (-y_1 - z_1) \mathbf{a}_1 + (-x_1 - z_1) \mathbf{a}_2 + (-x_1 - y_1) \mathbf{a}_3$	$=$	$-x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(16f)	Nb I
<b>B<sub>6</sub></b>	$= \left(\frac{1}{2} + y_1 - z_1\right) \mathbf{a}_1 + (x_1 - z_1) \mathbf{a}_2 + \left(\frac{1}{2} + x_1 + y_1\right) \mathbf{a}_3$	$=$	$x_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right) a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(16f)	Nb I
<b>B<sub>7</sub></b>	$= \left(\frac{1}{2} - x_1 - z_1\right) \mathbf{a}_1 + (y_1 - z_1) \mathbf{a}_2 + (-x_1 + y_1) \mathbf{a}_3$	$=$	$\left(-\frac{1}{4} + y_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_1\right) c \hat{\mathbf{z}}$	(16f)	Nb I
<b>B<sub>8</sub></b>	$= \left(\frac{1}{2} + x_1 - z_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_1 - z_1\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_1 - y_1\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} - y_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_1\right) c \hat{\mathbf{z}}$	(16f)	Nb I
<b>B<sub>9</sub></b>	$= (y_2 + z_2) \mathbf{a}_1 + (x_2 + z_2) \mathbf{a}_2 + (x_2 + y_2) \mathbf{a}_3$	$=$	$x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(16f)	Nb II
<b>B<sub>10</sub></b>	$= \left(\frac{1}{2} - y_2 + z_2\right) \mathbf{a}_1 + (-x_2 + z_2) \mathbf{a}_2 + \left(\frac{1}{2} - x_2 - y_2\right) \mathbf{a}_3$	$=$	$-x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(16f)	Nb II
<b>B<sub>11</sub></b>	$= \left(\frac{1}{2} + x_2 + z_2\right) \mathbf{a}_1 + (-y_2 + z_2) \mathbf{a}_2 + (x_2 - y_2) \mathbf{a}_3$	$=$	$\left(\frac{3}{4} - y_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_2\right) c \hat{\mathbf{z}}$	(16f)	Nb II
<b>B<sub>12</sub></b>	$= \left(\frac{1}{2} - x_2 + z_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2 + z_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_2 + y_2\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} + y_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_2\right) c \hat{\mathbf{z}}$	(16f)	Nb II
<b>B<sub>13</sub></b>	$= (-y_2 - z_2) \mathbf{a}_1 + (-x_2 - z_2) \mathbf{a}_2 + (-x_2 - y_2) \mathbf{a}_3$	$=$	$-x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(16f)	Nb II
<b>B<sub>14</sub></b>	$= \left(\frac{1}{2} + y_2 - z_2\right) \mathbf{a}_1 + (x_2 - z_2) \mathbf{a}_2 + \left(\frac{1}{2} + x_2 + y_2\right) \mathbf{a}_3$	$=$	$x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(16f)	Nb II
<b>B<sub>15</sub></b>	$= \left(\frac{1}{2} - x_2 - z_2\right) \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (-x_2 + y_2) \mathbf{a}_3$	$=$	$\left(-\frac{1}{4} + y_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_2\right) c \hat{\mathbf{z}}$	(16f)	Nb II
<b>B<sub>16</sub></b>	$= \left(\frac{1}{2} + x_2 - z_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2 - z_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_2 - y_2\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} - y_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_2\right) c \hat{\mathbf{z}}$	(16f)	Nb II
<b>B<sub>17</sub></b>	$= (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(16f)	O I
<b>B<sub>18</sub></b>	$= \left(\frac{1}{2} - y_3 + z_3\right) \mathbf{a}_1 + (-x_3 + z_3) \mathbf{a}_2 + \left(\frac{1}{2} - x_3 - y_3\right) \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(16f)	O I
<b>B<sub>19</sub></b>	$= \left(\frac{1}{2} + x_3 + z_3\right) \mathbf{a}_1 + (-y_3 + z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$\left(\frac{3}{4} - y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_3\right) c \hat{\mathbf{z}}$	(16f)	O I
<b>B<sub>20</sub></b>	$= \left(\frac{1}{2} - x_3 + z_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3 + z_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_3 + y_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} + y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_3\right) c \hat{\mathbf{z}}$	(16f)	O I
<b>B<sub>21</sub></b>	$= (-y_3 - z_3) \mathbf{a}_1 + (-x_3 - z_3) \mathbf{a}_2 + (-x_3 - y_3) \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(16f)	O I

$$\begin{aligned}
\mathbf{B}_{22} &= \begin{pmatrix} \frac{1}{2} + y_3 - z_3 \\ \frac{1}{2} + x_3 + y_3 \end{pmatrix} \mathbf{a}_1 + (x_3 - z_3) \mathbf{a}_2 + (x_3 - z_3) \mathbf{a}_2 + x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{23} &= \begin{pmatrix} \frac{1}{2} - x_3 - z_3 \\ -x_3 + y_3 \end{pmatrix} \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (-\frac{1}{4} + y_3) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_3\right) c \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{24} &= \begin{pmatrix} \frac{1}{2} + x_3 - z_3 \\ \frac{1}{2} - y_3 - z_3 \end{pmatrix} \mathbf{a}_1 + \left(\frac{1}{2} + x_3 - y_3\right) \mathbf{a}_3 = \left(\frac{1}{4} - y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_3\right) c \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{25} &= \begin{pmatrix} y_4 + z_4 \\ x_4 + y_4 \end{pmatrix} \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3 = x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{26} &= \begin{pmatrix} \frac{1}{2} - y_4 + z_4 \\ \frac{1}{2} - x_4 - y_4 \end{pmatrix} \mathbf{a}_1 + (-x_4 + z_4) \mathbf{a}_2 + (-x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{27} &= \begin{pmatrix} \frac{1}{2} + x_4 + z_4 \\ x_4 - y_4 \end{pmatrix} \mathbf{a}_1 + (-y_4 + z_4) \mathbf{a}_2 + \left(\frac{3}{4} - y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_4\right) c \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{28} &= \begin{pmatrix} \frac{1}{2} - x_4 + z_4 \\ \frac{1}{2} + y_4 + z_4 \end{pmatrix} \mathbf{a}_1 + \left(\frac{1}{2} - x_4 + y_4\right) \mathbf{a}_3 = \left(\frac{1}{4} + y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_4\right) c \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{29} &= \begin{pmatrix} -y_4 - z_4 \\ -x_4 - y_4 \end{pmatrix} \mathbf{a}_1 + (-x_4 - z_4) \mathbf{a}_2 + (-x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{30} &= \begin{pmatrix} \frac{1}{2} + y_4 - z_4 \\ \frac{1}{2} + x_4 + y_4 \end{pmatrix} \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{31} &= \begin{pmatrix} \frac{1}{2} - x_4 - z_4 \\ -x_4 + y_4 \end{pmatrix} \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (-\frac{1}{4} + y_4) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_4\right) c \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{32} &= \begin{pmatrix} \frac{1}{2} + x_4 - z_4 \\ \frac{1}{2} - y_4 - z_4 \end{pmatrix} \mathbf{a}_1 + \left(\frac{1}{2} + x_4 - y_4\right) \mathbf{a}_3 = \left(\frac{1}{4} - y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_4\right) c \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{33} &= \begin{pmatrix} y_5 + z_5 \\ x_5 + y_5 \end{pmatrix} \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + (x_5 + y_5) \mathbf{a}_3 = x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (16f) & \text{O III} \\
\mathbf{B}_{34} &= \begin{pmatrix} \frac{1}{2} - y_5 + z_5 \\ \frac{1}{2} - x_5 - y_5 \end{pmatrix} \mathbf{a}_1 + (-x_5 + z_5) \mathbf{a}_2 + (-x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (16f) & \text{O III} \\
\mathbf{B}_{35} &= \begin{pmatrix} \frac{1}{2} + x_5 + z_5 \\ x_5 - y_5 \end{pmatrix} \mathbf{a}_1 + (-y_5 + z_5) \mathbf{a}_2 + \left(\frac{3}{4} - y_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_5\right) c \hat{\mathbf{z}} & (16f) & \text{O III} \\
\mathbf{B}_{36} &= \begin{pmatrix} \frac{1}{2} - x_5 + z_5 \\ \frac{1}{2} + y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + \left(\frac{1}{2} - x_5 + y_5\right) \mathbf{a}_3 = \left(\frac{1}{4} + y_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_5\right) c \hat{\mathbf{z}} & (16f) & \text{O III} \\
\mathbf{B}_{37} &= \begin{pmatrix} -y_5 - z_5 \\ -x_5 - y_5 \end{pmatrix} \mathbf{a}_1 + (-x_5 - z_5) \mathbf{a}_2 + (-x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (16f) & \text{O III} \\
\mathbf{B}_{38} &= \begin{pmatrix} \frac{1}{2} + y_5 - z_5 \\ \frac{1}{2} + x_5 + y_5 \end{pmatrix} \mathbf{a}_1 + (x_5 - z_5) \mathbf{a}_2 + x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (16f) & \text{O III} \\
\mathbf{B}_{39} &= \begin{pmatrix} \frac{1}{2} - x_5 - z_5 \\ -x_5 + y_5 \end{pmatrix} \mathbf{a}_1 + (y_5 - z_5) \mathbf{a}_2 + (-\frac{1}{4} + y_5) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_5\right) c \hat{\mathbf{z}} & (16f) & \text{O III} \\
\mathbf{B}_{40} &= \begin{pmatrix} \frac{1}{2} + x_5 - z_5 \\ \frac{1}{2} - y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + \left(\frac{1}{2} + x_5 - y_5\right) \mathbf{a}_3 = \left(\frac{1}{4} - y_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_5\right) c \hat{\mathbf{z}} & (16f) & \text{O III} \\
\mathbf{B}_{41} &= \begin{pmatrix} y_6 + z_6 \\ x_6 + y_6 \end{pmatrix} \mathbf{a}_1 + (x_6 + z_6) \mathbf{a}_2 + (x_6 + y_6) \mathbf{a}_3 = x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (16f) & \text{O IV} \\
\mathbf{B}_{42} &= \begin{pmatrix} \frac{1}{2} - y_6 + z_6 \\ \frac{1}{2} - x_6 - y_6 \end{pmatrix} \mathbf{a}_1 + (-x_6 + z_6) \mathbf{a}_2 + (-x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (16f) & \text{O IV}
\end{aligned}$$

$$\mathbf{B}_{43} = \begin{pmatrix} \frac{1}{2} + x_6 + z_6 \\ (x_6 - y_6) \end{pmatrix} \mathbf{a}_1 + (-y_6 + z_6) \mathbf{a}_2 + \mathbf{a}_3 = \begin{pmatrix} \frac{3}{4} - y_6 \\ \frac{1}{4} + z_6 \end{pmatrix} a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_6\right) a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (16f) \quad \text{O IV}$$

$$\mathbf{B}_{44} = \begin{pmatrix} \frac{1}{2} - x_6 + z_6 \\ \frac{1}{2} + y_6 + z_6 \end{pmatrix} \mathbf{a}_1 + \left(\frac{1}{2} - x_6 + y_6\right) \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} + y_6 \\ \frac{1}{4} + z_6 \end{pmatrix} a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_6\right) a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (16f) \quad \text{O IV}$$

$$\mathbf{B}_{45} = \begin{pmatrix} -y_6 - z_6 \\ -x_6 - y_6 \end{pmatrix} \mathbf{a}_1 + (-x_6 - z_6) \mathbf{a}_2 + \mathbf{a}_3 = -x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} \quad (16f) \quad \text{O IV}$$

$$\mathbf{B}_{46} = \begin{pmatrix} \frac{1}{2} + y_6 - z_6 \\ \frac{1}{2} + x_6 + y_6 \end{pmatrix} \mathbf{a}_1 + (x_6 - z_6) \mathbf{a}_2 + \mathbf{a}_3 = x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} \quad (16f) \quad \text{O IV}$$

$$\mathbf{B}_{47} = \begin{pmatrix} \frac{1}{2} - x_6 - z_6 \\ -x_6 + y_6 \end{pmatrix} \mathbf{a}_1 + (y_6 - z_6) \mathbf{a}_2 + \mathbf{a}_3 = \begin{pmatrix} -\frac{1}{4} + y_6 \\ \frac{1}{4} - z_6 \end{pmatrix} a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_6\right) a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (16f) \quad \text{O IV}$$

$$\mathbf{B}_{48} = \begin{pmatrix} \frac{1}{2} + x_6 - z_6 \\ \frac{1}{2} - y_6 - z_6 \end{pmatrix} \mathbf{a}_1 + \left(\frac{1}{2} + x_6 - y_6\right) \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} - y_6 \\ \frac{1}{4} - z_6 \end{pmatrix} a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_6\right) a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (16f) \quad \text{O IV}$$

### References:

- R. Pynn, J. D. Axe, and R. Thomas, *Structural distortions in the low-temperature phase of NbO<sub>2</sub>*, Phys. Rev. B **13**, 2965–2975 (1976), doi:10.1103/PhysRevB.13.2965.

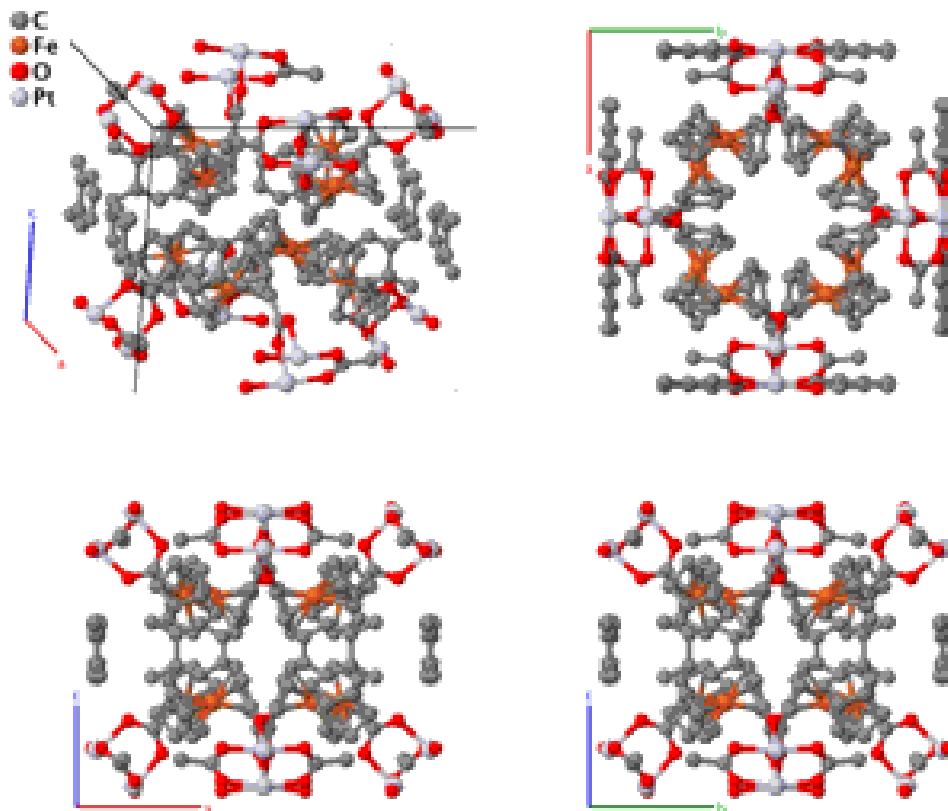
### Found in:

- A. A. Bolzan, C. Fong, B. J. Kennedy, and C. J. Howard, *A Powder Neutron Diffraction Study of Semiconducting and Metallic Niobium Dioxide*, J. Solid State Chem. **113**, 9–14 (1994), doi:10.1006/jssc.1994.1334.

### Geometry files:

- CIF: pp. 866
- POSCAR: pp. 866

# C<sub>17</sub>FeO<sub>4</sub>Pt Structure: A17BC4D\_tP184\_89\_17p\_p\_4p\_io



<b>Prototype</b>	:	C <sub>17</sub> FeO <sub>4</sub> Pt
<b>AFLOW prototype label</b>	:	A17BC4D_tP184_89_17p_p_4p_io
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP184
<b>Space group number</b>	:	89
<b>Space group symbol</b>	:	<i>P</i> 422
<b>AFLOW prototype command</b>	:	<pre>aflow --proto=A17BC4D_tP184_89_17p_p_4p_io --params=a, c/a, z1, x2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18, y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22, x23, y23, z23, x24, y24, z24</pre>

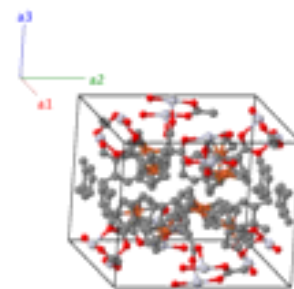
- Structures exhibiting space group #89 are quite rare. According to (Hoffmann, 2014), there are only two entries in the Inorganic Crystal Structure Database with space group #89; however, they are incorrectly classified. This structure is listed in the Cambridge Structure Database (ID=863010). Only the non-hydrogen atoms are listed.

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4i)	Pt I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + z_1 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + z_1 c \hat{\mathbf{z}}$	(4i)	Pt I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(4i)	Pt I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + -z_1 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + -z_1 c \hat{\mathbf{z}}$	(4i)	Pt I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$= x_2 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(4o)	Pt II
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$= -x_2 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(4o)	Pt II
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1 + x_2 \mathbf{a}_2$	$= \frac{1}{2} a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}}$	(4o)	Pt II
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1 - x_2 \mathbf{a}_2$	$= \frac{1}{2} a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}}$	(4o)	Pt II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8p)	C I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= -x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8p)	C I
$\mathbf{B}_{11}$	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= -y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8p)	C I
$\mathbf{B}_{12}$	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8p)	C I
$\mathbf{B}_{13}$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$= -x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(8p)	C I
$\mathbf{B}_{14}$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(8p)	C I
$\mathbf{B}_{15}$	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$= y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(8p)	C I
$\mathbf{B}_{16}$	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$= -y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(8p)	C I
$\mathbf{B}_{17}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8p)	C II
$\mathbf{B}_{18}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8p)	C II
$\mathbf{B}_{19}$	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= -y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8p)	C II
$\mathbf{B}_{20}$	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8p)	C II
$\mathbf{B}_{21}$	$= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$= -x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(8p)	C II
$\mathbf{B}_{22}$	$= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$= x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(8p)	C II
$\mathbf{B}_{23}$	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$= y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(8p)	C II
$\mathbf{B}_{24}$	$= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$= -y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(8p)	C II
$\mathbf{B}_{25}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8p)	C III
$\mathbf{B}_{26}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= -x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8p)	C III
$\mathbf{B}_{27}$	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= -y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8p)	C III











$$\begin{array}{llllll}
\mathbf{B}_{172} & = & y_{23} \mathbf{a}_1 - x_{23} \mathbf{a}_2 + z_{23} \mathbf{a}_3 & = & y_{23}a \hat{\mathbf{x}} - x_{23}a \hat{\mathbf{y}} + z_{23}c \hat{\mathbf{z}} & (8p) & \text{O III} \\
\mathbf{B}_{173} & = & -x_{23} \mathbf{a}_1 + y_{23} \mathbf{a}_2 - z_{23} \mathbf{a}_3 & = & -x_{23}a \hat{\mathbf{x}} + y_{23}a \hat{\mathbf{y}} - z_{23}c \hat{\mathbf{z}} & (8p) & \text{O III} \\
\mathbf{B}_{174} & = & x_{23} \mathbf{a}_1 - y_{23} \mathbf{a}_2 - z_{23} \mathbf{a}_3 & = & x_{23}a \hat{\mathbf{x}} - y_{23}a \hat{\mathbf{y}} - z_{23}c \hat{\mathbf{z}} & (8p) & \text{O III} \\
\mathbf{B}_{175} & = & y_{23} \mathbf{a}_1 + x_{23} \mathbf{a}_2 - z_{23} \mathbf{a}_3 & = & y_{23}a \hat{\mathbf{x}} + x_{23}a \hat{\mathbf{y}} - z_{23}c \hat{\mathbf{z}} & (8p) & \text{O III} \\
\mathbf{B}_{176} & = & -y_{23} \mathbf{a}_1 - x_{23} \mathbf{a}_2 - z_{23} \mathbf{a}_3 & = & -y_{23}a \hat{\mathbf{x}} - x_{23}a \hat{\mathbf{y}} - z_{23}c \hat{\mathbf{z}} & (8p) & \text{O III} \\
\mathbf{B}_{177} & = & x_{24} \mathbf{a}_1 + y_{24} \mathbf{a}_2 + z_{24} \mathbf{a}_3 & = & x_{24}a \hat{\mathbf{x}} + y_{24}a \hat{\mathbf{y}} + z_{24}c \hat{\mathbf{z}} & (8p) & \text{O IV} \\
\mathbf{B}_{178} & = & -x_{24} \mathbf{a}_1 - y_{24} \mathbf{a}_2 + z_{24} \mathbf{a}_3 & = & -x_{24}a \hat{\mathbf{x}} - y_{24}a \hat{\mathbf{y}} + z_{24}c \hat{\mathbf{z}} & (8p) & \text{O IV} \\
\mathbf{B}_{179} & = & -y_{24} \mathbf{a}_1 + x_{24} \mathbf{a}_2 + z_{24} \mathbf{a}_3 & = & -y_{24}a \hat{\mathbf{x}} + x_{24}a \hat{\mathbf{y}} + z_{24}c \hat{\mathbf{z}} & (8p) & \text{O IV} \\
\mathbf{B}_{180} & = & y_{24} \mathbf{a}_1 - x_{24} \mathbf{a}_2 + z_{24} \mathbf{a}_3 & = & y_{24}a \hat{\mathbf{x}} - x_{24}a \hat{\mathbf{y}} + z_{24}c \hat{\mathbf{z}} & (8p) & \text{O IV} \\
\mathbf{B}_{181} & = & -x_{24} \mathbf{a}_1 + y_{24} \mathbf{a}_2 - z_{24} \mathbf{a}_3 & = & -x_{24}a \hat{\mathbf{x}} + y_{24}a \hat{\mathbf{y}} - z_{24}c \hat{\mathbf{z}} & (8p) & \text{O IV} \\
\mathbf{B}_{182} & = & x_{24} \mathbf{a}_1 - y_{24} \mathbf{a}_2 - z_{24} \mathbf{a}_3 & = & x_{24}a \hat{\mathbf{x}} - y_{24}a \hat{\mathbf{y}} - z_{24}c \hat{\mathbf{z}} & (8p) & \text{O IV} \\
\mathbf{B}_{183} & = & y_{24} \mathbf{a}_1 + x_{24} \mathbf{a}_2 - z_{24} \mathbf{a}_3 & = & y_{24}a \hat{\mathbf{x}} + x_{24}a \hat{\mathbf{y}} - z_{24}c \hat{\mathbf{z}} & (8p) & \text{O IV} \\
\mathbf{B}_{184} & = & -y_{24} \mathbf{a}_1 - x_{24} \mathbf{a}_2 - z_{24} \mathbf{a}_3 & = & -y_{24}a \hat{\mathbf{x}} - x_{24}a \hat{\mathbf{y}} - z_{24}c \hat{\mathbf{z}} & (8p) & \text{O IV}
\end{array}$$

---

#### References:

- S. Tanaka and K. Mashima, *Interaction of Ferrocene Moieties Across a Square Pt<sub>4</sub> Unit: Synthesis, Characterization, and Electrochemical Properties of Carboxylate-Bridged Bimetallic Pt<sub>4</sub>Fe<sub>n</sub> (n = 2, 3, and 4) Complexes*, *Inorg. Chem.* **50**, 11384–11393 (2011), [doi:10.1021/ic201012m](https://doi.org/10.1021/ic201012m).

#### Found in:

- C. R. Groom, I. J. Bruno, M. P. Lightfoot, and S. C. Ward, *The Cambridge Structural Database*, *Acta Crystallogr. Sect. B Struct. Sci.* **72**, 171–179 (2016), [doi:10.1107/S2052520616003954](https://doi.org/10.1107/S2052520616003954).

- F. Hoffmann, *The Fascination of Crystals and Symmetry* (2014). 230 - The space group list project.

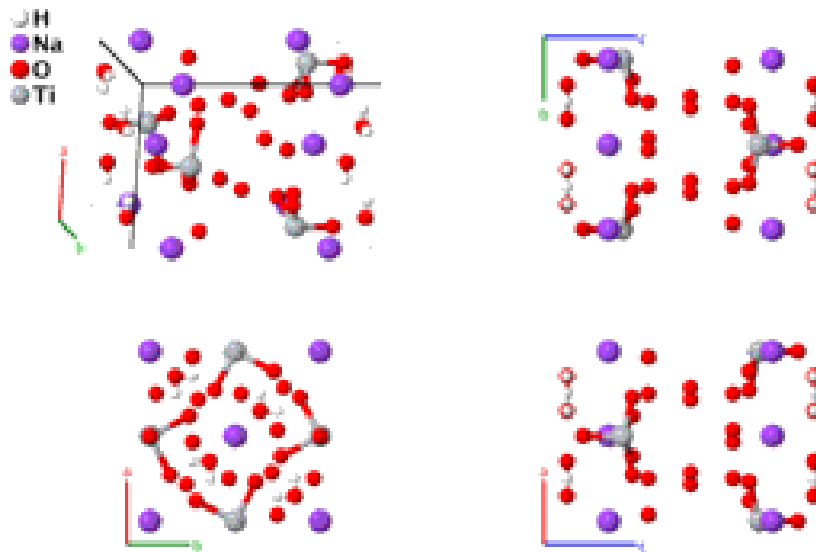
---

#### Geometry files:

- CIF: pp. [866](#)

- POSCAR: pp. [867](#)

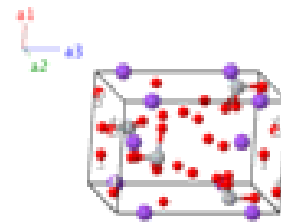
# Na<sub>4</sub>Ti<sub>2</sub>Si<sub>8</sub>O<sub>22</sub>[H<sub>2</sub>O]<sub>4</sub> Structure: A4B2C13D\_tP40\_90\_g\_d\_cef2g\_c



**Prototype** : Na<sub>4</sub>Ti<sub>2</sub>Si<sub>8</sub>O<sub>22</sub>[H<sub>2</sub>O]<sub>4</sub>  
**AFLOW prototype label** : A4B2C13D\_tP40\_90\_g\_d\_cef2g\_c  
**Strukturbericht designation** : None  
**Pearson symbol** : tP40  
**Space group number** : 90  
**Space group symbol** : *P4*<sub>2</sub>*1*2  
**AFLOW prototype command** : aflow --proto=A4B2C13D\_tP40\_90\_g\_d\_cef2g\_c  
 --params=*a*, *c/a*, *z*<sub>1</sub>, *z*<sub>2</sub>, *z*<sub>3</sub>, *x*<sub>4</sub>, *x*<sub>5</sub>, *x*<sub>6</sub>, *y*<sub>6</sub>, *z*<sub>6</sub>, *x*<sub>7</sub>, *y*<sub>7</sub>, *z*<sub>7</sub>, *x*<sub>8</sub>, *y*<sub>8</sub>, *z*<sub>8</sub>

Simple Tetragonal primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $\frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(2c)	O I
<b>B</b> <sub>2</sub>	= $\frac{1}{2} \mathbf{a}_1 + -z_1 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + -z_1 c \hat{\mathbf{z}}$	(2c)	O I
<b>B</b> <sub>3</sub>	= $\frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2c)	Ti
<b>B</b> <sub>4</sub>	= $\frac{1}{2} \mathbf{a}_1 + -z_2 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + -z_2 c \hat{\mathbf{z}}$	(2c)	Ti
<b>B</b> <sub>5</sub>	= $z_3 \mathbf{a}_3$	=	$z_3 c \hat{\mathbf{z}}$	(4d)	Na



- S. Ferdov, U. Kolitsch, C. Lengauer, E. Tillmanns, Z. Lin, and R. A. Sá Ferreira, *Refinement of the layered titanosilicate AM-1 from single-crystal X-ray diffraction data*, Acta Crystallogr. E **63**, i186–i186 (2007), [doi:10.1107/S160053680704812X](https://doi.org/10.1107/S160053680704812X).

**Found in:**

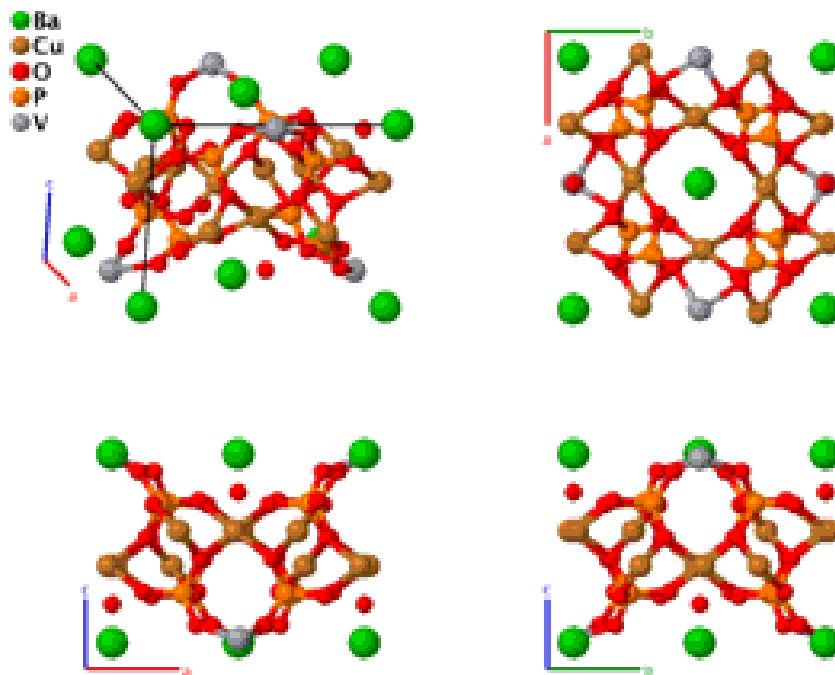
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [868](#)
- POSCAR: pp. [868](#)

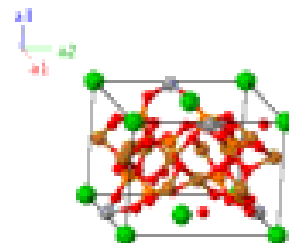
# BaCu<sub>4</sub>[VO][PO<sub>4</sub>]<sub>4</sub> Structure: AB4C17D4E\_tP54\_90\_a\_g\_c4g\_g\_c



**Prototype** : BaCu<sub>4</sub>[VO][PO<sub>4</sub>]<sub>4</sub>  
**AFLOW prototype label** : AB4C17D4E\_tP54\_90\_a\_g\_c4g\_g\_c  
**Strukturbericht designation** : None  
**Pearson symbol** : tP54  
**Space group number** : 90  
**Space group symbol** : *P42*<sub>1</sub>*2*  
**AFLOW prototype command** : `aflow --proto=AB4C17D4E_tP54_90_a_g_c4g_g_c`  
`--params=a, c/a, z2, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9`

Simple Tetragonal primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$	=	$0\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}}$	(2a)	Ba



$\mathbf{B}_{38}$	$=$	$-y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}}$	$(8g)$	O IV
$\mathbf{B}_{39}$	$=$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$x_8 a \hat{\mathbf{x}} + y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	$(8g)$	O V
$\mathbf{B}_{40}$	$=$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-x_8 a \hat{\mathbf{x}} - y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	$(8g)$	O V
$\mathbf{B}_{41}$	$=$	$(\frac{1}{2} - y_8) \mathbf{a}_1 + (\frac{1}{2} + x_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(\frac{1}{2} - y_8) a \hat{\mathbf{x}} + (\frac{1}{2} + x_8) a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	$(8g)$	O V
$\mathbf{B}_{42}$	$=$	$(\frac{1}{2} + y_8) \mathbf{a}_1 + (\frac{1}{2} - x_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(\frac{1}{2} + y_8) a \hat{\mathbf{x}} + (\frac{1}{2} - x_8) a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	$(8g)$	O V
$\mathbf{B}_{43}$	$=$	$(\frac{1}{2} - x_8) \mathbf{a}_1 + (\frac{1}{2} + y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$(\frac{1}{2} - x_8) a \hat{\mathbf{x}} + (\frac{1}{2} + y_8) a \hat{\mathbf{y}} - z_8 c \hat{\mathbf{z}}$	$(8g)$	O V
$\mathbf{B}_{44}$	$=$	$(\frac{1}{2} + x_8) \mathbf{a}_1 + (\frac{1}{2} - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$(\frac{1}{2} + x_8) a \hat{\mathbf{x}} + (\frac{1}{2} - y_8) a \hat{\mathbf{y}} - z_8 c \hat{\mathbf{z}}$	$(8g)$	O V
$\mathbf{B}_{45}$	$=$	$y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$y_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} - z_8 c \hat{\mathbf{z}}$	$(8g)$	O V
$\mathbf{B}_{46}$	$=$	$-y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-y_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} - z_8 c \hat{\mathbf{z}}$	$(8g)$	O V
$\mathbf{B}_{47}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$x_9 a \hat{\mathbf{x}} + y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	$(8g)$	P
$\mathbf{B}_{48}$	$=$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-x_9 a \hat{\mathbf{x}} - y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	$(8g)$	P
$\mathbf{B}_{49}$	$=$	$(\frac{1}{2} - y_9) \mathbf{a}_1 + (\frac{1}{2} + x_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(\frac{1}{2} - y_9) a \hat{\mathbf{x}} + (\frac{1}{2} + x_9) a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	$(8g)$	P
$\mathbf{B}_{50}$	$=$	$(\frac{1}{2} + y_9) \mathbf{a}_1 + (\frac{1}{2} - x_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(\frac{1}{2} + y_9) a \hat{\mathbf{x}} + (\frac{1}{2} - x_9) a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	$(8g)$	P
$\mathbf{B}_{51}$	$=$	$(\frac{1}{2} - x_9) \mathbf{a}_1 + (\frac{1}{2} + y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$(\frac{1}{2} - x_9) a \hat{\mathbf{x}} + (\frac{1}{2} + y_9) a \hat{\mathbf{y}} - z_9 c \hat{\mathbf{z}}$	$(8g)$	P
$\mathbf{B}_{52}$	$=$	$(\frac{1}{2} + x_9) \mathbf{a}_1 + (\frac{1}{2} - y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$(\frac{1}{2} + x_9) a \hat{\mathbf{x}} + (\frac{1}{2} - y_9) a \hat{\mathbf{y}} - z_9 c \hat{\mathbf{z}}$	$(8g)$	P
$\mathbf{B}_{53}$	$=$	$y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$y_9 a \hat{\mathbf{x}} + x_9 a \hat{\mathbf{y}} - z_9 c \hat{\mathbf{z}}$	$(8g)$	P
$\mathbf{B}_{54}$	$=$	$-y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-y_9 a \hat{\mathbf{x}} - x_9 a \hat{\mathbf{y}} - z_9 c \hat{\mathbf{z}}$	$(8g)$	P

---

#### References:

- S. Meyer and H. Müller-Buschbaum, *Cu<sub>4</sub>O<sub>12</sub>-Baugruppen aus planaren CuO<sub>4</sub>-Polygonen im Barium-Vanadyl-Oxocuprat(II)-phosphat Ba(VO)Cu<sub>4</sub>(PO<sub>4</sub>)<sub>4</sub>*, Z. Anorg. Allg. Chem. **623**, 1693–1698 (1997), [doi:10.1002/zaac.19976231103](https://doi.org/10.1002/zaac.19976231103).

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

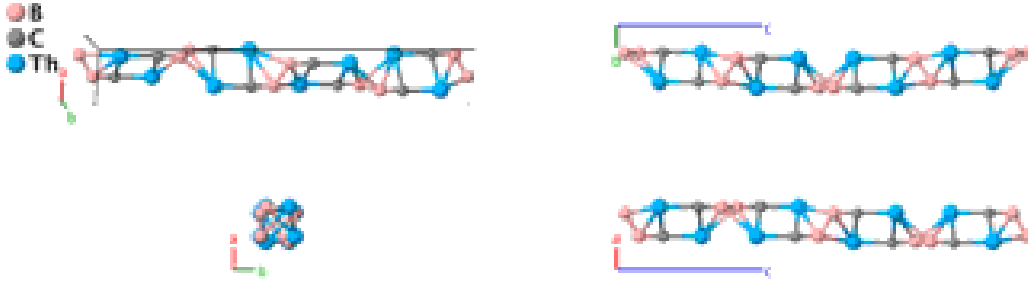
---

#### Geometry files:

- CIF: pp. [868](#)  
- POSCAR: pp. [869](#)



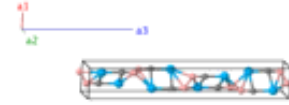
# ThBC Structure: ABC\_tP24\_91\_d\_d\_d



<b>Prototype</b>	:	ThBC
<b>AFLOW prototype label</b>	:	ABC_tP24_91_d_d_d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP24
<b>Space group number</b>	:	91
<b>Space group symbol</b>	:	$P4_122$
<b>AFLOW prototype command</b>	:	aflow --proto=ABC_tP24_91_d_d_d --params= $a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_3$	$-y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{1}{4} + z_1\right) \mathbf{a}_3$	$-y_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_1\right) c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_4$	$y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{3}{4} + z_1\right) \mathbf{a}_3$	$y_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_1\right) c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_5$	$-x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_6$	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_7$	$y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{3}{4} - z_1\right) \mathbf{a}_3$	$y_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \left(\frac{3}{4} - z_1\right) c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_8$	$-y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{1}{4} - z_1\right) \mathbf{a}_3$	$-y_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_1\right) c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_9$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8d)	C
$\mathbf{B}_{10}$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$-x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(8d)	C
$\mathbf{B}_{11}$	$-y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{4} + z_2\right) \mathbf{a}_3$	$-y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_2\right) c \hat{\mathbf{z}}$	(8d)	C
$\mathbf{B}_{12}$	$y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{3}{4} + z_2\right) \mathbf{a}_3$	$y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_2\right) c \hat{\mathbf{z}}$	(8d)	C
$\mathbf{B}_{13}$	$-x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$-x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(8d)	C
$\mathbf{B}_{14}$	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	$x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(8d)	C

$$\begin{aligned}
\mathbf{B}_{15} &= y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{3}{4} - z_2\right) \mathbf{a}_3 &= y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \left(\frac{3}{4} - z_2\right) c \hat{\mathbf{z}} && (8d) && \text{C} \\
\mathbf{B}_{16} &= -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{4} - z_2\right) \mathbf{a}_3 &= -y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_2\right) c \hat{\mathbf{z}} && (8d) && \text{C} \\
\mathbf{B}_{17} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{18} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{19} &= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{4} + z_3\right) \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_3\right) c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{20} &= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{3}{4} + z_3\right) \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_3\right) c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{21} &= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{22} &= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{23} &= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{3}{4} - z_3\right) \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{3}{4} - z_3\right) c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{24} &= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{4} - z_3\right) \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_3\right) c \hat{\mathbf{z}} && (8d) && \text{Th}
\end{aligned}$$

---

### References:

- P. Rogl, *The crystal structure of ThBC*, J. Nucl. Mat. **73**, 198–203 (1978), doi:10.1016/0022-3115(78)90560-3.

### Found in:

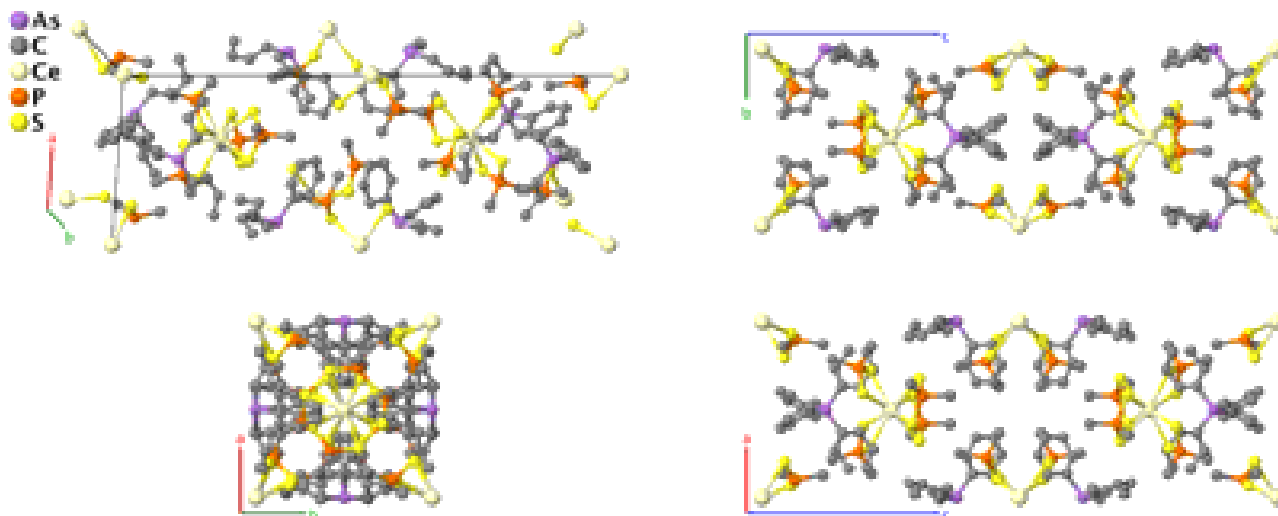
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. 869  
- POSCAR: pp. 869

# AsPh<sub>4</sub>CeS<sub>8</sub>P<sub>4</sub>Me<sub>8</sub> Structure: AB32CD4E8\_tP184\_93\_i\_16p\_af\_2p\_4p

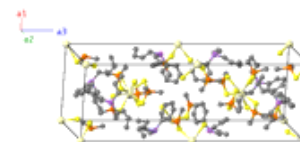


<b>Prototype</b>	:	AsPh <sub>4</sub> CeS <sub>8</sub> P <sub>4</sub> Me <sub>8</sub>
<b>AFLOW prototype label</b>	:	AB32CD4E8_tP184_93_i_16p_af_2p_4p
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP184
<b>Space group number</b>	:	93
<b>Space group symbol</b>	:	<i>P</i> 4 <sub>2</sub> 22
<b>AFLOW prototype command</b>	:	aflow --proto=AB32CD4E8_tP184_93_i_16p_af_2p_4p --params= <i>a, c/a, z</i> <sub>3, x</sub> <sub>4, y</sub> <sub>4, z</sub> <sub>4, x</sub> <sub>5, y</sub> <sub>5, z</sub> <sub>6, y</sub> <sub>6, z</sub> <sub>7, x</sub> <sub>7, y</sub> <sub>7, z</sub> <sub>8, x</sub> <sub>8, y</sub> <sub>8, z</sub> <sub>9, y</sub> <sub>9, z</sub> <sub>10, x</sub> <sub>10, y</sub> <sub>10, z</sub> <sub>11, x</sub> <sub>11, y</sub> <sub>11, z</sub> <sub>12, x</sub> <sub>12, y</sub> <sub>12, z</sub> <sub>13, x</sub> <sub>13, y</sub> <sub>13, z</sub> <sub>14, x</sub> <sub>14, y</sub> <sub>14, z</sub> <sub>15, x</sub> <sub>15, y</sub> <sub>15, z</sub> <sub>16, x</sub> <sub>16, y</sub> <sub>16, z</sub> <sub>17, x</sub> <sub>17, y</sub> <sub>17, z</sub> <sub>18, x</sub> <sub>18, y</sub> <sub>18, z</sub> <sub>19, x</sub> <sub>19, y</sub> <sub>19, z</sub> <sub>20, x</sub> <sub>20, y</sub> <sub>20, z</sub> <sub>21, x</sub> <sub>21, y</sub> <sub>21, z</sub> <sub>22, x</sub> <sub>22, y</sub> <sub>22, z</sub> <sub>23, x</sub> <sub>23, y</sub> <sub>23, z</sub> <sub>24, x</sub> <sub>24, y</sub> <sub>24, z</sub> <sub>25, x</sub> <sub>25, y</sub> <sub>25, z</sub>

- Structures exhibiting space group #93 are quite rare. According to (Hoffmann, 2014), there are no entries in the Inorganic Crystal Structure Database with space group #93. The hydrogen atoms are not included in this prototype. (Ph = Phenyl and Me = Methyl)

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= 0 <b>a</b> <sub>1</sub> + 0 <b>a</b> <sub>2</sub> + 0 <b>a</b> <sub>3</sub>	= 0 <b>x</b> + 0 <b>y</b> + 0 <b>z</b>	(2 <i>a</i> )	Ce I
<b>B</b> <sub>2</sub>	= $\frac{1}{2}$ <b>a</b> <sub>3</sub>	= $\frac{1}{2}$ <i>c</i> <b>z</b>	(2 <i>a</i> )	Ce I
<b>B</b> <sub>3</sub>	= $\frac{1}{2}$ <b>a</b> <sub>1</sub> + $\frac{1}{2}$ <b>a</b> <sub>2</sub> + $\frac{1}{4}$ <b>a</b> <sub>3</sub>	= $\frac{1}{2}$ <i>a</i> <b>x</b> + $\frac{1}{2}$ <i>a</i> <b>y</b> + $\frac{1}{4}$ <i>c</i> <b>z</b>	(2 <i>f</i> )	Ce II

$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	$(2f)$	Ce II
$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	$(4i)$	As
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	$(4i)$	As
$\mathbf{B}_7$	$=$	$\frac{1}{2} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	$(4i)$	As
$\mathbf{B}_8$	$=$	$\frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}}$	$(4i)$	As
$\mathbf{B}_9$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	$(8p)$	CI
$\mathbf{B}_{10}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	$(8p)$	CI
$\mathbf{B}_{11}$	$=$	$-y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$-y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	$(8p)$	CI
$\mathbf{B}_{12}$	$=$	$y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	$(8p)$	CI
$\mathbf{B}_{13}$	$=$	$-x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	$(8p)$	CI
$\mathbf{B}_{14}$	$=$	$x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	$(8p)$	CI
$\mathbf{B}_{15}$	$=$	$y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$=$	$y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	$(8p)$	CI
$\mathbf{B}_{16}$	$=$	$-y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$=$	$-y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	$(8p)$	CI
$\mathbf{B}_{17}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	$(8p)$	CII
$\mathbf{B}_{18}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	$(8p)$	CII
$\mathbf{B}_{19}$	$=$	$-y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	$(8p)$	CII
$\mathbf{B}_{20}$	$=$	$y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	$(8p)$	CII
$\mathbf{B}_{21}$	$=$	$-x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	$(8p)$	CII
$\mathbf{B}_{22}$	$=$	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	$(8p)$	CII
$\mathbf{B}_{23}$	$=$	$y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}}$	$(8p)$	CII
$\mathbf{B}_{24}$	$=$	$-y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}}$	$(8p)$	CII
$\mathbf{B}_{25}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	$(8p)$	CIII
$\mathbf{B}_{26}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	$(8p)$	CIII
$\mathbf{B}_{27}$	$=$	$-y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	$(8p)$	CIII
$\mathbf{B}_{28}$	$=$	$y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	$(8p)$	CIII
$\mathbf{B}_{29}$	$=$	$-x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	$(8p)$	CIII
$\mathbf{B}_{30}$	$=$	$x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	$(8p)$	CIII
$\mathbf{B}_{31}$	$=$	$y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(\frac{1}{2} - z_6\right) \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}}$	$(8p)$	CIII
$\mathbf{B}_{32}$	$=$	$-y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(\frac{1}{2} - z_6\right) \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}}$	$(8p)$	CIII
$\mathbf{B}_{33}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	$(8p)$	CIV
$\mathbf{B}_{34}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	$(8p)$	CIV
$\mathbf{B}_{35}$	$=$	$-y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	$=$	$-y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	$(8p)$	CIV
$\mathbf{B}_{36}$	$=$	$y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	$=$	$y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	$(8p)$	CIV
$\mathbf{B}_{37}$	$=$	$-x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}}$	$(8p)$	CIV
$\mathbf{B}_{38}$	$=$	$x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}}$	$(8p)$	CIV
$\mathbf{B}_{39}$	$=$	$y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(\frac{1}{2} - z_7\right) \mathbf{a}_3$	$=$	$y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_7\right) c \hat{\mathbf{z}}$	$(8p)$	CIV











$$\mathbf{B}_{184} = -y_{25} \mathbf{a}_1 - x_{25} \mathbf{a}_2 + \left(\frac{1}{2} - z_{25}\right) \mathbf{a}_3 = -y_{25}a \hat{\mathbf{x}} - x_{25}a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{25}\right)c \hat{\mathbf{z}} \quad (8p) \quad \text{S IV}$$

---

**References:**

- S. Spiliadis, A. A. Pinkerton, and D. Schwarzenbach, *Crystal and molecular structures of [AsPh<sub>4</sub>][Ln(S<sub>2</sub>PMe<sub>2</sub>)<sub>4</sub>](Ln = Ce or Tm) and their comparison with results obtained from paramagnetic nuclear magnetic resonance data in solution*, J. Chem. Soc. Dalton Trans. pp. 1809–1813 (1982), doi:[10.1039/DT9820001809](https://doi.org/10.1039/DT9820001809).

**Found in:**

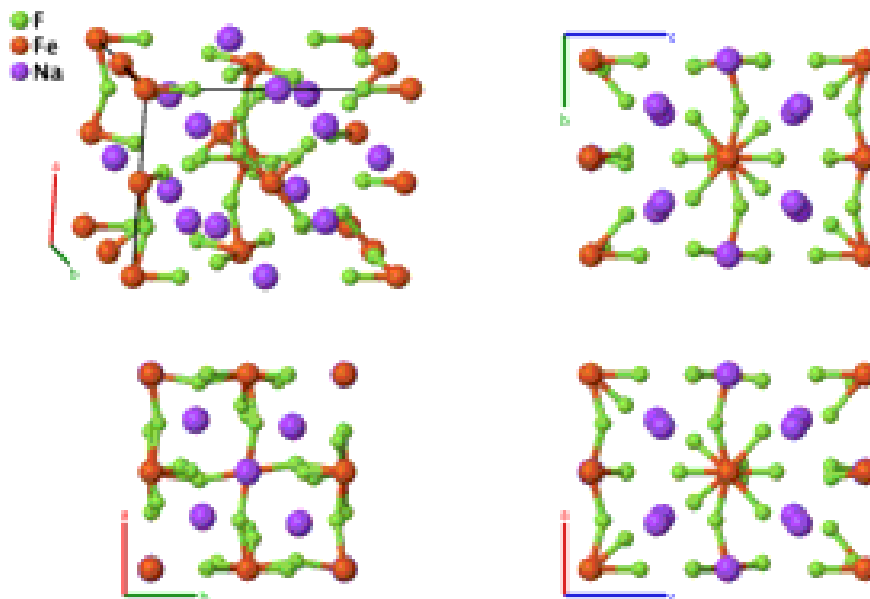
- F. Hoffmann, *The Fascination of Crystals and Symmetry* (2014). 230 - The space group list project.

---

**Geometry files:**

- CIF: pp. [870](#)
- POSCAR: pp. [870](#)

# Na<sub>5</sub>Fe<sub>3</sub>F<sub>14</sub> (High-temperature) Structure: A14B3C5\_tP44\_94\_c3g\_ad\_bg



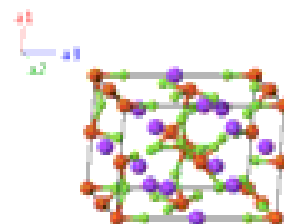
<b>Prototype</b>	:	Na <sub>5</sub> Fe <sub>3</sub> F <sub>14</sub>
<b>AFLOW prototype label</b>	:	A14B3C5_tP44_94_c3g_ad_bg
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP44
<b>Space group number</b>	:	94
<b>Space group symbol</b>	:	<i>P</i> 4 <sub>2</sub> 2 <sub>1</sub> 2
<b>AFLOW prototype command</b>	:	aflow --proto=A14B3C5_tP44_94_c3g_ad_bg --params= <i>a</i> , <i>c/a</i> , <i>z</i> <sub>3</sub> , <i>z</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>x</i> <sub>6</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub> , <i>x</i> <sub>7</sub> , <i>y</i> <sub>7</sub> , <i>z</i> <sub>7</sub> , <i>x</i> <sub>8</sub> , <i>y</i> <sub>8</sub> , <i>z</i> <sub>8</sub>

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type	
<b>B</b> <sub>1</sub>	=	0 <b>a</b> <sub>1</sub> + 0 <b>a</b> <sub>2</sub> + 0 <b>a</b> <sub>3</sub>	=	0 <b>x</b> <sub>̂</sub> + 0 <b>y</b> <sub>̂</sub> + 0 <b>z</b> <sub>̂</sub>	(2a)	Fe I
<b>B</b> <sub>2</sub>	=	$\frac{1}{2}$ <b>a</b> <sub>1</sub> + $\frac{1}{2}$ <b>a</b> <sub>2</sub> + $\frac{1}{2}$ <b>a</b> <sub>3</sub>	=	$\frac{1}{2}$ <b>a</b> <sub>1</sub> <b>x</b> <sub>̂</sub> + $\frac{1}{2}$ <b>a</b> <sub>2</sub> <b>y</b> <sub>̂</sub> + $\frac{1}{2}$ <b>c</b> <b>z</b> <sub>̂</sub>	(2a)	Fe I
<b>B</b> <sub>3</sub>	=	$\frac{1}{2}$ <b>a</b> <sub>3</sub>	=	$\frac{1}{2}$ <b>c</b> <b>z</b> <sub>̂</sub>	(2b)	Na I
<b>B</b> <sub>4</sub>	=	$\frac{1}{2}$ <b>a</b> <sub>1</sub> + $\frac{1}{2}$ <b>a</b> <sub>2</sub>	=	$\frac{1}{2}$ <b>a</b> <sub>1</sub> <b>x</b> <sub>̂</sub> + $\frac{1}{2}$ <b>a</b> <sub>2</sub> <b>y</b> <sub>̂</sub>	(2b)	Na I



$$\begin{aligned}
\mathbf{B}_{33} &= \begin{pmatrix} \frac{1}{2} - x_7 \\ \frac{1}{2} - z_7 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_7 \\ \frac{1}{2} - z_7 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= \begin{pmatrix} \frac{1}{2} - x_7 \\ \frac{1}{2} - z_7 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_7 \\ \frac{1}{2} - z_7 \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} & (8g) & \text{F IV} \\
\mathbf{B}_{34} &= \begin{pmatrix} \frac{1}{2} + x_7 \\ \frac{1}{2} - z_7 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - y_7 \\ \frac{1}{2} - z_7 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= \begin{pmatrix} \frac{1}{2} + x_7 \\ \frac{1}{2} - z_7 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - y_7 \\ \frac{1}{2} - z_7 \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} & (8g) & \text{F IV} \\
\mathbf{B}_{35} &= y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} & (8g) & \text{F IV} \\
\mathbf{B}_{36} &= -y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} & (8g) & \text{F IV} \\
\mathbf{B}_{37} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= x_8 a \hat{\mathbf{x}} + y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} & (8g) & \text{Na II} \\
\mathbf{B}_{38} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= -x_8 a \hat{\mathbf{x}} - y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} & (8g) & \text{Na II} \\
\mathbf{B}_{39} &= \begin{pmatrix} \frac{1}{2} - y_8 \\ \frac{1}{2} + z_8 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + x_8 \\ \frac{1}{2} + z_8 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= \begin{pmatrix} \frac{1}{2} - y_8 \\ \frac{1}{2} + z_8 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + x_8 \\ \frac{1}{2} + z_8 \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} & (8g) & \text{Na II} \\
\mathbf{B}_{40} &= \begin{pmatrix} \frac{1}{2} + y_8 \\ \frac{1}{2} + z_8 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - x_8 \\ \frac{1}{2} + z_8 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= \begin{pmatrix} \frac{1}{2} + y_8 \\ \frac{1}{2} + z_8 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - x_8 \\ \frac{1}{2} + z_8 \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} & (8g) & \text{Na II} \\
\mathbf{B}_{41} &= \begin{pmatrix} \frac{1}{2} - x_8 \\ \frac{1}{2} - z_8 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_8 \\ \frac{1}{2} - z_8 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= \begin{pmatrix} \frac{1}{2} - x_8 \\ \frac{1}{2} - z_8 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_8 \\ \frac{1}{2} - z_8 \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} & (8g) & \text{Na II} \\
\mathbf{B}_{42} &= \begin{pmatrix} \frac{1}{2} + x_8 \\ \frac{1}{2} - z_8 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - y_8 \\ \frac{1}{2} - z_8 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= \begin{pmatrix} \frac{1}{2} + x_8 \\ \frac{1}{2} - z_8 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - y_8 \\ \frac{1}{2} - z_8 \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} & (8g) & \text{Na II} \\
\mathbf{B}_{43} &= y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= y_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} - z_8 c \hat{\mathbf{z}} & (8g) & \text{Na II} \\
\mathbf{B}_{44} &= -y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -y_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} - z_8 c \hat{\mathbf{z}} & (8g) & \text{Na II}
\end{aligned}$$

---

#### References:

- M. Vlasse, F. Menil, C. Moriliere, J. M. Dance, A. Tressaud, and J. Portier, *Etude cristallographique et par effet Mössbauer du fluorure ferrimagnétique Na<sub>5</sub>Fe<sub>3</sub>F<sub>14</sub>γ*, J. Solid State Chem. **17**, 291–298 (1976), [doi:10.1016/0022-4596\(76\)90134-1](https://doi.org/10.1016/0022-4596(76)90134-1).

#### Found in:

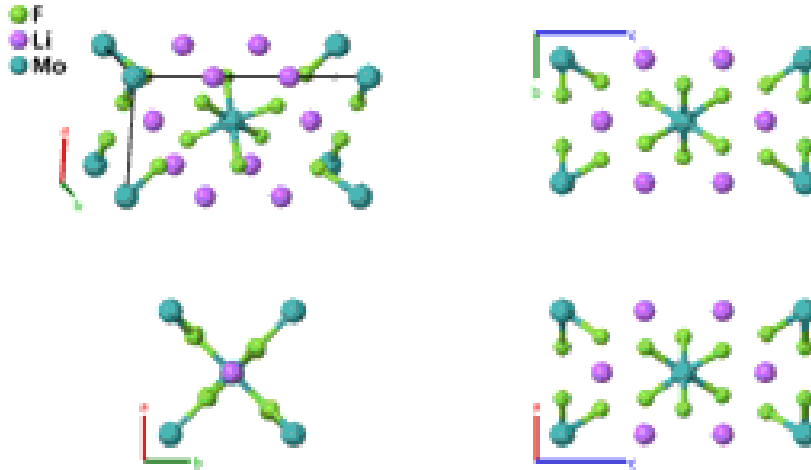
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [871](#)  
- POSCAR: pp. [871](#)

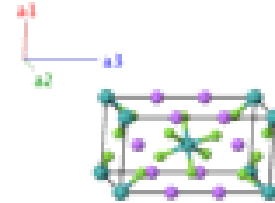
# Li<sub>2</sub>MoF<sub>6</sub> Structure: A6B2C\_tP18\_94\_eg\_c\_a



<b>Prototype</b>	:	Li <sub>2</sub> MoF <sub>6</sub>
<b>AFLOW prototype label</b>	:	A6B2C_tP18_94_eg_c_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP18
<b>Space group number</b>	:	94
<b>Space group symbol</b>	:	<i>P</i> 4 <sub>2</sub> 2 <sub>1</sub> 2
<b>AFLOW prototype command</b>	:	aflow --proto=A6B2C_tP18_94_eg_c_a --params= <i>a, c/a, z<sub>2</sub>, x<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub></i>

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2 <i>a</i> )	Mo
<b>B<sub>2</sub></b>	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2 <i>a</i> )	Mo
<b>B<sub>3</sub></b>	$z_2 \mathbf{a}_3$	=	$z_2 c \hat{\mathbf{z}}$	(4 <i>c</i> )	Li
<b>B<sub>4</sub></b>	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4 <i>c</i> )	Li
<b>B<sub>5</sub></b>	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(4 <i>c</i> )	Li
<b>B<sub>6</sub></b>	$-z_2 \mathbf{a}_3$	=	$-z_2 c \hat{\mathbf{z}}$	(4 <i>c</i> )	Li
<b>B<sub>7</sub></b>	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	=	$x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}}$	(4 <i>e</i> )	F I
<b>B<sub>8</sub></b>	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	=	$-x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}}$	(4 <i>e</i> )	F I

$$\begin{aligned}
\mathbf{B}_9 &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} && (4e) && \text{F I} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} && (4e) && \text{F I} \\
\mathbf{B}_{11} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (8g) && \text{F II} \\
\mathbf{B}_{12} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (8g) && \text{F II} \\
\mathbf{B}_{13} &= \left(\frac{1}{2} - y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} && (8g) && \text{F II} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} + y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} && (8g) && \text{F II} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} && (8g) && \text{F II} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} && (8g) && \text{F II} \\
\mathbf{B}_{17} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (8g) && \text{F II} \\
\mathbf{B}_{18} &= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (8g) && \text{F II}
\end{aligned}$$

---

#### References:

- G. Brunton, *The crystal structure of Li<sub>2</sub>MoF<sub>6</sub>*, Mater. Res. Bull. **6**, 555–560 (1971), doi:10.1016/0025-5408(71)90004-3.

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [872](#)  
- POSCAR: pp. [872](#)

# ThBC Structure: ABC\_tP24\_95\_d\_d\_d



<b>Prototype</b>	:	ThBC
<b>AFLOW prototype label</b>	:	ABC_tP24_95_d_d_d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP24
<b>Space group number</b>	:	95
<b>Space group symbol</b>	:	$P4_322$
<b>AFLOW prototype command</b>	:	aflow --proto=ABC_tP24_95_d_d_d --params= $a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

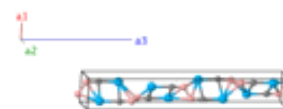
- This structure is the enantiomorph of the [ThBC \(ABC\\_tP24\\_91\\_d\\_d\\_d\) structure](#), and was generated by reflecting the coordinates of the space group #91 structure through the  $z = 0$  plane.

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_3$	$-y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{3}{4} + z_1\right) \mathbf{a}_3$	$-y_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_1\right) c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_4$	$y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{1}{4} + z_1\right) \mathbf{a}_3$	$y_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_1\right) c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_5$	$-x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_6$	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_7$	$y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{1}{4} - z_1\right) \mathbf{a}_3$	$y_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_1\right) c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_8$	$-y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{3}{4} - z_1\right) \mathbf{a}_3$	$-y_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \left(\frac{3}{4} - z_1\right) c \hat{\mathbf{z}}$	(8d)	B
$\mathbf{B}_9$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8d)	C
$\mathbf{B}_{10}$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$-x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(8d)	C
$\mathbf{B}_{11}$	$-y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{3}{4} + z_2\right) \mathbf{a}_3$	$-y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_2\right) c \hat{\mathbf{z}}$	(8d)	C
$\mathbf{B}_{12}$	$y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{4} + z_2\right) \mathbf{a}_3$	$y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_2\right) c \hat{\mathbf{z}}$	(8d)	C

$$\begin{aligned}
\mathbf{B}_{13} &= -x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} && (8d) && \text{C} \\
\mathbf{B}_{14} &= x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} && (8d) && \text{C} \\
\mathbf{B}_{15} &= y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{4} - z_2\right) \mathbf{a}_3 &= y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_2\right) c \hat{\mathbf{z}} && (8d) && \text{C} \\
\mathbf{B}_{16} &= -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{3}{4} - z_2\right) \mathbf{a}_3 &= -y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{3}{4} - z_2\right) c \hat{\mathbf{z}} && (8d) && \text{C} \\
\mathbf{B}_{17} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{18} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{19} &= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{3}{4} + z_3\right) \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{3}{4} + z_3\right) c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{20} &= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{4} + z_3\right) \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_3\right) c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{21} &= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{22} &= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{23} &= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{4} - z_3\right) \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_3\right) c \hat{\mathbf{z}} && (8d) && \text{Th} \\
\mathbf{B}_{24} &= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{3}{4} - z_3\right) \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{3}{4} - z_3\right) c \hat{\mathbf{z}} && (8d) && \text{Th}
\end{aligned}$$

---

### References:

- P. Rogl, *The crystal structure of ThBC*, J. Nucl. Mat. **73**, 198–203 (1978), doi:10.1016/0022-3115(78)90560-3.

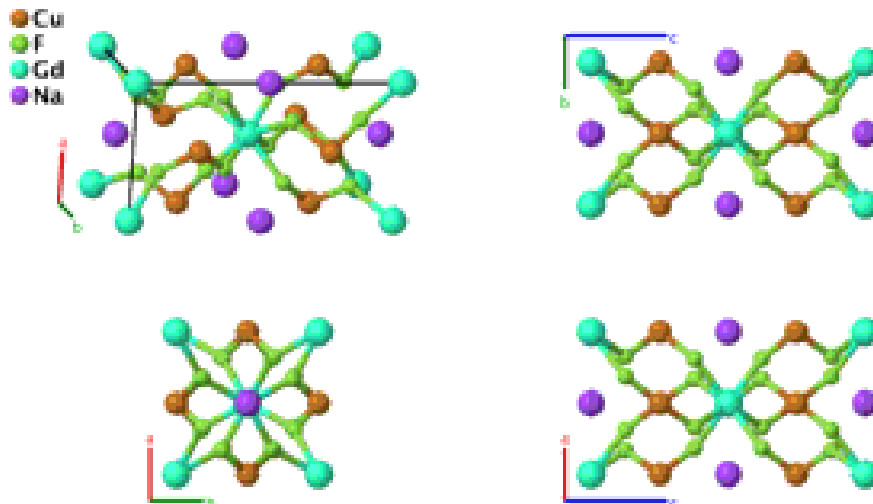
---

### Geometry files:

- CIF: pp. [872](#)  
- POSCAR: pp. [872](#)



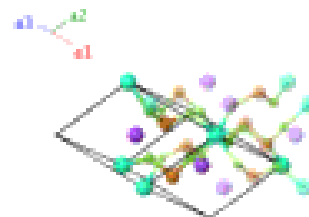
# NaGdCu<sub>2</sub>F<sub>8</sub> Structure: A2B8CD\_tI24\_97\_d\_k\_a\_b



**Prototype** : NaGdCu<sub>2</sub>F<sub>8</sub>  
**AFLOW prototype label** : A2B8CD\_tI24\_97\_d\_k\_a\_b  
**Strukturbericht designation** : None  
**Pearson symbol** : tI24  
**Space group number** : 97  
**Space group symbol** : *I422*  
**AFLOW prototype command** : aflow --proto=A2B8CD\_tI24\_97\_d\_k\_a\_b  
 --params=*a, c/a, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>*

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\
 \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$	$0\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}}$	(2 <i>a</i> )	Gd
<b>B<sub>2</sub></b> =	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$\frac{1}{2}c\hat{\mathbf{z}}$	(2 <i>b</i> )	Na
<b>B<sub>3</sub></b> =	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$\frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4 <i>d</i> )	Cu
<b>B<sub>4</sub></b> =	$\frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4 <i>d</i> )	Cu
<b>B<sub>5</sub></b> =	$(y_4 + z_4)\mathbf{a}_1 + (x_4 + z_4)\mathbf{a}_2 + (x_4 + y_4)\mathbf{a}_3$	$x_4a\hat{\mathbf{x}} + y_4a\hat{\mathbf{y}} + z_4c\hat{\mathbf{z}}$	(16 <i>k</i> )	F
<b>B<sub>6</sub></b> =	$(-y_4 + z_4)\mathbf{a}_1 + (-x_4 + z_4)\mathbf{a}_2 + (-x_4 - y_4)\mathbf{a}_3$	$-x_4a\hat{\mathbf{x}} - y_4a\hat{\mathbf{y}} + z_4c\hat{\mathbf{z}}$	(16 <i>k</i> )	F
<b>B<sub>7</sub></b> =	$(x_4 + z_4)\mathbf{a}_1 + (-y_4 + z_4)\mathbf{a}_2 + (x_4 - y_4)\mathbf{a}_3$	$-y_4a\hat{\mathbf{x}} + x_4a\hat{\mathbf{y}} + z_4c\hat{\mathbf{z}}$	(16 <i>k</i> )	F
<b>B<sub>8</sub></b> =	$(-x_4 + z_4)\mathbf{a}_1 + (y_4 + z_4)\mathbf{a}_2 + (-x_4 + y_4)\mathbf{a}_3$	$y_4a\hat{\mathbf{x}} - x_4a\hat{\mathbf{y}} + z_4c\hat{\mathbf{z}}$	(16 <i>k</i> )	F

$$\mathbf{B}_9 = (y_4 - z_4) \mathbf{a}_1 + (-x_4 - z_4) \mathbf{a}_2 + (-x_4 + y_4) \mathbf{a}_3 = -x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} \quad (16k) \quad \text{F}$$

$$\mathbf{B}_{10} = (-y_4 - z_4) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3 = x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} \quad (16k) \quad \text{F}$$

$$\mathbf{B}_{11} = (x_4 - z_4) \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3 = y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} \quad (16k) \quad \text{F}$$

$$\mathbf{B}_{12} = (-x_4 - z_4) \mathbf{a}_1 + (-y_4 - z_4) \mathbf{a}_2 + (-x_4 - y_4) \mathbf{a}_3 = -y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} \quad (16k) \quad \text{F}$$

---

**References:**

- C. De Nadaï, A. Demourgues, L. Lozano, P. Gravereau, and J. Grannec, *Structural investigations of new copper fluorides NaRECu<sub>2</sub>F<sub>8</sub> (RE<sup>3+</sup> = Sm<sup>3+</sup>, Eu<sup>3+</sup>, Gd<sup>3+</sup>, Y<sup>3+</sup>, Er<sup>3+</sup>, Yb<sup>3+</sup>)*, J. Mater. Chem. **8**, 2487–2491 (1998), [doi:10.1039/A803015D](https://doi.org/10.1039/A803015D).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

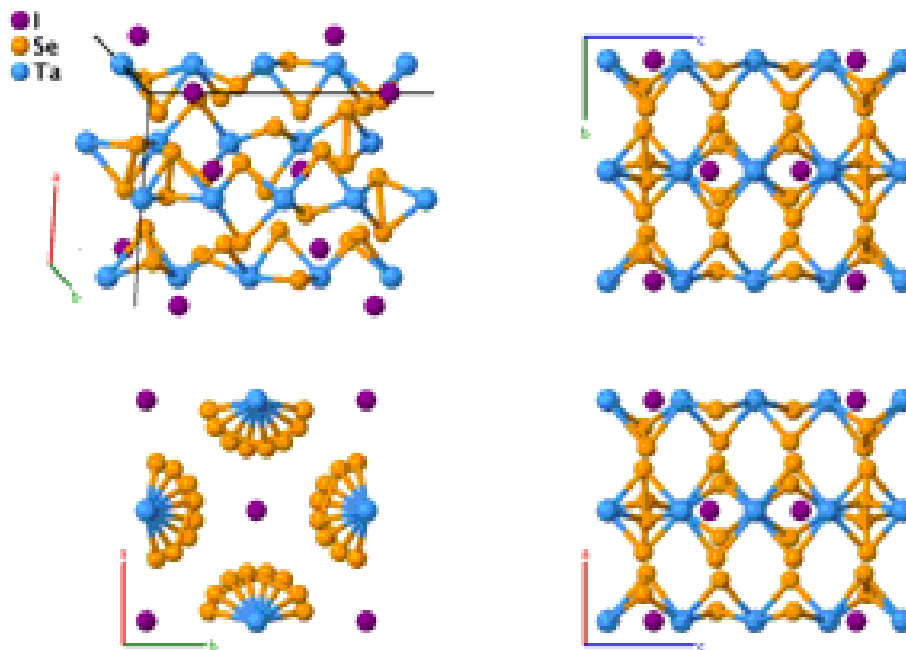
---

**Geometry files:**

- CIF: pp. [873](#)

- POSCAR: pp. [873](#)

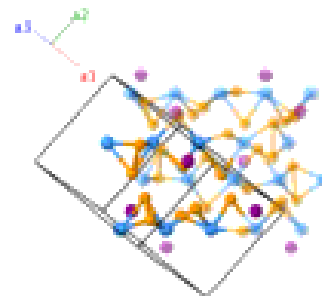
# Ta<sub>2</sub>Se<sub>8</sub>I Structure: AB8C2\_tI44\_97\_e\_2k\_cd



<b>Prototype</b>	:	Ta <sub>2</sub> Se <sub>8</sub> I
<b>AFLOW prototype label</b>	:	AB8C2_tI44_97_e_2k_cd
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI44
<b>Space group number</b>	:	97
<b>Space group symbol</b>	:	I422
<b>AFLOW prototype command</b>	:	aflow --proto=AB8C2_tI44_97_e_2k_cd --params=a, c/a, z3, x4, y4, z4, x5, y5, z5

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{y}}$	(4c)	Ta I
<b>B<sub>2</sub></b> =	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}}$	(4c)	Ta I
<b>B<sub>3</sub></b> =	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Ta II
<b>B<sub>4</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Ta II

$$\begin{aligned}
\mathbf{B}_5 &= z_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 &= z_3 c \hat{\mathbf{z}} & (4e) & \text{I} \\
\mathbf{B}_6 &= -z_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 &= -z_3 c \hat{\mathbf{z}} & (4e) & \text{I} \\
\mathbf{B}_7 &= (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16k) & \text{Se I} \\
\mathbf{B}_8 &= (-y_4 + z_4) \mathbf{a}_1 + (-x_4 + z_4) \mathbf{a}_2 + (-x_4 - y_4) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16k) & \text{Se I} \\
\mathbf{B}_9 &= (x_4 + z_4) \mathbf{a}_1 + (-y_4 + z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3 &= -y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16k) & \text{Se I} \\
\mathbf{B}_{10} &= (-x_4 + z_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + (-x_4 + y_4) \mathbf{a}_3 &= y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16k) & \text{Se I} \\
\mathbf{B}_{11} &= (y_4 - z_4) \mathbf{a}_1 + (-x_4 - z_4) \mathbf{a}_2 + (-x_4 + y_4) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16k) & \text{Se I} \\
\mathbf{B}_{12} &= (-y_4 - z_4) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16k) & \text{Se I} \\
\mathbf{B}_{13} &= (x_4 - z_4) \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3 &= y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16k) & \text{Se I} \\
\mathbf{B}_{14} &= (-x_4 - z_4) \mathbf{a}_1 + (-y_4 - z_4) \mathbf{a}_2 + (-x_4 - y_4) \mathbf{a}_3 &= -y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16k) & \text{Se I} \\
\mathbf{B}_{15} &= (y_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + (x_5 + y_5) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (16k) & \text{Se II} \\
\mathbf{B}_{16} &= (-y_5 + z_5) \mathbf{a}_1 + (-x_5 + z_5) \mathbf{a}_2 + (-x_5 - y_5) \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (16k) & \text{Se II} \\
\mathbf{B}_{17} &= (x_5 + z_5) \mathbf{a}_1 + (-y_5 + z_5) \mathbf{a}_2 + (x_5 - y_5) \mathbf{a}_3 &= -y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (16k) & \text{Se II} \\
\mathbf{B}_{18} &= (-x_5 + z_5) \mathbf{a}_1 + (y_5 + z_5) \mathbf{a}_2 + (-x_5 + y_5) \mathbf{a}_3 &= y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (16k) & \text{Se II} \\
\mathbf{B}_{19} &= (y_5 - z_5) \mathbf{a}_1 + (-x_5 - z_5) \mathbf{a}_2 + (-x_5 + y_5) \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (16k) & \text{Se II} \\
\mathbf{B}_{20} &= (-y_5 - z_5) \mathbf{a}_1 + (x_5 - z_5) \mathbf{a}_2 + (x_5 - y_5) \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (16k) & \text{Se II} \\
\mathbf{B}_{21} &= (x_5 - z_5) \mathbf{a}_1 + (y_5 - z_5) \mathbf{a}_2 + (x_5 + y_5) \mathbf{a}_3 &= y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (16k) & \text{Se II} \\
\mathbf{B}_{22} &= (-x_5 - z_5) \mathbf{a}_1 + (-y_5 - z_5) \mathbf{a}_2 + (-x_5 - y_5) \mathbf{a}_3 &= -y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (16k) & \text{Se II}
\end{aligned}$$

---

### References:

- P. Gressier, A. Meerschaut, L. Guemas, J. Rouxel, and P. Monceau, *Characterization of the new series of quasi one-dimensional compounds (MX<sub>4</sub>)<sub>n</sub>Y (M = Nb, Ta; X = S, Se; Y = Br, I)*, J. Solid State Chem. **51**, 141–151 (1984), doi:10.1016/0022-4596(84)90327-X.

### Found in:

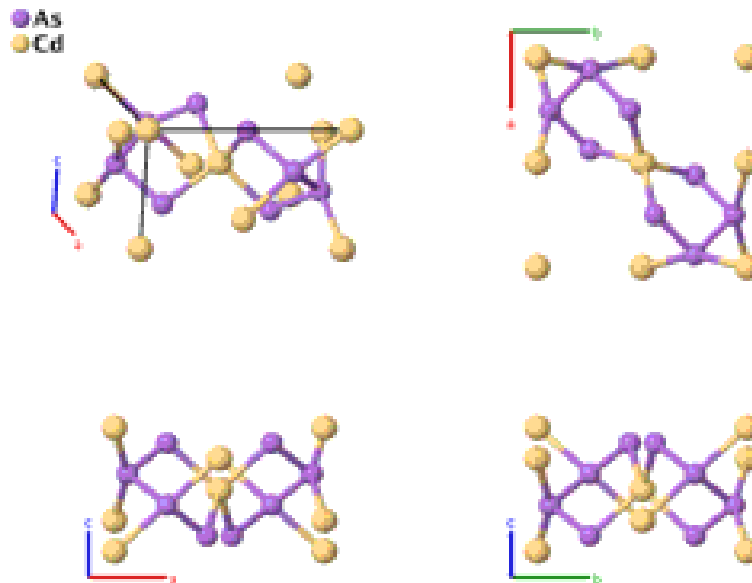
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. 873  
- POSCAR: pp. 874

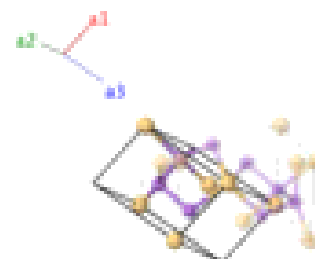
# CdAs<sub>2</sub> Structure: A2B\_tI12\_98\_f\_a



<b>Prototype</b>	:	CdAs <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_tI12_98_f_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI12
<b>Space group number</b>	:	98
<b>Space group symbol</b>	:	<i>I</i> 4 <sub>1</sub> 22
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_tI12_98_f_a --params=a, c/a, x <sub>2</sub>

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(4a)	Cd
<b>B<sub>2</sub></b>	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4a)	Cd
<b>B<sub>3</sub></b>	$\frac{3}{8} \mathbf{a}_1 + \left(\frac{1}{8} + x_2\right) \mathbf{a}_2 + \left(\frac{1}{4} + x_2\right) \mathbf{a}_3$	=	$x_2 a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{8} c \hat{\mathbf{z}}$	(8f)	As
<b>B<sub>4</sub></b>	$\frac{7}{8} \mathbf{a}_1 + \left(\frac{1}{8} - x_2\right) \mathbf{a}_2 + \left(\frac{3}{4} - x_2\right) \mathbf{a}_3$	=	$-x_2 a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{8} c \hat{\mathbf{z}}$	(8f)	As

$$\mathbf{B}_5 = \left(\frac{7}{8} + x_2\right) \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \left(\frac{1}{4} + x_2\right) \mathbf{a}_3 = \frac{3}{4}a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right)a \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}} \quad (8f) \quad \text{As}$$

$$\mathbf{B}_6 = \left(\frac{7}{8} - x_2\right) \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \left(\frac{3}{4} - x_2\right) \mathbf{a}_3 = \frac{1}{4}a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right)a \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}} \quad (8f) \quad \text{As}$$

---

**References:**

- V. N. Yakimovich, V. A. Rubtsov, and V. M. Trukhan, *Phase Relationships in the CdP<sub>4</sub>-ZnP<sub>2</sub>-CdAs<sub>2</sub>-ZnAs<sub>2</sub> System*, *Inorg. Mat.* **32**, 579–582 (1996).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

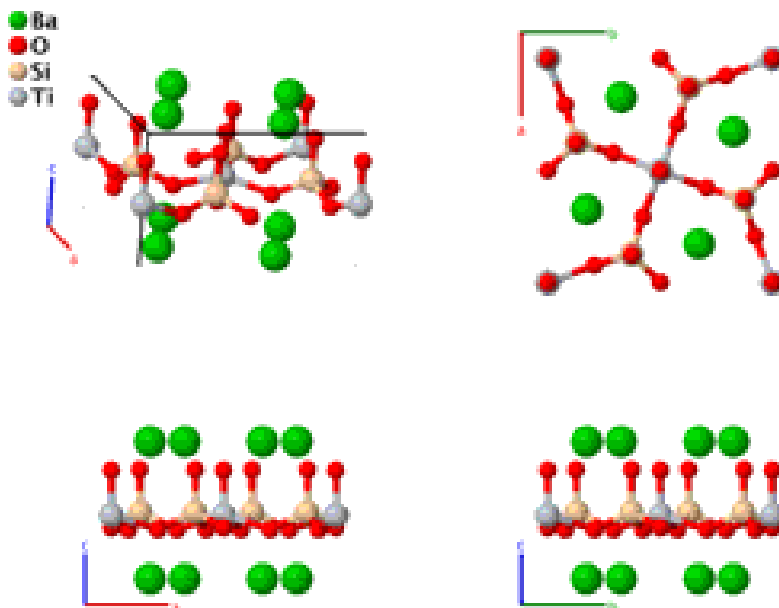
---

**Geometry files:**

- CIF: pp. [874](#)

- POSCAR: pp. [874](#)

# Fresnoite ( $\text{Ba}_2\text{TiSi}_2\text{O}_8$ ) Structure: A2B8C2D\_tP26\_100\_c\_abcd\_c\_a

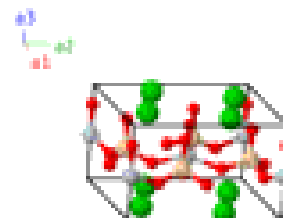


<b>Prototype</b>	:	$\text{Ba}_2\text{TiSi}_2\text{O}_8$
<b>AFLOW prototype label</b>	:	A2B8C2D_tP26_100_c_abcd_c_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP26
<b>Space group number</b>	:	100
<b>Space group symbol</b>	:	$P4bm$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B8C2D_tP26_100_c_abcd_c_a --params= $a, c/a, z_1, z_2, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, y_7, z_7$

- Found in the [Big Creek-Rush Creek sanbornite deposit](#), 5 miles NE of Trimmer, Fresno Co. California.

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= a \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$z_1 c \hat{z}$	(2a)	O I

$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_3$	$=$	$z_2 \mathbf{a}_3$	$=$	$z_2 c \hat{\mathbf{z}}$	(2a)	Ti
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2a)	Ti
$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + z_3 c \hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B}_7$	$=$	$x_4 \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4c)	Ba
$\mathbf{B}_8$	$=$	$-x_4 \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4c)	Ba
$\mathbf{B}_9$	$=$	$\left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4c)	Ba
$\mathbf{B}_{10}$	$=$	$\left(\frac{1}{2} + x_4\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4c)	Ba
$\mathbf{B}_{11}$	$=$	$x_5 \mathbf{a}_1 + \left(\frac{1}{2} + x_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{12}$	$=$	$-x_5 \mathbf{a}_1 + \left(\frac{1}{2} - x_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{13}$	$=$	$\left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{14}$	$=$	$\left(\frac{1}{2} + x_5\right) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{15}$	$=$	$x_6 \mathbf{a}_1 + \left(\frac{1}{2} + x_6\right) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4c)	Si
$\mathbf{B}_{16}$	$=$	$-x_6 \mathbf{a}_1 + \left(\frac{1}{2} - x_6\right) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4c)	Si
$\mathbf{B}_{17}$	$=$	$\left(\frac{1}{2} - x_6\right) \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_6\right) a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4c)	Si
$\mathbf{B}_{18}$	$=$	$\left(\frac{1}{2} + x_6\right) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_6\right) a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(4c)	Si
$\mathbf{B}_{19}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{20}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{21}$	$=$	$-y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{22}$	$=$	$y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{23}$	$=$	$\left(\frac{1}{2} + x_7\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_7\right) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_7\right) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{24}$	$=$	$\left(\frac{1}{2} - x_7\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_7\right) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_7\right) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{25}$	$=$	$\left(\frac{1}{2} - y_7\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_7\right) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - y_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_7\right) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{26}$	$=$	$\left(\frac{1}{2} + y_7\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_7\right) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + y_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_7\right) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8d)	O IV

---

### References:

- S. A. Markgraf, A. Halliya, A. S. Bhalla, R. E. Newnham, and C. T. Prewitt, *X-ray structure refinement and pyroelectric investigation of fersnoite, Ba<sub>2</sub>TiSi<sub>2</sub>O<sub>8</sub>*, *Ferroelectrics* **62**, 17–26 (1985), [doi:10.1080/00150198508017914](https://doi.org/10.1080/00150198508017914).

---

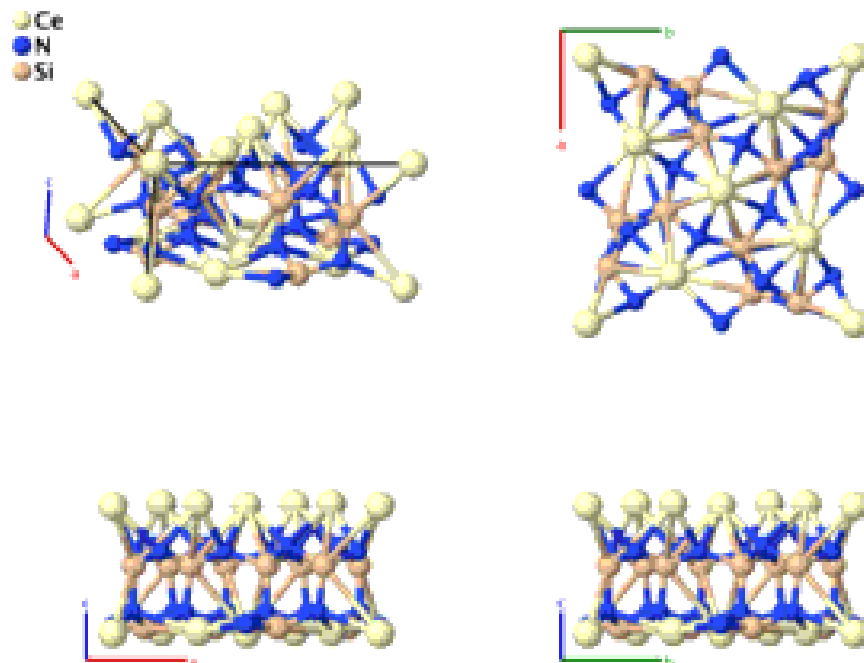
### Geometry files:

- CIF: pp. [874](#)

- POSCAR: pp. [875](#)



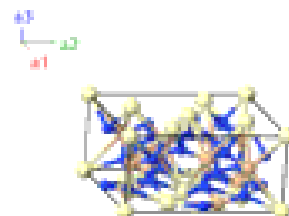
# Ce<sub>3</sub>Si<sub>6</sub>N<sub>11</sub> Structure: A3B11C6\_tP40\_100\_ac\_bc2d\_cd



<b>Prototype</b>	:	Ce <sub>3</sub> Si <sub>6</sub> N <sub>11</sub>
<b>AFLOW prototype label</b>	:	A3B11C6_tP40_100_ac_bc2d_cd
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP40
<b>Space group number</b>	:	100
<b>Space group symbol</b>	:	<i>P4bm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3B11C6_tP40_100_ac_bc2d_cd --params= <i>a, c/a, z<sub>1</sub>, z<sub>2</sub>, x<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub></i>

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(2a)	Ce I
<b>B<sub>2</sub></b>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(2a)	Ce I



$$\mathbf{B}_{39} = \left(\frac{1}{2} - y_8\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_8\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 = \left(\frac{1}{2} - y_8\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_8\right) a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} \quad (8d) \quad \text{Si II}$$

$$\mathbf{B}_{40} = \left(\frac{1}{2} + y_8\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_8\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 = \left(\frac{1}{2} + y_8\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_8\right) a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} \quad (8d) \quad \text{Si II}$$

---

**References:**

- M. Woike and W. Jeitschko, *Preparation and Crystal Structure of the Nitridosilicates  $Ln_3Si_6N_{11}$  ( $Ln = La, Ce, Pr, Nd, Sm$ ) and  $LnSi_3N_5$  ( $Ln = Ce, Pr, Nd$ )*, *Inorg. Chem.* **34**, 5105–5108 (1995), [doi:10.1021/ic00125a005](https://doi.org/10.1021/ic00125a005).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

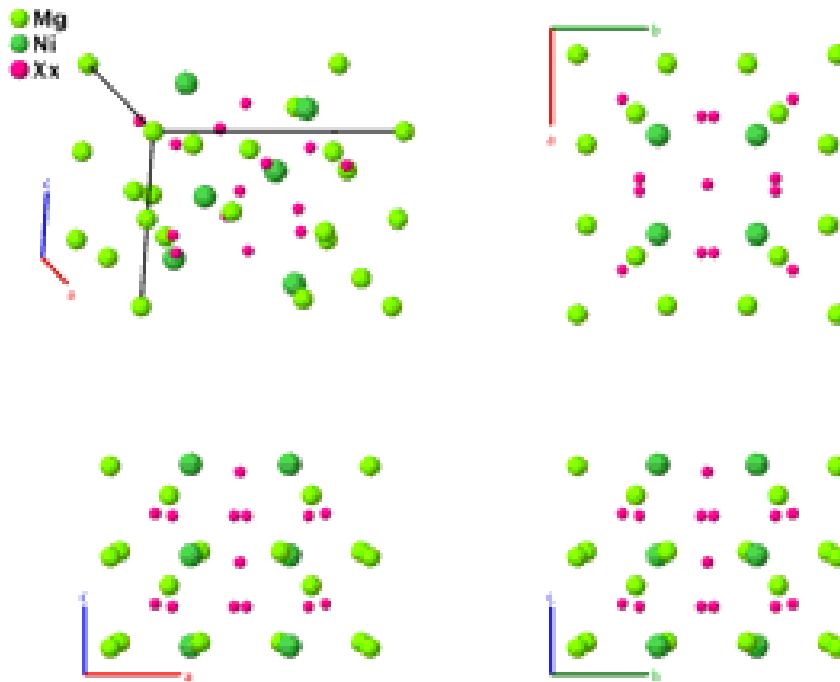
---

**Geometry files:**

- CIF: pp. [875](#)

- POSCAR: pp. [875](#)

# $\gamma$ -MgNiSn Structure: A7B7C2\_tP32\_101\_bde\_ade\_d

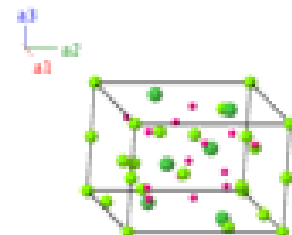


<b>Prototype</b>	:	$\gamma$ -MgNiSn
<b>AFLOW prototype label</b>	:	A7B7C2_tP32_101_bde_ade_d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP32
<b>Space group number</b>	:	101
<b>Space group symbol</b>	:	$P4_2cm$
<b>AFLOW prototype command</b>	:	aflow --proto=A7B7C2_tP32_101_bde_ade_d --params=a, c/a, z <sub>1</sub> , z <sub>2</sub> , x <sub>3</sub> , z <sub>3</sub> , x <sub>4</sub> , z <sub>4</sub> , x <sub>5</sub> , z <sub>5</sub> , x <sub>6</sub> , y <sub>6</sub> , z <sub>6</sub> , x <sub>7</sub> , y <sub>7</sub> , z <sub>7</sub>

- This is the  $\gamma$  phase of the Mg-Ni-Sn ternary system. The (2b), (8e) and (4d) Wyckoff positions are partially occupied and are represented by the labels M I, M II, and M III, respectively. Here, M I is 0.88Mg+0.12Ni, M II is 0.96Mg+0.05Ni, and M III is 0.88Sn+0.12Mg. The Jmol image does not distinguish between the different M labels and is represented by the "Xx" atoms.

**Simple Tetragonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(2a)	Mg I
<b>B</b> <sub>2</sub>	= $\left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$\left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Mg I
<b>B</b> <sub>3</sub>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2b)	M I
<b>B</b> <sub>4</sub>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(2b)	M I
<b>B</b> <sub>5</sub>	= $x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4d)	M II
<b>B</b> <sub>6</sub>	= $-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$-x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4d)	M II
<b>B</b> <sub>7</sub>	= $-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	=	$-x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4d)	M II
<b>B</b> <sub>8</sub>	= $x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	=	$x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4d)	M II
<b>B</b> <sub>9</sub>	= $x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4d)	Mg II
<b>B</b> <sub>10</sub>	= $-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$-x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4d)	Mg II
<b>B</b> <sub>11</sub>	= $-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	=	$-x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(4d)	Mg II
<b>B</b> <sub>12</sub>	= $x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	=	$x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(4d)	Mg II
<b>B</b> <sub>13</sub>	= $x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4d)	Ni
<b>B</b> <sub>14</sub>	= $-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$-x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4d)	Ni
<b>B</b> <sub>15</sub>	= $-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	=	$-x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(4d)	Ni
<b>B</b> <sub>16</sub>	= $x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	=	$x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(4d)	Ni
<b>B</b> <sub>17</sub>	= $x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8e)	M III
<b>B</b> <sub>18</sub>	= $-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$-x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8e)	M III
<b>B</b> <sub>19</sub>	= $-y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	=	$-y_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(8e)	M III
<b>B</b> <sub>20</sub>	= $y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	=	$y_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(8e)	M III
<b>B</b> <sub>21</sub>	= $x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	=	$x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(8e)	M III
<b>B</b> <sub>22</sub>	= $-x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3$	=	$-x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}}$	(8e)	M III
<b>B</b> <sub>23</sub>	= $-y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$-y_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8e)	M III
<b>B</b> <sub>24</sub>	= $y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$y_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8e)	M III
<b>B</b> <sub>25</sub>	= $x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8e)	Mg III
<b>B</b> <sub>26</sub>	= $-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8e)	Mg III
<b>B</b> <sub>27</sub>	= $-y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	=	$-y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(8e)	Mg III
<b>B</b> <sub>28</sub>	= $y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	=	$y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(8e)	Mg III
<b>B</b> <sub>29</sub>	= $x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(8e)	Mg III
<b>B</b> <sub>30</sub>	= $-x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}}$	(8e)	Mg III
<b>B</b> <sub>31</sub>	= $-y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$-y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8e)	Mg III
<b>B</b> <sub>32</sub>	= $y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(8e)	Mg III

#### References:

- M. Boudard, P. Bordet, H. Vincent, and F. Audebert, *The structure of the Y-phase in the Mg–Ni–Sn system*, J. Alloys Compd. **372**, 121–128 (2004), doi:10.1016/j.jallcom.2003.09.142.

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

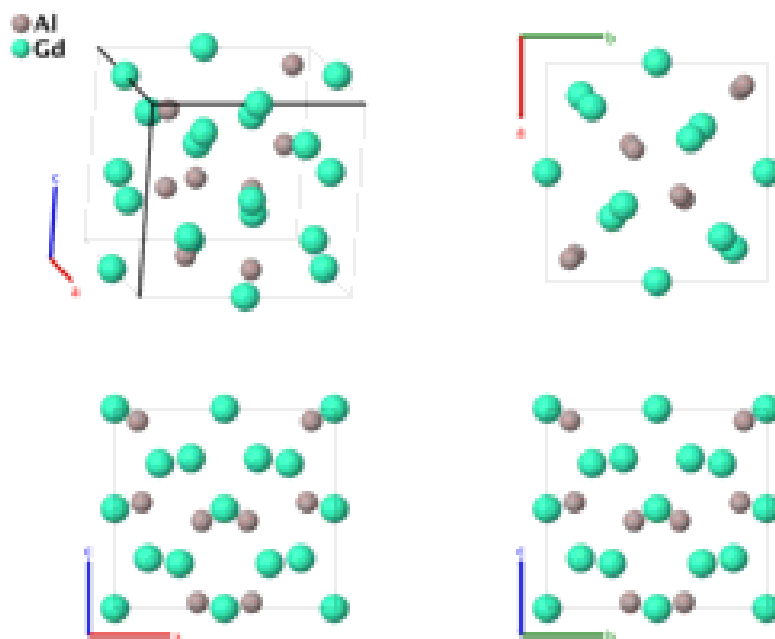
---

**Geometry files:**

- CIF: pp. [875](#)

- POSCAR: pp. [876](#)

# Gd<sub>3</sub>Al<sub>2</sub> Structure: A2B3\_tP20\_102\_2c\_b2c



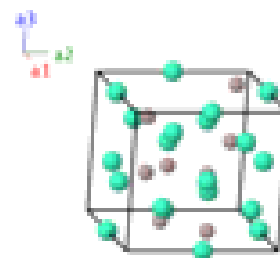
<b>Prototype</b>	:	Gd <sub>3</sub> Al <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B3_tP20_102_2c_b2c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP20
<b>Space group number</b>	:	102
<b>Space group symbol</b>	:	<i>P4<sub>2</sub>nm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3_tP20_102_2c_b2c --params= <i>a, c/a, z<sub>1</sub>, z<sub>2</sub>, z<sub>3</sub>, z<sub>4</sub>, z<sub>5</sub></i>

Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$\frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4b)	Gd I
<b>B<sub>2</sub></b> =	$\frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4b)	Gd I
<b>B<sub>3</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4b)	Gd I
<b>B<sub>4</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + z_1 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + z_1 c \hat{\mathbf{z}}$	(4b)	Gd I

$$\begin{aligned}
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (4c) & \text{Al I} \\
\mathbf{B}_6 &= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (4c) & \text{Al I} \\
\mathbf{B}_7 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4c) & \text{Al I} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4c) & \text{Al I} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4c) & \text{Al II} \\
\mathbf{B}_{10} &= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (4c) & \text{Al II} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4c) & \text{Al II} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4c) & \text{Al II} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (4c) & \text{Gd II} \\
\mathbf{B}_{14} &= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (4c) & \text{Gd II} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (4c) & \text{Gd II} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (4c) & \text{Gd II} \\
\mathbf{B}_{17} &= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (4c) & \text{Gd III} \\
\mathbf{B}_{18} &= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (4c) & \text{Gd III} \\
\mathbf{B}_{19} &= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (4c) & \text{Gd III} \\
\mathbf{B}_{20} &= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (4c) & \text{Gd III}
\end{aligned}$$

---

#### References:

- K. H. J. Buschow, *Rare earth-aluminium intermetallic compounds of the form  $RAl$  and  $R_3Al_2$* , *J. Less-Common Met.* **8**, 209–212 (1965), doi:10.1016/0022-5088(65)90047-0.

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

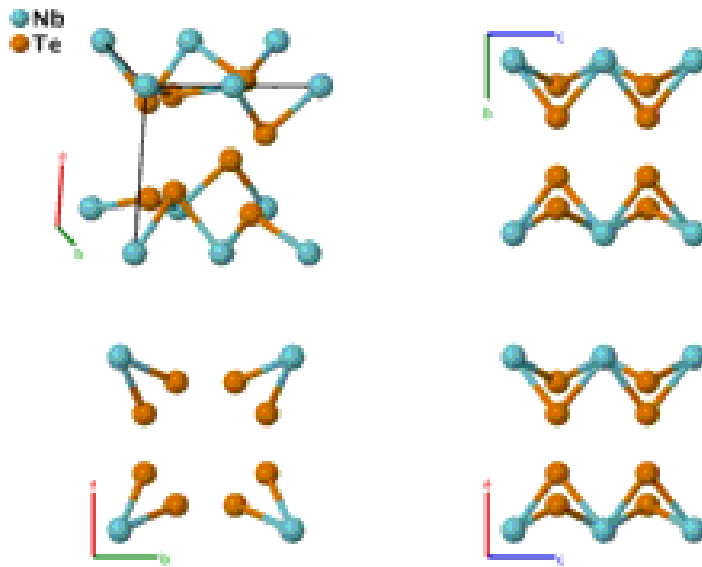
---

#### Geometry files:

- CIF: pp. 876  
- POSCAR: pp. 876



# NbTe<sub>4</sub> Structure: AB4\_tP10\_103\_a\_d



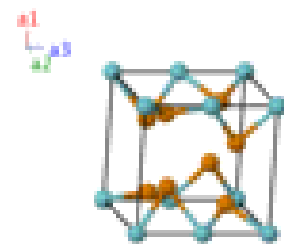
<b>Prototype</b>	:	NbTe <sub>4</sub>
<b>AFLOW prototype label</b>	:	AB4_tP10_103_a_d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP10
<b>Space group number</b>	:	103
<b>Space group symbol</b>	:	<i>P4cc</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB4_tP10_103_a_d --params=a, c/a, z <sub>1</sub> , x <sub>2</sub> , y <sub>2</sub> , z <sub>2</sub>

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$z_1 \mathbf{a}_3$	$z_1 c \hat{\mathbf{z}}$	(2a)	Nb
<b>B<sub>2</sub></b> =	$\left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Nb
<b>B<sub>3</sub></b> =	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8d)	Te
<b>B<sub>4</sub></b> =	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$-x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8d)	Te
<b>B<sub>5</sub></b> =	$-y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$-y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8d)	Te
<b>B<sub>6</sub></b> =	$y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8d)	Te

$$\mathbf{B}_7 = x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} \quad (8d) \quad \text{Te}$$

$$\mathbf{B}_8 = -x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} \quad (8d) \quad \text{Te}$$

$$\mathbf{B}_9 = -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = -y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} \quad (8d) \quad \text{Te}$$

$$\mathbf{B}_{10} = y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} \quad (8d) \quad \text{Te}$$

#### References:

- H. Böhm, *The high temperature modification of niobium tetratelluride NbTe<sub>4</sub>*, *Zeitschrift für Kristallographie - Crystalline Materials* **180**, 113–122 (1987), [doi:10.1524/zkri.1987.180.1-4.113](https://doi.org/10.1524/zkri.1987.180.1-4.113).

#### Found in:

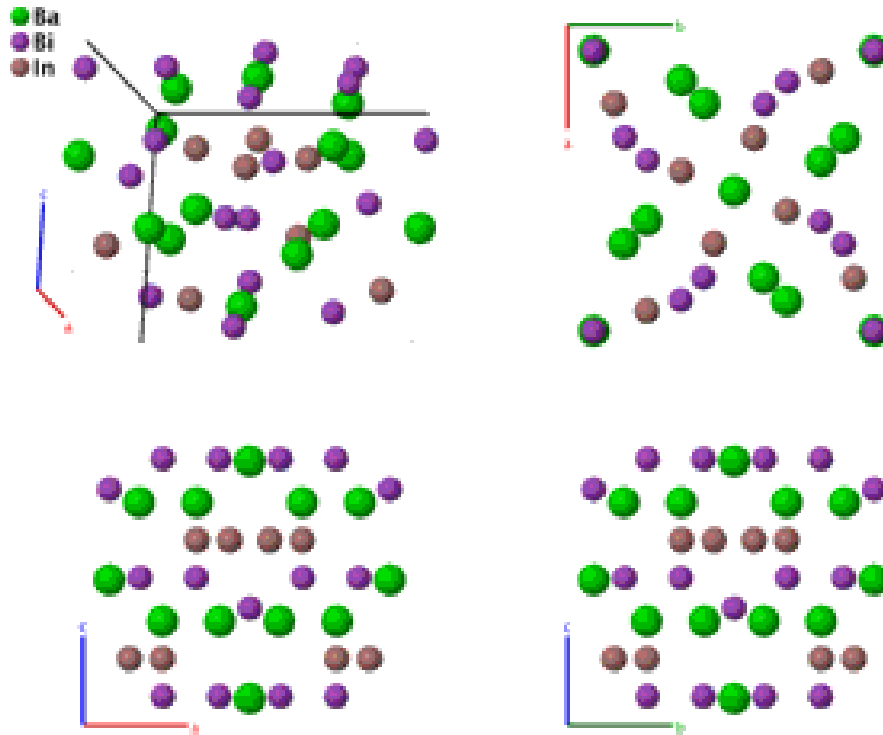
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. [877](#)

- POSCAR: pp. [877](#)

# Ba<sub>5</sub>In<sub>4</sub>Bi<sub>5</sub> Structure: A5B5C4\_tP28\_104\_ac\_ac\_c



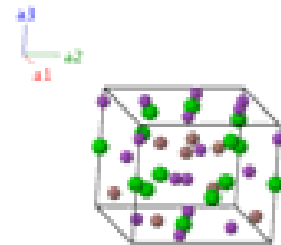
<b>Prototype</b>	:	Ba <sub>5</sub> In <sub>4</sub> Bi <sub>5</sub>
<b>AFLOW prototype label</b>	:	A5B5C4_tP28_104_ac_ac_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP28
<b>Space group number</b>	:	104
<b>Space group symbol</b>	:	<i>P4nc</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A5B5C4_tP28_104_ac_ac_c</code> <code>--params=a, c/a, z1, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5</code>

Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$z_1 c \hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Ba I



**References:**

- S. Ponou, T. F. Fässler, G. Tobías, E. Canadell, A. Cho, and S. C. Sevov, *Synthesis, Characterization, and Electronic Structure of  $Ba_5In_4Bi_5$ : An Acentric and One-Electron Deficient Phase*, Chem. Euro. J. **10**, 3615–3621 (2004), [doi:10.1002/chem.200306061](https://doi.org/10.1002/chem.200306061).

**Found in:**

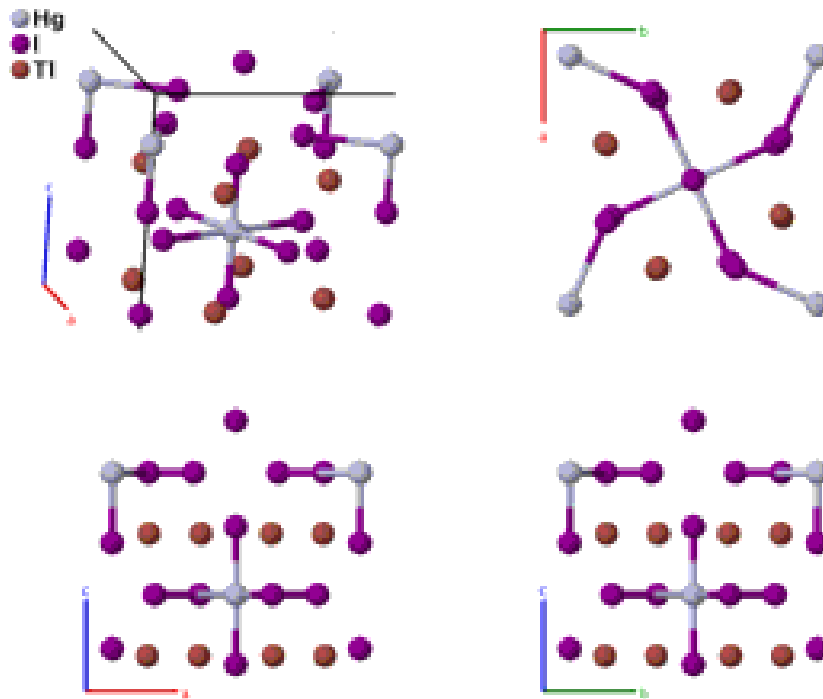
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [877](#)  
- POSCAR: pp. [877](#)

# Tl<sub>4</sub>HgI<sub>6</sub> Structure: AB6C4\_tP22\_104\_a\_2ac\_c

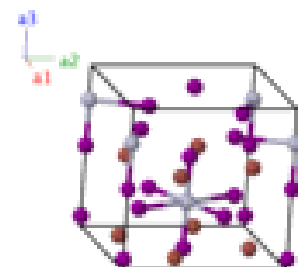


<b>Prototype</b>	:	Tl <sub>4</sub> HgI <sub>6</sub>
<b>AFLOW prototype label</b>	:	AB6C4_tP22_104_a_2ac_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP22
<b>Space group number</b>	:	104
<b>Space group symbol</b>	:	<i>P4nc</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB6C4_tP22_104_a_2ac_c --params=a, c/a, z <sub>1</sub> , z <sub>2</sub> , z <sub>3</sub> , x <sub>4</sub> , y <sub>4</sub> , z <sub>4</sub> , x <sub>5</sub> , y <sub>5</sub> , z <sub>5</sub>

- The second I site is reported with an occupancy 0.92.

**Simple Tetragonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= a \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	=	$z_1 \mathbf{a}_3$	=	$z_1 c \hat{z}$	(2a) Hg

$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Hg
$\mathbf{B}_3$	$=$	$z_2 \mathbf{a}_3$	$=$	$z_2 c \hat{\mathbf{z}}$	(2a)	II
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(2a)	II
$\mathbf{B}_5$	$=$	$z_3 \mathbf{a}_3$	$=$	$z_3 c \hat{\mathbf{z}}$	(2a)	II
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(2a)	II
$\mathbf{B}_7$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8c)	III
$\mathbf{B}_8$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8c)	III
$\mathbf{B}_9$	$=$	$-y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8c)	III
$\mathbf{B}_{10}$	$=$	$y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8c)	III
$\mathbf{B}_{11}$	$=$	$\left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(8c)	III
$\mathbf{B}_{12}$	$=$	$\left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(8c)	III
$\mathbf{B}_{13}$	$=$	$\left(\frac{1}{2} - y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(8c)	III
$\mathbf{B}_{14}$	$=$	$\left(\frac{1}{2} + y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(8c)	III
$\mathbf{B}_{15}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8c)	TI
$\mathbf{B}_{16}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8c)	TI
$\mathbf{B}_{17}$	$=$	$-y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8c)	TI
$\mathbf{B}_{18}$	$=$	$y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8c)	TI
$\mathbf{B}_{19}$	$=$	$\left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(8c)	TI
$\mathbf{B}_{20}$	$=$	$\left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(8c)	TI
$\mathbf{B}_{21}$	$=$	$\left(\frac{1}{2} - y_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - y_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(8c)	TI
$\mathbf{B}_{22}$	$=$	$\left(\frac{1}{2} + y_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + y_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(8c)	TI

#### References:

- D. V. Badikov, V. V. Badikov, G. M. Kuz'micheva, V. L. Panyutin, V. B. Rybakov, V. I. Chizhikov, G. S. Shevyrdyaeva, and E. S. Shcherbakova, *Growth and X-ray diffraction study of  $Tl_4HgI_6$  crystals*, *Inorg. Mat.* **40**, 314–320 (2004), [doi:10.1023/B:INMA.0000020535.59699.ff](https://doi.org/10.1023/B:INMA.0000020535.59699.ff).

#### Found in:

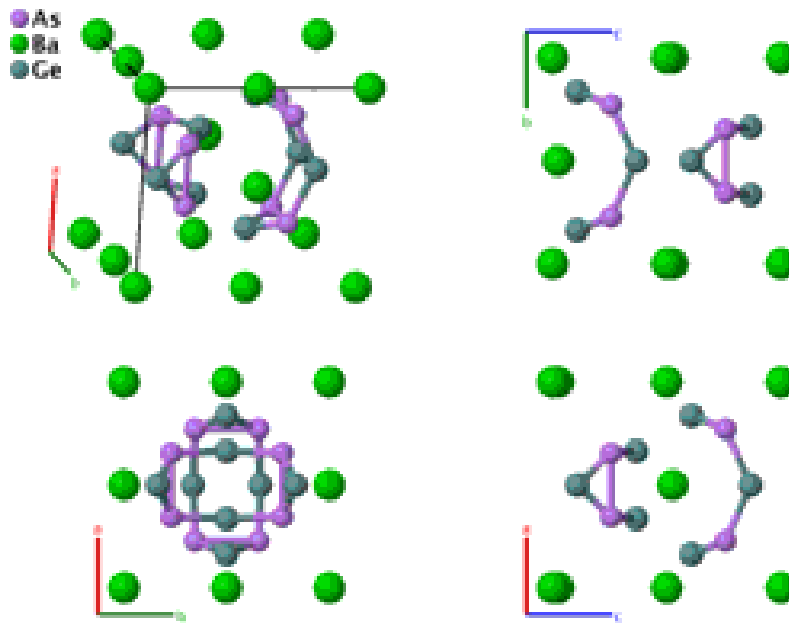
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. 878

- POSCAR: pp. 878

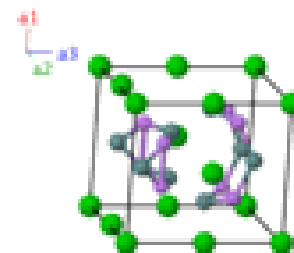
# BaGe<sub>2</sub>As<sub>2</sub> Structure: A2BC2\_tP20\_105\_f\_ac\_2e



**Prototype** : BaGe<sub>2</sub>As<sub>2</sub>  
**AFLOW prototype label** : A2BC2\_tP20\_105\_f\_ac\_2e  
**Strukturbericht designation** : None  
**Pearson symbol** : tP20  
**Space group number** : 105  
**Space group symbol** :  $P4_2mc$   
**AFLOW prototype command** : `aflow --proto=A2BC2_tP20_105_f_ac_2e`  
                                   `--params=a, c/a, z1, z2, x3, z3, x4, z4, x5, y5, z5`

**Simple Tetragonal primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$= z_1 c \hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B}_2$	$= \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2c)	Ba II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(2c)	Ba II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4e)	Ge I



$\mathbf{B}_6$	$=$	$-x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4e)	Ge I
$\mathbf{B}_7$	$=$	$\frac{1}{2} \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4e)	Ge I
$\mathbf{B}_8$	$=$	$\frac{1}{2} \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4e)	Ge I
$\mathbf{B}_9$	$=$	$x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4e)	Ge II
$\mathbf{B}_{10}$	$=$	$-x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4e)	Ge II
$\mathbf{B}_{11}$	$=$	$\frac{1}{2} \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(4e)	Ge II
$\mathbf{B}_{12}$	$=$	$\frac{1}{2} \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(4e)	Ge II
$\mathbf{B}_{13}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8f)	As
$\mathbf{B}_{14}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8f)	As
$\mathbf{B}_{15}$	$=$	$-y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(8f)	As
$\mathbf{B}_{16}$	$=$	$y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(8f)	As
$\mathbf{B}_{17}$	$=$	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8f)	As
$\mathbf{B}_{18}$	$=$	$-x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(8f)	As
$\mathbf{B}_{19}$	$=$	$-y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(8f)	As
$\mathbf{B}_{20}$	$=$	$y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(8f)	As

---

#### References:

- B. Eisenmann and H. Schäfer, *Zintlphasen mit binären Anionen: Zur Kenntnis von BaGe<sub>2</sub>P<sub>2</sub> und BaGe<sub>2</sub>As<sub>2</sub> / Zintl Phases with Binary Anions: BaGe<sub>2</sub>P<sub>2</sub> and BaGe<sub>2</sub>As<sub>2</sub>*, *Z. Naturforsch. B* **36**, 415–419 (1981), doi:10.1515/znb-1981-0403.

#### Found in:

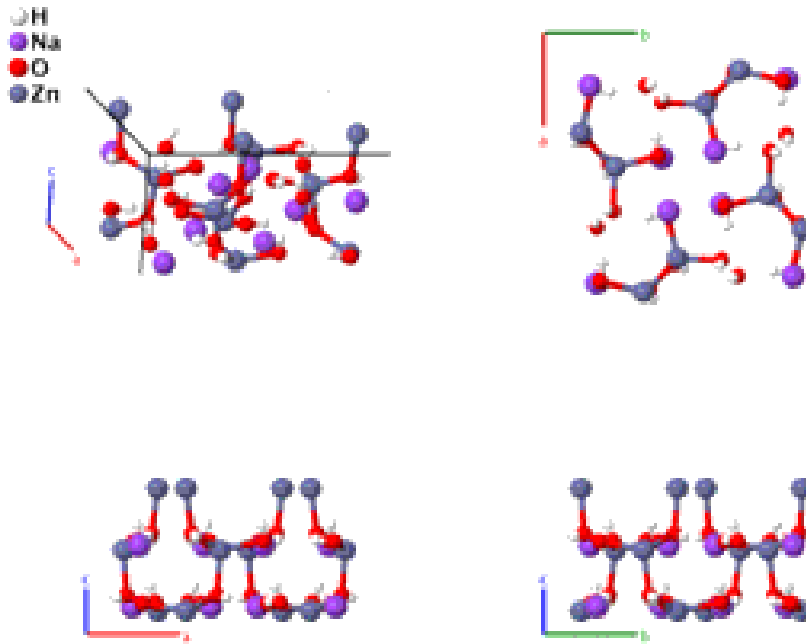
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 878  
 - POSCAR: pp. 878

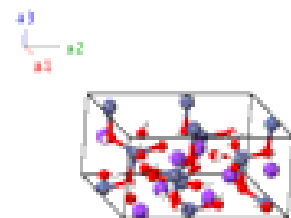
# NaZn[OH]<sub>3</sub> Structure: A3BC3D\_tP64\_106\_3c\_c\_3c\_c



<b>Prototype</b>	:	NaZn[OH] <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3BC3D_tP64_106_3c_c_3c_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP64
<b>Space group number</b>	:	106
<b>Space group symbol</b>	:	<i>P</i> 4 <sub>2</sub> <i>bc</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3BC3D_tP64_106_3c_c_3c_c --params= <i>a</i> , <i>c/a</i> , <i>x</i> <sub>1</sub> , <i>y</i> <sub>1</sub> , <i>z</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>y</i> <sub>2</sub> , <i>z</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>x</i> <sub>6</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub> , <i>x</i> <sub>7</sub> , <i>y</i> <sub>7</sub> , <i>z</i> <sub>7</sub> , <i>x</i> <sub>8</sub> , <i>y</i> <sub>8</sub> , <i>z</i> <sub>8</sub>

Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8c)	H I
<b>B<sub>2</sub></b>	= $-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$-x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8c)	H I





$$\mathbf{B}_{64} = \begin{pmatrix} \frac{1}{2} + y_8 \\ \frac{1}{2} + x_8 \\ \frac{1}{2} + z_8 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + x_8 \\ \frac{1}{2} + y_8 \\ \frac{1}{2} + z_8 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} + y_8 \\ \frac{1}{2} + x_8 \\ \frac{1}{2} + z_8 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + x_8 \\ \frac{1}{2} + y_8 \\ \frac{1}{2} + z_8 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} + y_8 \\ \frac{1}{2} + x_8 \\ \frac{1}{2} + z_8 \end{pmatrix} c \hat{\mathbf{z}} \quad (8c) \quad \text{Zn}$$

**References:**

- R. Stahl and H. Jacobs, *Synthese und Kristallstruktur von NaZn(OH)<sub>3</sub>·3H<sub>2</sub>O und NaZn(OH)<sub>3</sub>*, Z. Anorg. Allg. Chem. **624**, 25–29 (1998), doi:[10.1002/\(SICI\)1521-3749\(199801\)624:1<25::AID-ZAAC25>3.0.CO;2-8](https://doi.org/10.1002/(SICI)1521-3749(199801)624:1<25::AID-ZAAC25>3.0.CO;2-8).

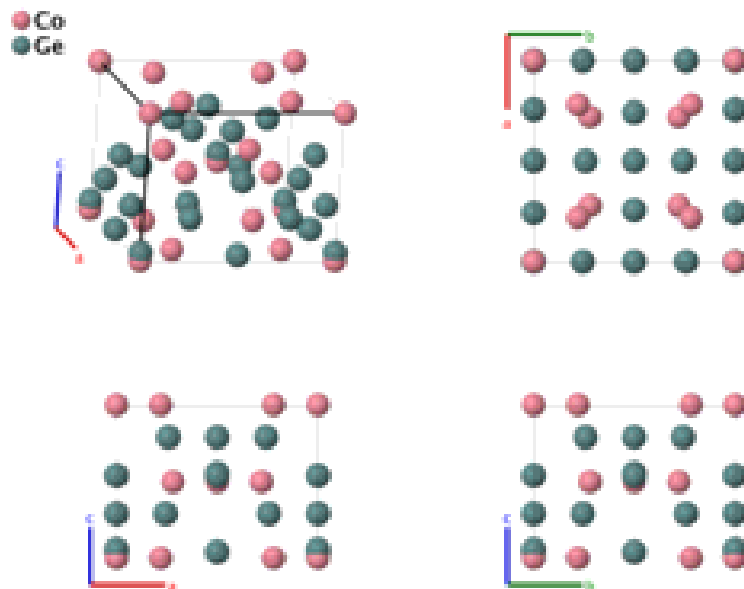
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [879](#)
- POSCAR: pp. [879](#)

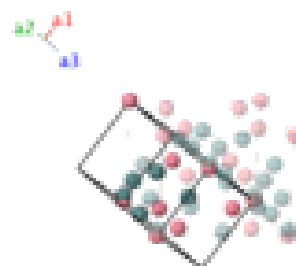
# Co<sub>5</sub>Ge<sub>7</sub> Structure: A5B7\_tI24\_107\_ac\_abd



<b>Prototype</b>	:	Co <sub>5</sub> Ge <sub>7</sub>
<b>AFLOW prototype label</b>	:	A5B7_tI24_107_ac_abd
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI24
<b>Space group number</b>	:	107
<b>Space group symbol</b>	:	<i>I4mm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A5B7_tI24_107_ac_abd --params= <i>a, c/a, z<sub>1</sub>, z<sub>2</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, z<sub>5</sub></i>

**Body-centered Tetragonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2$	$z_1 c \hat{\mathbf{z}}$	(2a)	Co I
<b>B<sub>2</sub></b> =	$z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	$z_2 c \hat{\mathbf{z}}$	(2a)	Ge I
<b>B<sub>3</sub></b> =	$\left(\frac{1}{2} + z_3\right) \mathbf{a}_1 + z_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4b)	Ge II
<b>B<sub>4</sub></b> =	$z_3 \mathbf{a}_1 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} + z_3 c \hat{\mathbf{z}}$	(4b)	Ge II
<b>B<sub>5</sub></b> =	$(x_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + 2x_4 \mathbf{a}_3$	$x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(8c)	Co II

$$\begin{aligned}
\mathbf{B}_6 &= (-x_4 + z_4) \mathbf{a}_1 + (-x_4 + z_4) \mathbf{a}_2 - 2x_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (8c) && \text{Co II} \\
\mathbf{B}_7 &= (x_4 + z_4) \mathbf{a}_1 + (-x_4 + z_4) \mathbf{a}_2 &= -x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (8c) && \text{Co II} \\
\mathbf{B}_8 &= (-x_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 &= x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (8c) && \text{Co II} \\
\mathbf{B}_9 &= z_5 \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + x_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + z_5 c \hat{\mathbf{z}} && (8d) && \text{Ge III} \\
\mathbf{B}_{10} &= z_5 \mathbf{a}_1 + (-x_5 + z_5) \mathbf{a}_2 - x_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + z_5 c \hat{\mathbf{z}} && (8d) && \text{Ge III} \\
\mathbf{B}_{11} &= (x_5 + z_5) \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (8d) && \text{Ge III} \\
\mathbf{B}_{12} &= (-x_5 + z_5) \mathbf{a}_1 + z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (8d) && \text{Ge III}
\end{aligned}$$

**References:**

- K. Schubert, T. R. Anantharaman, H. O. K. Ata, H. G. Meissner, M. Pötzschke, W. Rossteutscher, and E. Stolz, *Einige strukturelle Ergebnisse an metallischen Phasen (6)*, *Naturwissenschaften* **47**, 512 (1960), [doi:10.1007/BF00641115](https://doi.org/10.1007/BF00641115).

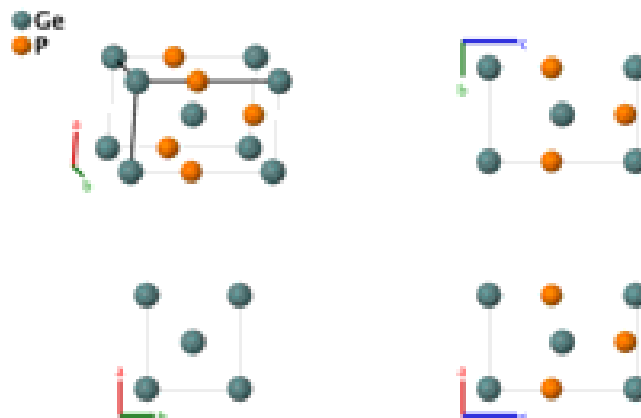
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [879](#)  
- POSCAR: pp. [880](#)

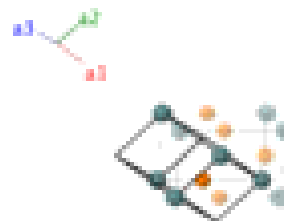
# GeP (High-pressure, superconducting) Structure: AB\_tI4\_107\_a\_a



<b>Prototype</b>	:	GeP
<b>AFLOW prototype label</b>	:	AB_tI4_107_a_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI4
<b>Space group number</b>	:	107
<b>Space group symbol</b>	:	$I4mm$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB_tI4_107_a_a --params=a, c/a, z1, z2</code>

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2$	$=$	$z_1 c \hat{\mathbf{z}}$	(2a)	Ge
$\mathbf{B}_2$	$= z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	$=$	$z_2 c \hat{\mathbf{z}}$	(2a)	P

## References:

- P. C. Donohue and H. S. Young, *Synthesis, structure, and superconductivity of new high pressure phases in the systems Ge-P and Ge-As*, J. Solid State Chem. **1**, 143–149 (1970), doi:[10.1016/0022-4596\(70\)90005-8](https://doi.org/10.1016/0022-4596(70)90005-8).

## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).



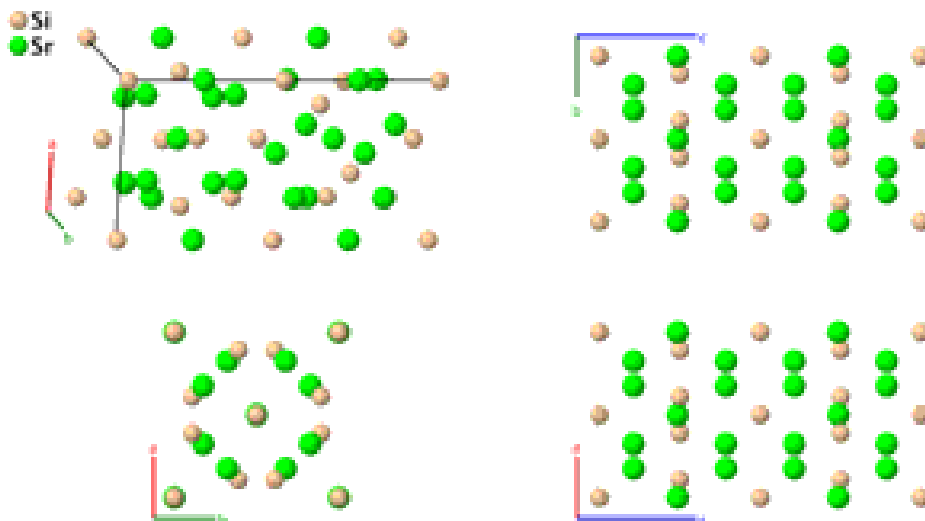
---

**Geometry files:**

- CIF: pp. [880](#)

- POSCAR: pp. [880](#)

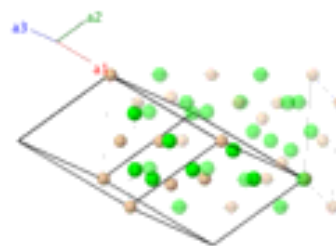
# Sr<sub>5</sub>Si<sub>3</sub> Structure: A3B5\_tI32\_108\_ac\_a2c



<b>Prototype</b>	:	Sr <sub>5</sub> Si <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B5_tI32_108_ac_a2c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI32
<b>Space group number</b>	:	108
<b>Space group symbol</b>	:	<i>I4cm</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A3B5_tI32_108_ac_a2c</code> <code>--params=a, c/a, z1, z2, x3, z3, x4, z4, x5, z5</code>

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2$	$z_1 c \hat{\mathbf{z}}$	(4a)	Si I
<b>B<sub>2</sub></b>	$\left(\frac{1}{2} + z_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_2$	$\left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4a)	Si I
<b>B<sub>3</sub></b>	$z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	$z_2 c \hat{\mathbf{z}}$	(4a)	Sr I
<b>B<sub>4</sub></b>	$\left(\frac{1}{2} + z_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_2$	$\left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4a)	Sr I
<b>B<sub>5</sub></b>	$\left(\frac{1}{2} + x_3 + z_3\right) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + \left(\frac{1}{2} + 2x_3\right) \mathbf{a}_3$	$x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8c)	Si II
<b>B<sub>6</sub></b>	$\left(\frac{1}{2} - x_3 + z_3\right) \mathbf{a}_1 + (-x_3 + z_3) \mathbf{a}_2 + \left(\frac{1}{2} - 2x_3\right) \mathbf{a}_3$	$-x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8c)	Si II

$$\mathbf{B}_7 = (x_3 + z_3) \mathbf{a}_1 + \left(\frac{1}{2} - x_3 + z_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} \quad (8c) \quad \text{Si II}$$

$$\mathbf{B}_8 = (-x_3 + z_3) \mathbf{a}_1 + \left(\frac{1}{2} + x_3 + z_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} \quad (8c) \quad \text{Si II}$$

$$\mathbf{B}_9 = \left(\frac{1}{2} + x_4 + z_4\right) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + \left(\frac{1}{2} + 2x_4\right) \mathbf{a}_3 = x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} \quad (8c) \quad \text{Sr II}$$

$$\mathbf{B}_{10} = \left(\frac{1}{2} - x_4 + z_4\right) \mathbf{a}_1 + (-x_4 + z_4) \mathbf{a}_2 + \left(\frac{1}{2} - 2x_4\right) \mathbf{a}_3 = -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} \quad (8c) \quad \text{Sr II}$$

$$\mathbf{B}_{11} = (x_4 + z_4) \mathbf{a}_1 + \left(\frac{1}{2} - x_4 + z_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} \quad (8c) \quad \text{Sr II}$$

$$\mathbf{B}_{12} = (-x_4 + z_4) \mathbf{a}_1 + \left(\frac{1}{2} + x_4 + z_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} \quad (8c) \quad \text{Sr II}$$

$$\mathbf{B}_{13} = \left(\frac{1}{2} + x_5 + z_5\right) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + \left(\frac{1}{2} + 2x_5\right) \mathbf{a}_3 = x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} \quad (8c) \quad \text{Sr III}$$

$$\mathbf{B}_{14} = \left(\frac{1}{2} - x_5 + z_5\right) \mathbf{a}_1 + (-x_5 + z_5) \mathbf{a}_2 + \left(\frac{1}{2} - 2x_5\right) \mathbf{a}_3 = -x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} \quad (8c) \quad \text{Sr III}$$

$$\mathbf{B}_{15} = (x_5 + z_5) \mathbf{a}_1 + \left(\frac{1}{2} - x_5 + z_5\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} \quad (8c) \quad \text{Sr III}$$

$$\mathbf{B}_{16} = (-x_5 + z_5) \mathbf{a}_1 + \left(\frac{1}{2} + x_5 + z_5\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} \quad (8c) \quad \text{Sr III}$$

#### References:

- G. Nagorsen, G. Rocktäschel, H. Schäfer, and A. Weiss, *Die Kristallstruktur der Phase Sr<sub>5</sub>Si<sub>3</sub>*, *Z. Naturforsch. B* **22**, 101–102 (1967), doi:10.1515/znb-1967-0122.

#### Found in:

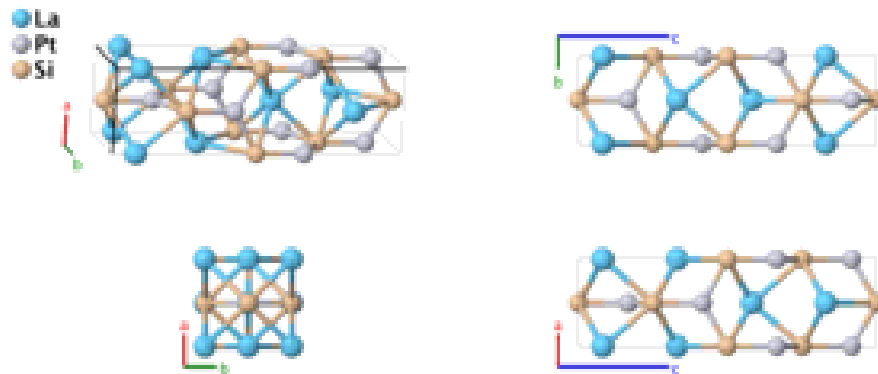
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. 880

- POSCAR: pp. 881

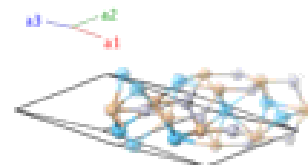
# LaPtSi Structure: ABC\_tI12\_109\_a\_a\_a



<b>Prototype</b>	:	LaPtSi
<b>AFLOW prototype label</b>	:	ABC_tI12_109_a_a_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI12
<b>Space group number</b>	:	109
<b>Space group symbol</b>	:	$I4_1md$
<b>AFLOW prototype command</b>	:	aflow --proto=ABC_tI12_109_a_a_a --params=a, c/a, z <sub>1</sub> , z <sub>2</sub> , z <sub>3</sub>

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2$	$=$	$z_1 c \hat{\mathbf{z}}$	(4a)	La
$\mathbf{B}_2$	$= \left(\frac{3}{4} + z_1\right) \mathbf{a}_1 + \left(\frac{1}{4} + z_1\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_1\right) c \hat{\mathbf{z}}$	(4a)	La
$\mathbf{B}_3$	$= z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	$=$	$z_2 c \hat{\mathbf{z}}$	(4a)	Pt
$\mathbf{B}_4$	$= \left(\frac{3}{4} + z_2\right) \mathbf{a}_1 + \left(\frac{1}{4} + z_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_2\right) c \hat{\mathbf{z}}$	(4a)	Pt
$\mathbf{B}_5$	$= z_3 \mathbf{a}_1 + z_3 \mathbf{a}_2$	$=$	$z_3 c \hat{\mathbf{z}}$	(4a)	Si
$\mathbf{B}_6$	$= \left(\frac{3}{4} + z_3\right) \mathbf{a}_1 + \left(\frac{1}{4} + z_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_3\right) c \hat{\mathbf{z}}$	(4a)	Si

## References:

- K. Klepp and E. Parthé, *RPtSi phases (R = La, Ce, Pr, Nd, Sm and Gd) with an ordered ThSi<sub>2</sub> derivative structure*, Acta Crystallogr. Sect. B Struct. Sci. **38**, 1105–1108 (1982), doi:10.1107/S056774088200507X.

## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

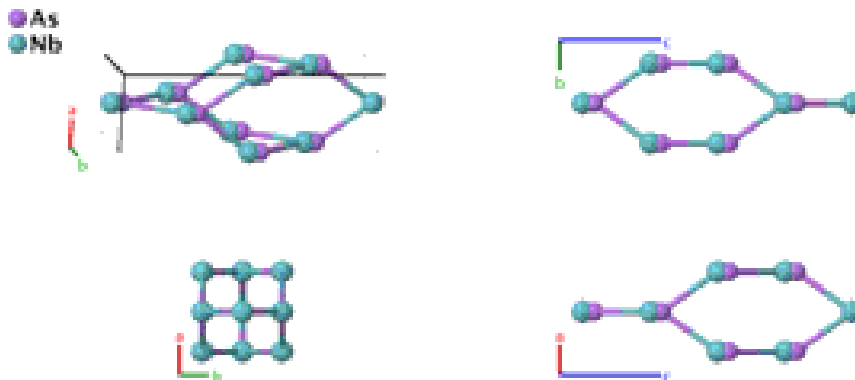
---

**Geometry files:**

- CIF: pp. [881](#)

- POSCAR: pp. [881](#)

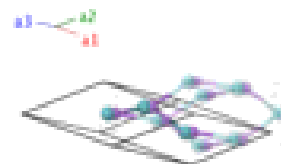
# NbAs Structure: AB\_tI8\_109\_a\_a



**Prototype** : NbAs  
**AFLOW prototype label** : AB\_tI8\_109\_a\_a  
**Strukturbericht designation** : None  
**Pearson symbol** : tI8  
**Space group number** : 109  
**Space group symbol** :  $I4_1md$   
**AFLOW prototype command** : `aflow --proto=AB_tI8_109_a_a --params=a, c/a, z1, z2`

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\
 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2$	=	$z_1 c \hat{\mathbf{z}}$	(4a)	As
$\mathbf{B}_2$	$\left(\frac{3}{4} + z_1\right) \mathbf{a}_1 + \left(\frac{1}{4} + z_1\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_1\right) c \hat{\mathbf{z}}$	(4a)	As
$\mathbf{B}_3$	$z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	=	$z_2 c \hat{\mathbf{z}}$	(4a)	Nb
$\mathbf{B}_4$	$\left(\frac{3}{4} + z_2\right) \mathbf{a}_1 + \left(\frac{1}{4} + z_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_2\right) c \hat{\mathbf{z}}$	(4a)	Nb

## References:

- S. Furuseth and A. Kjekshus, *On the Arsenides and Antimonides of Niobium*, Acta Chem. Scand. **18**, 1180–1195 (1964), [doi:10.3891/acta.chem.scand.18-1180](https://doi.org/10.3891/acta.chem.scand.18-1180).

## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

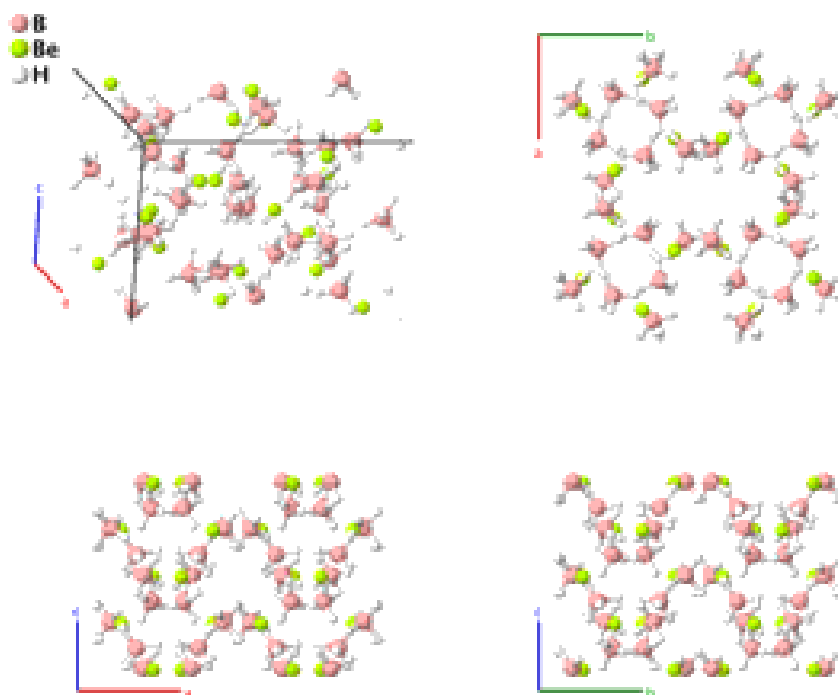
---

**Geometry files:**

- CIF: pp. [881](#)

- POSCAR: pp. [882](#)

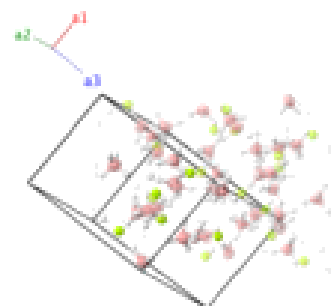
# Be[BH<sub>4</sub>]<sub>2</sub> Structure: A2BC8\_tI176\_110\_2b\_b\_8b



<b>Prototype</b>	:	Be[BH <sub>4</sub> ] <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2BC8_tI176_110_2b_b_8b
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI176
<b>Space group number</b>	:	110
<b>Space group symbol</b>	:	<i>I</i> 4 <sub>1</sub> <i>cd</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2BC8_tI176_110_2b_b_8b --params= <i>a</i> , <i>c/a</i> , <i>x</i> <sub>1</sub> , <i>y</i> <sub>1</sub> , <i>z</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>y</i> <sub>2</sub> , <i>z</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>x</i> <sub>6</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub> , <i>x</i> <sub>7</sub> , <i>y</i> <sub>7</sub> , <i>z</i> <sub>7</sub> , <i>x</i> <sub>8</sub> , <i>y</i> <sub>8</sub> , <i>z</i> <sub>8</sub> , <i>x</i> <sub>9</sub> , <i>y</i> <sub>9</sub> , <i>z</i> <sub>9</sub> , <i>x</i> <sub>10</sub> , <i>y</i> <sub>10</sub> , <i>z</i> <sub>10</sub> , <i>x</i> <sub>11</sub> , <i>y</i> <sub>11</sub> , <i>z</i> <sub>11</sub>

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= (y_1 + z_1) \mathbf{a}_1 + (x_1 + z_1) \mathbf{a}_2 + (x_1 + y_1) \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(16b)	B I









$$\begin{aligned}
\mathbf{B}_{65} &= (y_9 + z_9) \mathbf{a}_1 + (x_9 + z_9) \mathbf{a}_2 + (x_9 + y_9) \mathbf{a}_3 &= x_9 a \hat{\mathbf{x}} + y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}} & (16b) & \text{H VI} \\
\mathbf{B}_{66} &= (-y_9 + z_9) \mathbf{a}_1 + (-x_9 + z_9) \mathbf{a}_2 + (-x_9 - y_9) \mathbf{a}_3 &= -x_9 a \hat{\mathbf{x}} - y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}} & (16b) & \text{H VI} \\
\mathbf{B}_{67} &= \left(\frac{3}{4} + x_9 + z_9\right) \mathbf{a}_1 + \left(\frac{1}{4} - y_9 + z_9\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_9 - y_9\right) \mathbf{a}_3 &= -y_9 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_9\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_9\right) c \hat{\mathbf{z}} & (16b) & \text{H VI} \\
\mathbf{B}_{68} &= \left(\frac{3}{4} - x_9 + z_9\right) \mathbf{a}_1 + \left(\frac{1}{4} + y_9 + z_9\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_9 + y_9\right) \mathbf{a}_3 &= y_9 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_9\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_9\right) c \hat{\mathbf{z}} & (16b) & \text{H VI} \\
\mathbf{B}_{69} &= \left(\frac{1}{2} - y_9 + z_9\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_9 + z_9\right) \mathbf{a}_2 + (x_9 - y_9) \mathbf{a}_3 &= x_9 a \hat{\mathbf{x}} - y_9 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}} & (16b) & \text{H VI} \\
\mathbf{B}_{70} &= \left(\frac{1}{2} + y_9 + z_9\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_9 + z_9\right) \mathbf{a}_2 + (-x_9 + y_9) \mathbf{a}_3 &= -x_9 a \hat{\mathbf{x}} + y_9 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_9\right) c \hat{\mathbf{z}} & (16b) & \text{H VI} \\
\mathbf{B}_{71} &= \left(\frac{1}{4} - x_9 + z_9\right) \mathbf{a}_1 + \left(\frac{3}{4} - y_9 + z_9\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_9 - y_9\right) \mathbf{a}_3 &= \left(\frac{1}{2} - y_9\right) a \hat{\mathbf{x}} - x_9 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_9\right) c \hat{\mathbf{z}} & (16b) & \text{H VI} \\
\mathbf{B}_{72} &= \left(\frac{1}{4} + x_9 + z_9\right) \mathbf{a}_1 + \left(\frac{3}{4} + y_9 + z_9\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_9 + y_9\right) \mathbf{a}_3 &= \left(\frac{1}{2} + y_9\right) a \hat{\mathbf{x}} + x_9 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_9\right) c \hat{\mathbf{z}} & (16b) & \text{H VI} \\
\mathbf{B}_{73} &= (y_{10} + z_{10}) \mathbf{a}_1 + (x_{10} + z_{10}) \mathbf{a}_2 + (x_{10} + y_{10}) \mathbf{a}_3 &= x_{10} a \hat{\mathbf{x}} + y_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}} & (16b) & \text{H VII} \\
\mathbf{B}_{74} &= (-y_{10} + z_{10}) \mathbf{a}_1 + (-x_{10} + z_{10}) \mathbf{a}_2 + (-x_{10} - y_{10}) \mathbf{a}_3 &= -x_{10} a \hat{\mathbf{x}} - y_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}} & (16b) & \text{H VII} \\
\mathbf{B}_{75} &= \left(\frac{3}{4} + x_{10} + z_{10}\right) \mathbf{a}_1 + \left(\frac{1}{4} - y_{10} + z_{10}\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_{10} - y_{10}\right) \mathbf{a}_3 &= -y_{10} a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_{10}\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_{10}\right) c \hat{\mathbf{z}} & (16b) & \text{H VII} \\
\mathbf{B}_{76} &= \left(\frac{3}{4} - x_{10} + z_{10}\right) \mathbf{a}_1 + \left(\frac{1}{4} + y_{10} + z_{10}\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_{10} + y_{10}\right) \mathbf{a}_3 &= y_{10} a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_{10}\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_{10}\right) c \hat{\mathbf{z}} & (16b) & \text{H VII} \\
\mathbf{B}_{77} &= \left(\frac{1}{2} - y_{10} + z_{10}\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_{10} + z_{10}\right) \mathbf{a}_2 + (x_{10} - y_{10}) \mathbf{a}_3 &= x_{10} a \hat{\mathbf{x}} - y_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}} & (16b) & \text{H VII} \\
\mathbf{B}_{78} &= \left(\frac{1}{2} + y_{10} + z_{10}\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_{10} + z_{10}\right) \mathbf{a}_2 + (-x_{10} + y_{10}) \mathbf{a}_3 &= -x_{10} a \hat{\mathbf{x}} + y_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) c \hat{\mathbf{z}} & (16b) & \text{H VII} \\
\mathbf{B}_{79} &= \left(\frac{1}{4} - x_{10} + z_{10}\right) \mathbf{a}_1 + \left(\frac{3}{4} - y_{10} + z_{10}\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_{10} - y_{10}\right) \mathbf{a}_3 &= \left(\frac{1}{2} - y_{10}\right) a \hat{\mathbf{x}} - x_{10} a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_{10}\right) c \hat{\mathbf{z}} & (16b) & \text{H VII} \\
\mathbf{B}_{80} &= \left(\frac{1}{4} + x_{10} + z_{10}\right) \mathbf{a}_1 + \left(\frac{3}{4} + y_{10} + z_{10}\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_{10} + y_{10}\right) \mathbf{a}_3 &= \left(\frac{1}{2} + y_{10}\right) a \hat{\mathbf{x}} + x_{10} a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_{10}\right) c \hat{\mathbf{z}} & (16b) & \text{H VII} \\
\mathbf{B}_{81} &= (y_{11} + z_{11}) \mathbf{a}_1 + (x_{11} + z_{11}) \mathbf{a}_2 + (x_{11} + y_{11}) \mathbf{a}_3 &= x_{11} a \hat{\mathbf{x}} + y_{11} a \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}} & (16b) & \text{H VIII} \\
\mathbf{B}_{82} &= (-y_{11} + z_{11}) \mathbf{a}_1 + (-x_{11} + z_{11}) \mathbf{a}_2 + (-x_{11} - y_{11}) \mathbf{a}_3 &= -x_{11} a \hat{\mathbf{x}} - y_{11} a \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}} & (16b) & \text{H VIII} \\
\mathbf{B}_{83} &= \left(\frac{3}{4} + x_{11} + z_{11}\right) \mathbf{a}_1 + \left(\frac{1}{4} - y_{11} + z_{11}\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_{11} - y_{11}\right) \mathbf{a}_3 &= -y_{11} a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_{11}\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_{11}\right) c \hat{\mathbf{z}} & (16b) & \text{H VIII}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{84} &= \begin{pmatrix} \frac{3}{4} - x_{11} + z_{11} \\ \frac{1}{4} + y_{11} + z_{11} \\ \frac{1}{2} - x_{11} + y_{11} \end{pmatrix} \mathbf{a}_1 + &= y_{11}a\hat{\mathbf{x}} + \left(\frac{1}{2} - x_{11}\right)a\hat{\mathbf{y}} + \left(\frac{1}{4} + z_{11}\right)c\hat{\mathbf{z}} & (16b) & \text{H VIII} \\
\mathbf{B}_{85} &= \begin{pmatrix} \frac{1}{2} - y_{11} + z_{11} \\ \frac{1}{2} + x_{11} + z_{11} \\ x_{11} - y_{11} \end{pmatrix} \mathbf{a}_1 + &= x_{11}a\hat{\mathbf{x}} - y_{11}a\hat{\mathbf{y}} + \left(\frac{1}{2} + z_{11}\right)c\hat{\mathbf{z}} & (16b) & \text{H VIII} \\
\mathbf{B}_{86} &= \begin{pmatrix} \frac{1}{2} + y_{11} + z_{11} \\ \frac{1}{2} - x_{11} + z_{11} \\ -x_{11} + y_{11} \end{pmatrix} \mathbf{a}_1 + &= -x_{11}a\hat{\mathbf{x}} + y_{11}a\hat{\mathbf{y}} + \left(\frac{1}{2} + z_{11}\right)c\hat{\mathbf{z}} & (16b) & \text{H VIII} \\
\mathbf{B}_{87} &= \begin{pmatrix} \frac{1}{4} - x_{11} + z_{11} \\ \frac{3}{4} - y_{11} + z_{11} \\ \frac{1}{2} - x_{11} - y_{11} \end{pmatrix} \mathbf{a}_1 + &= \left(\frac{1}{2} - y_{11}\right)a\hat{\mathbf{x}} - x_{11}a\hat{\mathbf{y}} + \left(\frac{1}{4} + z_{11}\right)c\hat{\mathbf{z}} & (16b) & \text{H VIII} \\
\mathbf{B}_{88} &= \begin{pmatrix} \frac{1}{4} + x_{11} + z_{11} \\ \frac{3}{4} + y_{11} + z_{11} \\ \frac{1}{2} + x_{11} + y_{11} \end{pmatrix} \mathbf{a}_1 + &= \left(\frac{1}{2} + y_{11}\right)a\hat{\mathbf{x}} + x_{11}a\hat{\mathbf{y}} + \left(\frac{1}{4} + z_{11}\right)c\hat{\mathbf{z}} & (16b) & \text{H VIII}
\end{aligned}$$

---

#### References:

- D. S. Marynick and W. N. Lipscomb, *Crystal structure of beryllium borohydride*, *Inorg. Chem.* **11**, 820–823 (1972), [doi:10.1021/ic50110a033](https://doi.org/10.1021/ic50110a033).

#### Found in:

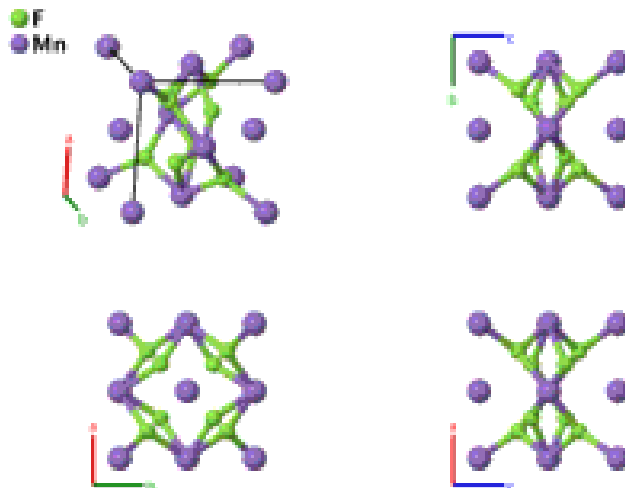
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [882](#)  
- POSCAR: pp. [882](#)

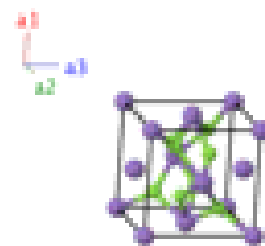
# MnF<sub>2</sub> Structure: A2B\_tP12\_111\_2n\_adf



<b>Prototype</b>	:	MnF <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_tP12_111_2n_adf
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP12
<b>Space group number</b>	:	111
<b>Space group symbol</b>	:	$P\bar{4}2m$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_tP12_111_2n_adf --params=a, c/a, x <sub>4</sub> , z <sub>4</sub> , x <sub>5</sub> , z <sub>5</sub>

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	= $0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Mn I
<b>B<sub>2</sub></b>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	= $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(1d)	Mn II
<b>B<sub>3</sub></b>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	= $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2f)	Mn III
<b>B<sub>4</sub></b>	= $\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	= $\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2f)	Mn III
<b>B<sub>5</sub></b>	= $x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	= $x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4n)	F I
<b>B<sub>6</sub></b>	= $-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	= $-x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4n)	F I
<b>B<sub>7</sub></b>	= $x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	= $x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(4n)	F I

$$\begin{aligned}
\mathbf{B}_8 &= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (4n) & \text{F I} \\
\mathbf{B}_9 &= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (4n) & \text{F II} \\
\mathbf{B}_{10} &= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (4n) & \text{F II} \\
\mathbf{B}_{11} &= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (4n) & \text{F II} \\
\mathbf{B}_{12} &= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (4n) & \text{F II}
\end{aligned}$$

---

**References:**

- T. Yagi, J. C. Jamieson, and P. B. Moore, *Polymorphism in MnF<sub>2</sub> (rutile type) at high pressures*, J. Geophys. Res. **84**, 1113–1115 (1979), [doi:10.1029/JB084iB03p01113](https://doi.org/10.1029/JB084iB03p01113).

**Found in:**

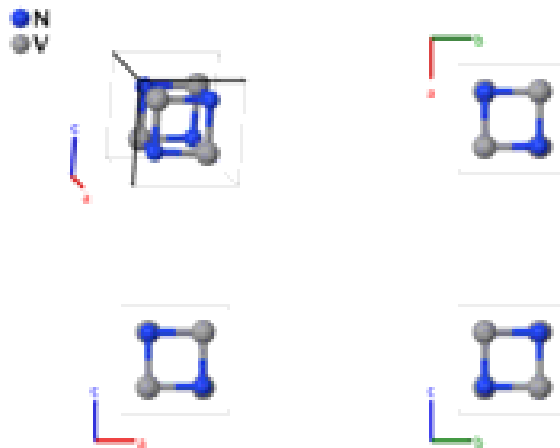
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [883](#)
- POSCAR: pp. [883](#)

# NV (Low-temperature) Structure: AB\_tP8\_111\_n\_n



<b>Prototype</b>	:	VN
<b>AFLOW prototype label</b>	:	AB_tP8_111_n_n
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP8
<b>Space group number</b>	:	111
<b>Space group symbol</b>	:	$P\bar{4}2m$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB_tP8_111_n_n --params=a, c/a, x1, z1, x2, z2</code>

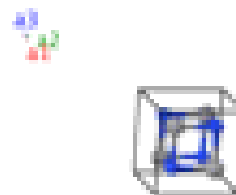
- FINDSYM identifies space group #111 for this structure (consistent with the reference); however, since  $c/a \approx 1$ , AFLOW-SYM and Platon identify #215. Lowering the tolerance value for AFLOW-SYM resolves the expected space group #111. Space groups #111 and #215 are both reasonable classifications since they are commensurate with sub-group relations.

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4n)	N
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4n)	N
$\mathbf{B}_3$	$= x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(4n)	N
$\mathbf{B}_4$	$= -x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(4n)	N



$$\begin{aligned}
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} && (4n) && \text{V} \\
\mathbf{B}_6 &= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} && (4n) && \text{V} \\
\mathbf{B}_7 &= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} && (4n) && \text{V} \\
\mathbf{B}_8 &= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} && (4n) && \text{V}
\end{aligned}$$

---

#### References:

- F. Kubel, W. Lengauer, K. Yvon, K. Knorr, and A. Junod, *Structural phase transition at 205 K in stoichiometric vanadium nitride*, Phys. Rev. B **38**, 12908 (1988), doi:[10.1103/PhysRevB.38.12908](https://doi.org/10.1103/PhysRevB.38.12908).
- H. T. Stokes and D. M. Hatch, *FINDSYM: Program for identifying the space group symmetry of a crystal*, J. Appl. Crystallogr. **38**, 237–238 (2005), doi:[10.1107/S0021889804031528](https://doi.org/10.1107/S0021889804031528).
- D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy, and S. Curtarolo, *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*, Acta Crystallogr. Sect. A **74**, 184–203 (2018), doi:[10.1107/S2053273318003066](https://doi.org/10.1107/S2053273318003066).
- A. L. Spek, *Single-crystal structure validation with the program PLATON*, J. Appl. Crystallogr. **36**, 7–13 (2003), doi:[10.1107/S0021889802022112](https://doi.org/10.1107/S0021889802022112).

#### Found in:

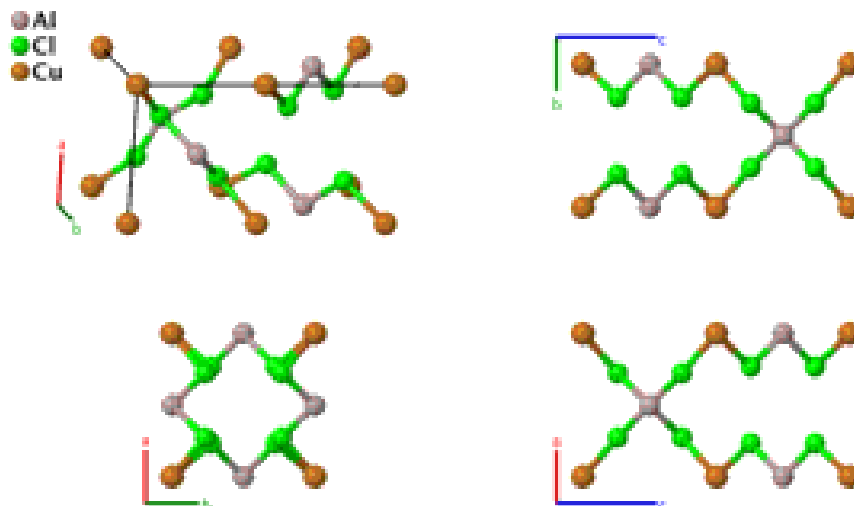
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [883](#)
- POSCAR: pp. [884](#)

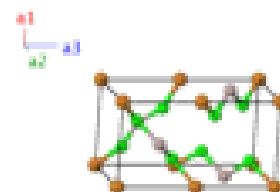
# $\alpha$ -CuAlCl<sub>4</sub> Structure: AB4C\_tP12\_112\_b\_n\_e



**Prototype** :  $\alpha$ -CuAlCl<sub>4</sub>  
**AFLOW prototype label** : AB4C\_tP12\_112\_b\_n\_e  
**Strukturbericht designation** : None  
**Pearson symbol** : tP12  
**Space group number** : 112  
**Space group symbol** :  $P\bar{4}2c$   
**AFLOW prototype command** : aflow --proto=AB4C\_tP12\_112\_b\_n\_e  
 --params= $a, c/a, x_3, y_3, z_3$

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2b)	Al
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2b)	Al
$\mathbf{B}_3$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2e)	Cu
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} c \hat{\mathbf{z}}$	(2e)	Cu
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8n)	Cl
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= -x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8n)	Cl
$\mathbf{B}_7$	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$= y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(8n)	Cl
$\mathbf{B}_8$	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$= -y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(8n)	Cl

$$\mathbf{B}_9 = -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = -x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} \quad (8n) \quad \text{Cl}$$

$$\mathbf{B}_{10} = x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} \quad (8n) \quad \text{Cl}$$

$$\mathbf{B}_{11} = -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = -y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \quad (8n) \quad \text{Cl}$$

$$\mathbf{B}_{12} = y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \quad (8n) \quad \text{Cl}$$

---

**References:**

- J. D. Martin, B. R. Leafblad, R. M. Sullivan, and P. D. Boyle,  *$\alpha$ - and  $\beta$ -CuAlCl<sub>4</sub>: Framework Construction Using Corner-Shared Tetrahedral Metal-Halide Building Blocks*, *Inorg. Chem.* **37**, 1341–1346 (1998), doi:[10.1021/ic971148v](https://doi.org/10.1021/ic971148v).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

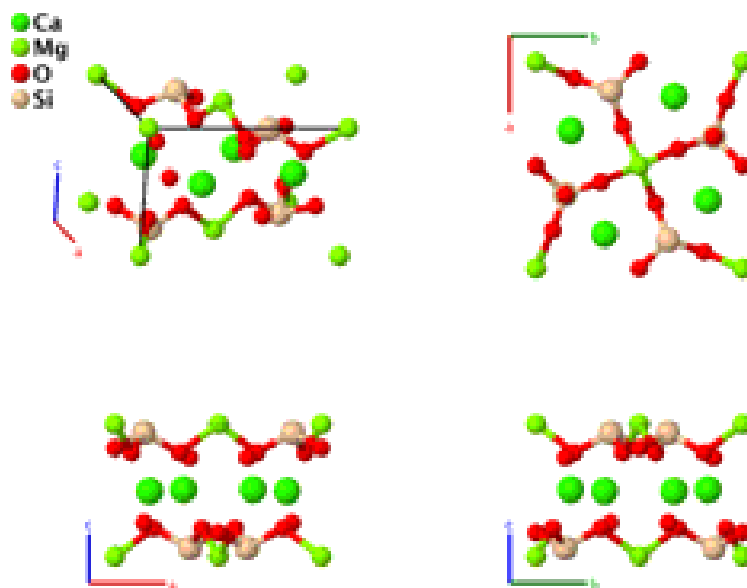
---

**Geometry files:**

- CIF: pp. [884](#)

- POSCAR: pp. [884](#)

# Akermanite ( $\text{Ca}_2\text{MgSi}_2\text{O}_7$ , $S5_3$ ) Structure: A2BC7D2\_tP24\_113\_e\_a\_cef\_e



<b>Prototype</b>	:	$\text{Ca}_2\text{MgSi}_2\text{O}_7$
<b>AFLOW prototype label</b>	:	A2BC7D2_tP24_113_e_a_cef_e
<b>Strukturbericht designation</b>	:	$S5_3$
<b>Pearson symbol</b>	:	tP24
<b>Space group number</b>	:	113
<b>Space group symbol</b>	:	$P\bar{4}2_1m$
<b>AFLOW prototype command</b>	:	aflow --proto=A2BC7D2_tP24_113_e_a_cef_e --params=a, c/a, z2, x3, z3, x4, z4, x5, z5, x6, y6, z6

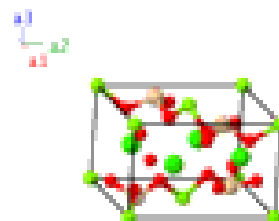
## Other compounds with this structure:

- (Ca,Na)<sub>2</sub>(Al,Mg,Fe)(Si,Al)<sub>2</sub>O<sub>7</sub> (melilite), (Ca,Na)<sub>2</sub>(Al,Mg,Fe)(Si<sub>2</sub>O<sub>7</sub>) (alumoakermanite), Ca<sub>2</sub>Al<sub>2</sub>SiO<sub>7</sub> (gehlenite), Ca<sub>2</sub>BeSi<sub>2</sub>O<sub>7</sub> (gugiaite), Ca<sub>2</sub>ZnSi<sub>2</sub>O<sub>7</sub> (hardystonite), Ca<sub>2</sub>B<sub>2</sub>SiO<sub>7</sub> (okayamalite), (Ca,Na)<sub>2</sub>(Mg,Al,Si)<sub>3</sub>O<sub>7</sub>, Sr<sub>2</sub>ZrSi<sub>2</sub>O<sub>7</sub>, Sr<sub>2</sub>MnGe<sub>2</sub>O<sub>7</sub>, Sr<sub>2</sub>MnGe<sub>2</sub>S<sub>6</sub>O

- Akermanite is an end point of the mineral melilite, which, like [thortveitite](#) ( $S2_1$ ), is a sorosilicate, a mineral containing isolated Si<sub>2</sub>O<sub>7</sub> or related groups. We have followed (Parthé, 1997) and use akermanite to represent the entire class of materials. We use the ambient pressure data from (Yang, 1997) to describe the structure.

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



---

**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	Mg
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(2a)	Mg
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + -z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + -z_2 c \hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4e)	Ca
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4e)	Ca
$\mathbf{B}_7$	$= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(4e)	Ca
$\mathbf{B}_8$	$= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(4e)	Ca
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{11}$	$= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{12}$	$= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + \left(\frac{1}{2} + x_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4e)	Si
$\mathbf{B}_{14}$	$= -x_5 \mathbf{a}_1 + \left(\frac{1}{2} - x_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4e)	Si
$\mathbf{B}_{15}$	$= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(4e)	Si
$\mathbf{B}_{16}$	$= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(4e)	Si
$\mathbf{B}_{17}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{18}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{19}$	$= y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{20}$	$= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{21}$	$= \left(\frac{1}{2} - x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_6\right) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{22}$	$= \left(\frac{1}{2} + x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{23}$	$= \left(\frac{1}{2} - y_6\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_6\right) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - y_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{24}$	$= \left(\frac{1}{2} + y_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_6\right) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + y_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(8f)	O III

---

**References:**

- H. Yang, R. M. Hazen, R. T. Downs, and L. W. Finger, *Structural change associated with the incommensurate-normal phase transition in akermanite, Ca<sub>2</sub>MgSi<sub>2</sub>O<sub>7</sub>, at high pressure*, Phys. Chem. Miner. **24**, 510–519 (1997),

[doi:10.1007/s002690050066](https://doi.org/10.1007/s002690050066).

- E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types*, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., [doi:10.1007/978-3-662-02909-1\\_3](https://doi.org/10.1007/978-3-662-02909-1_3).

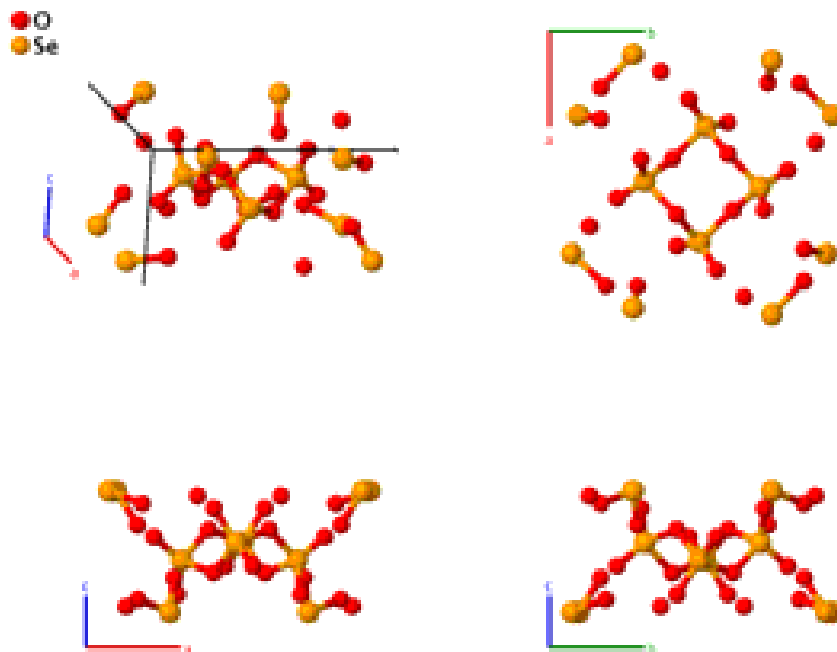
---

**Geometry files:**

- CIF: pp. 884

- POSCAR: pp. 885

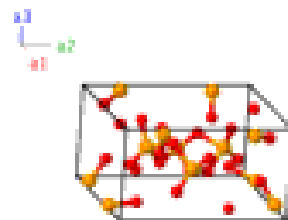
# SeO<sub>3</sub> Structure: A3B\_tP32\_114\_3e\_e



**Prototype** : SeO<sub>3</sub>  
**AFLOW prototype label** : A3B\_tP32\_114\_3e\_e  
**Strukturbericht designation** : None  
**Pearson symbol** : tP32  
**Space group number** : 114  
**Space group symbol** :  $P\bar{4}_21c$   
**AFLOW prototype command** : aflow --proto=A3B\_tP32\_114\_3e\_e  
 --params= $a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

Simple Tetragonal primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B}_3$	$= y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= y_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(8e)	O I



$$\mathbf{B}_{30} = \begin{pmatrix} \frac{1}{2} + x_4 \\ \frac{1}{2} - y_4 \\ \frac{1}{2} - z_4 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - y_4 \\ \frac{1}{2} - x_4 \\ \frac{1}{2} - z_4 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} + x_4 \\ \frac{1}{2} - y_4 \\ \frac{1}{2} - z_4 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - y_4 \\ \frac{1}{2} - x_4 \\ \frac{1}{2} - z_4 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} + x_4 \\ \frac{1}{2} - y_4 \\ \frac{1}{2} - z_4 \end{pmatrix} c \hat{\mathbf{z}} \quad (8e) \quad \text{Se}$$

$$\mathbf{B}_{31} = \begin{pmatrix} \frac{1}{2} - y_4 \\ \frac{1}{2} - x_4 \\ \frac{1}{2} + z_4 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - y_4 \\ \frac{1}{2} - x_4 \\ \frac{1}{2} + z_4 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} - y_4 \\ \frac{1}{2} - x_4 \\ \frac{1}{2} + z_4 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - y_4 \\ \frac{1}{2} - x_4 \\ \frac{1}{2} + z_4 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} - y_4 \\ \frac{1}{2} - x_4 \\ \frac{1}{2} + z_4 \end{pmatrix} c \hat{\mathbf{z}} \quad (8e) \quad \text{Se}$$

$$\mathbf{B}_{32} = \begin{pmatrix} \frac{1}{2} + y_4 \\ \frac{1}{2} + x_4 \\ \frac{1}{2} + z_4 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_4 \\ \frac{1}{2} + x_4 \\ \frac{1}{2} + z_4 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} + y_4 \\ \frac{1}{2} + x_4 \\ \frac{1}{2} + z_4 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_4 \\ \frac{1}{2} + x_4 \\ \frac{1}{2} + z_4 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} + y_4 \\ \frac{1}{2} + x_4 \\ \frac{1}{2} + z_4 \end{pmatrix} c \hat{\mathbf{z}} \quad (8e) \quad \text{Se}$$

#### References:

- F. C. Mijlhoff and C. H. MacGillavry, *Symmetry and unit-cell dimensions of selenium trioxide*, Acta Cryst. **15**, 620–620 (1962), doi:[10.1107/S0365110X62001644](https://doi.org/10.1107/S0365110X62001644).

#### Found in:

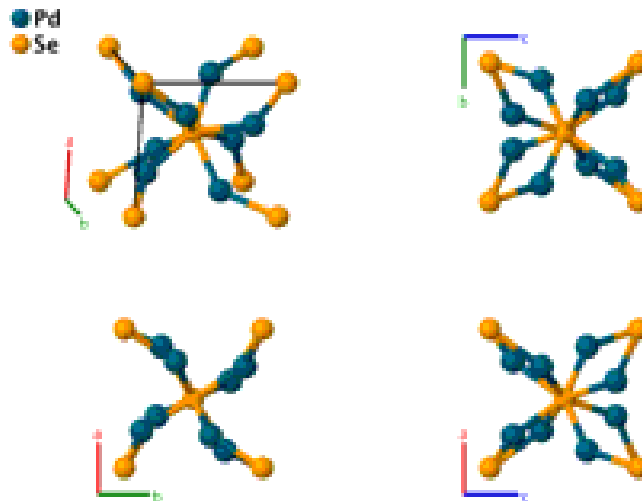
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. [885](#)
- POSCAR: pp. [885](#)



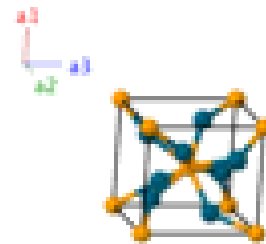
# Pd<sub>4</sub>Se Structure: A4B\_tP10\_114\_e\_a



<b>Prototype</b>	:	Pd <sub>4</sub> Se
<b>AFLOW prototype label</b>	:	A4B_tP10_114_e_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP10
<b>Space group number</b>	:	114
<b>Space group symbol</b>	:	$P\bar{4}2_1c$
<b>AFLOW prototype command</b>	:	aflow --proto=A4B_tP10_114_e_a --params= $a, c/a, x_2, y_2, z_2$

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	Se
<b>B<sub>2</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Se
<b>B<sub>3</sub></b> =	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8e)	Pd
<b>B<sub>4</sub></b> =	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$-x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8e)	Pd
<b>B<sub>5</sub></b> =	$y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(8e)	Pd
<b>B<sub>6</sub></b> =	$-y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(8e)	Pd

$$\mathbf{B}_7 = \begin{pmatrix} \frac{1}{2} - x_2 \\ \frac{1}{2} - z_2 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_2 \\ \frac{1}{2} - z_2 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 = \begin{pmatrix} \frac{1}{2} - x_2 \\ \frac{1}{2} - z_2 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_2 \\ \frac{1}{2} - z_2 \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (8e) \quad \text{Pd}$$

$$\mathbf{B}_8 = \begin{pmatrix} \frac{1}{2} + x_2 \\ \frac{1}{2} - z_2 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - y_2 \\ \frac{1}{2} - z_2 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 = \begin{pmatrix} \frac{1}{2} + x_2 \\ \frac{1}{2} - z_2 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - y_2 \\ \frac{1}{2} - z_2 \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (8e) \quad \text{Pd}$$

$$\mathbf{B}_9 = \begin{pmatrix} \frac{1}{2} - y_2 \\ \frac{1}{2} + z_2 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - x_2 \\ \frac{1}{2} + z_2 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 = \begin{pmatrix} \frac{1}{2} - y_2 \\ \frac{1}{2} + z_2 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - x_2 \\ \frac{1}{2} + z_2 \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (8e) \quad \text{Pd}$$

$$\mathbf{B}_{10} = \begin{pmatrix} \frac{1}{2} + y_2 \\ \frac{1}{2} + z_2 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + x_2 \\ \frac{1}{2} + z_2 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 = \begin{pmatrix} \frac{1}{2} + y_2 \\ \frac{1}{2} + z_2 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + x_2 \\ \frac{1}{2} + z_2 \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (8e) \quad \text{Pd}$$

#### References:

- F. Grønvold and E. Røst, *On the sulfides, selenides and tellurides of palladium*, Acta Chem. Scand. **10**, 1620–1634 (1956), [doi:10.3891/acta.chem.scand.10-1620](https://doi.org/10.3891/acta.chem.scand.10-1620).

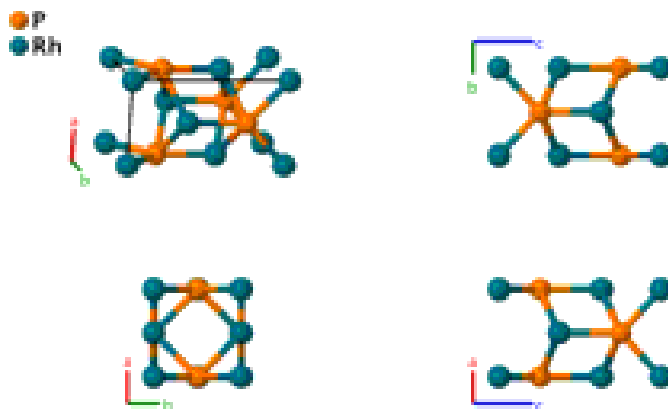
#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. [885](#)
- POSCAR: pp. [886](#)

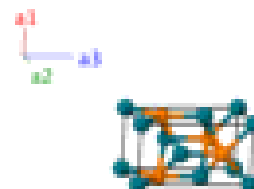
# Rh<sub>3</sub>P<sub>2</sub> Structure: A2B3\_tP5\_115\_g\_ag



<b>Prototype</b>	:	Rh <sub>3</sub> P <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B3_tP5_115_g_ag
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP5
<b>Space group number</b>	:	115
<b>Space group symbol</b>	:	$P\bar{4}m2$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3_tP5_115_g_ag --params=a, c/a, z <sub>2</sub> , z <sub>3</sub>

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Rh I
<b>B<sub>2</sub></b> =	$\frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2g)	P
<b>B<sub>3</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + -z_2 \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} + -z_2 c \hat{\mathbf{z}}$	(2g)	P
<b>B<sub>4</sub></b> =	$\frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2g)	Rh II
<b>B<sub>5</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + -z_3 \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} + -z_3 c \hat{\mathbf{z}}$	(2g)	Rh II

## References:

- E. H. El Ghadraoui, R. Guerin, and M. Sergent, *Diphosphure de trirhodium, Rh<sub>3</sub>P<sub>2</sub>: premier exemple d'une structure lacunaire ordonn e de type anti-PbFCl*, Acta Crystallogr. C **39**, 1493–1494 (1983), doi:10.1107/S0108270183009002.

## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

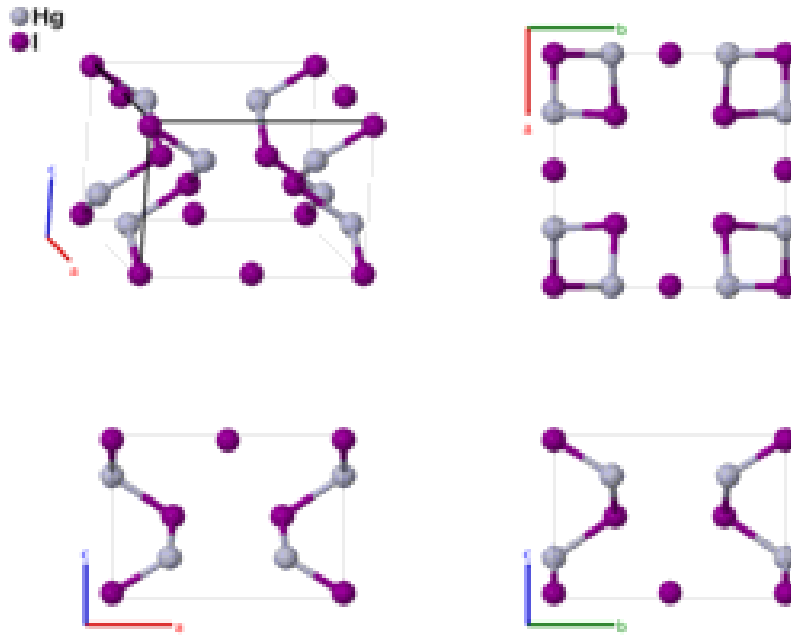
---

**Geometry files:**

- CIF: pp. [886](#)

- POSCAR: pp. [886](#)

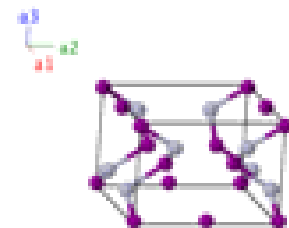
# HgI<sub>2</sub> Structure: AB2\_tP12\_115\_j\_egi



**Prototype** : HgI<sub>2</sub>  
**AFLOW prototype label** : AB2\_tP12\_115\_j\_egi  
**Strukturbericht designation** : None  
**Pearson symbol** : tP12  
**Space group number** : 115  
**Space group symbol** :  $P\bar{4}m2$   
**AFLOW prototype command** : `aflow --proto=AB2_tP12_115_j_egi`  
                                   `--params=a, c/a, z1, z2, x3, x4, z4`

**Simple Tetragonal primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$= z_1 c \hat{\mathbf{z}}$	(2e)	I I
$\mathbf{B}_2$	$= -z_1 \mathbf{a}_3$	$= -z_1 c \hat{\mathbf{z}}$	(2e)	I I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2g)	I II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + -z_2 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + -z_2 c \hat{\mathbf{z}}$	(2g)	I II

$$\begin{array}{llllll}
\mathbf{B}_5 & = & x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4i) & \text{I III} \\
\mathbf{B}_6 & = & -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & -x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4i) & \text{I III} \\
\mathbf{B}_7 & = & x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4i) & \text{I III} \\
\mathbf{B}_8 & = & -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & -x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4i) & \text{I III} \\
\mathbf{B}_9 & = & x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3 & = & x_4 a \hat{\mathbf{x}} + z_4 c \hat{\mathbf{z}} & (4j) & \text{Hg} \\
\mathbf{B}_{10} & = & -x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3 & = & -x_4 a \hat{\mathbf{x}} + z_4 c \hat{\mathbf{z}} & (4j) & \text{Hg} \\
\mathbf{B}_{11} & = & -x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 & = & -x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (4j) & \text{Hg} \\
\mathbf{B}_{12} & = & x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 & = & x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (4j) & \text{Hg}
\end{array}$$

### References:

- M. Hostettler, H. Birkedal, and D. Schwarzenbach, *The structure of orange HgI<sub>2</sub>. I. Polytypic layer structure*, Acta Crystallogr. Sect. B Struct. Sci. **58**, 903–913 (2002), doi:[10.1107/S010876810201618X](https://doi.org/10.1107/S010876810201618X).

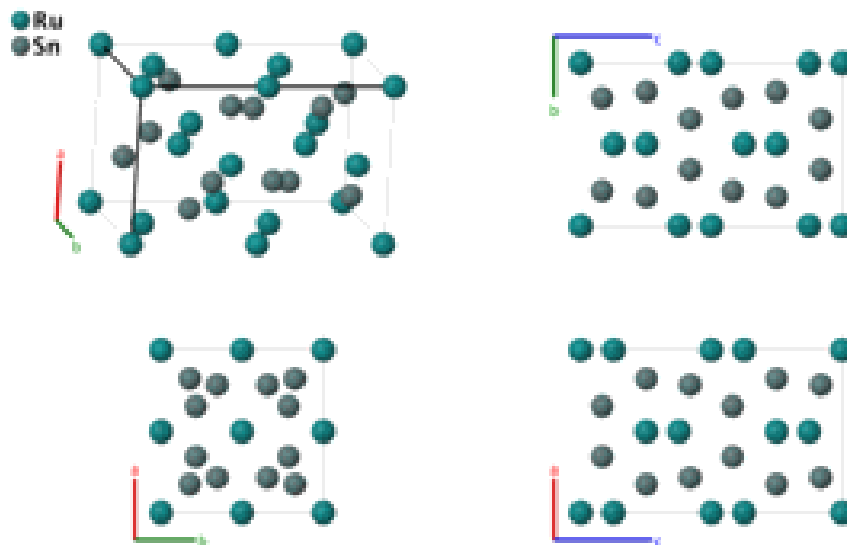
### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

### Geometry files:

- CIF: pp. [886](#)
- POSCAR: pp. [887](#)

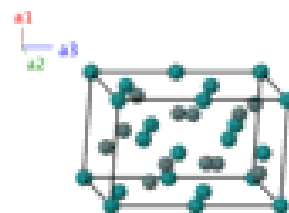
# Ru<sub>2</sub>Sn<sub>3</sub> Structure: A2B3\_tP20\_116\_bci\_fj



<b>Prototype</b>	:	Ru <sub>2</sub> Sn <sub>3</sub>
<b>AFLOW prototype label</b>	:	A2B3_tP20_116_bci_fj
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP20
<b>Space group number</b>	:	116
<b>Space group symbol</b>	:	$P\bar{4}c2$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3_tP20_116_bci_fj --params=a, c/a, x <sub>3</sub> , z <sub>4</sub> , x <sub>5</sub> , y <sub>5</sub> , z <sub>5</sub>

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2b)	Ru I
<b>B<sub>2</sub></b>	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2b)	Ru I
<b>B<sub>3</sub></b>	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2c)	Ru II
<b>B<sub>4</sub></b>	$= \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} c \hat{\mathbf{z}}$	(2c)	Ru II
<b>B<sub>5</sub></b>	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4f)	Sn I
<b>B<sub>6</sub></b>	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= -x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4f)	Sn I
<b>B<sub>7</sub></b>	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4f)	Sn I

$$\begin{array}{llllll}
\mathbf{B}_8 & = & -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 & = & -x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (4f) & \text{Sn I} \\
\mathbf{B}_9 & = & \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (4i) & \text{Ru III} \\
\mathbf{B}_{10} & = & \frac{1}{2} \mathbf{a}_1 + -z_4 \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + -z_4 c \hat{\mathbf{z}} & (4i) & \text{Ru III} \\
\mathbf{B}_{11} & = & \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (4i) & \text{Ru III} \\
\mathbf{B}_{12} & = & \frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (4i) & \text{Ru III} \\
\mathbf{B}_{13} & = & x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 & = & x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8j) & \text{Sn II} \\
\mathbf{B}_{14} & = & -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 & = & -x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8j) & \text{Sn II} \\
\mathbf{B}_{15} & = & y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 & = & y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (8j) & \text{Sn II} \\
\mathbf{B}_{16} & = & -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 & = & -y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (8j) & \text{Sn II} \\
\mathbf{B}_{17} & = & x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 & = & x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (8j) & \text{Sn II} \\
\mathbf{B}_{18} & = & -x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 & = & -x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (8j) & \text{Sn II} \\
\mathbf{B}_{19} & = & y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 & = & y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} & (8j) & \text{Sn II} \\
\mathbf{B}_{20} & = & -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 & = & -y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} & (8j) & \text{Sn II}
\end{array}$$

---

#### References:

- O. Schwomma, H. Nowotny, and A. Wittmann, *Untersuchungen im System: Ru–Sn*, *Monatsh. Chem.* **95**, 1538–1543 (1964), [doi:10.1007/BF00901709](https://doi.org/10.1007/BF00901709).

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

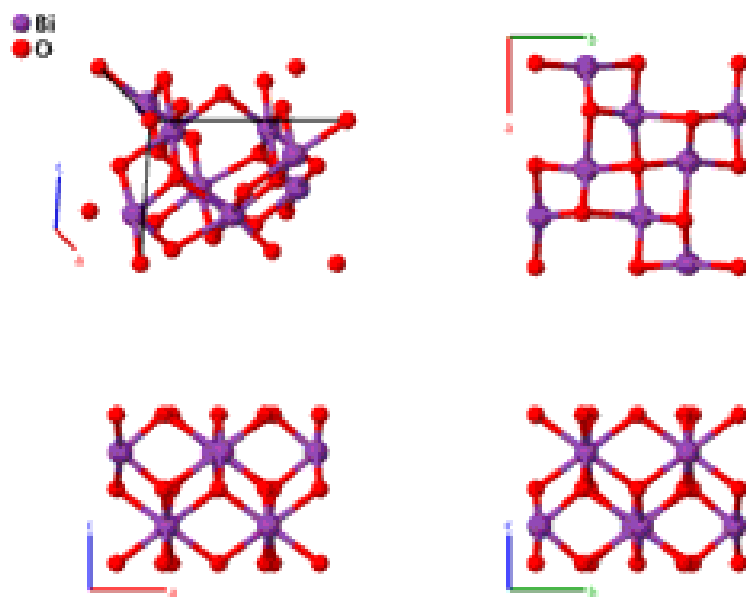
#### Geometry files:

- CIF: pp. [887](#)  
- POSCAR: pp. [887](#)



# $\beta$ -Bi<sub>2</sub>O<sub>3</sub> (High-temperature) Structure:

A2B3\_tP20\_117\_i\_adgh



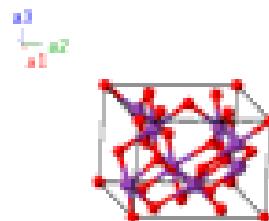
<b>Prototype</b>	:	$\beta$ -Bi <sub>2</sub> O <sub>3</sub>
<b>AFLOW prototype label</b>	:	A2B3_tP20_117_i_adgh
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP20
<b>Space group number</b>	:	117
<b>Space group symbol</b>	:	$P\bar{4}b2$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A2B3_tP20_117_i_adgh</code> <code>--params=a, c/a, x3, x4, x5, y5, z5</code>

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2d)	O II

$$\begin{array}{llllll}
\mathbf{B}_4 & = & \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}} & (2d) & \text{O II} \\
\mathbf{B}_5 & = & x_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 & = & x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} & (4g) & \text{O III} \\
\mathbf{B}_6 & = & -x_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 & = & -x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} & (4g) & \text{O III} \\
\mathbf{B}_7 & = & \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 & = & \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} & (4g) & \text{O III} \\
\mathbf{B}_8 & = & \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 & = & \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} & (4g) & \text{O III} \\
\mathbf{B}_9 & = & x_4 \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{O IV} \\
\mathbf{B}_{10} & = & -x_4 \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{O IV} \\
\mathbf{B}_{11} & = & \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{O IV} \\
\mathbf{B}_{12} & = & \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4h) & \text{O IV} \\
\mathbf{B}_{13} & = & x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 & = & x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8i) & \text{Bi} \\
\mathbf{B}_{14} & = & -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 & = & -x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8i) & \text{Bi} \\
\mathbf{B}_{15} & = & y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 & = & y_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (8i) & \text{Bi} \\
\mathbf{B}_{16} & = & -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 & = & -y_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (8i) & \text{Bi} \\
\mathbf{B}_{17} & = & \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3 & = & \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8i) & \text{Bi} \\
\mathbf{B}_{18} & = & \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3 & = & \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (8i) & \text{Bi} \\
\mathbf{B}_{19} & = & \left(\frac{1}{2} + y_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_5\right) \mathbf{a}_2 - z_5 \mathbf{a}_3 & = & \left(\frac{1}{2} + y_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (8i) & \text{Bi} \\
\mathbf{B}_{20} & = & \left(\frac{1}{2} - y_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_5\right) \mathbf{a}_2 - z_5 \mathbf{a}_3 & = & \left(\frac{1}{2} - y_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (8i) & \text{Bi}
\end{array}$$

---

#### References:

- L. G. Sillén, *X-ray studies on bismuth trioxide*, Ark. Kem. Mineral. Geol. **12A**, 1–15 (1937).

#### Found in:

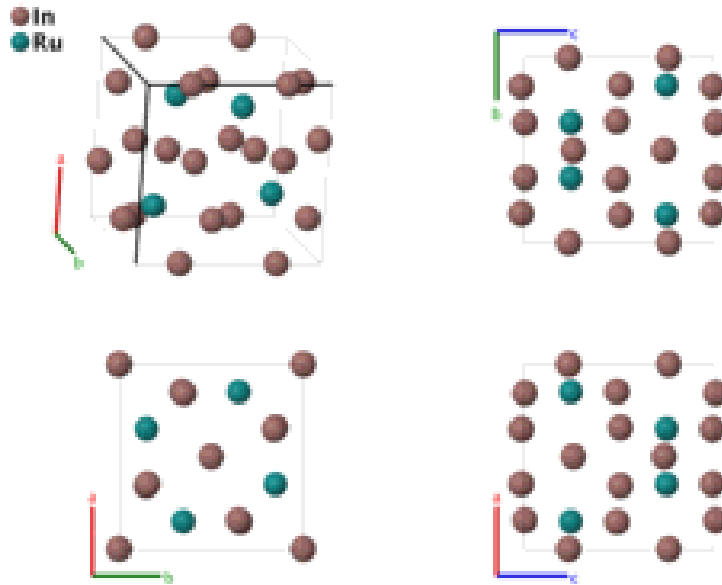
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [887](#)  
- POSCAR: pp. [888](#)

# RuIn<sub>3</sub> Structure: A3B\_tP16\_118\_ei\_f



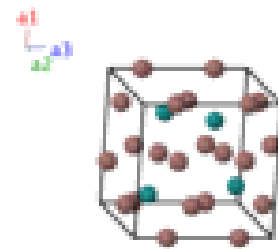
<b>Prototype</b>	:	RuIn <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B_tP16_118_ei_f
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP16
<b>Space group number</b>	:	118
<b>Space group symbol</b>	:	$P\bar{4}n2$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A3B_tP16_118_ei_f --params=a, c/a, z1, x2, x3, y3, z3</code>

**Simple Tetragonal primitive vectors:**

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1 =$	$z_1 \mathbf{a}_3$	$=$	$z_1 c \hat{\mathbf{z}}$	(4e)	In I
$\mathbf{B}_2 =$	$-z_1 \mathbf{a}_3$	$=$	$-z_1 c \hat{\mathbf{z}}$	(4e)	In I
$\mathbf{B}_3 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4e)	In I
$\mathbf{B}_4 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	(4e)	In I
$\mathbf{B}_5 =$	$x_2 \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4f)	Ru

$$\begin{aligned}
\mathbf{B}_6 &= -x_2 \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} && (4f) && \text{Ru} \\
\mathbf{B}_7 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} && (4f) && \text{Ru} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} && (4f) && \text{Ru} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} && (8i) && \text{In II} \\
\mathbf{B}_{10} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} && (8i) && \text{In II} \\
\mathbf{B}_{11} &= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} && (8i) && \text{In II} \\
\mathbf{B}_{12} &= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} && (8i) && \text{In II} \\
\mathbf{B}_{13} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} + && (8i) && \text{In II} \\
&\quad \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} + && (8i) && \text{In II} \\
&\quad \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} + y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + && (8i) && \text{In II} \\
&\quad \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} - y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + && (8i) && \text{In II} \\
&\quad \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}}
\end{aligned}$$

#### References:

- R. B. Roof, Z. Fisk, and J. L. Smith, *Crystal data for RuIn<sub>3</sub>*, Powder Diffraction **1**, 20–21 (1986), [doi:10.1017/S0885715600011234](https://doi.org/10.1017/S0885715600011234).

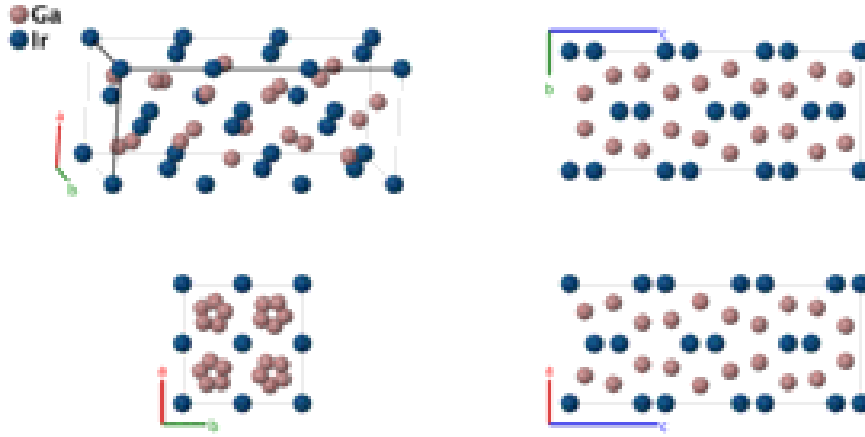
#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. [888](#)  
- POSCAR: pp. [888](#)

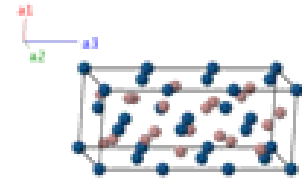
# Ir<sub>3</sub>Ga<sub>5</sub> Structure: A5B3\_tP32\_118\_g2i\_aceh



<b>Prototype</b>	:	Ir <sub>3</sub> Ga <sub>5</sub>
<b>AFLOW prototype label</b>	:	A5B3_tP32_118_g2i_aceh
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP32
<b>Space group number</b>	:	118
<b>Space group symbol</b>	:	$P\bar{4}n2$
<b>AFLOW prototype command</b>	:	aflow --proto=A5B3_tP32_118_g2i_aceh --params=a, c/a, z <sub>3</sub> , x <sub>4</sub> , z <sub>5</sub> , x <sub>6</sub> , y <sub>6</sub> , z <sub>6</sub> , x <sub>7</sub> , y <sub>7</sub> , z <sub>7</sub>

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	Ir I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Ir I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2c)	Ir II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2c)	Ir II
$\mathbf{B}_5$	$= z_3 \mathbf{a}_3$	$=$	$z_3 c \hat{\mathbf{z}}$	(4e)	Ir III
$\mathbf{B}_6$	$= -z_3 \mathbf{a}_3$	$=$	$-z_3 c \hat{\mathbf{z}}$	(4e)	Ir III
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4e)	Ir III
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}}$	(4e)	Ir III
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4g)	Ga I
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4g)	Ga I

$$\begin{aligned}
\mathbf{B}_{11} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} &(4g) & \text{Ga I} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} &(4g) & \text{Ga I} \\
\mathbf{B}_{13} &= \frac{1}{2} \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} &(4h) & \text{Ir IV} \\
\mathbf{B}_{14} &= \frac{1}{2} \mathbf{a}_1 + -z_5 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + -z_5 c \hat{\mathbf{z}} &(4h) & \text{Ir IV} \\
\mathbf{B}_{15} &= \frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} &(4h) & \text{Ir IV} \\
\mathbf{B}_{16} &= \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} &(4h) & \text{Ir IV} \\
\mathbf{B}_{17} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} &(8i) & \text{Ga II} \\
\mathbf{B}_{18} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= -x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} &(8i) & \text{Ga II} \\
\mathbf{B}_{19} &= y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= y_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} &(8i) & \text{Ga II} \\
\mathbf{B}_{20} &= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -y_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} &(8i) & \text{Ga II} \\
\mathbf{B}_{21} &= \left(\frac{1}{2} + x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_6\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_6\right) a \hat{\mathbf{y}} + &(8i) & \text{Ga II} \\
&\quad \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{22} &= \left(\frac{1}{2} - x_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_6\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) a \hat{\mathbf{y}} + &(8i) & \text{Ga II} \\
&\quad \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{23} &= \left(\frac{1}{2} + y_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_6\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + y_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{y}} + &(8i) & \text{Ga II} \\
&\quad \left(\frac{1}{2} - z_6\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{24} &= \left(\frac{1}{2} - y_6\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_6\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - y_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{y}} + &(8i) & \text{Ga II} \\
&\quad \left(\frac{1}{2} - z_6\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{25} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} &(8i) & \text{Ga III} \\
\mathbf{B}_{26} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= -x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} &(8i) & \text{Ga III} \\
\mathbf{B}_{27} &= y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} &(8i) & \text{Ga III} \\
\mathbf{B}_{28} &= -y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} &(8i) & \text{Ga III} \\
\mathbf{B}_{29} &= \left(\frac{1}{2} + x_7\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_7\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + x_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_7\right) a \hat{\mathbf{y}} + &(8i) & \text{Ga III} \\
&\quad \left(\frac{1}{2} + z_7\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{30} &= \left(\frac{1}{2} - x_7\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_7\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_7\right) a \hat{\mathbf{y}} + &(8i) & \text{Ga III} \\
&\quad \left(\frac{1}{2} + z_7\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{31} &= \left(\frac{1}{2} + y_7\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_7\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + y_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_7\right) a \hat{\mathbf{y}} + &(8i) & \text{Ga III} \\
&\quad \left(\frac{1}{2} - z_7\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_7\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{32} &= \left(\frac{1}{2} - y_7\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_7\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - y_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_7\right) a \hat{\mathbf{y}} + &(8i) & \text{Ga III} \\
&\quad \left(\frac{1}{2} - z_7\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_7\right) c \hat{\mathbf{z}}
\end{aligned}$$

#### References:

- H. Völlenkle, A. Wittmann, and H. Nowotny, *Die Kristallstrukturen von Rh<sub>10</sub>Ga<sub>17</sub> und Ir<sub>3</sub>Ga<sub>5</sub>*, *Monatsh. Chem.* **98**, 176–183 (1967), doi:10.1007/BF00901115.

#### Found in:

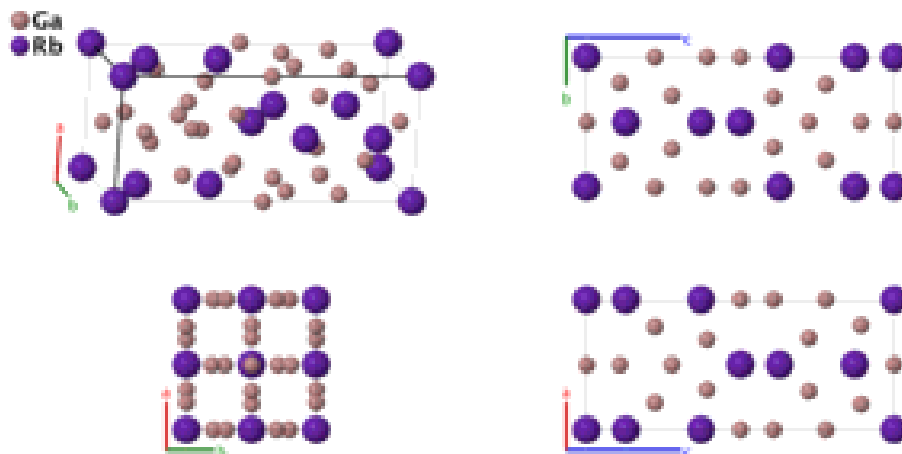
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. 888

- POSCAR: pp. [889](#)

# RbGa<sub>3</sub> Structure: A3B\_tI24\_119\_b2i\_af



<b>Prototype</b>	:	RbGa <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B_tI24_119_b2i_af
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI24
<b>Space group number</b>	:	119
<b>Space group symbol</b>	:	$I\bar{4}m2$
<b>AFLOW prototype command</b>	:	aflow --proto=A3B_tI24_119_b2i_af --params=a, c/a, z <sub>3</sub> , x <sub>4</sub> , z <sub>4</sub> , x <sub>5</sub> , z <sub>5</sub>

## Other compounds with this structure:

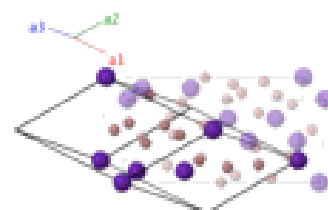
- CsGa<sub>3</sub>, KGa<sub>3</sub>

## Body-centered Tetragonal primitive vectors:

$$\mathbf{a}_1 = -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= 0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$	$= 0\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}}$	(2a)	Rb I
<b>B<sub>2</sub></b>	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$= \frac{1}{2}c\hat{\mathbf{z}}$	(2b)	Ga I
<b>B<sub>3</sub></b>	$= \left(\frac{1}{2} + z_3\right)\mathbf{a}_1 + z_3\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$= \frac{1}{2}a\hat{\mathbf{y}} + z_3c\hat{\mathbf{z}}$	(4f)	Rb II
<b>B<sub>4</sub></b>	$= -z_3\mathbf{a}_1 + \left(\frac{1}{2} - z_3\right)\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$= \frac{1}{2}a\hat{\mathbf{x}} - z_3c\hat{\mathbf{z}}$	(4f)	Rb II
<b>B<sub>5</sub></b>	$= z_4\mathbf{a}_1 + (x_4 + z_4)\mathbf{a}_2 + x_4\mathbf{a}_3$	$= x_4a\hat{\mathbf{x}} + z_4c\hat{\mathbf{z}}$	(8i)	Ga II
<b>B<sub>6</sub></b>	$= z_4\mathbf{a}_1 + (-x_4 + z_4)\mathbf{a}_2 - x_4\mathbf{a}_3$	$= -x_4a\hat{\mathbf{x}} + z_4c\hat{\mathbf{z}}$	(8i)	Ga II
<b>B<sub>7</sub></b>	$= (-x_4 - z_4)\mathbf{a}_1 - z_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$= -x_4a\hat{\mathbf{y}} - z_4c\hat{\mathbf{z}}$	(8i)	Ga II



$$\begin{aligned}
\mathbf{B}_8 &= (x_4 - z_4) \mathbf{a}_1 - z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8i) & \text{Ga II} \\
\mathbf{B}_9 &= z_5 \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + x_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{x}} + z_5 c \hat{\mathbf{z}} & (8i) & \text{Ga III} \\
\mathbf{B}_{10} &= z_5 \mathbf{a}_1 + (-x_5 + z_5) \mathbf{a}_2 - x_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{x}} + z_5 c \hat{\mathbf{z}} & (8i) & \text{Ga III} \\
\mathbf{B}_{11} &= (-x_5 - z_5) \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3 &= -x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (8i) & \text{Ga III} \\
\mathbf{B}_{12} &= (x_5 - z_5) \mathbf{a}_1 - z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3 &= x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (8i) & \text{Ga III}
\end{aligned}$$

---

**References:**

- R. G. Ling and C. Belin, *Preparation and Crystal Structure Determination of the New Intermetallic Compound RbGa<sub>3</sub>*, *Z. Anorg. Allg. Chem.* **480**, 181–185 (1981), [doi:10.1002/zaac.19814800923](https://doi.org/10.1002/zaac.19814800923).

**Found in:**

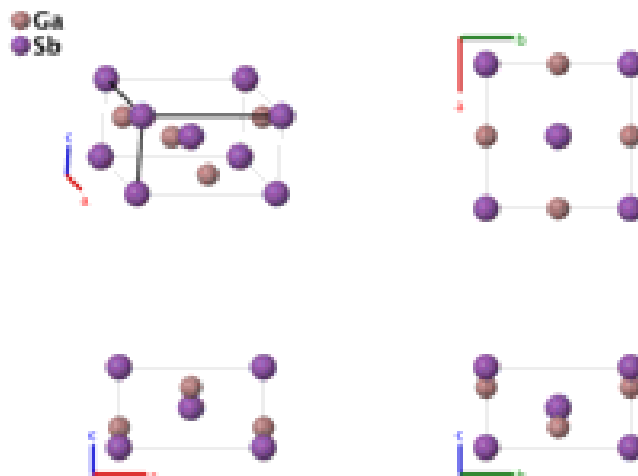
- P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), vol. III, chap. , p. 3545.

---

**Geometry files:**

- CIF: pp. [889](#)
- POSCAR: pp. [889](#)

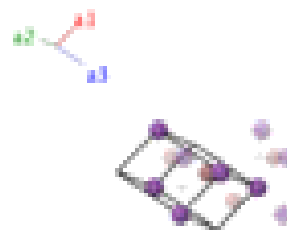
# GaSb Structure: AB\_tI4\_119\_c\_a



<b>Prototype</b>	:	GaSb
<b>AFLOW prototype label</b>	:	AB_tI4_119_c_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI4
<b>Space group number</b>	:	119
<b>Space group symbol</b>	:	$I\bar{4}m2$
<b>AFLOW prototype command</b>	:	aflow --proto=AB_tI4_119_c_a --params=a,c/a

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$	$= 0\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}}$	(2a)	Sb
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$= \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2c)	Ga

## References:

- T. R. R. McDonald, R. Sard, and E. Gregory, *Retention of GaSb (II) at low temperatures and one atmosphere pressure*, J. Appl. Phys. **36**, 1498–1499 (1965), [doi:10.1063/1.1714346](https://doi.org/10.1063/1.1714346).

## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

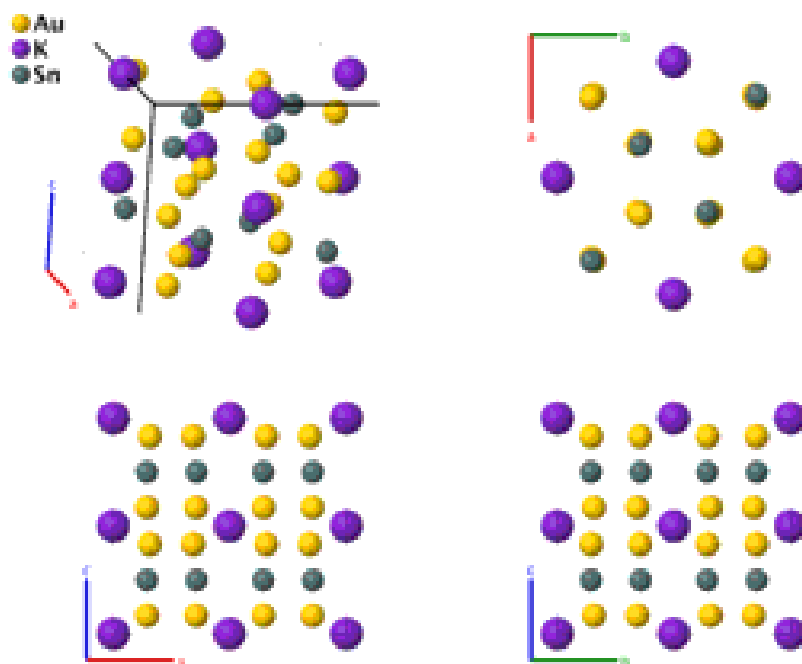
---

**Geometry files:**

- CIF: pp. [889](#)

- POSCAR: pp. [890](#)

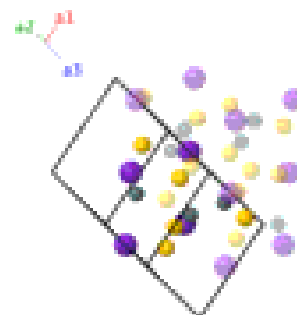
# KAu<sub>4</sub>Sn<sub>2</sub> Structure: A4BC2\_tI28\_120\_i\_d\_e



<b>Prototype</b>	:	KAu <sub>4</sub> Sn <sub>2</sub>
<b>AFLOW prototype label</b>	:	A4BC2_tI28_120_i_d_e
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI28
<b>Space group number</b>	:	120
<b>Space group symbol</b>	:	$I\bar{4}c2$
<b>AFLOW prototype command</b>	:	aflow --proto=A4BC2_tI28_120_i_d_e --params=a, c/a, x <sub>2</sub> , x <sub>3</sub> , y <sub>3</sub> , z <sub>3</sub>

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}}$	(4d)	K
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}}$	(4d)	K
$\mathbf{B}_3$	$= \left(\frac{1}{4} + x_2\right)\mathbf{a}_1 + \left(\frac{1}{4} + x_2\right)\mathbf{a}_2 + 2x_2\mathbf{a}_3$	$=$	$x_2a\hat{\mathbf{x}} + x_2a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(8e)	Sn
$\mathbf{B}_4$	$= \left(\frac{1}{4} - x_2\right)\mathbf{a}_1 + \left(\frac{1}{4} - x_2\right)\mathbf{a}_2 - 2x_2\mathbf{a}_3$	$=$	$-x_2a\hat{\mathbf{x}} - x_2a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(8e)	Sn

$$\begin{aligned}
\mathbf{B}_5 &= \left(\frac{3}{4} - x_2\right) \mathbf{a}_1 + \left(\frac{3}{4} + x_2\right) \mathbf{a}_2 &= x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8e) & \text{Sn} \\
\mathbf{B}_6 &= \left(\frac{3}{4} + x_2\right) \mathbf{a}_1 + \left(\frac{3}{4} - x_2\right) \mathbf{a}_2 &= -x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8e) & \text{Sn} \\
\mathbf{B}_7 &= (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (16i) & \text{Au} \\
\mathbf{B}_8 &= (-y_3 + z_3) \mathbf{a}_1 + (-x_3 + z_3) \mathbf{a}_2 + &= -x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (16i) & \text{Au} \\
&\quad (-x_3 - y_3) \mathbf{a}_3 \\
\mathbf{B}_9 &= (-x_3 - z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + &= y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (16i) & \text{Au} \\
&\quad (-x_3 + y_3) \mathbf{a}_3 \\
\mathbf{B}_{10} &= (x_3 - z_3) \mathbf{a}_1 + (-y_3 - z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (16i) & \text{Au} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} - y_3 + z_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_3 + z_3\right) \mathbf{a}_2 + &= x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (16i) & \text{Au} \\
&\quad (x_3 - y_3) \mathbf{a}_3 \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + y_3 + z_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3 + z_3\right) \mathbf{a}_2 + &= -x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (16i) & \text{Au} \\
&\quad (-x_3 + y_3) \mathbf{a}_3 \\
\mathbf{B}_{13} &= \left(\frac{1}{2} + x_3 - z_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3 - z_3\right) \mathbf{a}_2 + &= y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (16i) & \text{Au} \\
&\quad (x_3 + y_3) \mathbf{a}_3 \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_3 - z_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3 - z_3\right) \mathbf{a}_2 + &= -y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (16i) & \text{Au} \\
&\quad (-x_3 - y_3) \mathbf{a}_3
\end{aligned}$$

---

#### References:

- H.-D. Sinnen and H.-U. Schuster, *Darstellung und Struktur des  $\text{KAu}_4\text{Sn}_2$  / Preparation and Crystal Structure of  $\text{KAu}_4\text{Sn}_2$* , Z. Naturforsch. B **33**, 1077–1079 (1978), doi:10.1515/znb-1978-1004.

#### Found in:

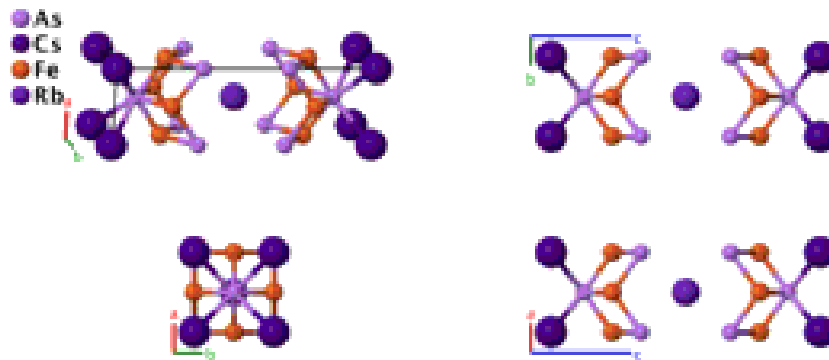
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 890  
- POSCAR: pp. 890

# CaRbFe<sub>4</sub>As<sub>4</sub> (Superconducting) Structure: A4BC4D\_tP10\_123\_gh\_a\_i\_d



<b>Prototype</b>	:	CsRbFe <sub>4</sub> As <sub>4</sub>
<b>AFLOW prototype label</b>	:	A4BC4D_tP10_123_gh_a_i_d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP10
<b>Space group number</b>	:	123
<b>Space group symbol</b>	:	<i>P4/mmm</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A4BC4D_tP10_123_gh_a_i_d --params=a, c/a, z3, z4, z5</code>

## Other compounds with this structure:

- CaKFe<sub>4</sub>As<sub>4</sub>, CaCsFe<sub>4</sub>As<sub>4</sub>, SrRbFe<sub>4</sub>As<sub>4</sub>, SrCsFe<sub>4</sub>As<sub>4</sub>, BaCsFe<sub>4</sub>As<sub>4</sub>

- These compounds form a family of stoichiometric superconductors with transition temperatures  $T_c$  ranging from 26–37 K.

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	= $0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Cs
<b>B<sub>2</sub></b>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	= $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(1d)	Rb
<b>B<sub>3</sub></b>	= $z_3 \mathbf{a}_3$	= $z_3 c \hat{\mathbf{z}}$	(2g)	As I
<b>B<sub>4</sub></b>	= $-z_3 \mathbf{a}_3$	= $-z_3 c \hat{\mathbf{z}}$	(2g)	As I
<b>B<sub>5</sub></b>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	= $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(2h)	As II

$$\begin{aligned}
\mathbf{B}_6 &= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (2h) && \text{As II} \\
\mathbf{B}_7 &= \frac{1}{2} \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (4i) && \text{Fe} \\
\mathbf{B}_8 &= \frac{1}{2} \mathbf{a}_1 + z_5 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + z_5 c \hat{\mathbf{z}} && (4i) && \text{Fe} \\
\mathbf{B}_9 &= \frac{1}{2} \mathbf{a}_2 - z_5 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} && (4i) && \text{Fe} \\
\mathbf{B}_{10} &= \frac{1}{2} \mathbf{a}_1 + -z_5 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + -z_5 c \hat{\mathbf{z}} && (4i) && \text{Fe}
\end{aligned}$$

---

### References:

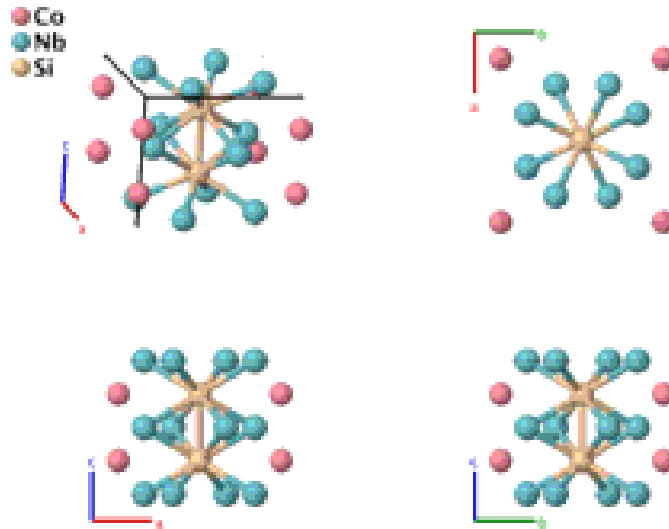
- A. Iyo, K. Kawashima, T. Kinjo, T. Nishio, S. Ishida, H. Fujihisa, Y. Gotoh, K. Kihou, H. Eisaki, and Y. Yoshida, *New-Structure-Type Fe-Based Superconductors: CaFe<sub>4</sub>As<sub>4</sub> (A = K, Rb, Cs) and SrFe<sub>4</sub>As<sub>4</sub> (A = Rb, Cs)*, J. Am. Chem. Soc. **138**, 3410–3415 (2016), doi:[10.1021/jacs.5b12571](https://doi.org/10.1021/jacs.5b12571).

---

### Geometry files:

- CIF: pp. [890](#)  
- POSCAR: pp. [891](#)

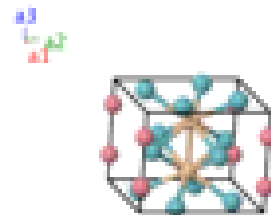
# Nb<sub>4</sub>CoSi Structure: AB4C\_tP12\_124\_a\_m\_c



**Prototype** : Nb<sub>4</sub>CoSi  
**AFLOW prototype label** : AB4C\_tP12\_124\_a\_m\_c  
**Strukturbericht designation** : None  
**Pearson symbol** : tP12  
**Space group number** : 124  
**Space group symbol** : *P4/mcc*  
**AFLOW prototype command** : `aflow --proto=AB4C_tP12_124_a_m_c --params=a, c/a, x3, y3`

Simple Tetragonal primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $\frac{1}{4} \mathbf{a}_3$	= $\frac{1}{4} c \hat{\mathbf{z}}$	(2a)	Co
<b>B</b> <sub>2</sub>	= $\frac{3}{4} \mathbf{a}_3$	= $\frac{3}{4} c \hat{\mathbf{z}}$	(2a)	Co
<b>B</b> <sub>3</sub>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	= $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2c)	Si
<b>B</b> <sub>4</sub>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	= $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2c)	Si
<b>B</b> <sub>5</sub>	= $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	= $x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}}$	(8m)	Nb
<b>B</b> <sub>6</sub>	= $-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	= $-x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}}$	(8m)	Nb



$$\begin{aligned}
\mathbf{B}_7 &= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 &= -y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} & (8m) & \text{Nb} \\
\mathbf{B}_8 &= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 &= y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} & (8m) & \text{Nb} \\
\mathbf{B}_9 &= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8m) & \text{Nb} \\
\mathbf{B}_{10} &= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8m) & \text{Nb} \\
\mathbf{B}_{11} &= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8m) & \text{Nb} \\
\mathbf{B}_{12} &= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8m) & \text{Nb}
\end{aligned}$$

---

**References:**

- E. I. Gladyshevskii and Y. B. Kuz'ma, *The compounds Nb<sub>4</sub>FeSi, Nb<sub>4</sub>CoSi, Nb<sub>4</sub>NiSi and their crystal structures*, J. Struct. Chem. **6**, 60–63 (1965), doi:10.1007/BF00743870.

**Found in:**

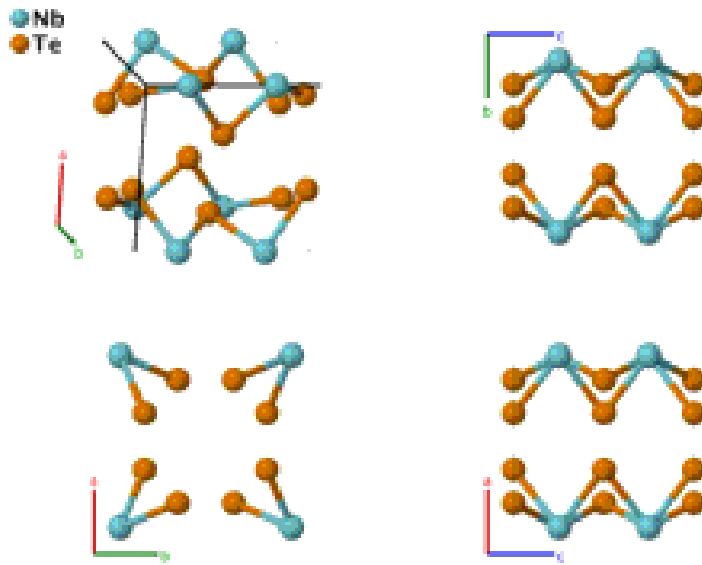
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [891](#)  
- POSCAR: pp. [891](#)

# NbTe<sub>4</sub> Structure: AB4\_tP10\_124\_a\_m



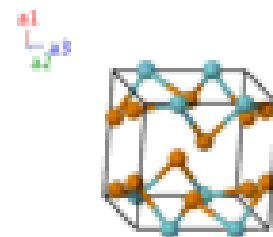
**Prototype** : NbTe<sub>4</sub>  
**AFLOW prototype label** : AB4\_tP10\_124\_a\_m  
**Strukturbericht designation** : None  
**Pearson symbol** : tP10  
**Space group number** : 124  
**Space group symbol** : *P4/mcc*  
**AFLOW prototype command** : aflow --proto=AB4\_tP10\_124\_a\_m  
 --params=a, c/a, x<sub>2</sub>, y<sub>2</sub>

Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $\frac{1}{4} \mathbf{a}_3$	= $\frac{1}{4} c \hat{\mathbf{z}}$	(2a)	Nb
<b>B</b> <sub>2</sub>	= $\frac{3}{4} \mathbf{a}_3$	= $\frac{3}{4} c \hat{\mathbf{z}}$	(2a)	Nb
<b>B</b> <sub>3</sub>	= $x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	= $x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}}$	(8m)	Te
<b>B</b> <sub>4</sub>	= $-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	= $-x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}}$	(8m)	Te
<b>B</b> <sub>5</sub>	= $-y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	= $-y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}}$	(8m)	Te
<b>B</b> <sub>6</sub>	= $y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	= $y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}}$	(8m)	Te

$$\mathbf{B}_7 = -x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \quad (8m) \quad \text{Te}$$

$$\mathbf{B}_8 = x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \quad (8m) \quad \text{Te}$$

$$\mathbf{B}_9 = y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \quad (8m) \quad \text{Te}$$

$$\mathbf{B}_{10} = -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \quad (8m) \quad \text{Te}$$

---

**References:**

- K. Selte and A. Kjekshus, *On the crystal structure of NbTe<sub>4</sub>*, Acta Chem. Scand. **18**, 690–696 (1964), [doi:10.3891/acta.chem.scand.18-0690](https://doi.org/10.3891/acta.chem.scand.18-0690).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

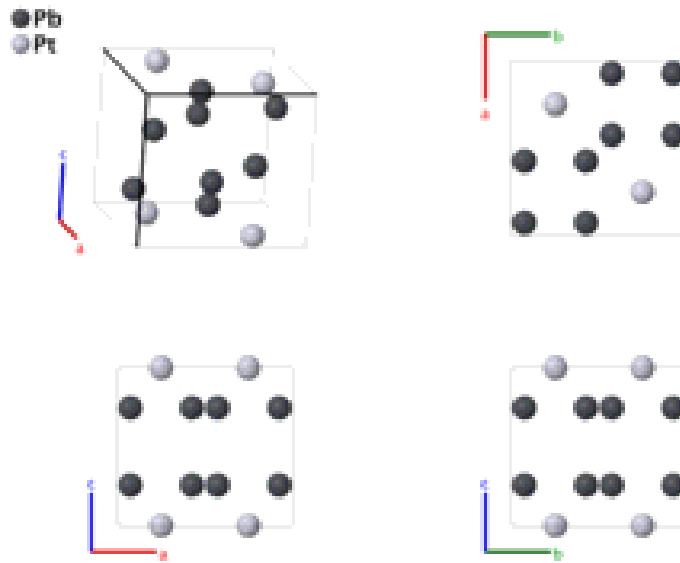
---

**Geometry files:**

- CIF: pp. [891](#)

- POSCAR: pp. [892](#)

# PtPb<sub>4</sub> Structure: A4B\_tP10\_125\_m\_a



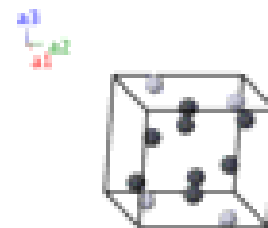
<b>Prototype</b>	:	PtPb <sub>4</sub>
<b>AFLOW prototype label</b>	:	A4B_tP10_125_m_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP10
<b>Space group number</b>	:	125
<b>Space group symbol</b>	:	<i>P4/nbm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A4B_tP10_125_m_a --params= <i>a, c/a, x<sub>2</sub>, z<sub>2</sub></i>

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	= $\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(2 <i>a</i> )	Pt
<b>B<sub>2</sub></b>	= $\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	= $\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(2 <i>a</i> )	Pt
<b>B<sub>3</sub></b>	= $x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	= $x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8 <i>m</i> )	Pb
<b>B<sub>4</sub></b>	= $(\frac{1}{2} - x_2) \mathbf{a}_1 + (\frac{1}{2} + x_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	= $(\frac{1}{2} - x_2) a \hat{\mathbf{x}} + (\frac{1}{2} + x_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8 <i>m</i> )	Pb
<b>B<sub>5</sub></b>	= $(\frac{1}{2} + x_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	= $(\frac{1}{2} + x_2) a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8 <i>m</i> )	Pb

$$\mathbf{B}_6 = -x_2 \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + z_2 \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} \quad (8m) \quad \text{Pb}$$

$$\mathbf{B}_7 = \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3 = \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} \quad (8m) \quad \text{Pb}$$

$$\mathbf{B}_8 = x_2 \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 - z_2 \mathbf{a}_3 = x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} \quad (8m) \quad \text{Pb}$$

$$\mathbf{B}_9 = -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} \quad (8m) \quad \text{Pb}$$

$$\mathbf{B}_{10} = \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 - z_2 \mathbf{a}_3 = \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} \quad (8m) \quad \text{Pb}$$

### References:

- R. Graham, G. C. S. Waghorn, and P. T. Davies, *An X-ray investigation of the lead-platinum system*, Acta Cryst. **7**, 634–635 (1954).

### Found in:

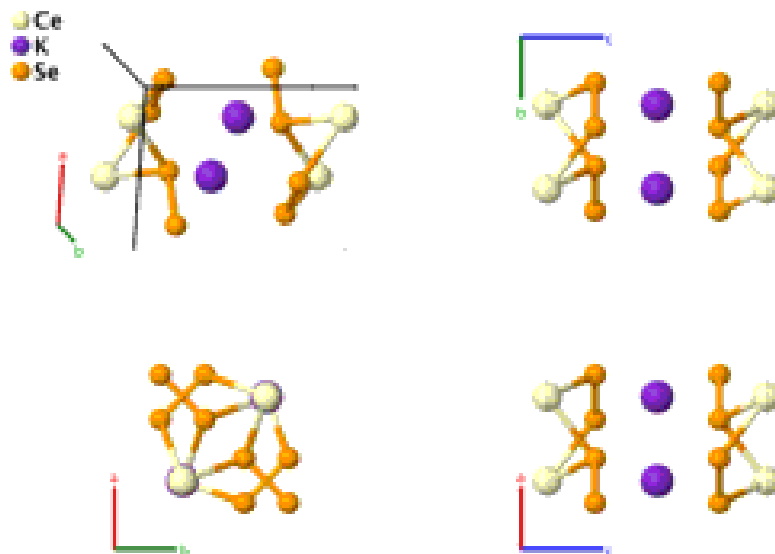
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

### Geometry files:

- CIF: pp. [892](#)

- POSCAR: pp. [892](#)

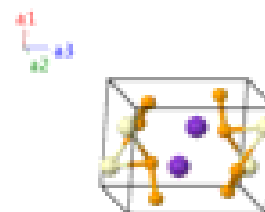
# KCeSe<sub>4</sub> Structure: ABC4\_tP12\_125\_a\_b\_m



<b>Prototype</b>	:	KCeSe <sub>4</sub>
<b>AFLOW prototype label</b>	:	ABC4_tP12_125_a_b_m
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP12
<b>Space group number</b>	:	125
<b>Space group symbol</b>	:	<i>P4/nbm</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=ABC4_tP12_125_a_b_m --params=a, c/a, x3, z3</code>

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(2a)	Ce
<b>B<sub>2</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(2a)	Ce
<b>B<sub>3</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2b)	K
<b>B<sub>4</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2b)	K
<b>B<sub>5</sub></b>	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8m)	Se
<b>B<sub>6</sub></b>	$= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(8m)	Se

$$\begin{aligned}
\mathbf{B}_7 &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8m) & \text{Se} \\
\mathbf{B}_8 &= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8m) & \text{Se} \\
\mathbf{B}_9 &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8m) & \text{Se} \\
\mathbf{B}_{10} &= x_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8m) & \text{Se} \\
\mathbf{B}_{11} &= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8m) & \text{Se} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8m) & \text{Se}
\end{aligned}$$

---

**References:**

- A. C. Sutorik and M. G. Kanatzidis, *KCeSe<sub>4</sub>: A New Solid-State Lanthanide Polychalcogenide*, *Angew. Chem. Int. Ed.* **31**, 1594–1596 (1992), [doi:10.1002/anie.199215941](https://doi.org/10.1002/anie.199215941).

**Found in:**

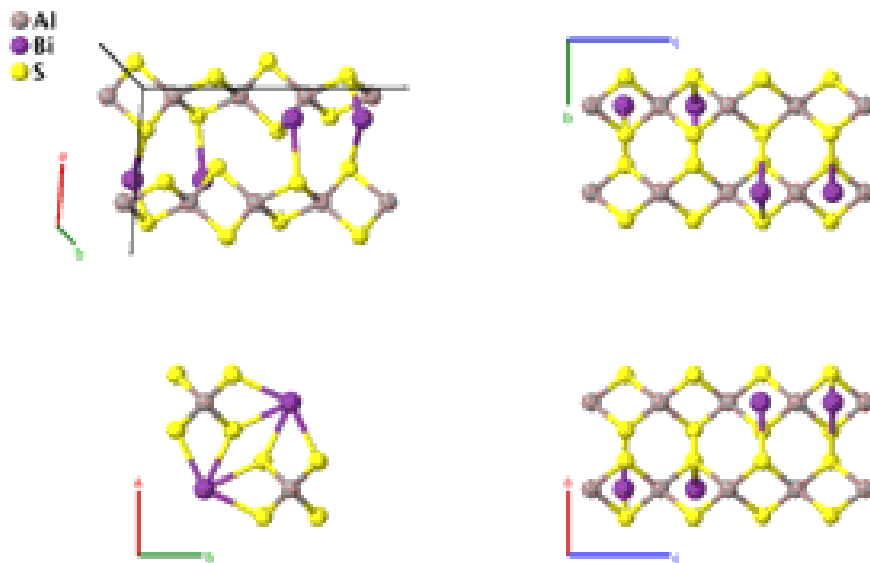
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [892](#)
- POSCAR: pp. [893](#)

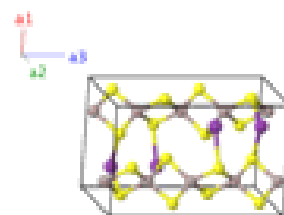
# BiAl<sub>2</sub>S<sub>4</sub> Structure: A2BC4\_tP28\_126\_cd\_e\_k



<b>Prototype</b>	:	BiAl <sub>2</sub> S <sub>4</sub>
<b>AFLOW prototype label</b>	:	A2BC4_tP28_126_cd_e_k
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP28
<b>Space group number</b>	:	126
<b>Space group symbol</b>	:	<i>P4/nnc</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2BC4_tP28_126_cd_e_k --params=a, c/a, z <sub>3</sub> , x <sub>4</sub> , y <sub>4</sub> , z <sub>4</sub>

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Al I
<b>B<sub>2</sub></b>	= $\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Al I
<b>B<sub>3</sub></b>	= $\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Al I
<b>B<sub>4</sub></b>	= $\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Al I
<b>B<sub>5</sub></b>	= $\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(4d)	Al II
<b>B<sub>6</sub></b>	= $\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	=	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(4d)	Al II



$\mathbf{B}_7$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4d)	Al II
$\mathbf{B}_8$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4d)	Al II
$\mathbf{B}_9$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4e)	Bi
$\mathbf{B}_{10}$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}}$	(4e)	Bi
$\mathbf{B}_{11}$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(4e)	Bi
$\mathbf{B}_{12}$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(4e)	Bi
$\mathbf{B}_{13}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{14}$	$=$	$\left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{15}$	$=$	$\left(\frac{1}{2} - y_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - y_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{16}$	$=$	$y_4 \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$y_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{17}$	$=$	$\left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{18}$	$=$	$x_4 \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{19}$	$=$	$y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$=$	$y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{20}$	$=$	$\left(\frac{1}{2} - y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 +$ $\left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{21}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{22}$	$=$	$\left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{23}$	$=$	$\left(\frac{1}{2} + y_4\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + y_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{24}$	$=$	$-y_4 \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-y_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{25}$	$=$	$\left(\frac{1}{2} + x_4\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{26}$	$=$	$-x_4 \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{27}$	$=$	$-y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$-y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(16k)	S
$\mathbf{B}_{28}$	$=$	$\left(\frac{1}{2} + y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 +$ $\left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(16k)	S

---

#### References:

- H. Kalpen, W. Hönle, M. Somer, U. Schwarz, K. Peters, H. G. von Schnering, and R. Blachnik, *Bismut(II)-chalkogenometallate(III)  $Bi_2M_4X_8$ , Verbindungen mit  $Bi^{4+}$ -Hanteln ( $M = Al, Ga$ ;  $X = S, Se$ )*, Z. Anorg. Allg. Chem. **624**, 1137–1147 (1998), doi:10.1002/(SICI)1521-3749(199807)624:7<1137::AID-ZAAC1137>3.0.CO;2-B.

#### Found in:

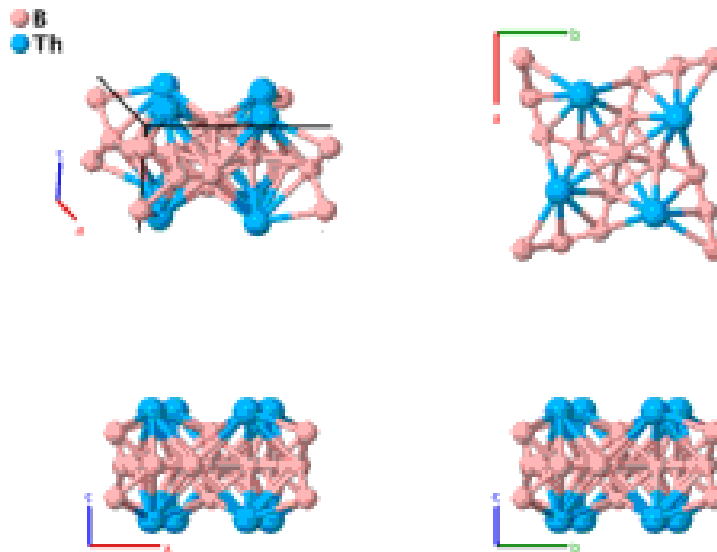
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [893](#)  
- POSCAR: pp. [893](#)

# ThB<sub>4</sub> (*D*1<sub>e</sub>) Structure: A4B\_tP20\_127\_ehj\_g



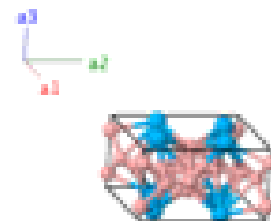
<b>Prototype</b>	:	ThB <sub>4</sub>
<b>AFLOW prototype label</b>	:	A4B_tP20_127_ehj_g
<b>Strukturbericht designation</b>	:	<i>D</i> 1 <sub>e</sub>
<b>Pearson symbol</b>	:	tP20
<b>Space group number</b>	:	127
<b>Space group symbol</b>	:	<i>P</i> 4/ <i>mbm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A4B_tP20_127_ehj_g --params= <i>a, c/a, z<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub></i>

## Other compounds with this structure:

- B<sub>4</sub>Ce, B<sub>4</sub>U, B<sub>4</sub>Y

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(4e)	B I
<b>B</b> <sub>2</sub>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(4e)	B I

$\mathbf{B}_3$	$= -z_1 \mathbf{a}_3$	$=$	$-z_1 c \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2$	$=$	$x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}}$	(4g)	Th
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2$	$=$	$-x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}}$	(4g)	Th
$\mathbf{B}_7$	$= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$\left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}}$	(4g)	Th
$\mathbf{B}_8$	$= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$\left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}}$	(4g)	Th
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	B II
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	B II
$\mathbf{B}_{11}$	$= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	B II
$\mathbf{B}_{12}$	$= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	B II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{15}$	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{16}$	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{17}$	$= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{18}$	$= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{19}$	$= \left(\frac{1}{2} + y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{20}$	$= \left(\frac{1}{2} - y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III

---

#### References:

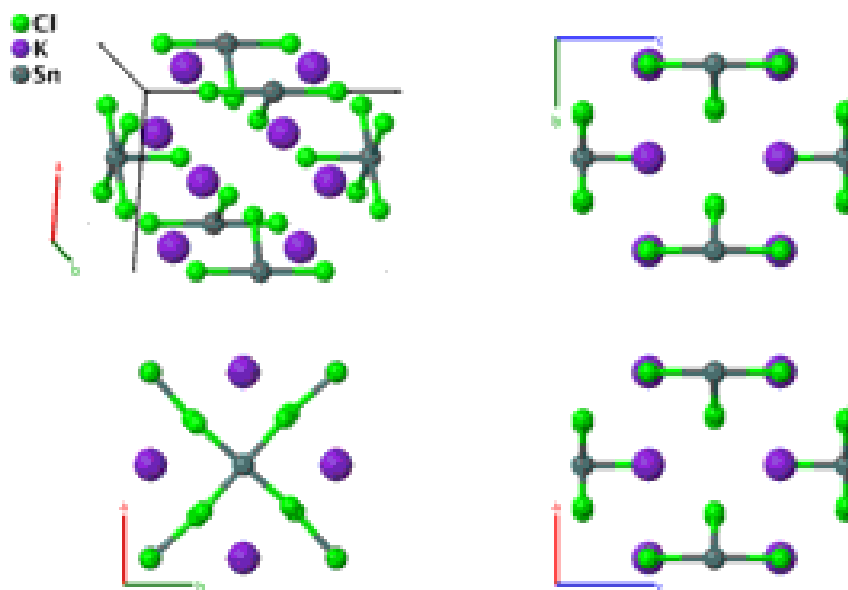
- A. Zalkin and D. H. Templeton, *The Crystal Structures of CeB<sub>4</sub>, ThB<sub>4</sub>, and UB<sub>4</sub>*, J. Chem. Phys. **18**, 391 (1950), [doi:10.1063/1.1747637](https://doi.org/10.1063/1.1747637).

---

#### Geometry files:

- CIF: pp. 893  
- POSCAR: pp. 894

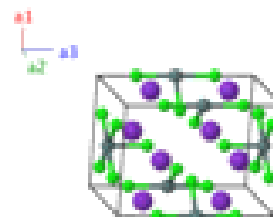
# K<sub>2</sub>SnCl<sub>6</sub> (Low-temperature) Structure: A6B2C\_tP18\_128\_eh\_d\_b



<b>Prototype</b>	:	K <sub>2</sub> SnCl <sub>6</sub>
<b>AFLOW prototype label</b>	:	A6B2C_tP18_128_eh_d_b
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP18
<b>Space group number</b>	:	128
<b>Space group symbol</b>	:	<i>P4/mnc</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A6B2C_tP18_128_eh_d_b --params=a, c/a, z3, x4, y4</code>

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} c \hat{\mathbf{z}}$	(2b)	Sn
<b>B<sub>2</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(2b)	Sn
<b>B<sub>3</sub></b> =	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	K
<b>B<sub>4</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	K
<b>B<sub>5</sub></b> =	$\frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	K

$$\begin{aligned}
\mathbf{B}_6 &= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}} & (4d) & \text{K} \\
\mathbf{B}_7 &= z_3 \mathbf{a}_3 &= z_3 c \hat{\mathbf{z}} & (4e) & \text{Cl I} \\
\mathbf{B}_8 &= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (4e) & \text{Cl I} \\
\mathbf{B}_9 &= -z_3 \mathbf{a}_3 &= -z_3 c \hat{\mathbf{z}} & (4e) & \text{Cl I} \\
\mathbf{B}_{10} &= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (4e) & \text{Cl I} \\
\mathbf{B}_{11} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 &= x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} & (8h) & \text{Cl II} \\
\mathbf{B}_{12} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 &= -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} & (8h) & \text{Cl II} \\
\mathbf{B}_{13} &= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 &= -y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} & (8h) & \text{Cl II} \\
\mathbf{B}_{14} &= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 &= y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} & (8h) & \text{Cl II} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{Cl II} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{Cl II} \\
\mathbf{B}_{17} &= \left(\frac{1}{2} + y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{Cl II} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} - y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{Cl II}
\end{aligned}$$

---

#### References:

- H. Boysen and A. W. Hewat, *A neutron powder investigation of the structural changes in  $K_2\text{SnCl}_6$* , Acta Crystallogr. Sect. B Struct. Sci. **34**, 1412–1418 (1978), doi:10.1107/S0567740878005816.

#### Found in:

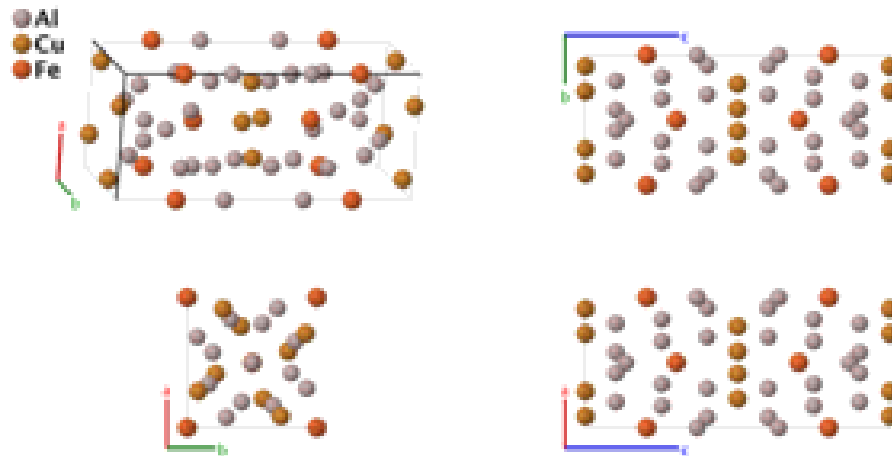
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [894](#)  
- POSCAR: pp. [894](#)

# FeCu<sub>2</sub>Al<sub>7</sub> (*E9<sub>a</sub>*) Structure: A7B2C\_tP40\_128\_egi\_h\_e



<b>Prototype</b>	:	FeCu <sub>2</sub> Al <sub>7</sub>
<b>AFLOW prototype label</b>	:	A7B2C_tP40_128_egi_h_e
<b>Strukturbericht designation</b>	:	<i>E9<sub>a</sub></i>
<b>Pearson symbol</b>	:	tP40
<b>Space group number</b>	:	128
<b>Space group symbol</b>	:	<i>P4/mnc</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A7B2C_tP40_128_egi_h_e --params= <i>a, c/a, z1, z2, x3, x4, y4, x5, y5, z5</i>

## Other compounds with this structure:

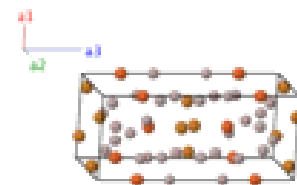
- T(CoCuAl), an alloy with an approximate composition of Co<sub>2</sub>Cu<sub>4.9</sub>Al<sub>17.7</sub>, NiCu<sub>3</sub>Al<sub>6</sub>

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(4 <i>e</i> )	Al I
<b>B<sub>2</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	(4 <i>e</i> )	Al I
<b>B<sub>3</sub></b> =	$-z_1 \mathbf{a}_3$	=	$-z_1 c \hat{\mathbf{z}}$	(4 <i>e</i> )	Al I
<b>B<sub>4</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4 <i>e</i> )	Al I
<b>B<sub>5</sub></b> =	$z_2 \mathbf{a}_3$	=	$z_2 c \hat{\mathbf{z}}$	(4 <i>e</i> )	Fe
<b>B<sub>6</sub></b> =	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(4 <i>e</i> )	Fe
<b>B<sub>7</sub></b> =	$-z_2 \mathbf{a}_3$	=	$-z_2 c \hat{\mathbf{z}}$	(4 <i>e</i> )	Fe



$$\mathbf{B}_{39} = \begin{pmatrix} \frac{1}{2} - y_5 \\ \frac{1}{2} + z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - x_5 \\ \frac{1}{2} + z_5 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 = \begin{pmatrix} \frac{1}{2} - y_5 \\ \frac{1}{2} + z_5 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - x_5 \\ \frac{1}{2} + z_5 \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

$$\mathbf{B}_{40} = \begin{pmatrix} \frac{1}{2} + y_5 \\ \frac{1}{2} + z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + x_5 \\ \frac{1}{2} + z_5 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 = \begin{pmatrix} \frac{1}{2} + y_5 \\ \frac{1}{2} + z_5 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + x_5 \\ \frac{1}{2} + z_5 \end{pmatrix} a \hat{\mathbf{y}} + c \hat{\mathbf{z}} \quad (16i) \quad \text{Al III}$$

**References:**

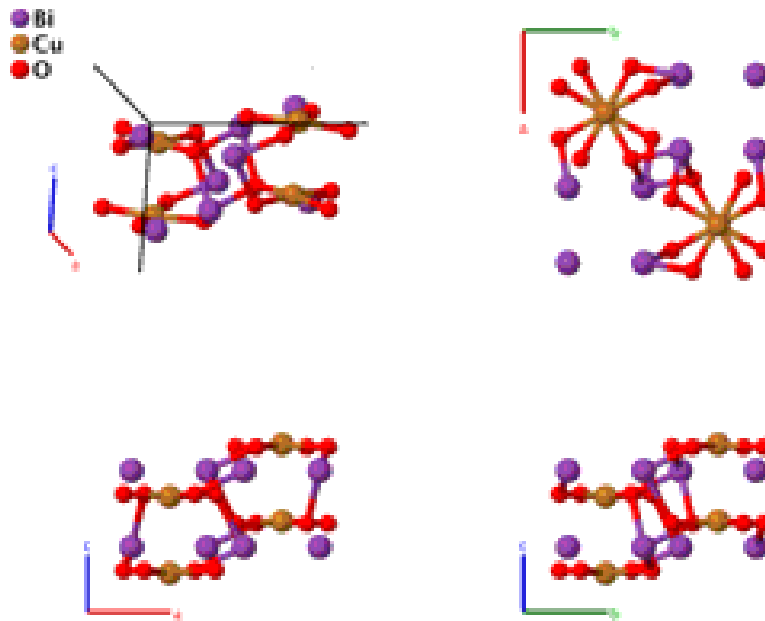
- M. G. Bown and P. J. Brown, *The structure of FeCu<sub>2</sub>Al<sub>7</sub> and T(CoCuAl)*, Acta Cryst. **9**, 911–914 (1956), [doi:10.1107/S0365110X56002576](https://doi.org/10.1107/S0365110X56002576).

**Geometry files:**

- CIF: pp. [895](#)  
 - POSCAR: pp. [895](#)



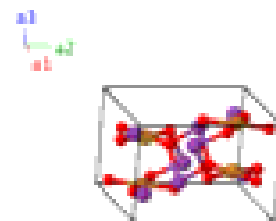
# CuBi<sub>2</sub>O<sub>4</sub> Structure: A2BC4\_tP28\_130\_f\_c\_g



**Prototype** : CuBi<sub>2</sub>O<sub>4</sub>  
**AFLOW prototype label** : A2BC4\_tP28\_130\_f\_c\_g  
**Strukturbericht designation** : None  
**Pearson symbol** : tP28  
**Space group number** : 130  
**Space group symbol** : *P4/ncc*  
**AFLOW prototype command** : `aflow --proto=A2BC4_tP28_130_f_c_g`  
                                   `--params=a, c/a, z1, x2, x3, y3, z3`

**Simple Tetragonal primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4c)	Cu
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	(4c)	Cu
$\mathbf{B}_3$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(4c)	Cu
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4c)	Cu

$$\begin{aligned}
\mathbf{B}_5 &= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8f) & \text{Bi} \\
\mathbf{B}_6 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8f) & \text{Bi} \\
\mathbf{B}_7 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8f) & \text{Bi} \\
\mathbf{B}_8 &= -x_2 \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8f) & \text{Bi} \\
\mathbf{B}_9 &= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8f) & \text{Bi} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8f) & \text{Bi} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8f) & \text{Bi} \\
\mathbf{B}_{12} &= x_2 \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8f) & \text{Bi} \\
\mathbf{B}_{13} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} - y_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{16} &= y_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{17} &= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{19} &= \left(\frac{1}{2} + y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + & (16g) & \text{O} \\
&\quad \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{20} &= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{21} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{22} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{23} &= \left(\frac{1}{2} + y_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{24} &= -y_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{25} &= x_3 \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{26} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (16g) & \text{O} \\
\mathbf{B}_{27} &= \left(\frac{1}{2} - y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + & (16g) & \text{O} \\
&\quad \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{28} &= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (16g) & \text{O}
\end{aligned}$$

---

### References:

- J.-C. Boivin, J. Trehoux, and D. Thomas, *Étude structurale de CuBi<sub>2</sub>O<sub>4</sub>*, Bull. Soc. fr. Mineral. Crystallogr. **99**, 193–196 (1976).

### Found in:

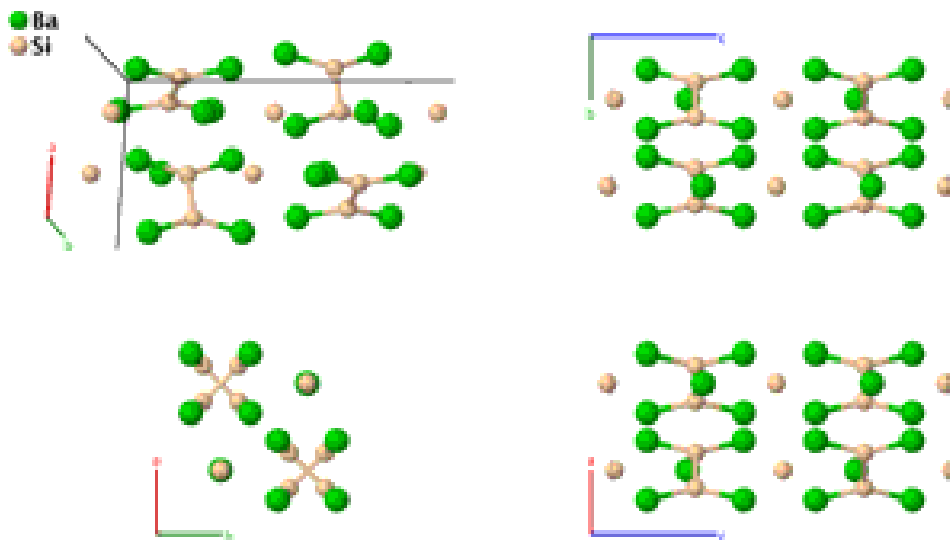
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. [895](#)  
- POSCAR: pp. [896](#)

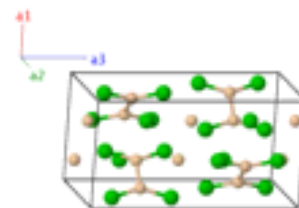
# Ba<sub>5</sub>Si<sub>3</sub> Structure: A5B3\_tP32\_130\_cg\_cf



**Prototype** : Ba<sub>5</sub>Si<sub>3</sub>  
**AFLOW prototype label** : A5B3\_tP32\_130\_cg\_cf  
**Strukturbericht designation** : None  
**Pearson symbol** : tP32  
**Space group number** : 130  
**Space group symbol** : *P4/ncc*  
**AFLOW prototype command** : aflow --proto=A5B3\_tP32\_130\_cg\_cf  
 --params=*a, c/a, z<sub>1</sub>, z<sub>2</sub>, x<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>*

## Simple Tetragonal primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(4c)	Ba I
<b>B<sub>2</sub></b> =	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) c \hat{\mathbf{z}}$	(4c)	Ba I
<b>B<sub>3</sub></b> =	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - z_1 c \hat{\mathbf{z}}$	(4c)	Ba I
<b>B<sub>4</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(4c)	Ba I
<b>B<sub>5</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4c)	Si I
<b>B<sub>6</sub></b> =	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(4c)	Si I
<b>B<sub>7</sub></b> =	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(4c)	Si I

$$\begin{aligned}
\mathbf{B}_8 &= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (4c) & \text{Si I} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8f) & \text{Si II} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8f) & \text{Si II} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8f) & \text{Si II} \\
\mathbf{B}_{12} &= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8f) & \text{Si II} \\
\mathbf{B}_{13} &= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8f) & \text{Si II} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8f) & \text{Si II} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8f) & \text{Si II} \\
\mathbf{B}_{16} &= x_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8f) & \text{Si II} \\
\mathbf{B}_{17} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{18} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{19} &= \left(\frac{1}{2} - y_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{20} &= y_4 \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + z_4 \mathbf{a}_3 &= y_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{21} &= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{22} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{23} &= \left(\frac{1}{2} + y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + &= \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + & (16g) & \text{Ba II} \\
&\quad \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{24} &= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= -y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{25} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{26} &= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{27} &= \left(\frac{1}{2} + y_4\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{28} &= -y_4 \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -y_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{29} &= x_4 \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{30} &= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (16g) & \text{Ba II} \\
\mathbf{B}_{31} &= \left(\frac{1}{2} - y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + & (16g) & \text{Ba II} \\
&\quad \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &\quad \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{32} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (16g) & \text{Ba II}
\end{aligned}$$

---

### References:

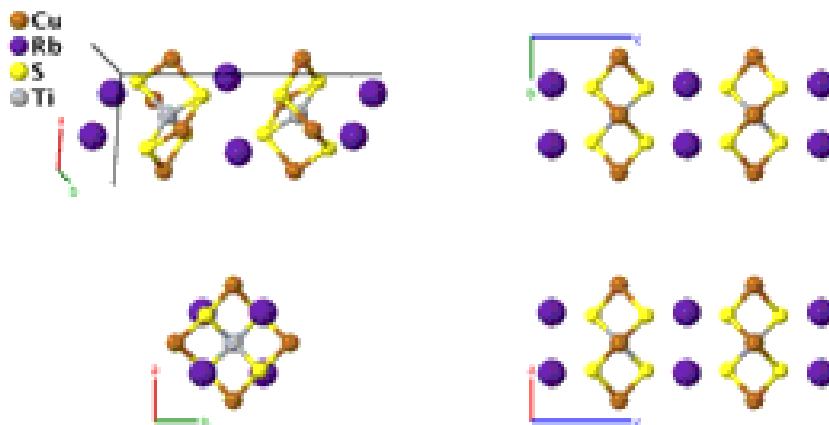
- R. Nesper and F. Zürcher, *Refinement of the crystal structure of pentabarium trisilicide, Ba<sub>5</sub>Si<sub>3</sub>*, Z. Kristallogr. B **214**, 20 (1966), doi:10.1515/ncrs-1999-0113.

---

### Geometry files:

- CIF: pp. 896  
- POSCAR: pp. 896

# Rb<sub>2</sub>TiCu<sub>2</sub>S<sub>4</sub> Structure: A2B2C4D\_tP18\_132\_e\_i\_o\_d



<b>Prototype</b>	:	Rb <sub>2</sub> TiCu <sub>2</sub> Se <sub>4</sub>
<b>AFLOW prototype label</b>	:	A2B2C4D_tP18_132_e_i_o_d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP18
<b>Space group number</b>	:	132
<b>Space group symbol</b>	:	<i>P4</i> <sub>2</sub> / <i>mcm</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A2B2C4D_tP18_132_e_i_o_d --params=a, c/a, x<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub></code>

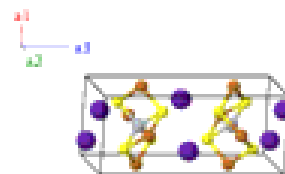
## Other compounds with this structure:

- Cs<sub>2</sub>TiAg<sub>2</sub>S<sub>4</sub>, Cs<sub>2</sub>TiCu<sub>2</sub>Se<sub>4</sub>

- The atomic positions for this structure are not given in the main text, but are provided as a Crystallographic Information File (CIF), ic001346d.cif.

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub> =	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2 <i>d</i> )	Ti
<b>B</b> <sub>2</sub> =	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2 <i>d</i> )	Ti
<b>B</b> <sub>3</sub> =	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4 <i>e</i> )	Cu
<b>B</b> <sub>4</sub> =	$\frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4 <i>e</i> )	Cu
<b>B</b> <sub>5</sub> =	$\frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4 <i>e</i> )	Cu

$$\begin{aligned}
\mathbf{B}_6 &= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}} & (4e) & \text{Cu} \\
\mathbf{B}_7 &= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 &= x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} & (4i) & \text{Rb} \\
\mathbf{B}_8 &= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 &= -x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} & (4i) & \text{Rb} \\
\mathbf{B}_9 &= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4i) & \text{Rb} \\
\mathbf{B}_{10} &= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4i) & \text{Rb} \\
\mathbf{B}_{11} &= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8o) & \text{S} \\
\mathbf{B}_{12} &= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8o) & \text{S} \\
\mathbf{B}_{13} &= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (8o) & \text{S} \\
\mathbf{B}_{14} &= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (8o) & \text{S} \\
\mathbf{B}_{15} &= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (8o) & \text{S} \\
\mathbf{B}_{16} &= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (8o) & \text{S} \\
\mathbf{B}_{17} &= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8o) & \text{S} \\
\mathbf{B}_{18} &= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8o) & \text{S}
\end{aligned}$$

---

#### References:

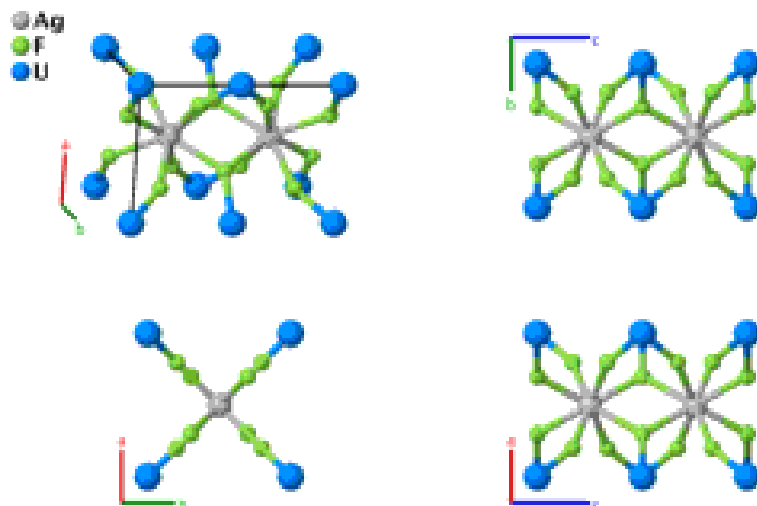
- F. Q. Huang and J. A. Ibers, *New Layered Materials: Syntheses, Structures, and Optical Properties of  $K_2TiCu_2S_4$ ,  $Rb_2TiCu_2S_4$ ,  $Rb_2TiAg_2S_4$ ,  $Cs_2TiAg_2S_4$ , and  $Cs_2TiCu_2Se_4$* , Inorg. Chem. **40**, 2602–2607 (2001), [doi:10.1021/ic001346d](https://doi.org/10.1021/ic001346d).

---

#### Geometry files:

- CIF: pp. [896](#)  
- POSCAR: pp. [897](#)

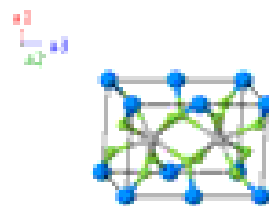
# AgUF<sub>6</sub> Structure: AB6C\_tP16\_132\_d\_io\_a



**Prototype** : AgUF<sub>6</sub>  
**AFLOW prototype label** : AB6C\_tP16\_132\_d\_io\_a  
**Strukturbericht designation** : None  
**Pearson symbol** : tP16  
**Space group number** : 132  
**Space group symbol** : *P4<sub>2</sub>/mcm*  
**AFLOW prototype command** : aflow --proto=AB6C\_tP16\_132\_d\_io\_a  
 --params=*a, c/a, x<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub>*

## Simple Tetragonal primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	U
<b>B</b> <sub>2</sub>	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} c \hat{\mathbf{z}}$	(2a)	U
<b>B</b> <sub>3</sub>	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2d)	Ag
<b>B</b> <sub>4</sub>	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2d)	Ag
<b>B</b> <sub>5</sub>	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	=	$x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}}$	(4i)	FI
<b>B</b> <sub>6</sub>	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	=	$-x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}}$	(4i)	FI
<b>B</b> <sub>7</sub>	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4i)	FI

$$\begin{array}{llllll}
\mathbf{B}_8 & = & x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4i) & \text{F I} \\
\mathbf{B}_9 & = & x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 & = & x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8o) & \text{F II} \\
\mathbf{B}_{10} & = & -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 & = & -x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (8o) & \text{F II} \\
\mathbf{B}_{11} & = & -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 & = & -x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (8o) & \text{F II} \\
\mathbf{B}_{12} & = & x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 & = & x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (8o) & \text{F II} \\
\mathbf{B}_{13} & = & -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 & = & -x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (8o) & \text{F II} \\
\mathbf{B}_{14} & = & x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 & = & x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} & (8o) & \text{F II} \\
\mathbf{B}_{15} & = & x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 & = & x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8o) & \text{F II} \\
\mathbf{B}_{16} & = & -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 & = & -x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (8o) & \text{F II}
\end{array}$$

---

### References:

- P. Charpin, *Structure cristalline des hexafluorures complexes d'uranium V et d'argent de potassium d'ammonium de rubidium ou de thallium*, C. R. Hebd. Séances Acad. Sci. **260**, 1914–1916 (1965).

### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

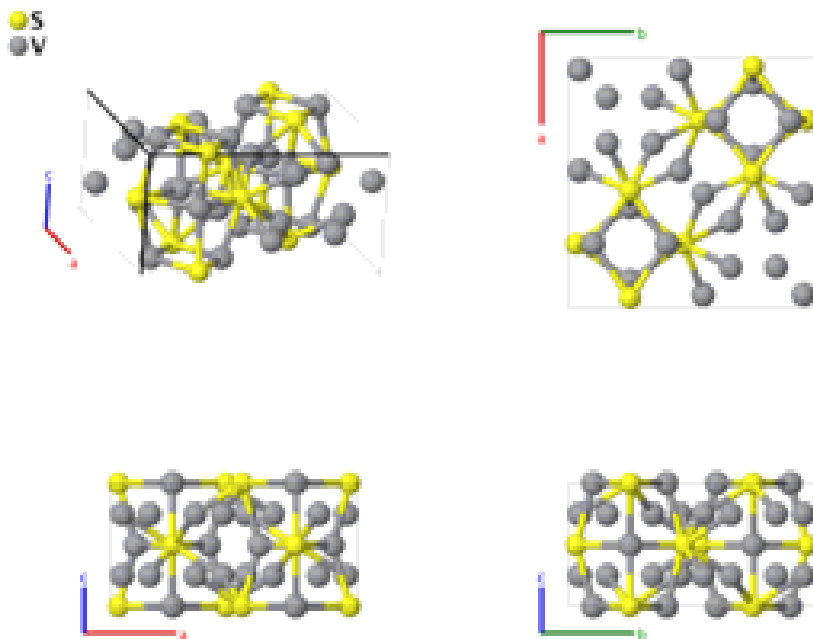
---

### Geometry files:

- CIF: pp. [897](#)  
- POSCAR: pp. [897](#)



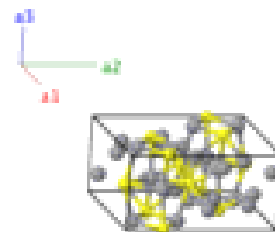
# $\beta$ -V<sub>3</sub>S Structure: AB3\_tP32\_133\_h\_i2j



<b>Prototype</b>	:	$\beta$ -V <sub>3</sub> S
<b>AFLOW prototype label</b>	:	AB3_tP32_133_h_i2j
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP32
<b>Space group number</b>	:	133
<b>Space group symbol</b>	:	$P4_2/nbc$
<b>AFLOW prototype command</b>	:	aflow --proto=AB3_tP32_133_h_i2j --params= $a, c/a, x_1, x_2, x_3, x_4$

Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$x_1 a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(8h)	S
$\mathbf{B}_2$	$= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(8h)	S
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	S

$\mathbf{B}_4$	$=$	$\frac{1}{4} \mathbf{a}_1 + \left(\frac{1}{2} - x_1\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	S
$\mathbf{B}_5$	$=$	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$-x_1 a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(8h)	S
$\mathbf{B}_6$	$=$	$\left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(8h)	S
$\mathbf{B}_7$	$=$	$\frac{3}{4} \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	S
$\mathbf{B}_8$	$=$	$\frac{3}{4} \mathbf{a}_1 + \left(\frac{1}{2} + x_1\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	S
$\mathbf{B}_9$	$=$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$x_2 a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	V I
$\mathbf{B}_{10}$	$=$	$\left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	V I
$\mathbf{B}_{11}$	$=$	$\frac{1}{4} \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}}$	(8i)	V I
$\mathbf{B}_{12}$	$=$	$\frac{1}{4} \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}}$	(8i)	V I
$\mathbf{B}_{13}$	$=$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_2 a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	V I
$\mathbf{B}_{14}$	$=$	$\left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	V I
$\mathbf{B}_{15}$	$=$	$\frac{3}{4} \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}}$	(8i)	V I
$\mathbf{B}_{16}$	$=$	$\frac{3}{4} \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}}$	(8i)	V I
$\mathbf{B}_{17}$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{18}$	$=$	$\left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{19}$	$=$	$\left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{20}$	$=$	$x_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{21}$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{22}$	$=$	$\left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{23}$	$=$	$\left(\frac{1}{2} + x_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{24}$	$=$	$-x_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{25}$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B}_{26}$	$=$	$\left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B}_{27}$	$=$	$\left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B}_{28}$	$=$	$x_4 \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B}_{29}$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B}_{30}$	$=$	$\left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B}_{31}$	$=$	$\left(\frac{1}{2} + x_4\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B}_{32}$	$=$	$-x_4 \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	V III

---

#### References:

- B. Pedersen and F. Grønvold, *The crystal structures of  $\alpha$ -V<sub>3</sub>S and  $\beta$ -V<sub>3</sub>S*, *Acta Cryst.* **12**, 1022–1027 (1959), [doi:10.1107/S0365110X59002869](https://doi.org/10.1107/S0365110X59002869).

#### Found in:

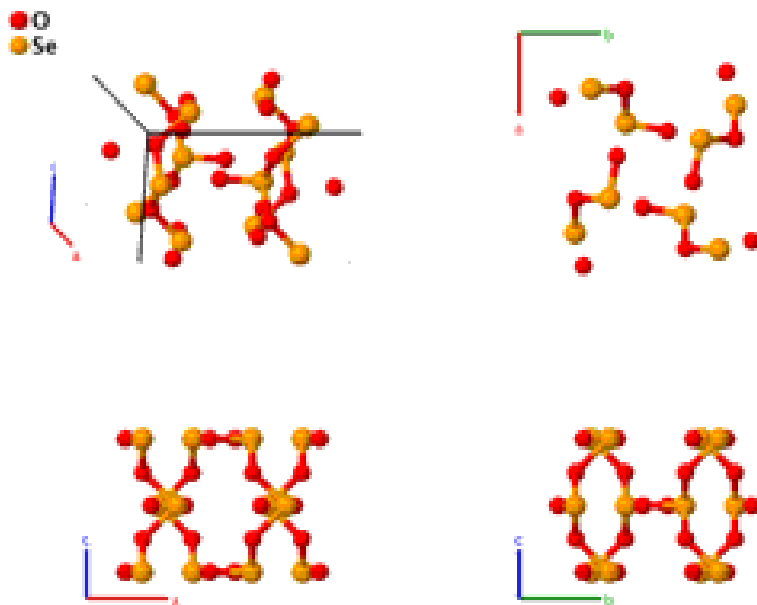
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [897](#)
- POSCAR: pp. [898](#)

# Downeyite (SeO<sub>2</sub>, C47) Structure: A2B\_tP24\_135\_gh\_h



<b>Prototype</b>	:	SeO <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_tP24_135_gh_h
<b>Strukturbericht designation</b>	:	C47
<b>Pearson symbol</b>	:	tP24
<b>Space group number</b>	:	135
<b>Space group symbol</b>	:	<i>P4<sub>2</sub>/mbc</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_tP24_135_gh_h --params= <i>a, c/a, x<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub></i>

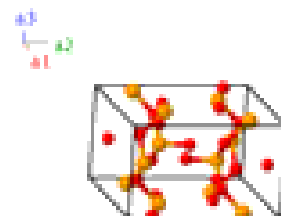
- Data for this structure was taken at 139 K.

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= x_1 \mathbf{a}_1 + \left(\frac{1}{2} + x_1\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8g)	O I

$$\begin{aligned}
\mathbf{B}_2 &= -x_1 \mathbf{a}_1 + \left(\frac{1}{2} - x_1\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -x_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_3 &= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_4 &= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_5 &= -x_1 \mathbf{a}_1 + \left(\frac{1}{2} - x_1\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -x_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_6 &= x_1 \mathbf{a}_1 + \left(\frac{1}{2} + x_1\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= x_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_7 &= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_8 &= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_9 &= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 &= x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} & (8h) & \text{O II} \\
\mathbf{B}_{10} &= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 &= -x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} & (8h) & \text{O II} \\
\mathbf{B}_{11} &= -y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -y_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{O II} \\
\mathbf{B}_{12} &= y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= y_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{O II} \\
\mathbf{B}_{13} &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{y}} & (8h) & \text{O II} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{y}} & (8h) & \text{O II} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} + y_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{O II} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} - y_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{O II} \\
\mathbf{B}_{17} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 &= x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} & (8h) & \text{Se} \\
\mathbf{B}_{18} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 &= -x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} & (8h) & \text{Se} \\
\mathbf{B}_{19} &= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{Se} \\
\mathbf{B}_{20} &= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{Se} \\
\mathbf{B}_{21} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} & (8h) & \text{Se} \\
\mathbf{B}_{22} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} & (8h) & \text{Se} \\
\mathbf{B}_{23} &= \left(\frac{1}{2} + y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{Se} \\
\mathbf{B}_{24} &= \left(\frac{1}{2} - y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{Se}
\end{aligned}$$

---

#### References:

- K. Ståhl, J. P. Legros, and J. Galy, *The crystal structure of SeO<sub>2</sub> at 139 and 286 K*, *Kristallografiya* **202**, 99–107 (1992), [doi:10.1524/zkri.1992.202.14.99](https://doi.org/10.1524/zkri.1992.202.14.99).

#### Found in:

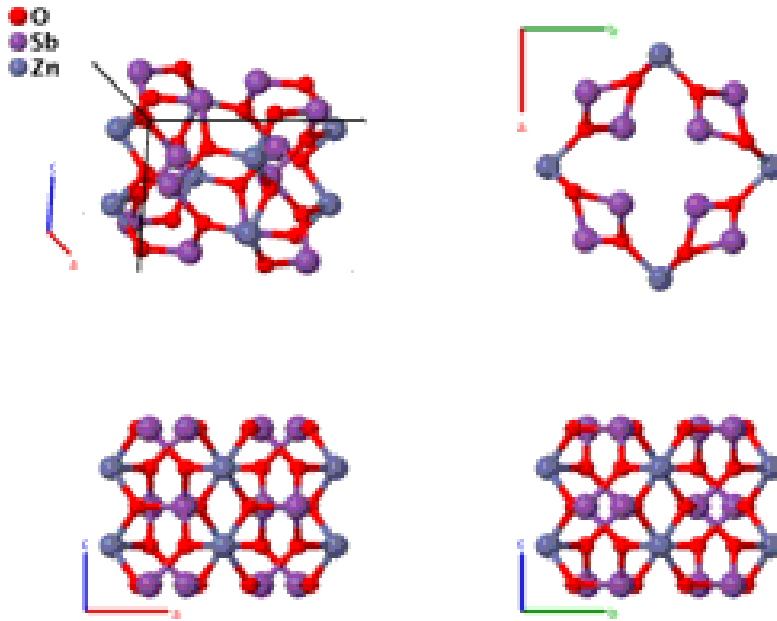
- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, *Am. Mineral.* **88**, 247–250 (2003).

---

#### Geometry files:

- CIF: pp. [898](#)  
- POSCAR: pp. [898](#)

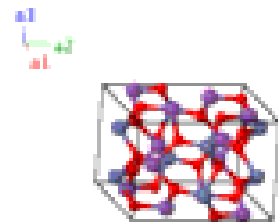
# ZnSb<sub>2</sub>O<sub>4</sub> Structure: A4B2C\_tP28\_135\_gh\_h\_d



**Prototype** : ZnSb<sub>2</sub>O<sub>4</sub>  
**AFLOW prototype label** : A4B2C\_tP28\_135\_gh\_h\_d  
**Strukturbericht designation** : None  
**Pearson symbol** : tP28  
**Space group number** : 135  
**Space group symbol** :  $P4_2/mbc$   
**AFLOW prototype command** : `aflow --proto=A4B2C_tP28_135_gh_h_d --params=a, c/a, x2, x3, y3, x4, y4`

Simple Tetragonal primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Zn
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Zn
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Zn
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Zn

$$\begin{array}{llll}
\mathbf{B}_5 & = & x_2 \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 & = & x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_6 & = & -x_2 \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 & = & -x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_7 & = & \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 & = & \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_8 & = & \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 & = & \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_9 & = & -x_2 \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 & = & -x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_{10} & = & x_2 \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 & = & x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_{11} & = & \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 & = & \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_{12} & = & \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 & = & \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8g) & \text{OI} \\
\mathbf{B}_{13} & = & x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 & = & x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} & (8h) & \text{O II} \\
\mathbf{B}_{14} & = & -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 & = & -x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} & (8h) & \text{O II} \\
\mathbf{B}_{15} & = & -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & -y_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{O II} \\
\mathbf{B}_{16} & = & y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & y_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{O II} \\
\mathbf{B}_{17} & = & \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 & = & \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} & (8h) & \text{O II} \\
\mathbf{B}_{18} & = & \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 & = & \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} & (8h) & \text{O II} \\
\mathbf{B}_{19} & = & \left(\frac{1}{2} + y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{O II} \\
\mathbf{B}_{20} & = & \left(\frac{1}{2} - y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{O II} \\
\mathbf{B}_{21} & = & x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 & = & x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} & (8h) & \text{Sb} \\
\mathbf{B}_{22} & = & -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 & = & -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} & (8h) & \text{Sb} \\
\mathbf{B}_{23} & = & -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & -y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{Sb} \\
\mathbf{B}_{24} & = & y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{Sb} \\
\mathbf{B}_{25} & = & \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 & = & \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{y}} & (8h) & \text{Sb} \\
\mathbf{B}_{26} & = & \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 & = & \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{y}} & (8h) & \text{Sb} \\
\mathbf{B}_{27} & = & \left(\frac{1}{2} + y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{Sb} \\
\mathbf{B}_{28} & = & \left(\frac{1}{2} - y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (8h) & \text{Sb}
\end{array}$$

---

#### References:

- S. Ståhl, *The crystal structure of ZnSb<sub>2</sub>O<sub>4</sub> and isomorphous compounds*, Ark. Kem. Mineral. Geol. **17B**, 1–7 (1943).

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

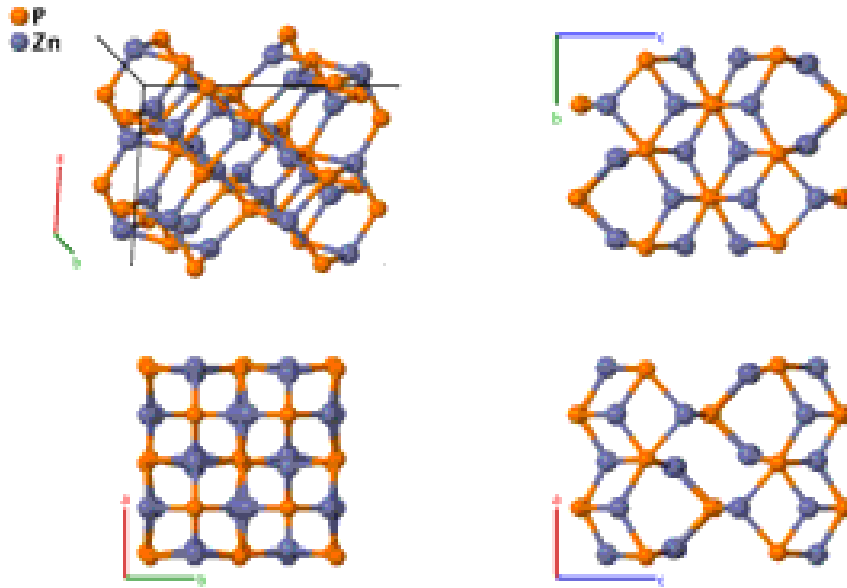
---

#### Geometry files:

- CIF: pp. [899](#)

- POSCAR: pp. [899](#)

# Zn<sub>3</sub>P<sub>2</sub> (*D*5<sub>9</sub>) Structure: A2B3\_tP40\_137\_cdf\_3g



<b>Prototype</b>	: Zn <sub>3</sub> P <sub>2</sub>
<b>AFLOW prototype label</b>	: A2B3_tP40_137_cdf_3g
<b>Strukturbericht designation</b>	: <i>D</i> 5 <sub>9</sub>
<b>Pearson symbol</b>	: tP40
<b>Space group number</b>	: 137
<b>Space group symbol</b>	: <i>P</i> 4 <sub>2</sub> / <i>nmc</i>
<b>AFLOW prototype command</b>	: aflow --proto=A2B3_tP40_137_cdf_3g --params= <i>a</i> , <i>c/a</i> , <i>z</i> <sub>1</sub> , <i>z</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub>

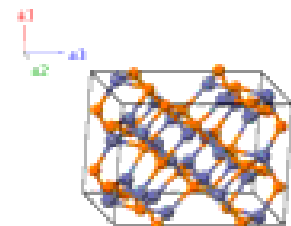
## Other compounds with this structure:

- $\alpha$ -As<sub>2</sub>Cd<sub>3</sub>,  $\alpha$ -As<sub>2</sub>Zn<sub>3</sub>, Cd<sub>3</sub>P<sub>2</sub>

- (Stackelberg, 1935) gives the atomic positions in the first setting of space group *P*4<sub>2</sub>/*nmc* #137. We have changed this to the second setting, placing the origin of the system at the inversion site. On page 803, (Pearson, 1958) gives the space group as *P*4<sub>2</sub>/*mmc* #131, but it is correctly given as *P*4<sub>2</sub>/*nmc* on page 111.

## Simple Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
---------------------	-----------------------	------------------	-----------





$$\begin{aligned}
\mathbf{B}_{37} &= \frac{3}{4} \mathbf{a}_1 + \left(\frac{1}{2} + y_6\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_6\right) a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} & (8g) & \quad \text{Zn III} \\
\mathbf{B}_{38} &= \frac{3}{4} \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} & (8g) & \quad \text{Zn III} \\
\mathbf{B}_{39} &= \left(\frac{1}{2} + y_6\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_6\right) \mathbf{a}_3 &= \left(\frac{1}{2} + y_6\right) a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}} & (8g) & \quad \text{Zn III} \\
\mathbf{B}_{40} &= -y_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_6\right) \mathbf{a}_3 &= -y_6 a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) c \hat{\mathbf{z}} & (8g) & \quad \text{Zn III}
\end{aligned}$$

**References:**

- M. v. Stackelberg and R. Paulu, *Untersuchungen an den Phosphiden und Arseniden des Zinks und Cadmiums. Das  $Zn_3P_2$ -Gitter*, Z. Phys. Chem. B **28**, 427–460 (1935), doi:10.1515/zpch-1935-2841.

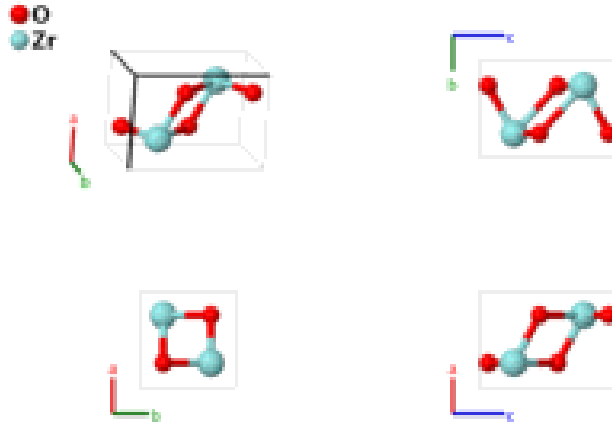
**Found in:**

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).  
- W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

**Geometry files:**

- CIF: pp. [899](#)  
- POSCAR: pp. [900](#)

# ZrO<sub>2</sub> (High-temperature) Structure: A2B\_tP6\_137\_d\_a



<b>Prototype</b>	:	ZrO <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_tP6_137_d_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP6
<b>Space group number</b>	:	137
<b>Space group symbol</b>	:	<i>P4<sub>2</sub>/nmc</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A2B_tP6_137_d_a --params=a, c/a, z<sub>2</sub></code>

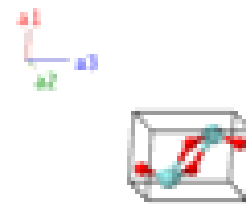
- ZrO<sub>2</sub> (pp. 443) and HgI<sub>2</sub> (pp. 447) have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2a)	Zr
<b>B<sub>2</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2a)	Zr
<b>B<sub>3</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4d)	O
<b>B<sub>4</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right)c \hat{\mathbf{z}}$	(4d)	O
<b>B<sub>5</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$= \frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(4d)	O
<b>B<sub>6</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	$= \frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right)c \hat{\mathbf{z}}$	(4d)	O

---

**References:**

- G. Teufer, *The crystal structure of tetragonal ZrO<sub>2</sub>*, *Acta Cryst.* **15**, 1187–1187 (1962),  
[doi:10.1107/S0365110X62003114](https://doi.org/10.1107/S0365110X62003114).

**Found in:**

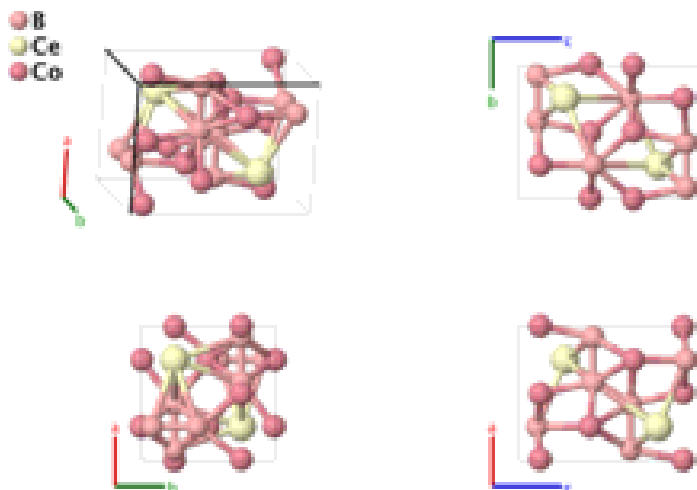
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [900](#)  
- POSCAR: pp. [900](#)

# CeCo<sub>4</sub>B<sub>4</sub> Structure: A4BC4\_tP18\_137\_g\_b\_g



**Prototype** : CeCo<sub>4</sub>B<sub>4</sub>  
**AFLOW prototype label** : A4BC4\_tP18\_137\_g\_b\_g  
**Strukturbericht designation** : None  
**Pearson symbol** : tP18  
**Space group number** : 137  
**Space group symbol** :  $P4_2/nmc$   
**AFLOW prototype command** : `aflow --proto=A4BC4_tP18_137_g_b_g --params=a, c/a, y2, z2, y3, z3`

## Simple Tetragonal primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2b)	Ce
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2b)	Ce
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8g)	B
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(8g)	B
$\mathbf{B}_5$	$= \left(\frac{1}{2} - y_2\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(8g)	B
$\mathbf{B}_6$	$= y_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= y_2 a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(8g)	B
$\mathbf{B}_7$	$= \frac{3}{4} \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(8g)	B
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(8g)	B

$$\begin{aligned}
\mathbf{B}_9 &= \left(\frac{1}{2} + y_2\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} & (8g) & \text{B} \\
\mathbf{B}_{10} &= -y_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 = -y_2 a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} & (8g) & \text{B} \\
\mathbf{B}_{11} &= \frac{1}{4} \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = \frac{1}{4} a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8g) & \text{Co} \\
\mathbf{B}_{12} &= \frac{1}{4} \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 = \frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (8g) & \text{Co} \\
\mathbf{B}_{13} &= \left(\frac{1}{2} - y_3\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (8g) & \text{Co} \\
\mathbf{B}_{14} &= y_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = y_3 a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (8g) & \text{Co} \\
\mathbf{B}_{15} &= \frac{3}{4} \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 = \frac{3}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8g) & \text{Co} \\
\mathbf{B}_{16} &= \frac{3}{4} \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = \frac{3}{4} a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} & (8g) & \text{Co} \\
\mathbf{B}_{17} &= \left(\frac{1}{2} + y_3\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (8g) & \text{Co} \\
\mathbf{B}_{18} &= -y_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = -y_3 a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} & (8g) & \text{Co}
\end{aligned}$$

---

### References:

- Y. B. Kuzma and N. S. Bilonizhko, *Crystal structure of the compounds CeCo<sub>4</sub>B<sub>4</sub> and its analogs*, Sov. Phys. Crystallogr. **16**, 897–898 (1972).

### Found in:

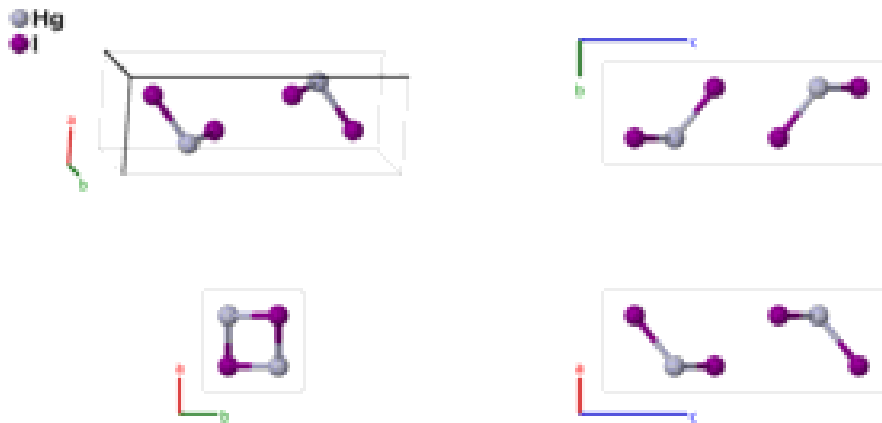
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. [900](#)  
- POSCAR: pp. [901](#)

# HgI<sub>2</sub> (C13) Structure: AB2\_tP6\_137\_a\_d



<b>Prototype</b>	:	HgI <sub>2</sub>
<b>AFLOW prototype label</b>	:	AB2_tP6_137_a_d
<b>Strukturbericht designation</b>	:	C13
<b>Pearson symbol</b>	:	tP6
<b>Space group number</b>	:	137
<b>Space group symbol</b>	:	<i>P4<sub>2</sub>/nmc</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB2_tP6_137_a_d --params=a, c/a, z<sub>2</sub></code>

- The CIF and POSCAR files contain the data at room temperature, 293 K. ZrO<sub>2</sub> (pp. 443) and HgI<sub>2</sub> (pp. 447) have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2a)	Hg
<b>B<sub>2</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2a)	Hg
<b>B<sub>3</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4d)	I
<b>B<sub>4</sub></b>	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4d)	I
<b>B<sub>5</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(4d)	I
<b>B<sub>6</sub></b>	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(4d)	I

---

**References:**

- D. Schwarzenbach, H. Birkedal, M. Hostettler, and P. Fischer, *Neutron diffraction investigation of the temperature dependence of crystal structure and thermal motions of red HgI<sub>2</sub>*, Acta Crystallogr. Sect. B Struct. Sci. **63**, 826–835 (2007), [doi:10.1107/S0108768107043327](https://doi.org/10.1107/S0108768107043327).

**Found in:**

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

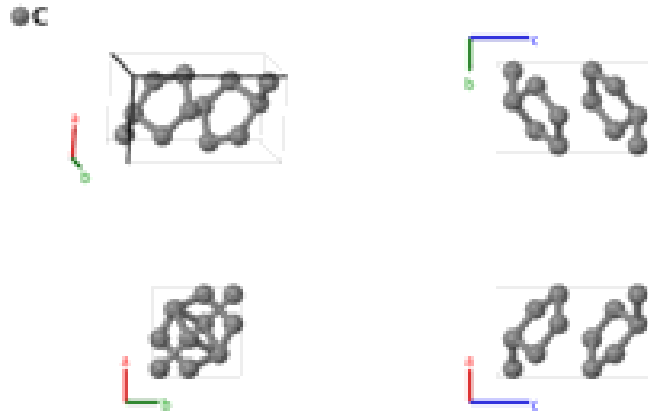
---

**Geometry files:**

- CIF: pp. [901](#)  
- POSCAR: pp. [901](#)



# C (T12 Group IV) Structure: A\_tP12\_138\_bi



<b>Prototype</b>	:	C
<b>AFLOW prototype label</b>	:	A_tP12_138_bi
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tP12
<b>Space group number</b>	:	138
<b>Space group symbol</b>	:	$P4_2/ncm$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A_tP12_138_bi --params=a, c/a, x2, z2</code>

## Other elements with this structure:

- Si, Ge

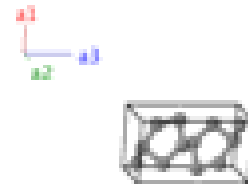
- This is a tetragonal allotrope of the diamond structure found computationally in C, Si, and Ge. The authors state “The T12 polymorph naturally accounts for the experimental  $d$  spacings and Raman spectra of synthesized metastable Ge and Si-XIII phases with long-puzzling unknown structures, respectively.”

## Simple Tetragonal primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4b)	CI
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4b)	CI
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4b)	CI

$$\begin{aligned}
\mathbf{B}_4 &= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (4b) & \text{C I} \\
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (8i) & \text{C II} \\
\mathbf{B}_6 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + z_2 \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (8i) & \text{C II} \\
\mathbf{B}_7 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (8i) & \text{C II} \\
\mathbf{B}_8 &= x_2 \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (8i) & \text{C II} \\
\mathbf{B}_9 &= -x_2 \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} & (8i) & \text{C II} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} & (8i) & \text{C II} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 - z_2 \mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} & (8i) & \text{C II} \\
\mathbf{B}_{12} &= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} & (8i) & \text{C II}
\end{aligned}$$

---

### References:

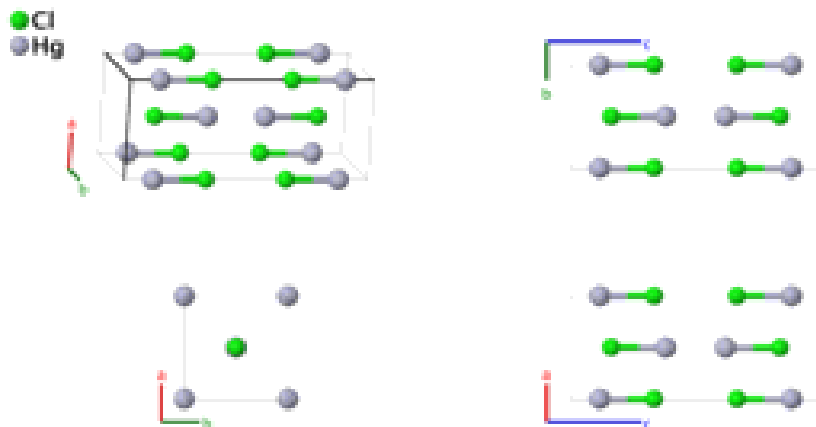
- Z. Zhao, F. Tian, X. Dong, Q. Li, Q. Wang, H. Wang, X. Zhong, B. Xu, D. Yu, J. He, H.-T. Wang, Y. Ma, and Y. Tian, *Tetragonal Allotrope of Group 14 Elements*, *J. Am. Chem. Soc.* **134**, 12362–12365 (2012), doi:10.1021/ja304380p.

---

### Geometry files:

- CIF: pp. 901  
- POSCAR: pp. 902

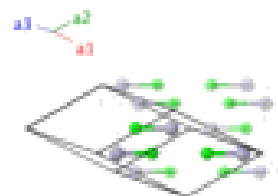
# Calomel (Hg<sub>2</sub>Cl<sub>2</sub>, *D*3<sub>1</sub>) Structure: AB\_tI8\_139\_e\_e



<b>Prototype</b>	:	Hg <sub>2</sub> Cl <sub>2</sub>
<b>AFLOW prototype label</b>	:	AB_tI8_139_e_e
<b>Strukturbericht designation</b>	:	<i>D</i> 3 <sub>1</sub>
<b>Pearson symbol</b>	:	tI8
<b>Space group number</b>	:	139
<b>Space group symbol</b>	:	<i>I</i> 4/ <i>mmm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB_tI8_139_e_e --params= <i>a, c/a, z<sub>1</sub>, z<sub>2</sub></i>

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2$	=	$z_1 c \hat{\mathbf{z}}$	(4e)	Cl
<b>B<sub>2</sub></b>	= $-z_1 \mathbf{a}_1 - z_1 \mathbf{a}_2$	=	$-z_1 c \hat{\mathbf{z}}$	(4e)	Cl
<b>B<sub>3</sub></b>	= $z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	=	$z_2 c \hat{\mathbf{z}}$	(4e)	Hg
<b>B<sub>4</sub></b>	= $-z_2 \mathbf{a}_1 - z_2 \mathbf{a}_2$	=	$-z_2 c \hat{\mathbf{z}}$	(4e)	Hg

## References:

- N. J. Calos, C. H. L. Kennard, and R. L. Davis, *The structure of calomel, Hg<sub>2</sub>Cl<sub>2</sub>, derived from neutron powder data*, *Z. Kristallogr.* **187**, 305–307 (1989), doi:[10.1524/zkri.1989.187.14.305](https://doi.org/10.1524/zkri.1989.187.14.305).

## Found in:

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, *Am. Mineral.* **88**, 247–250 (2003).

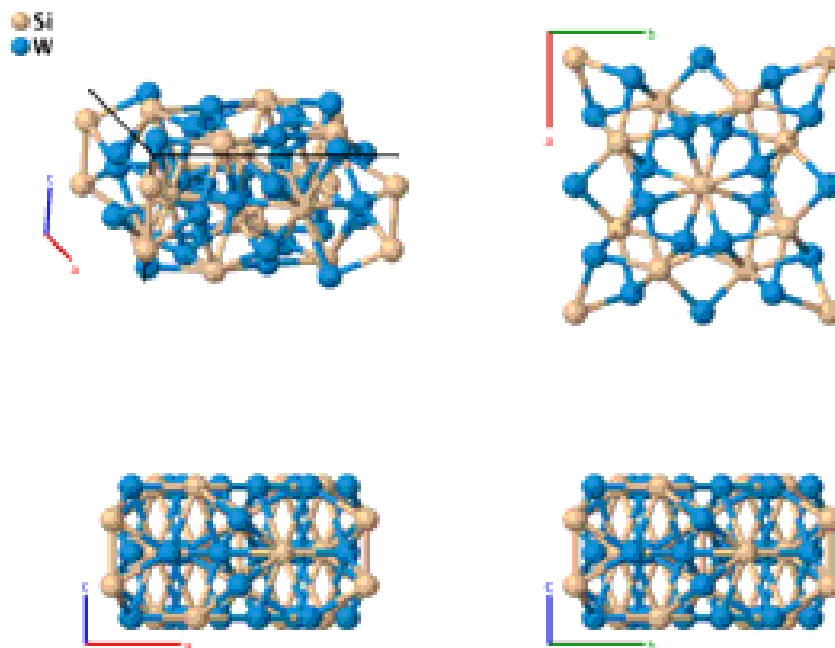
---

**Geometry files:**

- CIF: pp. [902](#)

- POSCAR: pp. [902](#)

# W<sub>5</sub>Si<sub>3</sub> (*D*8<sub>*m*</sub>) Structure: A3B5\_tI32\_140\_ah\_bk



<b>Prototype</b>	:	W <sub>5</sub> Si <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B5_tI32_140_ah_bk
<b>Strukturbericht designation</b>	:	<i>D</i> 8 <sub><i>m</i></sub>
<b>Pearson symbol</b>	:	tI32
<b>Space group number</b>	:	140
<b>Space group symbol</b>	:	<i>I</i> 4/ <i>mcm</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A3B5_tI32_140_ah_bk</code> <code>--params=<i>a</i>, <i>c/a</i>, <i>x</i><sub>3</sub>, <i>x</i><sub>4</sub>, <i>y</i><sub>4</sub></code>

## Other compounds with this structure:

- Cr<sub>5</sub>Ge<sub>3</sub>, Cr<sub>5</sub>Si<sub>3</sub>, Mo<sub>5</sub>Si<sub>3</sub>, Nb<sub>5</sub>Si<sub>3</sub>, Ta<sub>5</sub>Si<sub>3</sub>, V<sub>5</sub>Si<sub>3</sub>

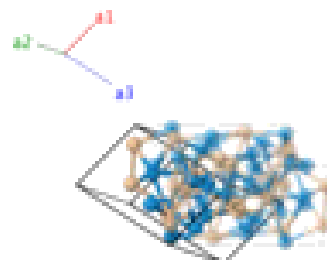
- (Pearson, 1958) refers to this as the “T1 phase.”

## Body-centered Tetragonal primitive vectors:

$$\mathbf{a}_1 = -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} c \hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B}_3$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4b)	W I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4b)	W I
$\mathbf{B}_5$	$= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + 2x_3\right) \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}}$	(8h)	Si II
$\mathbf{B}_6$	$= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} - 2x_3\right) \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}}$	(8h)	Si II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}}$	(8h)	Si II
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}}$	(8h)	Si II
$\mathbf{B}_9$	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}}$	(16k)	W II
$\mathbf{B}_{10}$	$= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + (-x_4 - y_4) \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}}$	(16k)	W II
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	$=$	$-y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}}$	(16k)	W II
$\mathbf{B}_{12}$	$= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + (-x_4 + y_4) \mathbf{a}_3$	$=$	$y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}}$	(16k)	W II
$\mathbf{B}_{13}$	$= \left(\frac{1}{2} + y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + (-x_4 + y_4) \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(16k)	W II
$\mathbf{B}_{14}$	$= \left(\frac{1}{2} - y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(16k)	W II
$\mathbf{B}_{15}$	$= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4\right) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	$=$	$y_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(16k)	W II
$\mathbf{B}_{16}$	$= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_4\right) \mathbf{a}_2 + (-x_4 - y_4) \mathbf{a}_3$	$=$	$-y_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(16k)	W II

---

#### References:

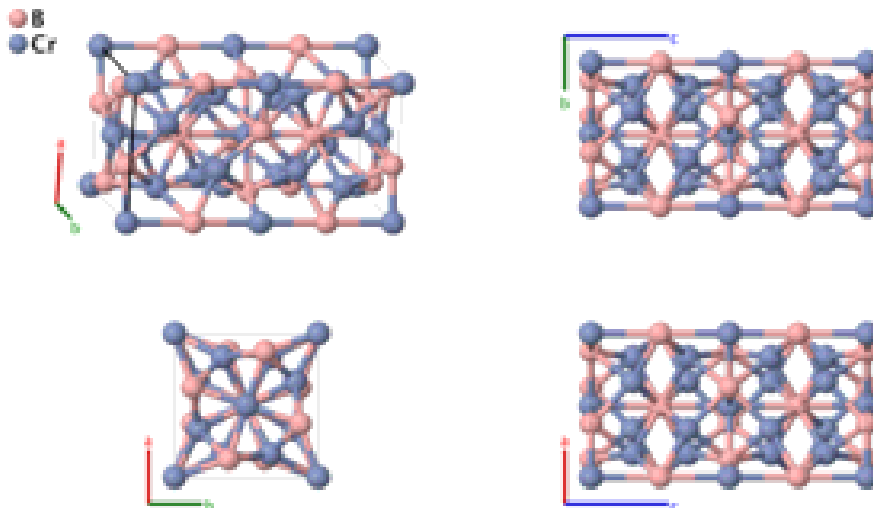
- B. Aronsson, *The Crystal Structure of Mo<sub>5</sub>Si<sub>3</sub> and W<sub>5</sub>Si<sub>3</sub>*, Acta Chem. Scand. **9**, 1107–1110 (1955), [doi:10.3891/acta.chem.scand.09-1107](https://doi.org/10.3891/acta.chem.scand.09-1107).

---

#### Geometry files:

- CIF: pp. 902  
- POSCAR: pp. 903

# Cr<sub>5</sub>B<sub>3</sub> (*D*8<sub>*l*</sub>) Structure: A3B5\_tI32\_140\_ah\_cl



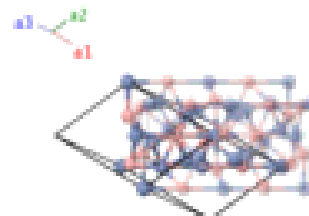
<b>Prototype</b>	:	Cr <sub>5</sub> B <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B5_tI32_140_ah_cl
<b>Strukturbericht designation</b>	:	<i>D</i> 8 <sub><i>l</i></sub>
<b>Pearson symbol</b>	:	tI32
<b>Space group number</b>	:	140
<b>Space group symbol</b>	:	<i>I</i> 4/ <i>mcm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3B5_tI32_140_ah_cl --params= <i>a</i> , <i>c/a</i> , <i>x</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>z</i> <sub>4</sub>

## Other compounds with this structure:

- Eu<sub>5</sub>Ge<sub>3</sub>, Pr<sub>5</sub>Si<sub>3</sub>, Ta<sub>5</sub>Ge<sub>3</sub>, Nb<sub>5</sub>Si<sub>3</sub>, Ta<sub>5</sub>Si<sub>3</sub>, EuIrGe<sub>2</sub>, Fe<sub>5</sub>PB<sub>2</sub>, Fe<sub>5</sub>SiB<sub>2</sub>, Fe<sub>4</sub>CoPB<sub>2</sub>, Fe<sub>4</sub>MnPB<sub>2</sub>, Fe<sub>4</sub>CoSiB<sub>2</sub>, Fe<sub>4</sub>MnSiB<sub>2</sub>, Mo<sub>5</sub>SiB<sub>2</sub>, Sr<sub>5</sub>In<sub>3</sub>, Gd<sub>5</sub>CoSi<sub>2</sub>, Ca<sub>5</sub>Si<sub>3</sub>,
- We have been unable to obtain a copy of (Bertaut, 1953), so we use the data found online from (Downs, 2003). Although Cr<sub>5</sub>B<sub>3</sub> is universally regarded as the prototype for *D*8<sub>*l*</sub>, it appears that no determination of the internal parameters has ever been made. The values found in (Bertaut, 1953) seem to be reasonable choices.

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	=	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	=	$\frac{1}{4} c \hat{\mathbf{z}}$	(4 <i>a</i> ) B I

$$\begin{aligned}
\mathbf{B}_2 &= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 &= \frac{3}{4} c \hat{\mathbf{z}} & (4a) & \text{B I} \\
\mathbf{B}_3 &= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3 &= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}} & (4c) & \text{Cr I} \\
\mathbf{B}_4 &= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 &= \frac{1}{2} c \hat{\mathbf{z}} & (4c) & \text{Cr I} \\
\mathbf{B}_5 &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + 2x_3\right) \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} & (8h) & \text{B II} \\
\mathbf{B}_6 &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} - 2x_3\right) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} & (8h) & \text{B II} \\
\mathbf{B}_7 &= x_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} & (8h) & \text{B II} \\
\mathbf{B}_8 &= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} & (8h) & \text{B II} \\
\mathbf{B}_9 &= \left(\frac{1}{2} + x_4 + z_4\right) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + \left(\frac{1}{2} + 2x_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16l) & \text{Cr II} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_4 + z_4\right) \mathbf{a}_1 + (-x_4 + z_4) \mathbf{a}_2 + \left(\frac{1}{2} - 2x_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16l) & \text{Cr II} \\
\mathbf{B}_{11} &= (x_4 + z_4) \mathbf{a}_1 + \left(\frac{1}{2} - x_4 + z_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16l) & \text{Cr II} \\
\mathbf{B}_{12} &= (-x_4 + z_4) \mathbf{a}_1 + \left(\frac{1}{2} + x_4 + z_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (16l) & \text{Cr II} \\
\mathbf{B}_{13} &= (x_4 - z_4) \mathbf{a}_1 + \left(\frac{1}{2} - x_4 - z_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16l) & \text{Cr II} \\
\mathbf{B}_{14} &= (-x_4 - z_4) \mathbf{a}_1 + \left(\frac{1}{2} + x_4 - z_4\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16l) & \text{Cr II} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} + x_4 - z_4\right) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + \left(\frac{1}{2} + 2x_4\right) \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16l) & \text{Cr II} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} - x_4 - z_4\right) \mathbf{a}_1 + (-x_4 - z_4) \mathbf{a}_2 + \left(\frac{1}{2} - 2x_4\right) \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} & (16l) & \text{Cr II}
\end{aligned}$$

---

#### References:

- F. Bertaut and P. Blum, *Etude des borures de chrome*, C. R. Hebd. Séances Acad. Sci. **236**, 1055–1056 (1953).

#### Found in:

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

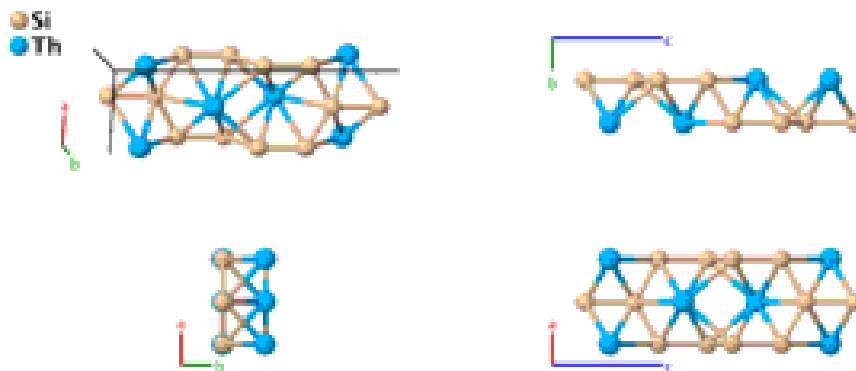
---

#### Geometry files:

- CIF: pp. [903](#)  
- POSCAR: pp. [903](#)



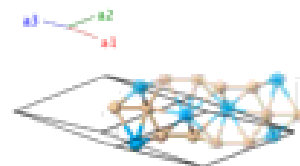
# $\alpha$ -ThSi<sub>2</sub> (*C<sub>c</sub>*) Structure: A2B\_tI12\_141\_e\_a



<b>Prototype</b>	:	$\alpha$ -ThSi <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_tI12_141_e_a
<b>Strukturbericht designation</b>	:	<i>C<sub>c</sub></i>
<b>Pearson symbol</b>	:	tI12
<b>Space group number</b>	:	141
<b>Space group symbol</b>	:	<i>I</i> 4 <sub>1</sub> / <i>amd</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_tI12_141_e_a --params= <i>a, c/a, z<sub>2</sub></i>

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$\frac{7}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$\frac{3}{4}a\hat{\mathbf{y}} + \frac{1}{8}c\hat{\mathbf{z}}$	(4 <i>a</i> )	Th
<b>B<sub>2</sub></b>	$\frac{1}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}} + \frac{3}{8}c\hat{\mathbf{z}}$	(4 <i>a</i> )	Th
<b>B<sub>3</sub></b>	$(\frac{1}{4} + z_2)\mathbf{a}_1 + z_2\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$\frac{1}{4}a\hat{\mathbf{y}} + z_2c\hat{\mathbf{z}}$	(8 <i>e</i> )	Si
<b>B<sub>4</sub></b>	$z_2\mathbf{a}_1 + (\frac{1}{4} + z_2)\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + (-\frac{1}{4} + z_2)c\hat{\mathbf{z}}$	(8 <i>e</i> )	Si
<b>B<sub>5</sub></b>	$(\frac{3}{4} - z_2)\mathbf{a}_1 - z_2\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$\frac{3}{4}a\hat{\mathbf{y}} - z_2c\hat{\mathbf{z}}$	(8 <i>e</i> )	Si
<b>B<sub>6</sub></b>	$-z_2\mathbf{a}_1 + (\frac{3}{4} - z_2)\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}} + (\frac{1}{4} - z_2)c\hat{\mathbf{z}}$	(8 <i>e</i> )	Si

## References:

- G. Brauer and A. Mitius, *Die Kristallstruktur des Thoriumsilicids ThSi<sub>2</sub>*, Z. Anorg. Allg. Chem. **249**, 325–339 (1942), doi:10.1002/zaac.19422490401.

## Found in:

- W. B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys* (Wiley Interscience, New York, London, Sydney, Toronto, 1972).

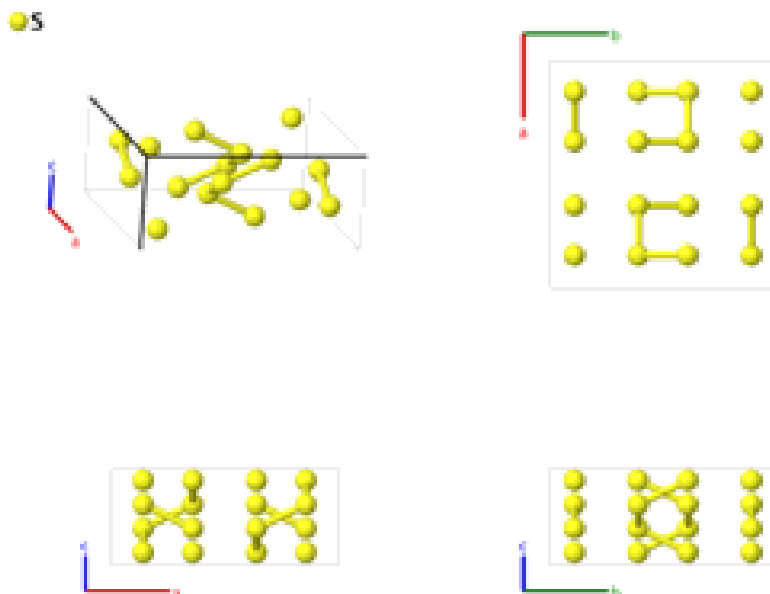
---

**Geometry files:**

- CIF: pp. [904](#)

- POSCAR: pp. [904](#)

# S-III Structure: A\_tI16\_142\_f



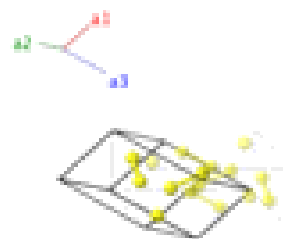
<b>Prototype</b>	:	S
<b>AFLOW prototype label</b>	:	A_tI16_142_f
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	tI16
<b>Space group number</b>	:	142
<b>Space group symbol</b>	:	$I4_1/acd$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A_tI16_142_f --params=a, c/a, x<sub>1</sub></code>

## Other elements with this structure:

- Se (Se-VII, prepared at 450 K and 20 GPa)
- The S-III phase is found when sulfur is pressurized above 36 GPa at 300 K. At 300 K it is stable up to 83 GPa.
- This data was taken at 12 GPa and 300 K.

## Body-centered Tetragonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \begin{pmatrix} \frac{3}{8} + x_1 \\ \frac{1}{4} + 2x_1 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{8} + x_1 \\ \frac{1}{4} - 2x_1 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_1\right) a \hat{\mathbf{y}} + \frac{1}{8} c \hat{\mathbf{z}}$	(16f)	S
$\mathbf{B}_2$	$= \begin{pmatrix} \frac{3}{8} - x_1 \\ \frac{1}{4} - 2x_1 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{8} - x_1 \\ \frac{1}{4} + 2x_1 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_1\right) a \hat{\mathbf{y}} + \frac{1}{8} c \hat{\mathbf{z}}$	(16f)	S
$\mathbf{B}_3$	$= \left(\frac{1}{8} + x_1\right) \mathbf{a}_1 + \left(\frac{3}{8} - x_1\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_1\right) a \hat{\mathbf{y}} - \frac{1}{8} c \hat{\mathbf{z}}$	(16f)	S
$\mathbf{B}_4$	$= \left(\frac{1}{8} - x_1\right) \mathbf{a}_1 + \left(\frac{3}{8} + x_1\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_1\right) a \hat{\mathbf{y}} + \frac{7}{8} c \hat{\mathbf{z}}$	(16f)	S
$\mathbf{B}_5$	$= \begin{pmatrix} \frac{5}{8} - x_1 \\ \frac{3}{4} - 2x_1 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{7}{8} - x_1 \\ \frac{3}{4} + 2x_1 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$= \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_1\right) a \hat{\mathbf{y}} + \frac{3}{8} c \hat{\mathbf{z}}$	(16f)	S
$\mathbf{B}_6$	$= \begin{pmatrix} \frac{5}{8} + x_1 \\ \frac{3}{4} + 2x_1 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{7}{8} + x_1 \\ \frac{3}{4} - 2x_1 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$= \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_1\right) a \hat{\mathbf{y}} + \frac{3}{8} c \hat{\mathbf{z}}$	(16f)	S
$\mathbf{B}_7$	$= \left(\frac{7}{8} - x_1\right) \mathbf{a}_1 + \left(\frac{5}{8} + x_1\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_1\right) a \hat{\mathbf{y}} + \frac{5}{8} c \hat{\mathbf{z}}$	(16f)	S
$\mathbf{B}_8$	$= \left(\frac{7}{8} + x_1\right) \mathbf{a}_1 + \left(\frac{5}{8} - x_1\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_1\right) a \hat{\mathbf{y}} + \frac{5}{8} c \hat{\mathbf{z}}$	(16f)	S

---

### References:

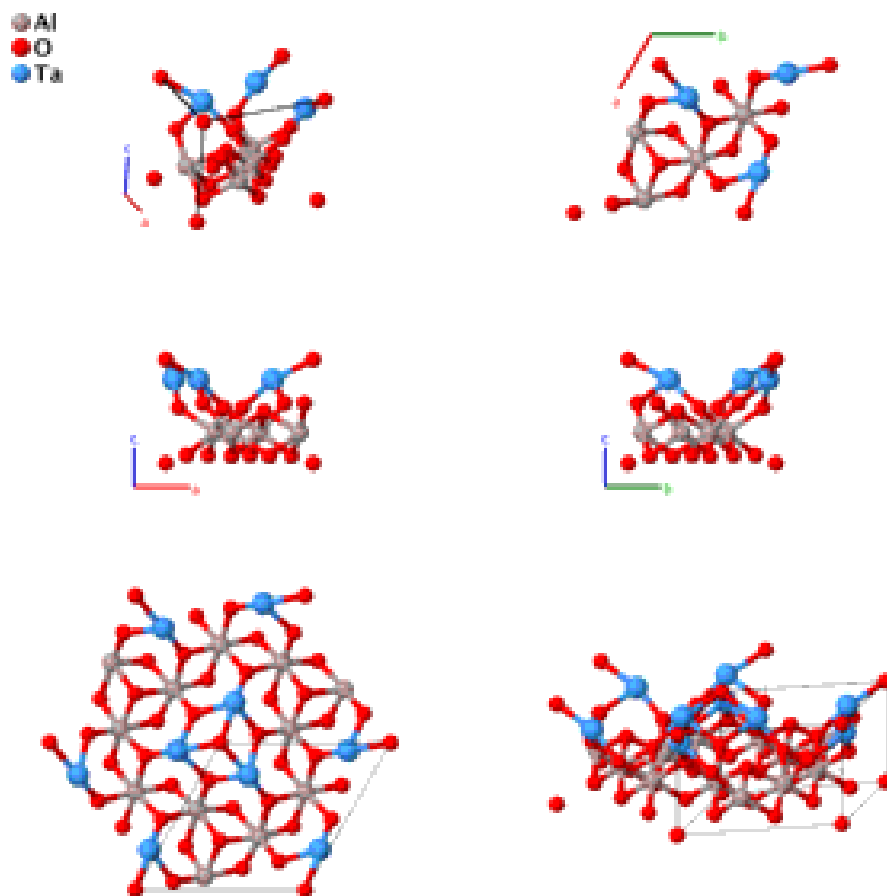
- O. Degtyareva, E. Gregoryanz, M. Somayazulu, P. Dera, H. Mao, and R. J. Hemley, *Novel chain structures in group VI elements*, Nat. Mater. **4**, 152–155 (2005), [doi:10.1038/nmat1294](https://doi.org/10.1038/nmat1294).

---

### Geometry files:

- CIF: pp. [904](#)  
- POSCAR: pp. [905](#)

# Simpsonite (Ta<sub>3</sub>Al<sub>4</sub>O<sub>13</sub>[OH]) Structure: A4B14C3\_hP21\_143\_bd\_ac4d\_d

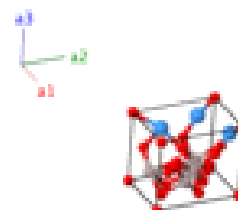


<b>Prototype</b>	: Ta <sub>3</sub> Al <sub>4</sub> O <sub>13</sub> [OH]
<b>AFLOW prototype label</b>	: A4B14C3_hP21_143_bd_ac4d_d
<b>Strukturbericht designation</b>	: None
<b>Pearson symbol</b>	: hP21
<b>Space group number</b>	: 143
<b>Space group symbol</b>	: <i>P</i> 3
<b>AFLOW prototype command</b>	: aflow --proto=A4B14C3_hP21_143_bd_ac4d_d --params= <i>a</i> , <i>c/a</i> , <i>z</i> <sub>1</sub> , <i>z</i> <sub>2</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>x</i> <sub>6</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub> , <i>x</i> <sub>7</sub> , <i>y</i> <sub>7</sub> , <i>z</i> <sub>7</sub> , <i>x</i> <sub>8</sub> , <i>y</i> <sub>8</sub> , <i>z</i> <sub>8</sub> , <i>x</i> <sub>9</sub> , <i>y</i> <sub>9</sub> , <i>z</i> <sub>9</sub>

- The OH molecule is centered on the (1c) site; however, it is only listed as O in this prototype.

## Trigonal Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



---

**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates		Wyckoff Position	Atom Type
$\mathbf{B}_1$	=	$z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(1a)	O I
$\mathbf{B}_2$	=	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(1b)	Al I
$\mathbf{B}_3$	=	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(1c)	O II
$\mathbf{B}_4$	=	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(3d)	Al II
$\mathbf{B}_5$	=	$-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(\frac{1}{2} x_4 - y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(3d)	Al II
$\mathbf{B}_6$	=	$(-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(-x_4 + \frac{1}{2} y_4) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(3d)	Al II
$\mathbf{B}_7$	=	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(3d)	O III
$\mathbf{B}_8$	=	$-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(\frac{1}{2} x_5 - y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(3d)	O III
$\mathbf{B}_9$	=	$(-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(-x_5 + \frac{1}{2} y_5) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(3d)	O III
$\mathbf{B}_{10}$	=	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$\frac{1}{2} (x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_6 + y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(3d)	O IV
$\mathbf{B}_{11}$	=	$-y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(\frac{1}{2} x_6 - y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(3d)	O IV
$\mathbf{B}_{12}$	=	$(-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(-x_6 + \frac{1}{2} y_6) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(3d)	O IV
$\mathbf{B}_{13}$	=	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$\frac{1}{2} (x_7 + y_7) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_7 + y_7) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(3d)	O V
$\mathbf{B}_{14}$	=	$-y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(\frac{1}{2} x_7 - y_7) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(3d)	O V
$\mathbf{B}_{15}$	=	$(-x_7 + y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(-x_7 + \frac{1}{2} y_7) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(3d)	O V
$\mathbf{B}_{16}$	=	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$\frac{1}{2} (x_8 + y_8) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_8 + y_8) a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(3d)	O VI
$\mathbf{B}_{17}$	=	$-y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(\frac{1}{2} x_8 - y_8) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(3d)	O VI
$\mathbf{B}_{18}$	=	$(-x_8 + y_8) \mathbf{a}_1 - x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(-x_8 + \frac{1}{2} y_8) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(3d)	O VI
$\mathbf{B}_{19}$	=	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$\frac{1}{2} (x_9 + y_9) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_9 + y_9) a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(3d)	Ta
$\mathbf{B}_{20}$	=	$-y_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(\frac{1}{2} x_9 - y_9) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(3d)	Ta
$\mathbf{B}_{21}$	=	$(-x_9 + y_9) \mathbf{a}_1 - x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(-x_9 + \frac{1}{2} y_9) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(3d)	Ta

---

**References:**

- T. S. Ercit, F. C. Hawthorne, and P. Cerny, *The crystal structure of alumotantite; its relation to the structures of simpsonite and the (Al, Ga)(Ta, Nb) O<sub>4</sub> compounds*, Can. Mineral. **30**, 653–662 (1992).

**Found in:**

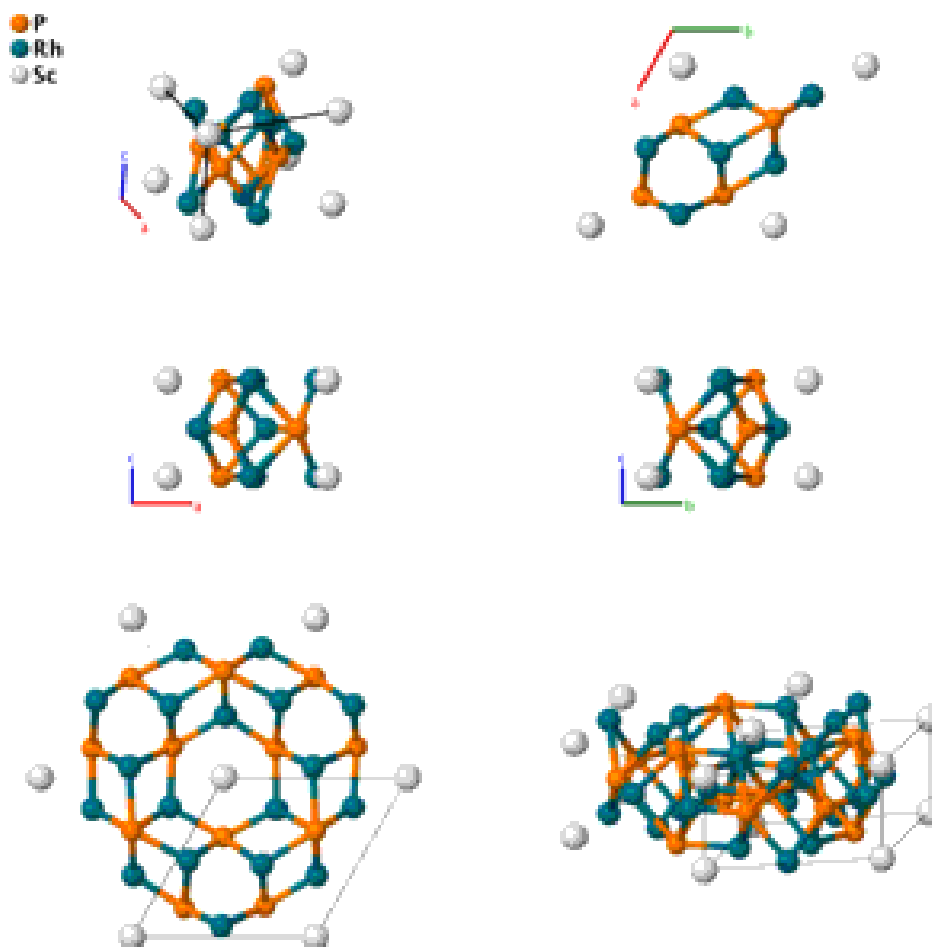
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. 905
- POSCAR: pp. 905

# ScRh<sub>6</sub>P<sub>4</sub> Structure: A4B6C\_hP11\_143\_bd\_2d\_a



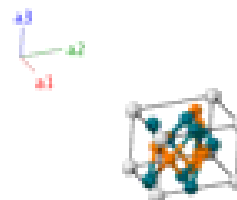
<b>Prototype</b>	:	ScRh <sub>6</sub> P <sub>4</sub>
<b>AFLOW prototype label</b>	:	A4B6C_hP11_143_bd_2d_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP11
<b>Space group number</b>	:	143
<b>Space group symbol</b>	:	<i>P</i> 3
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A4B6C_hP11_143_bd_2d_a --params=a, c/a, z1, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5</code>

- While FINDSYM identifies space group #143 for this structure (consistent with the reference), AFLOW-SYM and Platon identify #174 and #187, respectively. Lowering the tolerance value for AFLOW-SYM resolves the expected space group #143. Space groups #143, #174, and #187 are reasonable classifications since they are commensurate with subgroup relations.

---

**Trigonal Hexagonal primitive vectors:**

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



---

**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$= z_1 c \hat{\mathbf{z}}$	(1a)	Sc
$\mathbf{B}_2$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(1b)	P I
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_3 + y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(3d)	P II
$\mathbf{B}_4$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(\frac{1}{2} x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(3d)	P II
$\mathbf{B}_5$	$= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(-x_3 + \frac{1}{2} y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(3d)	P II
$\mathbf{B}_6$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(3d)	Rh I
$\mathbf{B}_7$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(3d)	Rh I
$\mathbf{B}_8$	$= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(3d)	Rh I
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= \frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(3d)	Rh II
$\mathbf{B}_{10}$	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= \left(\frac{1}{2} x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(3d)	Rh II
$\mathbf{B}_{11}$	$= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= \left(-x_5 + \frac{1}{2} y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(3d)	Rh II

---

**References:**

- U. Pfannenschmidt, U. C. Rodewald, and R. Pöttgen, *Bismuth flux crystal growth of  $RERh_6P_4$  ( $RE = Sc, Yb, Lu$ ): new phosphides with a superstructure of the  $LiCo_6P_4$  type*, *Monatsh. Chem.* **142**, 219–224 (2011), [doi:10.1007/s00706-011-0450-5](https://doi.org/10.1007/s00706-011-0450-5).
- H. T. Stokes and D. M. Hatch, *FINDSYM: Program for identifying the space group symmetry of a crystal*, *J. Appl. Crystallogr.* **38**, 237–238 (2005), [doi:10.1107/S0021889804031528](https://doi.org/10.1107/S0021889804031528).
- D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy, and S. Curtarolo, *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*, *Acta Crystallogr. Sect. A* **74**, 184–203 (2018), [doi:10.1107/S2053273318003066](https://doi.org/10.1107/S2053273318003066).
- A. L. Spek, *Single-crystal structure validation with the program PLATON*, *J. Appl. Crystallogr.* **36**, 7–13 (2003), [doi:10.1107/S0021889802022112](https://doi.org/10.1107/S0021889802022112).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

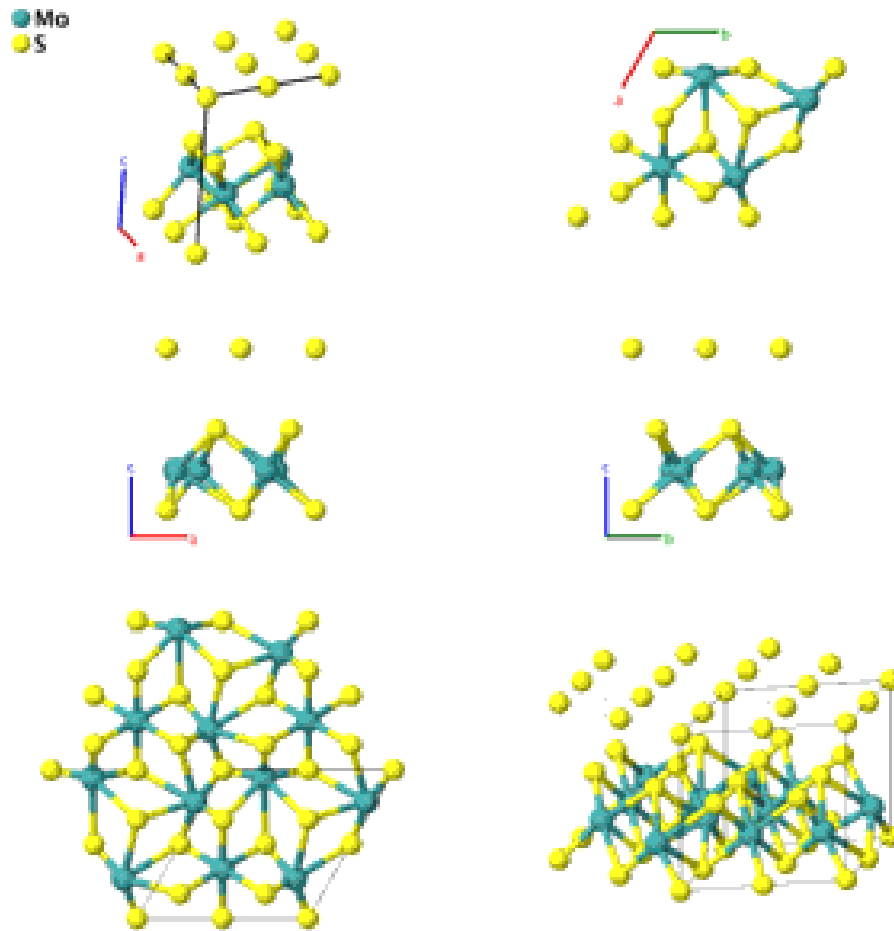
---

**Geometry files:**

- CIF: pp. [905](#)
- POSCAR: pp. [906](#)



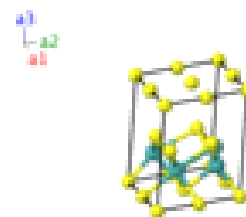
# MoS<sub>2</sub> Structure: AB2\_hP12\_143\_cd\_ab2d



<b>Prototype</b>	:	MoS <sub>2</sub>
<b>AFLOW prototype label</b>	:	AB2_hP12_143_cd_ab2d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP12
<b>Space group number</b>	:	143
<b>Space group symbol</b>	:	<i>P</i> 3
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB2_hP12_143_cd_ab2d</code> <code>--params=<i>a, c/a, z1, z2, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6</i></code>

**Trigonal Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates		Wyckoff Position	Atom Type
$\mathbf{B}_1$	=	$z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(1a)	S I
$\mathbf{B}_2$	=	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(1b)	S II
$\mathbf{B}_3$	=	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(1c)	Mo I
$\mathbf{B}_4$	=	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(3d)	Mo II
$\mathbf{B}_5$	=	$-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(3d)	Mo II
$\mathbf{B}_6$	=	$(-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(3d)	Mo II
$\mathbf{B}_7$	=	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(3d)	S III
$\mathbf{B}_8$	=	$-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\left(\frac{1}{2} x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(3d)	S III
$\mathbf{B}_9$	=	$(-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\left(-x_5 + \frac{1}{2} y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(3d)	S III
$\mathbf{B}_{10}$	=	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$\frac{1}{2} (x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_6 + y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(3d)	S IV
$\mathbf{B}_{11}$	=	$-y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$\left(\frac{1}{2} x_6 - y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(3d)	S IV
$\mathbf{B}_{12}$	=	$(-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$\left(-x_6 + \frac{1}{2} y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(3d)	S IV

---

#### References:

- K. E. Dungey, M. D. Curtis, and J. E. Penner-Hahn, *Structural characterization and thermal stability of MoS<sub>2</sub> intercalation compounds*, Chem. Mater. **10**, 2152–2161 (1998), doi:10.1021/cm980034u.

#### Found in:

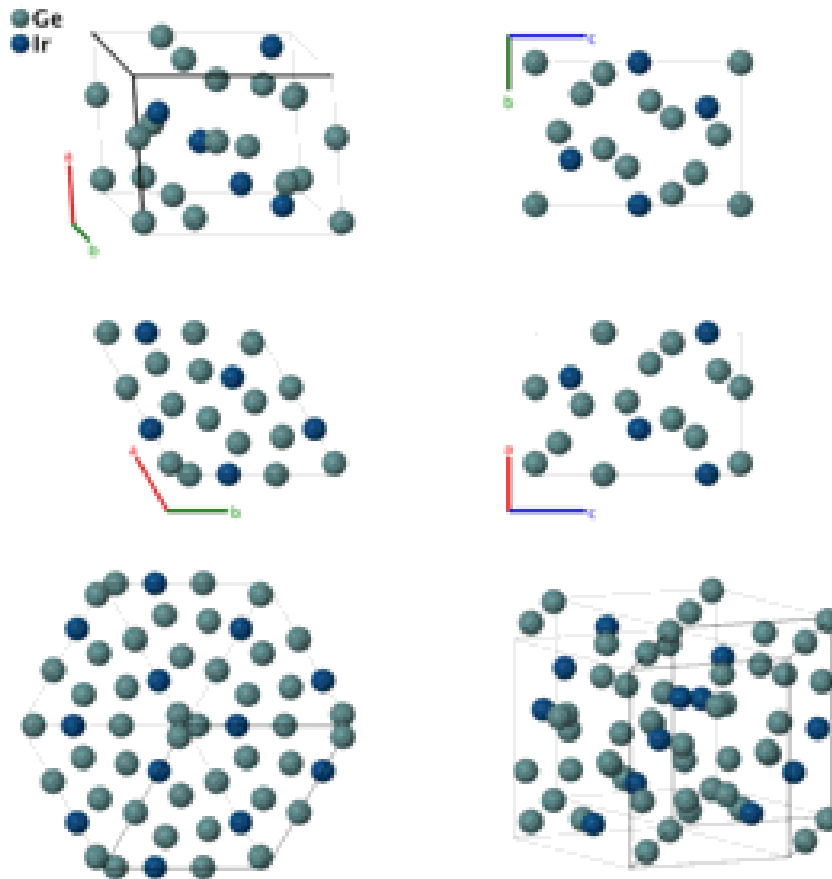
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 906
- POSCAR: pp. 906

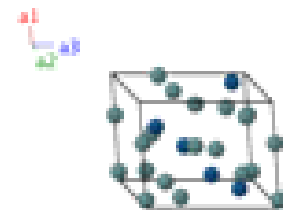
# IrGe<sub>4</sub> Structure: A4B\_hP15\_144\_4a\_a



**Prototype** : IrGe<sub>4</sub>  
**AFLOW prototype label** : A4B\_hP15\_144\_4a\_a  
**Strukturbericht designation** : None  
**Pearson symbol** : hP15  
**Space group number** : 144  
**Space group symbol** :  $P3_1$   
**AFLOW prototype command** : `aflow --proto=A4B_hP15_144_4a_a`  
`--params=a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5`

**Trigonal Hexagonal primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type

$$\begin{aligned}
\mathbf{B}_1 &= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3 = \frac{1}{2}(x_1 + y_1)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_1 + y_1)a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}} & (3a) & \text{Ge I} \\
\mathbf{B}_2 &= -y_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + \left(\frac{1}{3} + z_1\right) \mathbf{a}_3 = \left(\frac{1}{2}x_1 - y_1\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_1 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_1\right)c \hat{\mathbf{z}} & (3a) & \text{Ge I} \\
\mathbf{B}_3 &= (-x_1 + y_1) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{2}{3} + z_1\right) \mathbf{a}_3 = \left(-x_1 + \frac{1}{2}y_1\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_1 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_1\right)c \hat{\mathbf{z}} & (3a) & \text{Ge I} \\
\mathbf{B}_4 &= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 = \frac{1}{2}(x_2 + y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_2 + y_2)a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (3a) & \text{Ge II} \\
\mathbf{B}_5 &= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{1}{3} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2}x_2 - y_2\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_2\right)c \hat{\mathbf{z}} & (3a) & \text{Ge II} \\
\mathbf{B}_6 &= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{2}{3} + z_2\right) \mathbf{a}_3 = \left(-x_2 + \frac{1}{2}y_2\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_2\right)c \hat{\mathbf{z}} & (3a) & \text{Ge II} \\
\mathbf{B}_7 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = \frac{1}{2}(x_3 + y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3)a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (3a) & \text{Ge III} \\
\mathbf{B}_8 &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{1}{3} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2}x_3 - y_3\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_3\right)c \hat{\mathbf{z}} & (3a) & \text{Ge III} \\
\mathbf{B}_9 &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{2}{3} + z_3\right) \mathbf{a}_3 = \left(-x_3 + \frac{1}{2}y_3\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_3\right)c \hat{\mathbf{z}} & (3a) & \text{Ge III} \\
\mathbf{B}_{10} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = \frac{1}{2}(x_4 + y_4)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_4 + y_4)a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (3a) & \text{Ge IV} \\
\mathbf{B}_{11} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{1}{3} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2}x_4 - y_4\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_4\right)c \hat{\mathbf{z}} & (3a) & \text{Ge IV} \\
\mathbf{B}_{12} &= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{2}{3} + z_4\right) \mathbf{a}_3 = \left(-x_4 + \frac{1}{2}y_4\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_4\right)c \hat{\mathbf{z}} & (3a) & \text{Ge IV} \\
\mathbf{B}_{13} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \frac{1}{2}(x_5 + y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5)a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (3a) & \text{Ir} \\
\mathbf{B}_{14} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{1}{3} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2}x_5 - y_5\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_5\right)c \hat{\mathbf{z}} & (3a) & \text{Ir} \\
\mathbf{B}_{15} &= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{2}{3} + z_5\right) \mathbf{a}_3 = \left(-x_5 + \frac{1}{2}y_5\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_5\right)c \hat{\mathbf{z}} & (3a) & \text{Ir}
\end{aligned}$$

---

#### References:

- K. Schubert, S. Bhan, T. K. Biswas, K. Frank, and P. K. Panday, *Einige Strukturdaten metallischer Phasen*, *Naturwissenschaften* **55**, 542–543 (1968), doi:10.1007/BF00660131.

#### Found in:

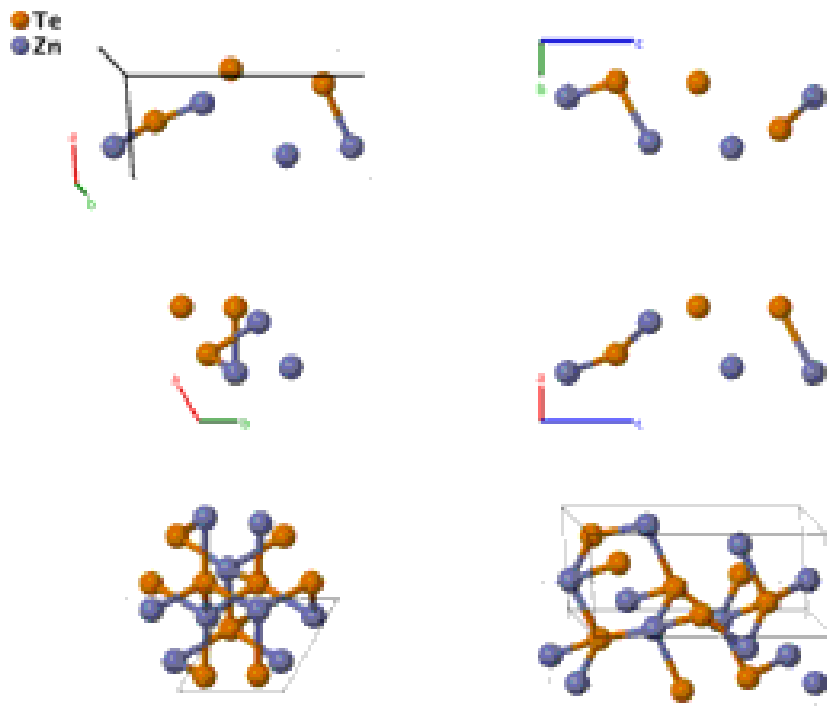
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 906  
- POSCAR: pp. 907

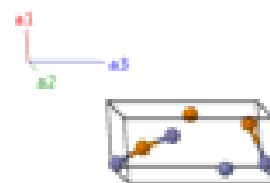
# TeZn (High-pressure) Structure: AB\_hP6\_144\_a\_a



<b>Prototype</b>	:	ZnTe
<b>AFLOW prototype label</b>	:	AB_hP6_144_a_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP6
<b>Space group number</b>	:	144
<b>Space group symbol</b>	:	$P3_1$
<b>AFLOW prototype command</b>	:	aflow --proto=AB_hP6_144_a_a --params=a, c/a, x <sub>1</sub> , y <sub>1</sub> , z <sub>1</sub> , x <sub>2</sub> , y <sub>2</sub> , z <sub>2</sub>

## Trigonal Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$\frac{1}{2} (x_1 + y_1) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_1 + y_1) a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(3a)	Te
$\mathbf{B}_2$	$-y_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + \left(\frac{1}{3} + z_1\right) \mathbf{a}_3$	$\left(\frac{1}{2} x_1 - y_1\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_1\right) c \hat{\mathbf{z}}$	(3a)	Te

$$\mathbf{B}_3 = (-x_1 + y_1) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{2}{3} + z_1\right) \mathbf{a}_3 = \left(-x_1 + \frac{1}{2}y_1\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_1a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_1\right)c \hat{\mathbf{z}} \quad (3a) \quad \text{Te}$$

$$\mathbf{B}_4 = x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 = \frac{1}{2}(x_2 + y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_2 + y_2)a \hat{\mathbf{y}} + z_2c \hat{\mathbf{z}} \quad (3a) \quad \text{Zn}$$

$$\mathbf{B}_5 = -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{1}{3} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2}x_2 - y_2\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_2\right)c \hat{\mathbf{z}} \quad (3a) \quad \text{Zn}$$

$$\mathbf{B}_6 = (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{2}{3} + z_2\right) \mathbf{a}_3 = \left(-x_2 + \frac{1}{2}y_2\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_2\right)c \hat{\mathbf{z}} \quad (3a) \quad \text{Zn}$$

#### References:

- K. Kusaba and D. J. Weidner, *Structure of high pressure phase I in ZnTe*, in *AIP Conference Proceedings* (1994), vol. 309, pp. 553–556, [doi:10.1063/1.46096](https://doi.org/10.1063/1.46096).

#### Found in:

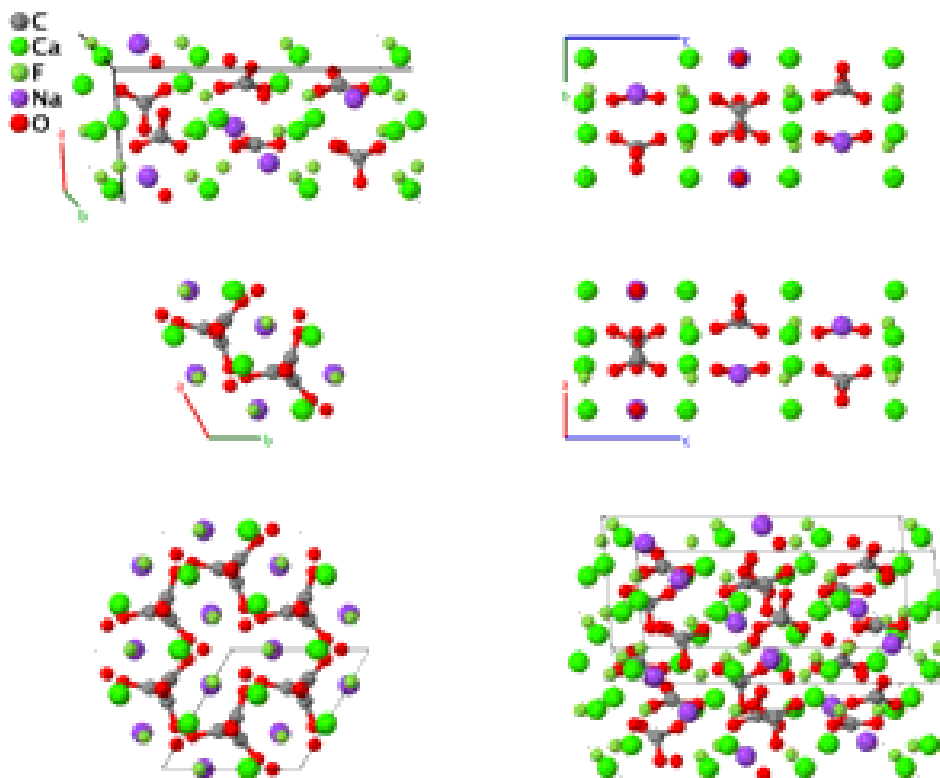
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. [907](#)  
 - POSCAR: pp. [907](#)

# Sheldrickite (NaCa<sub>3</sub>[CO<sub>3</sub>]<sub>2</sub>F<sub>3</sub>[H<sub>2</sub>O]) Structure:

A2B3C3DE7\_hP48\_145\_2a\_3a\_3a\_a\_7a

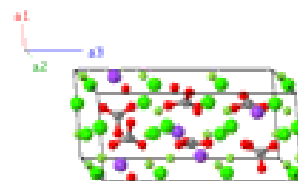


<b>Prototype</b>	:	NaCa <sub>3</sub> [CO <sub>3</sub> ] <sub>2</sub> F <sub>3</sub> [H <sub>2</sub> O]
<b>AFLOW prototype label</b>	:	A2B3C3DE7_hP48_145_2a_3a_3a_a_7a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP48
<b>Space group number</b>	:	145
<b>Space group symbol</b>	:	<i>P</i> 3 <sub>2</sub>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3C3DE7_hP48_145_2a_3a_3a_a_7a --params= <i>a</i> , <i>c/a</i> , <i>x</i> <sub>1</sub> , <i>y</i> <sub>1</sub> , <i>z</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>y</i> <sub>2</sub> , <i>z</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>x</i> <sub>6</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub> , <i>x</i> <sub>7</sub> , <i>y</i> <sub>7</sub> , <i>z</i> <sub>7</sub> , <i>x</i> <sub>8</sub> , <i>y</i> <sub>8</sub> , <i>z</i> <sub>8</sub> , <i>x</i> <sub>9</sub> , <i>y</i> <sub>9</sub> , <i>z</i> <sub>9</sub> , <i>x</i> <sub>10</sub> , <i>y</i> <sub>10</sub> , <i>z</i> <sub>10</sub> , <i>x</i> <sub>11</sub> , <i>y</i> <sub>11</sub> , <i>z</i> <sub>11</sub> , <i>x</i> <sub>12</sub> , <i>y</i> <sub>12</sub> , <i>z</i> <sub>12</sub> , <i>x</i> <sub>13</sub> , <i>y</i> <sub>13</sub> , <i>z</i> <sub>13</sub> , <i>x</i> <sub>14</sub> , <i>y</i> <sub>14</sub> , <i>z</i> <sub>14</sub> , <i>x</i> <sub>15</sub> , <i>y</i> <sub>15</sub> , <i>z</i> <sub>15</sub> , <i>x</i> <sub>16</sub> , <i>y</i> <sub>16</sub> , <i>z</i> <sub>16</sub>

- The H<sub>2</sub>O molecule is centered on one of the (3a) sites; however, it is only listed as O in this prototype.

**Trigonal Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}(x_1 + y_1)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_1 + y_1)a \hat{\mathbf{y}} + z_1c \hat{\mathbf{z}}$	(3a)	C I
$\mathbf{B}_2$	$= -y_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + \left(\frac{2}{3} + z_1\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2}x_1 - y_1\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_1a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_1\right)c \hat{\mathbf{z}}$	(3a)	C I
$\mathbf{B}_3$	$= (-x_1 + y_1) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{1}{3} + z_1\right) \mathbf{a}_3$	$=$	$\left(-x_1 + \frac{1}{2}y_1\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_1a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_1\right)c \hat{\mathbf{z}}$	(3a)	C I
$\mathbf{B}_4$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}(x_2 + y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_2 + y_2)a \hat{\mathbf{y}} + z_2c \hat{\mathbf{z}}$	(3a)	C II
$\mathbf{B}_5$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{2}{3} + z_2\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2}x_2 - y_2\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_2\right)c \hat{\mathbf{z}}$	(3a)	C II
$\mathbf{B}_6$	$= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{3} + z_2\right) \mathbf{a}_3$	$=$	$\left(-x_2 + \frac{1}{2}y_2\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_2\right)c \hat{\mathbf{z}}$	(3a)	C II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}(x_3 + y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3)a \hat{\mathbf{y}} + z_3c \hat{\mathbf{z}}$	(3a)	Ca I
$\mathbf{B}_8$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{2}{3} + z_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2}x_3 - y_3\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_3\right)c \hat{\mathbf{z}}$	(3a)	Ca I
$\mathbf{B}_9$	$= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{3} + z_3\right) \mathbf{a}_3$	$=$	$\left(-x_3 + \frac{1}{2}y_3\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_3\right)c \hat{\mathbf{z}}$	(3a)	Ca I
$\mathbf{B}_{10}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}(x_4 + y_4)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_4 + y_4)a \hat{\mathbf{y}} + z_4c \hat{\mathbf{z}}$	(3a)	Ca II
$\mathbf{B}_{11}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{2}{3} + z_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2}x_4 - y_4\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_4\right)c \hat{\mathbf{z}}$	(3a)	Ca II
$\mathbf{B}_{12}$	$= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{3} + z_4\right) \mathbf{a}_3$	$=$	$\left(-x_4 + \frac{1}{2}y_4\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_4\right)c \hat{\mathbf{z}}$	(3a)	Ca II
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}(x_5 + y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5)a \hat{\mathbf{y}} + z_5c \hat{\mathbf{z}}$	(3a)	Ca III
$\mathbf{B}_{14}$	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{2}{3} + z_5\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2}x_5 - y_5\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_5\right)c \hat{\mathbf{z}}$	(3a)	Ca III
$\mathbf{B}_{15}$	$= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{3} + z_5\right) \mathbf{a}_3$	$=$	$\left(-x_5 + \frac{1}{2}y_5\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_5\right)c \hat{\mathbf{z}}$	(3a)	Ca III
$\mathbf{B}_{16}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}(x_6 + y_6)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_6 + y_6)a \hat{\mathbf{y}} + z_6c \hat{\mathbf{z}}$	(3a)	F I
$\mathbf{B}_{17}$	$= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \left(\frac{2}{3} + z_6\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2}x_6 - y_6\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_6a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_6\right)c \hat{\mathbf{z}}$	(3a)	F I
$\mathbf{B}_{18}$	$= (-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(\frac{1}{3} + z_6\right) \mathbf{a}_3$	$=$	$\left(-x_6 + \frac{1}{2}y_6\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_6a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_6\right)c \hat{\mathbf{z}}$	(3a)	F I
$\mathbf{B}_{19}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}(x_7 + y_7)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_7 + y_7)a \hat{\mathbf{y}} + z_7c \hat{\mathbf{z}}$	(3a)	F II
$\mathbf{B}_{20}$	$= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \left(\frac{2}{3} + z_7\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2}x_7 - y_7\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_7a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_7\right)c \hat{\mathbf{z}}$	(3a)	F II



$$\begin{aligned}
\mathbf{B}_{21} &= (-x_7 + y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(\frac{1}{3} + z_7\right) \mathbf{a}_3 = \left(-x_7 + \frac{1}{2}y_7\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_7 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_7\right) c \hat{\mathbf{z}} & (3a) & \text{F II} \\
\mathbf{B}_{22} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = \frac{1}{2}(x_8 + y_8) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_8 + y_8) a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} & (3a) & \text{F III} \\
\mathbf{B}_{23} &= -y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + \left(\frac{2}{3} + z_8\right) \mathbf{a}_3 = \left(\frac{1}{2}x_8 - y_8\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_8 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_8\right) c \hat{\mathbf{z}} & (3a) & \text{F III} \\
\mathbf{B}_{24} &= (-x_8 + y_8) \mathbf{a}_1 - x_8 \mathbf{a}_2 + \left(\frac{1}{3} + z_8\right) \mathbf{a}_3 = \left(-x_8 + \frac{1}{2}y_8\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_8 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_8\right) c \hat{\mathbf{z}} & (3a) & \text{F III} \\
\mathbf{B}_{25} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = \frac{1}{2}(x_9 + y_9) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_9 + y_9) a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}} & (3a) & \text{Na} \\
\mathbf{B}_{26} &= -y_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + \left(\frac{2}{3} + z_9\right) \mathbf{a}_3 = \left(\frac{1}{2}x_9 - y_9\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_9 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_9\right) c \hat{\mathbf{z}} & (3a) & \text{Na} \\
\mathbf{B}_{27} &= (-x_9 + y_9) \mathbf{a}_1 - x_9 \mathbf{a}_2 + \left(\frac{1}{3} + z_9\right) \mathbf{a}_3 = \left(-x_9 + \frac{1}{2}y_9\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_9 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_9\right) c \hat{\mathbf{z}} & (3a) & \text{Na} \\
\mathbf{B}_{28} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \frac{1}{2}(x_{10} + y_{10}) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_{10} + y_{10}) a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}} & (3a) & \text{O I} \\
\mathbf{B}_{29} &= -y_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + \left(\frac{2}{3} + z_{10}\right) \mathbf{a}_3 = \left(\frac{1}{2}x_{10} - y_{10}\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_{10} a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_{10}\right) c \hat{\mathbf{z}} & (3a) & \text{O I} \\
\mathbf{B}_{30} &= (-x_{10} + y_{10}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 + \left(\frac{1}{3} + z_{10}\right) \mathbf{a}_3 = \left(-x_{10} + \frac{1}{2}y_{10}\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_{10} a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_{10}\right) c \hat{\mathbf{z}} & (3a) & \text{O I} \\
\mathbf{B}_{31} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = \frac{1}{2}(x_{11} + y_{11}) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_{11} + y_{11}) a \hat{\mathbf{y}} + z_{11} c \hat{\mathbf{z}} & (3a) & \text{O II} \\
\mathbf{B}_{32} &= -y_{11} \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 + \left(\frac{2}{3} + z_{11}\right) \mathbf{a}_3 = \left(\frac{1}{2}x_{11} - y_{11}\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_{11} a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_{11}\right) c \hat{\mathbf{z}} & (3a) & \text{O II} \\
\mathbf{B}_{33} &= (-x_{11} + y_{11}) \mathbf{a}_1 - x_{11} \mathbf{a}_2 + \left(\frac{1}{3} + z_{11}\right) \mathbf{a}_3 = \left(-x_{11} + \frac{1}{2}y_{11}\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_{11} a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_{11}\right) c \hat{\mathbf{z}} & (3a) & \text{O II} \\
\mathbf{B}_{34} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \frac{1}{2}(x_{12} + y_{12}) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_{12} + y_{12}) a \hat{\mathbf{y}} + z_{12} c \hat{\mathbf{z}} & (3a) & \text{O III} \\
\mathbf{B}_{35} &= -y_{12} \mathbf{a}_1 + (x_{12} - y_{12}) \mathbf{a}_2 + \left(\frac{2}{3} + z_{12}\right) \mathbf{a}_3 = \left(\frac{1}{2}x_{12} - y_{12}\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_{12} a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_{12}\right) c \hat{\mathbf{z}} & (3a) & \text{O III} \\
\mathbf{B}_{36} &= (-x_{12} + y_{12}) \mathbf{a}_1 - x_{12} \mathbf{a}_2 + \left(\frac{1}{3} + z_{12}\right) \mathbf{a}_3 = \left(-x_{12} + \frac{1}{2}y_{12}\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_{12} a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_{12}\right) c \hat{\mathbf{z}} & (3a) & \text{O III} \\
\mathbf{B}_{37} &= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 = \frac{1}{2}(x_{13} + y_{13}) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_{13} + y_{13}) a \hat{\mathbf{y}} + z_{13} c \hat{\mathbf{z}} & (3a) & \text{O IV} \\
\mathbf{B}_{38} &= -y_{13} \mathbf{a}_1 + (x_{13} - y_{13}) \mathbf{a}_2 + \left(\frac{2}{3} + z_{13}\right) \mathbf{a}_3 = \left(\frac{1}{2}x_{13} - y_{13}\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_{13} a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_{13}\right) c \hat{\mathbf{z}} & (3a) & \text{O IV} \\
\mathbf{B}_{39} &= (-x_{13} + y_{13}) \mathbf{a}_1 - x_{13} \mathbf{a}_2 + \left(\frac{1}{3} + z_{13}\right) \mathbf{a}_3 = \left(-x_{13} + \frac{1}{2}y_{13}\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_{13} a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_{13}\right) c \hat{\mathbf{z}} & (3a) & \text{O IV} \\
\mathbf{B}_{40} &= x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3 = \frac{1}{2}(x_{14} + y_{14}) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_{14} + y_{14}) a \hat{\mathbf{y}} + z_{14} c \hat{\mathbf{z}} & (3a) & \text{O V}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{41} &= -y_{14} \mathbf{a}_1 + (x_{14} - y_{14}) \mathbf{a}_2 + \left(\frac{2}{3} + z_{14}\right) \mathbf{a}_3 = \left(\frac{1}{2}x_{14} - y_{14}\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_{14}a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_{14}\right)c \hat{\mathbf{z}} & (3a) & \text{O V} \\
\mathbf{B}_{42} &= (-x_{14} + y_{14}) \mathbf{a}_1 - x_{14} \mathbf{a}_2 + \left(\frac{1}{3} + z_{14}\right) \mathbf{a}_3 = \left(-x_{14} + \frac{1}{2}y_{14}\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_{14}a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_{14}\right)c \hat{\mathbf{z}} & (3a) & \text{O V} \\
\mathbf{B}_{43} &= x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 = \frac{1}{2}(x_{15} + y_{15})a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_{15} + y_{15})a \hat{\mathbf{y}} + z_{15}c \hat{\mathbf{z}} & (3a) & \text{O VI} \\
\mathbf{B}_{44} &= -y_{15} \mathbf{a}_1 + (x_{15} - y_{15}) \mathbf{a}_2 + \left(\frac{2}{3} + z_{15}\right) \mathbf{a}_3 = \left(\frac{1}{2}x_{15} - y_{15}\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_{15}a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_{15}\right)c \hat{\mathbf{z}} & (3a) & \text{O VI} \\
\mathbf{B}_{45} &= (-x_{15} + y_{15}) \mathbf{a}_1 - x_{15} \mathbf{a}_2 + \left(\frac{1}{3} + z_{15}\right) \mathbf{a}_3 = \left(-x_{15} + \frac{1}{2}y_{15}\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_{15}a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_{15}\right)c \hat{\mathbf{z}} & (3a) & \text{O VI} \\
\mathbf{B}_{46} &= x_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3 = \frac{1}{2}(x_{16} + y_{16})a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_{16} + y_{16})a \hat{\mathbf{y}} + z_{16}c \hat{\mathbf{z}} & (3a) & \text{O VII} \\
\mathbf{B}_{47} &= -y_{16} \mathbf{a}_1 + (x_{16} - y_{16}) \mathbf{a}_2 + \left(\frac{2}{3} + z_{16}\right) \mathbf{a}_3 = \left(\frac{1}{2}x_{16} - y_{16}\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_{16}a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_{16}\right)c \hat{\mathbf{z}} & (3a) & \text{O VII} \\
\mathbf{B}_{48} &= (-x_{16} + y_{16}) \mathbf{a}_1 - x_{16} \mathbf{a}_2 + \left(\frac{1}{3} + z_{16}\right) \mathbf{a}_3 = \left(-x_{16} + \frac{1}{2}y_{16}\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_{16}a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_{16}\right)c \hat{\mathbf{z}} & (3a) & \text{O VII}
\end{aligned}$$

---

#### References:

- J. D. Grice, R. A. Gault, and J. Van Velthuisen, *Sheldrickite, a new sodium-calcium-fluorocarbonate mineral species from Mont Saint-Hilaire, Quebec*, Can. Mineral. **35**, 181–187 (1997).

#### Found in:

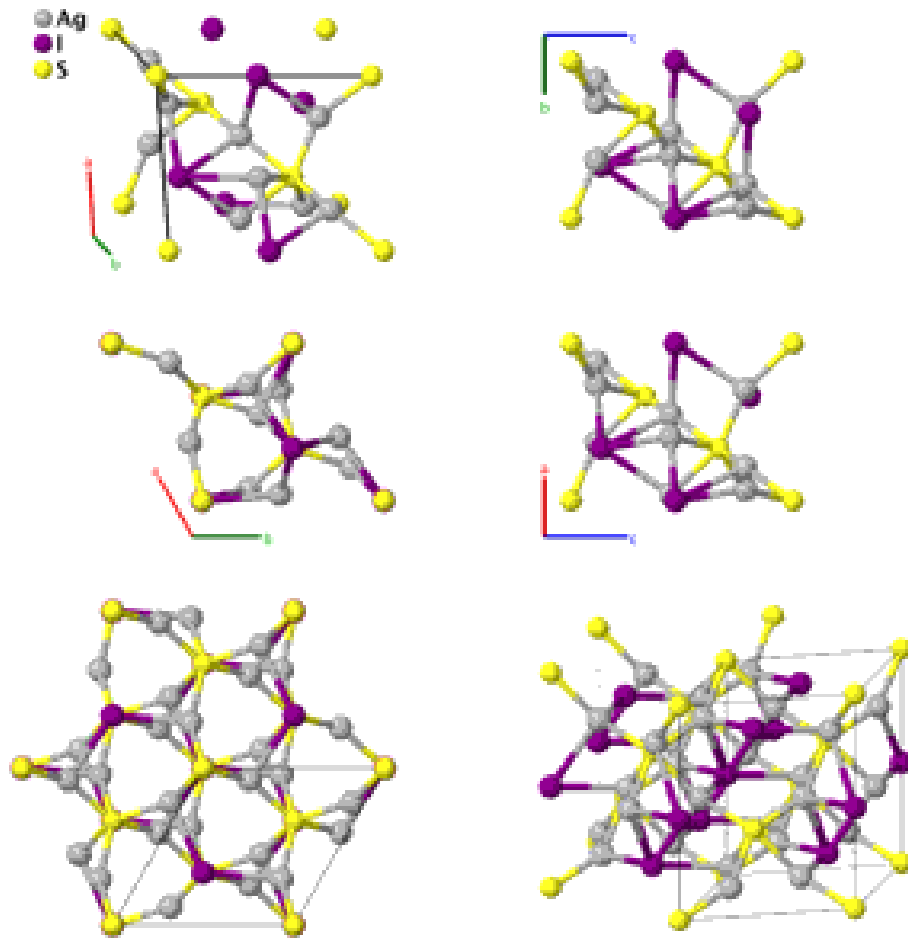
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [907](#)  
- POSCAR: pp. [907](#)

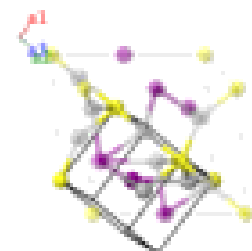
# $\gamma$ -Ag<sub>3</sub>SI (Low-temperature) Structure: A3BC\_hR5\_146\_b\_a\_a



<b>Prototype</b>	:	$\gamma$ -Ag <sub>3</sub> SI
<b>AFLOW prototype label</b>	:	A3BC_hR5_146_b_a_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hR5
<b>Space group number</b>	:	146
<b>Space group symbol</b>	:	<i>R</i> 3
<b>AFLOW prototype command</b>	:	aflow --proto=A3BC_hR5_146_b_a_a [--hex] --params= <i>a, c/a, x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub></i>

## Rhombohedral primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1 = x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3 =$	$x_1 c \hat{\mathbf{z}}$	(1a)	I
$\mathbf{B}_2 = x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3 =$	$x_2 c \hat{\mathbf{z}}$	(1a)	S
$\mathbf{B}_3 = x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 =$	$\frac{1}{2} (x_3 - z_3) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_3 + \frac{1}{\sqrt{3}} y_3 - \frac{1}{2\sqrt{3}} z_3 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_3 + y_3 + z_3) c \hat{\mathbf{z}}$	(3b)	Ag
$\mathbf{B}_4 = z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3 =$	$\frac{1}{2} (-y_3 + z_3) a \hat{\mathbf{x}} + \left( \frac{1}{\sqrt{3}} x_3 - \frac{1}{2\sqrt{3}} y_3 - \frac{1}{2\sqrt{3}} z_3 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_3 + y_3 + z_3) c \hat{\mathbf{z}}$	(3b)	Ag
$\mathbf{B}_5 = y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3 =$	$\frac{1}{2} (-x_3 + y_3) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_3 - \frac{1}{2\sqrt{3}} y_3 + \frac{1}{\sqrt{3}} z_3 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_3 + y_3 + z_3) c \hat{\mathbf{z}}$	(3b)	Ag

#### References:

- S. Hoshino, T. Sakuma, and Y. Fujii, *A Structural Phase Transition in Superionic Conductor Ag<sub>3</sub>SI*, J. Phys. Soc. Jpn. **47**, 1252–1259 (1979), doi:10.1143/JPSJ.47.1252.

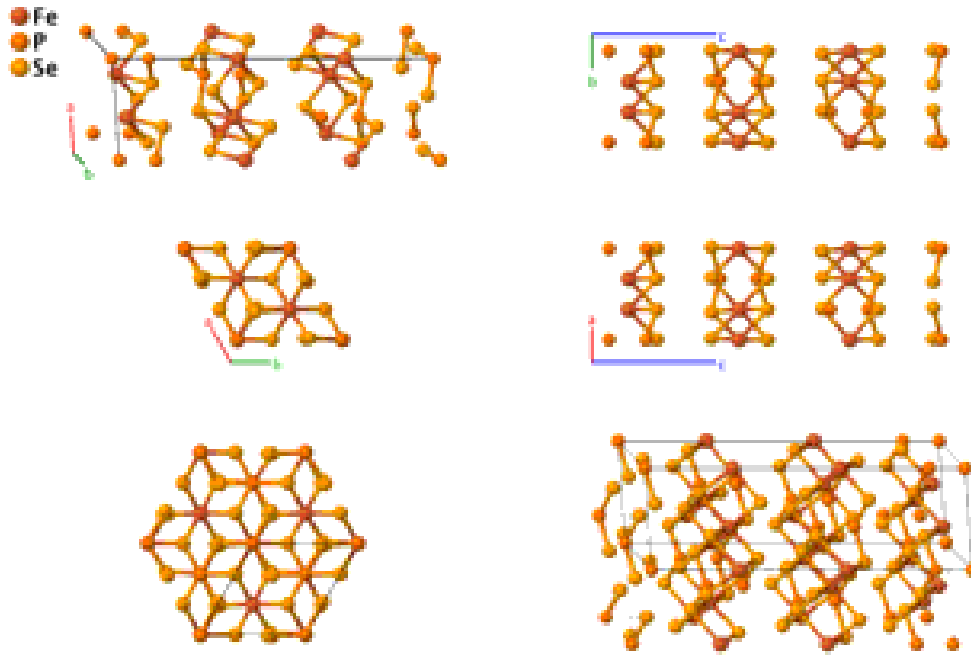
#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. 908
- POSCAR: pp. 908

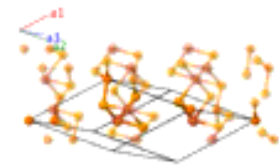
# FePSe<sub>3</sub> Structure: ABC3\_hR10\_146\_2a\_2a\_2b



**Prototype** : FePSe<sub>3</sub>  
**AFLOW prototype label** : ABC3\_hR10\_146\_2a\_2a\_2b  
**Strukturbericht designation** : None  
**Pearson symbol** : hR10  
**Space group number** : 146  
**Space group symbol** : *R*3  
**AFLOW prototype command** : aflow --proto=ABC3\_hR10\_146\_2a\_2a\_2b [--hex]  
 --params=*a, c/a, x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, x<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>*

## Rhombohedral primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\
 \mathbf{a}_3 &= -\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3 =$	$x_1 c \hat{\mathbf{z}}$	(1a)	Fe I
<b>B<sub>2</sub></b>	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3 =$	$x_2 c \hat{\mathbf{z}}$	(1a)	Fe II
<b>B<sub>3</sub></b>	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3 =$	$x_3 c \hat{\mathbf{z}}$	(1a)	P I
<b>B<sub>4</sub></b>	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 =$	$x_4 c \hat{\mathbf{z}}$	(1a)	P II
<b>B<sub>5</sub></b>	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 =$	$\frac{1}{2} (x_5 - z_5) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_5 + \frac{1}{\sqrt{3}} y_5 - \frac{1}{2\sqrt{3}} z_5 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_5 + y_5 + z_5) c \hat{\mathbf{z}}$	(3b)	Se I

$$\mathbf{B}_6 = z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3 = \frac{1}{2}(-y_5 + z_5) a \hat{\mathbf{x}} + \left( \frac{1}{\sqrt{3}}x_5 - \frac{1}{2\sqrt{3}}y_5 - \frac{1}{2\sqrt{3}}z_5 \right) a \hat{\mathbf{y}} + \frac{1}{3}(x_5 + y_5 + z_5) c \hat{\mathbf{z}} \quad (3b) \quad \text{Se I}$$

$$\mathbf{B}_7 = y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3 = \frac{1}{2}(-x_5 + y_5) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}}x_5 - \frac{1}{2\sqrt{3}}y_5 + \frac{1}{\sqrt{3}}z_5 \right) a \hat{\mathbf{y}} + \frac{1}{3}(x_5 + y_5 + z_5) c \hat{\mathbf{z}} \quad (3b) \quad \text{Se I}$$

$$\mathbf{B}_8 = x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \frac{1}{2}(x_6 - z_6) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}}x_6 + \frac{1}{\sqrt{3}}y_6 - \frac{1}{2\sqrt{3}}z_6 \right) a \hat{\mathbf{y}} + \frac{1}{3}(x_6 + y_6 + z_6) c \hat{\mathbf{z}} \quad (3b) \quad \text{Se II}$$

$$\mathbf{B}_9 = z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3 = \frac{1}{2}(-y_6 + z_6) a \hat{\mathbf{x}} + \left( \frac{1}{\sqrt{3}}x_6 - \frac{1}{2\sqrt{3}}y_6 - \frac{1}{2\sqrt{3}}z_6 \right) a \hat{\mathbf{y}} + \frac{1}{3}(x_6 + y_6 + z_6) c \hat{\mathbf{z}} \quad (3b) \quad \text{Se II}$$

$$\mathbf{B}_{10} = y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3 = \frac{1}{2}(-x_6 + y_6) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}}x_6 - \frac{1}{2\sqrt{3}}y_6 + \frac{1}{\sqrt{3}}z_6 \right) a \hat{\mathbf{y}} + \frac{1}{3}(x_6 + y_6 + z_6) c \hat{\mathbf{z}} \quad (3b) \quad \text{Se II}$$

#### References:

- W. Klungen, G. Eulenberger, and H. Hahn, *Über die Kristallstrukturen von Fe<sub>2</sub>P<sub>2</sub>Se<sub>6</sub> und Fe<sub>2</sub>P<sub>2</sub>S<sub>6</sub>*, Z. Anorg. Allg. Chem. **401**, 97–112 (1973), doi:10.1002/zaac.19734010113.

#### Found in:

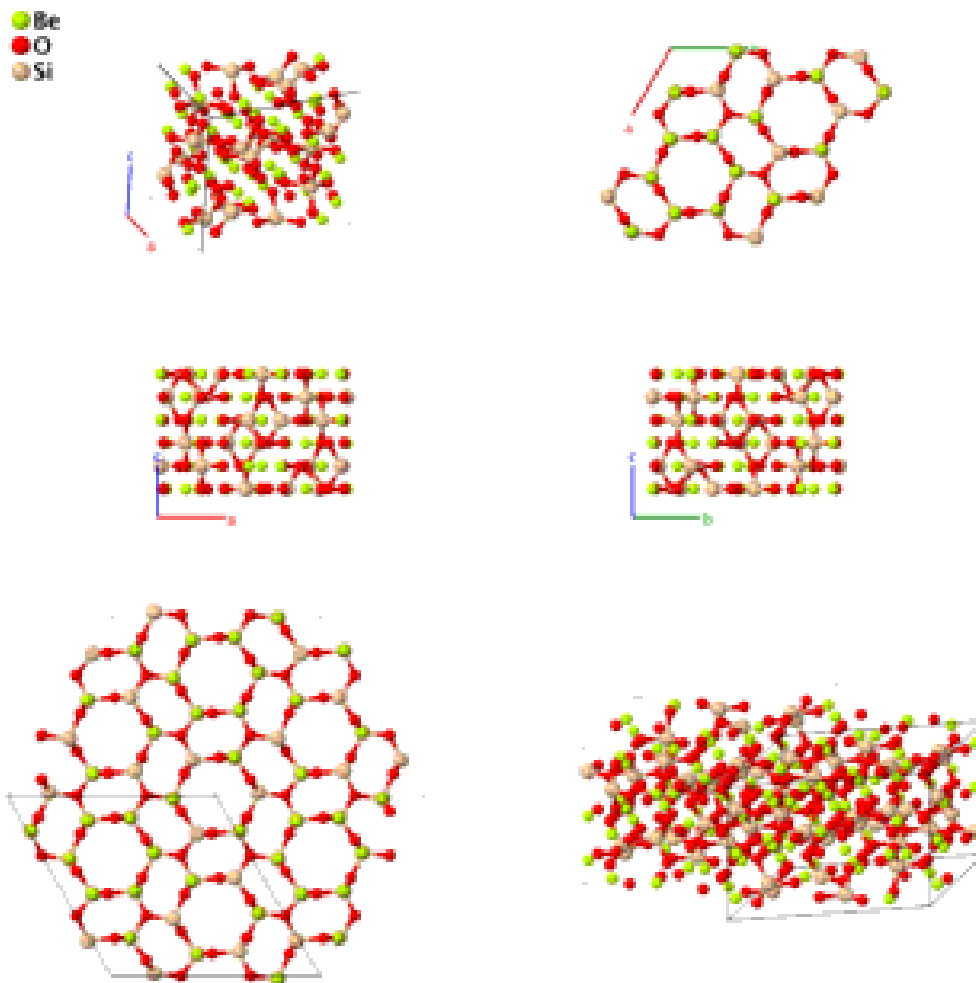
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. 908
- POSCAR: pp. 909

# Phenakite ( $\text{Be}_2\text{SiO}_4$ , $S 1_3$ ) Structure: A2B4C\_hR42\_148\_2f\_4f\_f

---



<b>Prototype</b>	:	$\text{Be}_2\text{SiO}_4$
<b>AFLOW prototype label</b>	:	A2B4C_hR42_148_2f_4f_f
<b>Strukturbericht designation</b>	:	$S 1_3$
<b>Pearson symbol</b>	:	hR42
<b>Space group number</b>	:	148
<b>Space group symbol</b>	:	$R\bar{3}$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B4C_hR42_148_2f_4f_f [--hex] --params= $a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

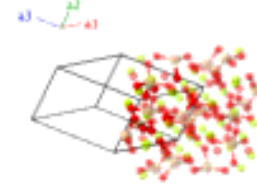
---

## Other compounds with this structure:

- $\text{Zn}_2\text{SiO}_4$  (willemite),  $(\text{Zn,Mn})_2\text{SiO}_4$  (troostite),  $\text{LiZnPO}_4$

## Rhombohedral primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{2} (x_1 - z_1) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_1 + \frac{1}{\sqrt{3}} y_1 - \frac{1}{2\sqrt{3}} z_1 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_1 + y_1 + z_1) c \hat{\mathbf{z}}$	(6f)	Be I
$\mathbf{B}_2$	$z_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	$= \frac{1}{2} (-y_1 + z_1) a \hat{\mathbf{x}} + \left( \frac{1}{\sqrt{3}} x_1 - \frac{1}{2\sqrt{3}} y_1 - \frac{1}{2\sqrt{3}} z_1 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_1 + y_1 + z_1) c \hat{\mathbf{z}}$	(6f)	Be I
$\mathbf{B}_3$	$y_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$= \frac{1}{2} (-x_1 + y_1) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_1 - \frac{1}{2\sqrt{3}} y_1 + \frac{1}{\sqrt{3}} z_1 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_1 + y_1 + z_1) c \hat{\mathbf{z}}$	(6f)	Be I
$\mathbf{B}_4$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= \frac{1}{2} (-x_1 + z_1) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_1 - \frac{1}{\sqrt{3}} y_1 + \frac{1}{2\sqrt{3}} z_1 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_1 + y_1 + z_1) c \hat{\mathbf{z}}$	(6f)	Be I
$\mathbf{B}_5$	$-z_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	$= \frac{1}{2} (y_1 - z_1) a \hat{\mathbf{x}} + \left( -\frac{1}{\sqrt{3}} x_1 + \frac{1}{2\sqrt{3}} y_1 + \frac{1}{2\sqrt{3}} z_1 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_1 + y_1 + z_1) c \hat{\mathbf{z}}$	(6f)	Be I
$\mathbf{B}_6$	$-y_1 \mathbf{a}_1 - z_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$= \frac{1}{2} (x_1 - y_1) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_1 + \frac{1}{2\sqrt{3}} y_1 - \frac{1}{\sqrt{3}} z_1 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_1 + y_1 + z_1) c \hat{\mathbf{z}}$	(6f)	Be I
$\mathbf{B}_7$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2} (x_2 - z_2) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_2 + \frac{1}{\sqrt{3}} y_2 - \frac{1}{2\sqrt{3}} z_2 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_2 + y_2 + z_2) c \hat{\mathbf{z}}$	(6f)	Be II
$\mathbf{B}_8$	$z_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + y_2 \mathbf{a}_3$	$= \frac{1}{2} (-y_2 + z_2) a \hat{\mathbf{x}} + \left( \frac{1}{\sqrt{3}} x_2 - \frac{1}{2\sqrt{3}} y_2 - \frac{1}{2\sqrt{3}} z_2 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_2 + y_2 + z_2) c \hat{\mathbf{z}}$	(6f)	Be II
$\mathbf{B}_9$	$y_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$= \frac{1}{2} (-x_2 + y_2) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_2 - \frac{1}{2\sqrt{3}} y_2 + \frac{1}{\sqrt{3}} z_2 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_2 + y_2 + z_2) c \hat{\mathbf{z}}$	(6f)	Be II
$\mathbf{B}_{10}$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$= \frac{1}{2} (-x_2 + z_2) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_2 - \frac{1}{\sqrt{3}} y_2 + \frac{1}{2\sqrt{3}} z_2 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_2 + y_2 + z_2) c \hat{\mathbf{z}}$	(6f)	Be II
$\mathbf{B}_{11}$	$-z_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - y_2 \mathbf{a}_3$	$= \frac{1}{2} (y_2 - z_2) a \hat{\mathbf{x}} + \left( -\frac{1}{\sqrt{3}} x_2 + \frac{1}{2\sqrt{3}} y_2 + \frac{1}{2\sqrt{3}} z_2 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_2 + y_2 + z_2) c \hat{\mathbf{z}}$	(6f)	Be II
$\mathbf{B}_{12}$	$-y_2 \mathbf{a}_1 - z_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$= \frac{1}{2} (x_2 - y_2) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_2 + \frac{1}{2\sqrt{3}} y_2 - \frac{1}{\sqrt{3}} z_2 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_2 + y_2 + z_2) c \hat{\mathbf{z}}$	(6f)	Be II
$\mathbf{B}_{13}$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2} (x_3 - z_3) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_3 + \frac{1}{\sqrt{3}} y_3 - \frac{1}{2\sqrt{3}} z_3 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_3 + y_3 + z_3) c \hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B}_{14}$	$z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$= \frac{1}{2} (-y_3 + z_3) a \hat{\mathbf{x}} + \left( \frac{1}{\sqrt{3}} x_3 - \frac{1}{2\sqrt{3}} y_3 - \frac{1}{2\sqrt{3}} z_3 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_3 + y_3 + z_3) c \hat{\mathbf{z}}$	(6f)	O I



$$\begin{aligned}
\mathbf{B}_{15} &= y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3 = \frac{1}{2}(-x_3 + y_3) a \hat{\mathbf{x}} + & (6f) & \quad \text{O I} \\
&\quad \left(-\frac{1}{2\sqrt{3}}x_3 - \frac{1}{2\sqrt{3}}y_3 + \frac{1}{\sqrt{3}}z_3\right) a \hat{\mathbf{y}} + \\
&\quad \frac{1}{3}(x_3 + y_3 + z_3) c \hat{\mathbf{z}} \\
\mathbf{B}_{16} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = \frac{1}{2}(-x_3 + z_3) a \hat{\mathbf{x}} + \left(\frac{1}{2\sqrt{3}}x_3 - \frac{1}{\sqrt{3}}y_3 + \frac{1}{2\sqrt{3}}z_3\right) a \hat{\mathbf{y}} - & (6f) & \quad \text{O I} \\
&\quad \frac{1}{3}(x_3 + y_3 + z_3) c \hat{\mathbf{z}} \\
\mathbf{B}_{17} &= -z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3 = \frac{1}{2}(y_3 - z_3) a \hat{\mathbf{x}} + \left(-\frac{1}{\sqrt{3}}x_3 + \frac{1}{2\sqrt{3}}y_3 + \frac{1}{2\sqrt{3}}z_3\right) a \hat{\mathbf{y}} - & (6f) & \quad \text{O I} \\
&\quad \frac{1}{3}(x_3 + y_3 + z_3) c \hat{\mathbf{z}} \\
\mathbf{B}_{18} &= -y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3 = \frac{1}{2}(x_3 - y_3) a \hat{\mathbf{x}} + \left(\frac{1}{2\sqrt{3}}x_3 + \frac{1}{2\sqrt{3}}y_3 - \frac{1}{\sqrt{3}}z_3\right) a \hat{\mathbf{y}} - & (6f) & \quad \text{O I} \\
&\quad \frac{1}{3}(x_3 + y_3 + z_3) c \hat{\mathbf{z}} \\
\mathbf{B}_{19} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = \frac{1}{2}(x_4 - z_4) a \hat{\mathbf{x}} + \left(-\frac{1}{2\sqrt{3}}x_4 + \frac{1}{\sqrt{3}}y_4 - \frac{1}{2\sqrt{3}}z_4\right) a \hat{\mathbf{y}} + & (6f) & \quad \text{O II} \\
&\quad \frac{1}{3}(x_4 + y_4 + z_4) c \hat{\mathbf{z}} \\
\mathbf{B}_{20} &= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3 = \frac{1}{2}(-y_4 + z_4) a \hat{\mathbf{x}} + \left(\frac{1}{\sqrt{3}}x_4 - \frac{1}{2\sqrt{3}}y_4 - \frac{1}{2\sqrt{3}}z_4\right) a \hat{\mathbf{y}} + & (6f) & \quad \text{O II} \\
&\quad \frac{1}{3}(x_4 + y_4 + z_4) c \hat{\mathbf{z}} \\
\mathbf{B}_{21} &= y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 = \frac{1}{2}(-x_4 + y_4) a \hat{\mathbf{x}} + & (6f) & \quad \text{O II} \\
&\quad \left(-\frac{1}{2\sqrt{3}}x_4 - \frac{1}{2\sqrt{3}}y_4 + \frac{1}{\sqrt{3}}z_4\right) a \hat{\mathbf{y}} + \\
&\quad \frac{1}{3}(x_4 + y_4 + z_4) c \hat{\mathbf{z}} \\
\mathbf{B}_{22} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = \frac{1}{2}(-x_4 + z_4) a \hat{\mathbf{x}} + \left(\frac{1}{2\sqrt{3}}x_4 - \frac{1}{\sqrt{3}}y_4 + \frac{1}{2\sqrt{3}}z_4\right) a \hat{\mathbf{y}} - & (6f) & \quad \text{O II} \\
&\quad \frac{1}{3}(x_4 + y_4 + z_4) c \hat{\mathbf{z}} \\
\mathbf{B}_{23} &= -z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3 = \frac{1}{2}(y_4 - z_4) a \hat{\mathbf{x}} + \left(-\frac{1}{\sqrt{3}}x_4 + \frac{1}{2\sqrt{3}}y_4 + \frac{1}{2\sqrt{3}}z_4\right) a \hat{\mathbf{y}} - & (6f) & \quad \text{O II} \\
&\quad \frac{1}{3}(x_4 + y_4 + z_4) c \hat{\mathbf{z}} \\
\mathbf{B}_{24} &= -y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3 = \frac{1}{2}(x_4 - y_4) a \hat{\mathbf{x}} + \left(\frac{1}{2\sqrt{3}}x_4 + \frac{1}{2\sqrt{3}}y_4 - \frac{1}{\sqrt{3}}z_4\right) a \hat{\mathbf{y}} - & (6f) & \quad \text{O II} \\
&\quad \frac{1}{3}(x_4 + y_4 + z_4) c \hat{\mathbf{z}} \\
\mathbf{B}_{25} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \frac{1}{2}(x_5 - z_5) a \hat{\mathbf{x}} + \left(-\frac{1}{2\sqrt{3}}x_5 + \frac{1}{\sqrt{3}}y_5 - \frac{1}{2\sqrt{3}}z_5\right) a \hat{\mathbf{y}} + & (6f) & \quad \text{O III} \\
&\quad \frac{1}{3}(x_5 + y_5 + z_5) c \hat{\mathbf{z}} \\
\mathbf{B}_{26} &= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3 = \frac{1}{2}(-y_5 + z_5) a \hat{\mathbf{x}} + \left(\frac{1}{\sqrt{3}}x_5 - \frac{1}{2\sqrt{3}}y_5 - \frac{1}{2\sqrt{3}}z_5\right) a \hat{\mathbf{y}} + & (6f) & \quad \text{O III} \\
&\quad \frac{1}{3}(x_5 + y_5 + z_5) c \hat{\mathbf{z}} \\
\mathbf{B}_{27} &= y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3 = \frac{1}{2}(-x_5 + y_5) a \hat{\mathbf{x}} + & (6f) & \quad \text{O III} \\
&\quad \left(-\frac{1}{2\sqrt{3}}x_5 - \frac{1}{2\sqrt{3}}y_5 + \frac{1}{\sqrt{3}}z_5\right) a \hat{\mathbf{y}} + \\
&\quad \frac{1}{3}(x_5 + y_5 + z_5) c \hat{\mathbf{z}} \\
\mathbf{B}_{28} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = \frac{1}{2}(-x_5 + z_5) a \hat{\mathbf{x}} + \left(\frac{1}{2\sqrt{3}}x_5 - \frac{1}{\sqrt{3}}y_5 + \frac{1}{2\sqrt{3}}z_5\right) a \hat{\mathbf{y}} - & (6f) & \quad \text{O III} \\
&\quad \frac{1}{3}(x_5 + y_5 + z_5) c \hat{\mathbf{z}} \\
\mathbf{B}_{29} &= -z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3 = \frac{1}{2}(y_5 - z_5) a \hat{\mathbf{x}} + \left(-\frac{1}{\sqrt{3}}x_5 + \frac{1}{2\sqrt{3}}y_5 + \frac{1}{2\sqrt{3}}z_5\right) a \hat{\mathbf{y}} - & (6f) & \quad \text{O III} \\
&\quad \frac{1}{3}(x_5 + y_5 + z_5) c \hat{\mathbf{z}} \\
\mathbf{B}_{30} &= -y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3 = \frac{1}{2}(x_5 - y_5) a \hat{\mathbf{x}} + \left(\frac{1}{2\sqrt{3}}x_5 + \frac{1}{2\sqrt{3}}y_5 - \frac{1}{\sqrt{3}}z_5\right) a \hat{\mathbf{y}} - & (6f) & \quad \text{O III} \\
&\quad \frac{1}{3}(x_5 + y_5 + z_5) c \hat{\mathbf{z}} \\
\mathbf{B}_{31} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \frac{1}{2}(x_6 - z_6) a \hat{\mathbf{x}} + \left(-\frac{1}{2\sqrt{3}}x_6 + \frac{1}{\sqrt{3}}y_6 - \frac{1}{2\sqrt{3}}z_6\right) a \hat{\mathbf{y}} + & (6f) & \quad \text{O IV} \\
&\quad \frac{1}{3}(x_6 + y_6 + z_6) c \hat{\mathbf{z}} \\
\mathbf{B}_{32} &= z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3 = \frac{1}{2}(-y_6 + z_6) a \hat{\mathbf{x}} + \left(\frac{1}{\sqrt{3}}x_6 - \frac{1}{2\sqrt{3}}y_6 - \frac{1}{2\sqrt{3}}z_6\right) a \hat{\mathbf{y}} + & (6f) & \quad \text{O IV} \\
&\quad \frac{1}{3}(x_6 + y_6 + z_6) c \hat{\mathbf{z}}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{33} &= y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3 = \frac{1}{2} (-x_6 + y_6) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_6 - \frac{1}{2\sqrt{3}} y_6 + \frac{1}{\sqrt{3}} z_6 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_6 + y_6 + z_6) c \hat{\mathbf{z}} & (6f) & \text{O IV} \\
\mathbf{B}_{34} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = \frac{1}{2} (-x_6 + z_6) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_6 - \frac{1}{\sqrt{3}} y_6 + \frac{1}{2\sqrt{3}} z_6 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_6 + y_6 + z_6) c \hat{\mathbf{z}} & (6f) & \text{O IV} \\
\mathbf{B}_{35} &= -z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - y_6 \mathbf{a}_3 = \frac{1}{2} (y_6 - z_6) a \hat{\mathbf{x}} + \left( -\frac{1}{\sqrt{3}} x_6 + \frac{1}{2\sqrt{3}} y_6 + \frac{1}{2\sqrt{3}} z_6 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_6 + y_6 + z_6) c \hat{\mathbf{z}} & (6f) & \text{O IV} \\
\mathbf{B}_{36} &= -y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3 = \frac{1}{2} (x_6 - y_6) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_6 + \frac{1}{2\sqrt{3}} y_6 - \frac{1}{\sqrt{3}} z_6 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_6 + y_6 + z_6) c \hat{\mathbf{z}} & (6f) & \text{O IV} \\
\mathbf{B}_{37} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = \frac{1}{2} (x_7 - z_7) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_7 + \frac{1}{\sqrt{3}} y_7 - \frac{1}{2\sqrt{3}} z_7 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_7 + y_7 + z_7) c \hat{\mathbf{z}} & (6f) & \text{Si} \\
\mathbf{B}_{38} &= z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3 = \frac{1}{2} (-y_7 + z_7) a \hat{\mathbf{x}} + \left( \frac{1}{\sqrt{3}} x_7 - \frac{1}{2\sqrt{3}} y_7 - \frac{1}{2\sqrt{3}} z_7 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_7 + y_7 + z_7) c \hat{\mathbf{z}} & (6f) & \text{Si} \\
\mathbf{B}_{39} &= y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3 = \frac{1}{2} (-x_7 + y_7) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_7 - \frac{1}{2\sqrt{3}} y_7 + \frac{1}{\sqrt{3}} z_7 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_7 + y_7 + z_7) c \hat{\mathbf{z}} & (6f) & \text{Si} \\
\mathbf{B}_{40} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 = \frac{1}{2} (-x_7 + z_7) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_7 - \frac{1}{\sqrt{3}} y_7 + \frac{1}{2\sqrt{3}} z_7 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_7 + y_7 + z_7) c \hat{\mathbf{z}} & (6f) & \text{Si} \\
\mathbf{B}_{41} &= -z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - y_7 \mathbf{a}_3 = \frac{1}{2} (y_7 - z_7) a \hat{\mathbf{x}} + \left( -\frac{1}{\sqrt{3}} x_7 + \frac{1}{2\sqrt{3}} y_7 + \frac{1}{2\sqrt{3}} z_7 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_7 + y_7 + z_7) c \hat{\mathbf{z}} & (6f) & \text{Si} \\
\mathbf{B}_{42} &= -y_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3 = \frac{1}{2} (x_7 - y_7) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_7 + \frac{1}{2\sqrt{3}} y_7 - \frac{1}{\sqrt{3}} z_7 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_7 + y_7 + z_7) c \hat{\mathbf{z}} & (6f) & \text{Si}
\end{aligned}$$

---

### References:

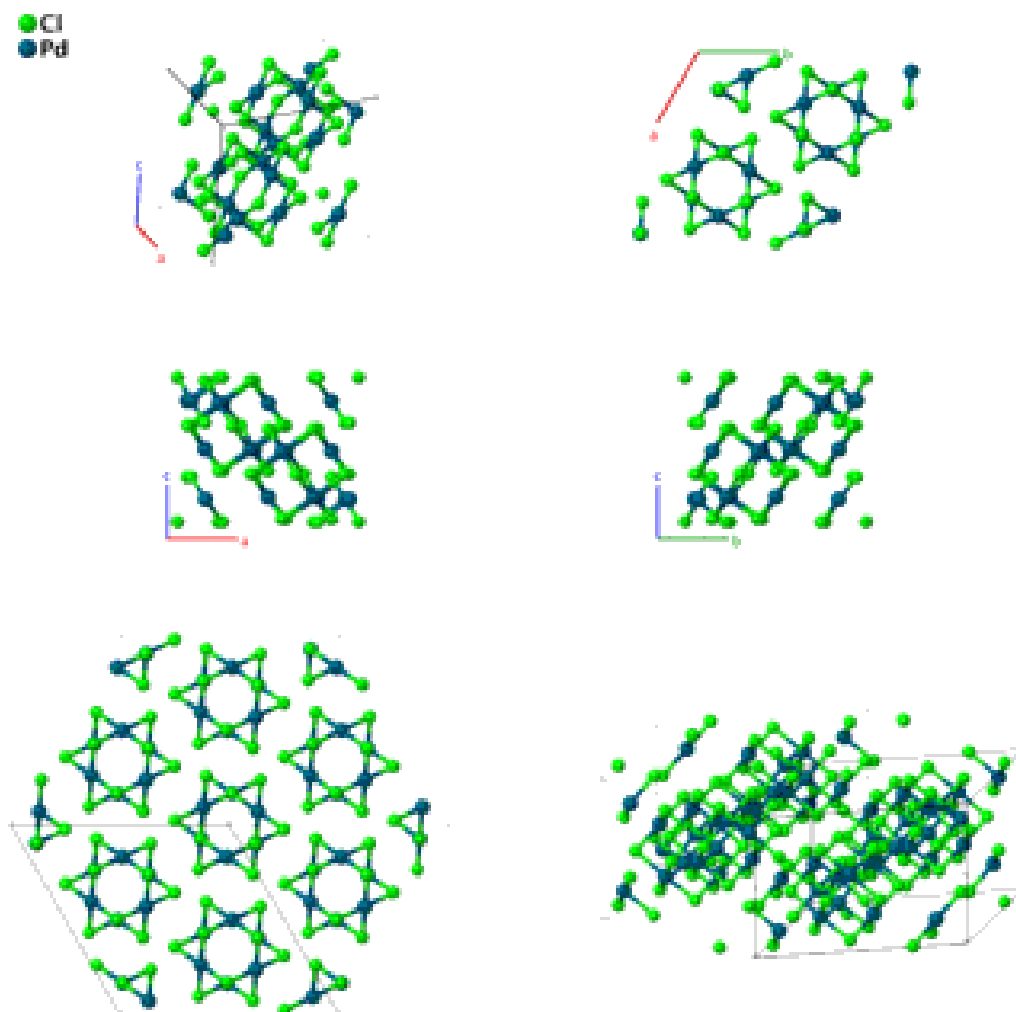
- R. M. Hazen and L. W. Finger, *High-Temperature Crystal Chemistry of Phenakite (Be<sub>2</sub>SiO<sub>4</sub>) and Chrysoberyl (BeAl<sub>2</sub>O<sub>4</sub>)*, Phys. Chem. Miner. **14**, 426–434 (1987), [doi:10.1007/BF00628819](https://doi.org/10.1007/BF00628819).

---

### Geometry files:

- CIF: pp. [909](#)  
- POSCAR: pp. [909](#)

# $\beta$ -PdCl<sub>2</sub> Structure: A2B\_hR18\_148\_2f\_f

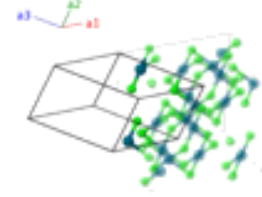


<b>Prototype</b>	:	$\beta$ -PdCl <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_hR18_148_2f_f
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hR18
<b>Space group number</b>	:	148
<b>Space group symbol</b>	:	$R\bar{3}$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A2B_hR18_148_2f_f [--hex]</code> <code>--params=a, c/a, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub></code>

- (Dell'Amico, 1996) did the original assessment of the crystal structure of  $\beta$ -PdCl<sub>2</sub>, but it is difficult to determine the Wyckoff positions from this paper. We relied on (Villars, 2010) for the Wyckoff positions.

## Rhombohedral primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{2} (x_1 - z_1) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_1 + \frac{1}{\sqrt{3}} y_1 - \frac{1}{2\sqrt{3}} z_1 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_1 + y_1 + z_1) c \hat{\mathbf{z}}$	(6f)	Cl I
$\mathbf{B}_2$	$z_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	$= \frac{1}{2} (-y_1 + z_1) a \hat{\mathbf{x}} + \left( \frac{1}{\sqrt{3}} x_1 - \frac{1}{2\sqrt{3}} y_1 - \frac{1}{2\sqrt{3}} z_1 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_1 + y_1 + z_1) c \hat{\mathbf{z}}$	(6f)	Cl I
$\mathbf{B}_3$	$y_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$= \frac{1}{2} (-x_1 + y_1) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_1 - \frac{1}{2\sqrt{3}} y_1 + \frac{1}{\sqrt{3}} z_1 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_1 + y_1 + z_1) c \hat{\mathbf{z}}$	(6f)	Cl I
$\mathbf{B}_4$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= \frac{1}{2} (-x_1 + z_1) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_1 - \frac{1}{\sqrt{3}} y_1 + \frac{1}{2\sqrt{3}} z_1 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_1 + y_1 + z_1) c \hat{\mathbf{z}}$	(6f)	Cl I
$\mathbf{B}_5$	$-z_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	$= \frac{1}{2} (y_1 - z_1) a \hat{\mathbf{x}} + \left( -\frac{1}{\sqrt{3}} x_1 + \frac{1}{2\sqrt{3}} y_1 + \frac{1}{2\sqrt{3}} z_1 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_1 + y_1 + z_1) c \hat{\mathbf{z}}$	(6f)	Cl I
$\mathbf{B}_6$	$-y_1 \mathbf{a}_1 - z_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$= \frac{1}{2} (x_1 - y_1) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_1 + \frac{1}{2\sqrt{3}} y_1 - \frac{1}{\sqrt{3}} z_1 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_1 + y_1 + z_1) c \hat{\mathbf{z}}$	(6f)	Cl I
$\mathbf{B}_7$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2} (x_2 - z_2) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_2 + \frac{1}{\sqrt{3}} y_2 - \frac{1}{2\sqrt{3}} z_2 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_2 + y_2 + z_2) c \hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B}_8$	$z_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + y_2 \mathbf{a}_3$	$= \frac{1}{2} (-y_2 + z_2) a \hat{\mathbf{x}} + \left( \frac{1}{\sqrt{3}} x_2 - \frac{1}{2\sqrt{3}} y_2 - \frac{1}{2\sqrt{3}} z_2 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_2 + y_2 + z_2) c \hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B}_9$	$y_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$= \frac{1}{2} (-x_2 + y_2) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_2 - \frac{1}{2\sqrt{3}} y_2 + \frac{1}{\sqrt{3}} z_2 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_2 + y_2 + z_2) c \hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B}_{10}$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$= \frac{1}{2} (-x_2 + z_2) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_2 - \frac{1}{\sqrt{3}} y_2 + \frac{1}{2\sqrt{3}} z_2 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_2 + y_2 + z_2) c \hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B}_{11}$	$-z_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - y_2 \mathbf{a}_3$	$= \frac{1}{2} (y_2 - z_2) a \hat{\mathbf{x}} + \left( -\frac{1}{\sqrt{3}} x_2 + \frac{1}{2\sqrt{3}} y_2 + \frac{1}{2\sqrt{3}} z_2 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_2 + y_2 + z_2) c \hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B}_{12}$	$-y_2 \mathbf{a}_1 - z_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$= \frac{1}{2} (x_2 - y_2) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_2 + \frac{1}{2\sqrt{3}} y_2 - \frac{1}{\sqrt{3}} z_2 \right) a \hat{\mathbf{y}} - \frac{1}{3} (x_2 + y_2 + z_2) c \hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B}_{13}$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2} (x_3 - z_3) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_3 + \frac{1}{\sqrt{3}} y_3 - \frac{1}{2\sqrt{3}} z_3 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_3 + y_3 + z_3) c \hat{\mathbf{z}}$	(6f)	Pd
$\mathbf{B}_{14}$	$z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$= \frac{1}{2} (-y_3 + z_3) a \hat{\mathbf{x}} + \left( \frac{1}{\sqrt{3}} x_3 - \frac{1}{2\sqrt{3}} y_3 - \frac{1}{2\sqrt{3}} z_3 \right) a \hat{\mathbf{y}} + \frac{1}{3} (x_3 + y_3 + z_3) c \hat{\mathbf{z}}$	(6f)	Pd

$$\begin{aligned}
\mathbf{B}_{15} &= y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3 = \frac{1}{2} (-x_3 + y_3) a \hat{\mathbf{x}} + & (6f) & \text{Pd} \\
&\quad \left( -\frac{1}{2\sqrt{3}} x_3 - \frac{1}{2\sqrt{3}} y_3 + \frac{1}{\sqrt{3}} z_3 \right) a \hat{\mathbf{y}} + \\
&\quad \frac{1}{3} (x_3 + y_3 + z_3) c \hat{\mathbf{z}} \\
\mathbf{B}_{16} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = \frac{1}{2} (-x_3 + z_3) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_3 - \frac{1}{\sqrt{3}} y_3 + \frac{1}{2\sqrt{3}} z_3 \right) a \hat{\mathbf{y}} - & (6f) & \text{Pd} \\
&\quad \frac{1}{3} (x_3 + y_3 + z_3) c \hat{\mathbf{z}} \\
\mathbf{B}_{17} &= -z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3 = \frac{1}{2} (y_3 - z_3) a \hat{\mathbf{x}} + \left( -\frac{1}{\sqrt{3}} x_3 + \frac{1}{2\sqrt{3}} y_3 + \frac{1}{2\sqrt{3}} z_3 \right) a \hat{\mathbf{y}} - & (6f) & \text{Pd} \\
&\quad \frac{1}{3} (x_3 + y_3 + z_3) c \hat{\mathbf{z}} \\
\mathbf{B}_{18} &= -y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3 = \frac{1}{2} (x_3 - y_3) a \hat{\mathbf{x}} + \left( \frac{1}{2\sqrt{3}} x_3 + \frac{1}{2\sqrt{3}} y_3 - \frac{1}{\sqrt{3}} z_3 \right) a \hat{\mathbf{y}} - & (6f) & \text{Pd} \\
&\quad \frac{1}{3} (x_3 + y_3 + z_3) c \hat{\mathbf{z}}
\end{aligned}$$

---

### References:

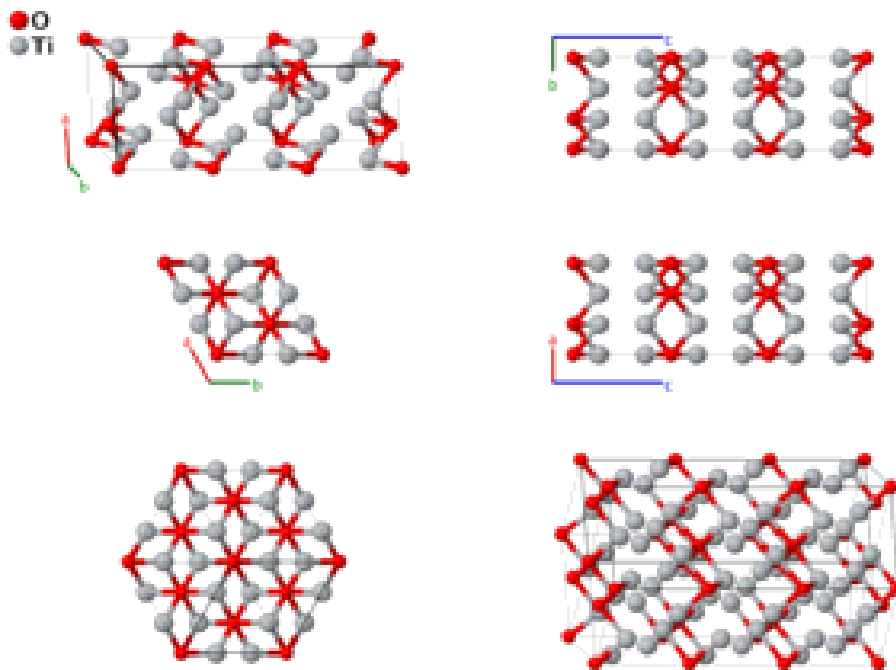
- D. B. Dell'Amico, F. Calderazzo, F. Marchetti, and S. Ramello, *Molecular Structure of [Pd<sub>6</sub>Cl<sub>12</sub>] in Single Crystals Chemically Grown at Room Temperature*, *Angew. Chem. Int. Ed.* **35**, 1331–1333 (1996), [doi:10.1002/anie.199613311](https://doi.org/10.1002/anie.199613311).
- P. Villars and K. Cenzual, eds., *Structure Types* (Springer, Berlin, Heidelberg, 2010), *Landolt-Börnstein – Group III Condensed Matter*, vol. 43A8, chap. Part 8: SpaceGroups (156) P3m1 – (148) R-3, [doi:10.1007/978-3-540-70892-6\\_423](https://doi.org/10.1007/978-3-540-70892-6_423).

---

### Geometry files:

- CIF: pp. [909](#)
- POSCAR: pp. [910](#)

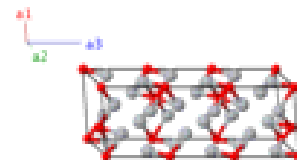
# Ti<sub>3</sub>O (Room-temperature) Structure: AB3\_hP24\_149\_acgi\_31



<b>Prototype</b>	:	Ti <sub>3</sub> O
<b>AFLOW prototype label</b>	:	AB3_hP24_149_acgi_31
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP24
<b>Space group number</b>	:	149
<b>Space group symbol</b>	:	<i>P</i> 312
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB3_hP24_149_acgi_31</code> <code>--params=<i>a</i>, <i>c/a</i>, <i>z</i><sub>3</sub>, <i>z</i><sub>4</sub>, <i>x</i><sub>5</sub>, <i>y</i><sub>5</sub>, <i>z</i><sub>5</sub>, <i>x</i><sub>6</sub>, <i>y</i><sub>6</sub>, <i>z</i><sub>6</sub>, <i>x</i><sub>7</sub>, <i>y</i><sub>7</sub>, <i>z</i><sub>7</sub></code>

## Trigonal Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	O I
<b>B<sub>2</sub></b>	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}}$	(1c)	O II
<b>B<sub>3</sub></b>	$z_3 \mathbf{a}_3$	=	$z_3 c \hat{\mathbf{z}}$	(2g)	O III
<b>B<sub>4</sub></b>	$-z_3 \mathbf{a}_3$	=	$-z_3 c \hat{\mathbf{z}}$	(2g)	O III

$$\begin{aligned}
\mathbf{B}_5 &= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (2i) && \text{O IV} \\
\mathbf{B}_6 &= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (2i) && \text{O IV} \\
\mathbf{B}_7 &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (6l) && \text{Ti I} \\
\mathbf{B}_8 &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \left(\frac{1}{2} x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (6l) && \text{Ti I} \\
\mathbf{B}_9 &= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \left(-x_5 + \frac{1}{2} y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} && (6l) && \text{Ti I} \\
\mathbf{B}_{10} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -\frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} && (6l) && \text{Ti I} \\
\mathbf{B}_{11} &= (-x_5 + y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= \left(-\frac{1}{2} x_5 + y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} && (6l) && \text{Ti I} \\
\mathbf{B}_{12} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 &= \left(x_5 - \frac{1}{2} y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} && (6l) && \text{Ti I} \\
\mathbf{B}_{13} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \frac{1}{2} (x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_6 + y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} && (6l) && \text{Ti II} \\
\mathbf{B}_{14} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \left(\frac{1}{2} x_6 - y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} && (6l) && \text{Ti II} \\
\mathbf{B}_{15} &= (-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \left(-x_6 + \frac{1}{2} y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} && (6l) && \text{Ti II} \\
\mathbf{B}_{16} &= -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -\frac{1}{2} (x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_6 + y_6) a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} && (6l) && \text{Ti II} \\
\mathbf{B}_{17} &= (-x_6 + y_6) \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= \left(-\frac{1}{2} x_6 + y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} && (6l) && \text{Ti II} \\
\mathbf{B}_{18} &= x_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= \left(x_6 - \frac{1}{2} y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}} && (6l) && \text{Ti II} \\
\mathbf{B}_{19} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= \frac{1}{2} (x_7 + y_7) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_7 + y_7) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} && (6l) && \text{Ti III} \\
\mathbf{B}_{20} &= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= \left(\frac{1}{2} x_7 - y_7\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} && (6l) && \text{Ti III} \\
\mathbf{B}_{21} &= (-x_7 + y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= \left(-x_7 + \frac{1}{2} y_7\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} && (6l) && \text{Ti III} \\
\mathbf{B}_{22} &= -y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -\frac{1}{2} (x_7 + y_7) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_7 + y_7) a \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} && (6l) && \text{Ti III} \\
\mathbf{B}_{23} &= (-x_7 + y_7) \mathbf{a}_1 + y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= \left(-\frac{1}{2} x_7 + y_7\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_7 a \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} && (6l) && \text{Ti III} \\
\mathbf{B}_{24} &= x_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3 &= \left(x_7 - \frac{1}{2} y_7\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_7 a \hat{\mathbf{y}} - z_7 c \hat{\mathbf{z}} && (6l) && \text{Ti III}
\end{aligned}$$

---

#### References:

- A. Jostsons and A. S. Malin, *The ordered structure of Ti<sub>3</sub>O*, Acta Crystallogr. Sect. B Struct. Sci. **24**, 211–213 (1968), doi:10.1107/S0567740868001974.

#### Found in:

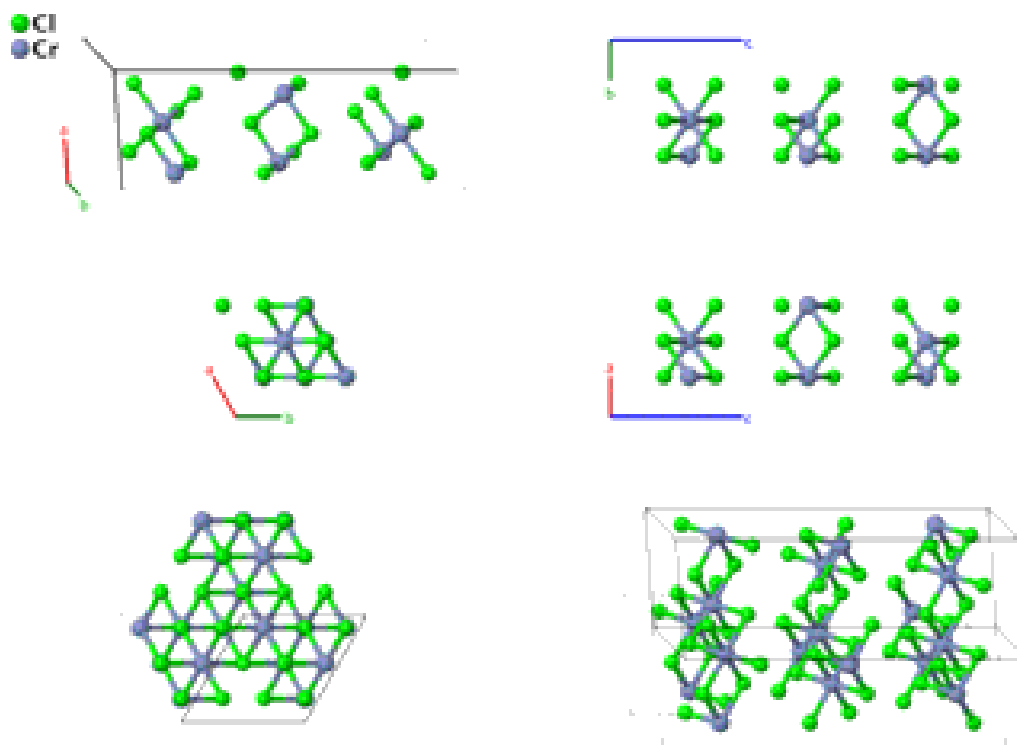
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 910  
- POSCAR: pp. 910

# CrCl<sub>3</sub> Structure: A3B\_hP24\_153\_3c\_2b

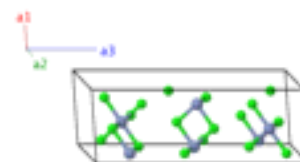


<b>Prototype</b>	:	CrCl <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B_hP24_153_3c_2b
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP24
<b>Space group number</b>	:	153
<b>Space group symbol</b>	:	$P3_212$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A3B_hP24_153_3c_2b</code> <code>--params=a, c/a, x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub></code>

- This structure is the enantiomorph of the [CrCl<sub>3</sub> \(D<sub>0</sub><sub>4</sub>, A3B\\_hP24\\_151\\_3c\\_2a\) structure](#), and was generated by reflecting the coordinates of the space group #151 structure through the  $z = 0$  plane.

## Trigonal Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{6} \mathbf{a}_3$	$= -\sqrt{3}x_1 a \hat{\mathbf{y}} + \frac{1}{6} c \hat{\mathbf{z}}$	(3b)	Cr I
$\mathbf{B}_2$	$= x_1 \mathbf{a}_1 + 2x_1 \mathbf{a}_2 + \frac{5}{6} \mathbf{a}_3$	$= \frac{3}{2}x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_1 a \hat{\mathbf{y}} + \frac{5}{6} c \hat{\mathbf{z}}$	(3b)	Cr I



$$\begin{aligned}
\mathbf{B}_3 &= -2x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -\frac{3}{2}x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_1 a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(3b) & \text{Cr I} \\
\mathbf{B}_4 &= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{6} \mathbf{a}_3 &= -\sqrt{3}x_2 a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}} &(3b) & \text{Cr II} \\
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{5}{6} \mathbf{a}_3 &= \frac{3}{2}x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \frac{5}{6}c \hat{\mathbf{z}} &(3b) & \text{Cr II} \\
\mathbf{B}_6 &= -2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -\frac{3}{2}x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(3b) & \text{Cr II} \\
\mathbf{B}_7 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + &(6c) & \text{Cl I} \\
& & \frac{\sqrt{3}}{2}(-x_3 + y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & & \\
\mathbf{B}_8 &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{2}{3} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2}x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + &(6c) & \text{Cl I} \\
& & \left(\frac{2}{3} + z_3\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_9 &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{3} + z_3\right) \mathbf{a}_3 &= \left(-x_3 + \frac{1}{2}y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + &(6c) & \text{Cl I} \\
& & \left(\frac{1}{3} + z_3\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{10} &= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{3} - z_3\right) \mathbf{a}_3 &= -\frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + &(6c) & \text{Cl I} \\
& & \frac{\sqrt{3}}{2}(-x_3 + y_3) a \hat{\mathbf{y}} + \left(\frac{1}{3} - z_3\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{11} &= (-x_3 + y_3) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{2}{3} - z_3\right) \mathbf{a}_3 &= \left(-\frac{1}{2}x_3 + y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + &(6c) & \text{Cl I} \\
& & \left(\frac{2}{3} - z_3\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{12} &= x_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3 &= \left(x_3 - \frac{1}{2}y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} &(6c) & \text{Cl I} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \frac{1}{2}(x_4 + y_4) a \hat{\mathbf{x}} + &(6c) & \text{Cl II} \\
& & \frac{\sqrt{3}}{2}(-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & & \\
\mathbf{B}_{14} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{2}{3} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2}x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + &(6c) & \text{Cl II} \\
& & \left(\frac{2}{3} + z_4\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{15} &= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{3} + z_4\right) \mathbf{a}_3 &= \left(-x_4 + \frac{1}{2}y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} + &(6c) & \text{Cl II} \\
& & \left(\frac{1}{3} + z_4\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{16} &= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{3} - z_4\right) \mathbf{a}_3 &= -\frac{1}{2}(x_4 + y_4) a \hat{\mathbf{x}} + &(6c) & \text{Cl II} \\
& & \frac{\sqrt{3}}{2}(-x_4 + y_4) a \hat{\mathbf{y}} + \left(\frac{1}{3} - z_4\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{17} &= (-x_4 + y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{2}{3} - z_4\right) \mathbf{a}_3 &= \left(-\frac{1}{2}x_4 + y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + &(6c) & \text{Cl II} \\
& & \left(\frac{2}{3} - z_4\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{18} &= x_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \left(x_4 - \frac{1}{2}y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} &(6c) & \text{Cl II} \\
\mathbf{B}_{19} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + &(6c) & \text{Cl III} \\
& & \frac{\sqrt{3}}{2}(-x_5 + y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & & \\
\mathbf{B}_{20} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{2}{3} + z_5\right) \mathbf{a}_3 &= \left(\frac{1}{2}x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + &(6c) & \text{Cl III} \\
& & \left(\frac{2}{3} + z_5\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{21} &= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{3} + z_5\right) \mathbf{a}_3 &= \left(-x_5 + \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + &(6c) & \text{Cl III} \\
& & \left(\frac{1}{3} + z_5\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{22} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{3} - z_5\right) \mathbf{a}_3 &= -\frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + &(6c) & \text{Cl III} \\
& & \frac{\sqrt{3}}{2}(-x_5 + y_5) a \hat{\mathbf{y}} + \left(\frac{1}{3} - z_5\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{23} &= (-x_5 + y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{2}{3} - z_5\right) \mathbf{a}_3 &= \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + &(6c) & \text{Cl III} \\
& & \left(\frac{2}{3} - z_5\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{24} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 &= \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} &(6c) & \text{Cl III}
\end{aligned}$$

## References:

- N. Wooster, *The Structure of Chromium Trichloride CrCl<sub>3</sub>*, *Zeitschrift für Kristallographie - Crystalline Materials* **74**, 363–374 (1930), doi:10.1524/zkri.1930.74.1.363.

**Found in:**

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

---

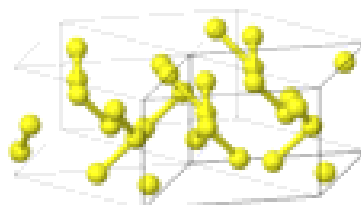
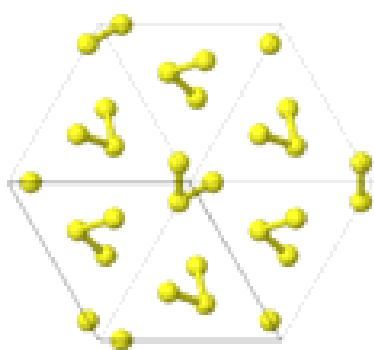
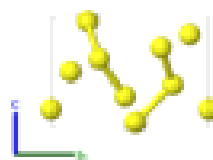
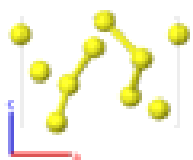
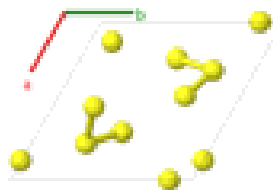
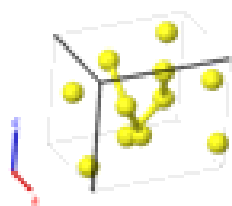
**Geometry files:**

- CIF: pp. [911](#)

- POSCAR: pp. [911](#)

# S-II Structure: A\_hP9\_154\_bc

● S

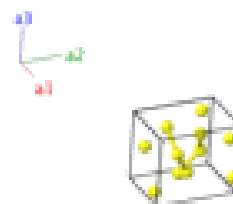


<b>Prototype</b>	:	S
<b>AFLOW prototype label</b>	:	A_hP9_154_bc
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP9
<b>Space group number</b>	:	154
<b>Space group symbol</b>	:	$P3_21$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A_hP9_154_bc --params=a, c/a, x1, x2, y2, z2</code>

- The S-II phase is found when sulfur heated and pressurized above 3 GPa. This data was taken at 5.8 GPa and 800 K.

**Trigonal Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{6} \mathbf{a}_3$	$=$	$\frac{1}{2}x_1 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_1 a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3b)	S I
$\mathbf{B}_2$	$= x_1 \mathbf{a}_2 + \frac{5}{6} \mathbf{a}_3$	$=$	$\frac{1}{2}x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_1 a \hat{\mathbf{y}} + \frac{5}{6}c \hat{\mathbf{z}}$	(3b)	S I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_1 a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3b)	S I
$\mathbf{B}_4$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}(x_2 + y_2) a \hat{\mathbf{x}} +$ $\frac{\sqrt{3}}{2}(-x_2 + y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6c)	S II
$\mathbf{B}_5$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{2}{3} + z_2\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2}x_2 - y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} +$ $\left(\frac{2}{3} + z_2\right) c \hat{\mathbf{z}}$	(6c)	S II
$\mathbf{B}_6$	$= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{3} + z_2\right) \mathbf{a}_3$	$=$	$\left(-x_2 + \frac{1}{2}y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} +$ $\left(\frac{1}{3} + z_2\right) c \hat{\mathbf{z}}$	(6c)	S II
$\mathbf{B}_7$	$= y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}(x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_2 - y_2) a \hat{\mathbf{y}} -$ $z_2 c \hat{\mathbf{z}}$	(6c)	S II
$\mathbf{B}_8$	$= (x_2 - y_2) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{3} - z_2\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2}x_2 - y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} +$ $\left(\frac{1}{3} - z_2\right) c \hat{\mathbf{z}}$	(6c)	S II
$\mathbf{B}_9$	$= -x_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + \left(\frac{2}{3} - z_2\right) \mathbf{a}_3$	$=$	$\left(-x_2 + \frac{1}{2}y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} +$ $\left(\frac{2}{3} - z_2\right) c \hat{\mathbf{z}}$	(6c)	S II

---

#### References:

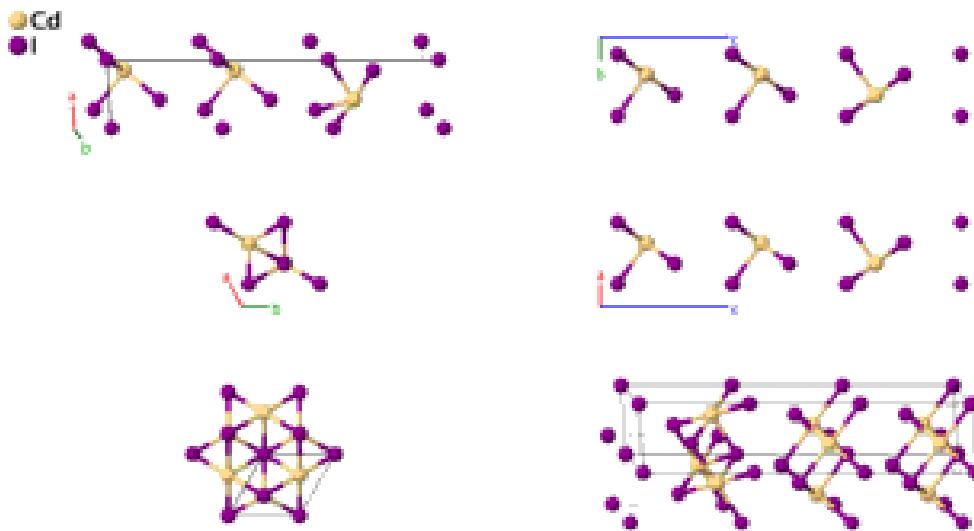
- O. Degtyareva, E. Gregoryanz, M. Somayazulu, P. Dera, H. Mao, and R. J. Hemley, *Novel chain structures in group VI elements*, Nat. Mater. **4**, 152–155 (2005), doi:10.1038/nmat1294.

---

#### Geometry files:

- CIF: pp. 911  
- POSCAR: pp. 911

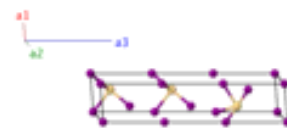
# CdI<sub>2</sub> (Polytype 6H<sub>1</sub>) Structure: AB2\_hP9\_156\_b2c\_3a2bc



<b>Prototype</b>	:	CdI <sub>2</sub>
<b>AFLOW prototype label</b>	:	AB2_hP9_156_b2c_3a2bc
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP9
<b>Space group number</b>	:	156
<b>Space group symbol</b>	:	<i>P3m1</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB2_hP9_156_b2c_3a2bc --params= <i>a, c/a, z<sub>1</sub>, z<sub>2</sub>, z<sub>3</sub>, z<sub>4</sub>, z<sub>5</sub>, z<sub>6</sub>, z<sub>7</sub>, z<sub>8</sub>, z<sub>9</sub></i>

## Trigonal Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(1a)	I I
<b>B<sub>2</sub></b>	= $z_2 \mathbf{a}_3$	=	$z_2 c \hat{\mathbf{z}}$	(1a)	I II
<b>B<sub>3</sub></b>	= $z_3 \mathbf{a}_3$	=	$z_3 c \hat{\mathbf{z}}$	(1a)	I III
<b>B<sub>4</sub></b>	= $\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(1b)	Cd I
<b>B<sub>5</sub></b>	= $\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(1b)	I IV
<b>B<sub>6</sub></b>	= $\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(1b)	I V
<b>B<sub>7</sub></b>	= $\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(1c)	Cd II
<b>B<sub>8</sub></b>	= $\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(1c)	Cd III

$$\mathbf{B}_9 = \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_9 \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}} \quad (1c) \quad \text{I VI}$$

---

**References:**

- R. S. Mitchell, *Polytypism of Cadmium Iodide and its Relationship to Screw Dislocations: I. Cadmium Iodide Polytypes*, *Zeitschrift für Kristallographie - Crystalline Materials* **108**, 296–315 (1956), [doi:10.1524/zkri.1956.108.3-4.296](https://doi.org/10.1524/zkri.1956.108.3-4.296).

**Found in:**

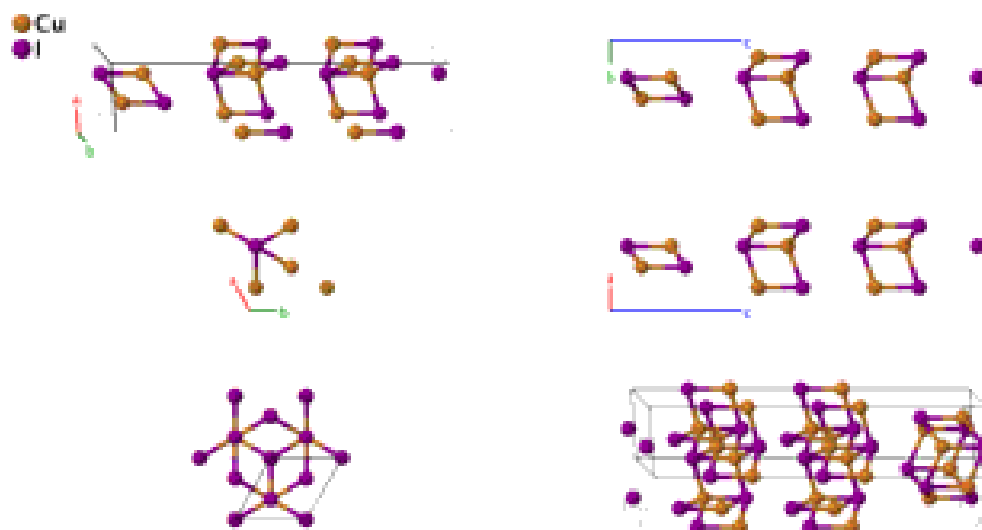
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [911](#)
- POSCAR: pp. [912](#)

# CuI Structure: AB\_hP12\_156\_2ab3c\_2ab3c



<b>Prototype</b>	:	CuI
<b>AFLOW prototype label</b>	:	AB_hP12_156_2ab3c_2ab3c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP12
<b>Space group number</b>	:	156
<b>Space group symbol</b>	:	$P3m1$
<b>AFLOW prototype command</b>	:	aflow --proto=AB_hP12_156_2ab3c_2ab3c --params= $a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8, z_9, z_{10}, z_{11}, z_{12}$

## Trigonal Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$= z_1 c \hat{\mathbf{z}}$	(1a)	Cu I
$\mathbf{B}_2$	$= z_2 \mathbf{a}_3$	$= z_2 c \hat{\mathbf{z}}$	(1a)	Cu II
$\mathbf{B}_3$	$= z_3 \mathbf{a}_3$	$= z_3 c \hat{\mathbf{z}}$	(1a)	I I
$\mathbf{B}_4$	$= z_4 \mathbf{a}_3$	$= z_4 c \hat{\mathbf{z}}$	(1a)	I II
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(1b)	Cu III
$\mathbf{B}_6$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(1b)	I III
$\mathbf{B}_7$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}}$	(1c)	Cu IV
$\mathbf{B}_8$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_8 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}}$	(1c)	Cu V
$\mathbf{B}_9$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_9 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}}$	(1c)	Cu VI

$$\mathbf{B}_{10} = \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + z_{10}\mathbf{a}_3 = \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2\sqrt{3}}a\hat{\mathbf{y}} + z_{10}c\hat{\mathbf{z}} \quad (1c) \quad \text{I IV}$$

$$\mathbf{B}_{11} = \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + z_{11}\mathbf{a}_3 = \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2\sqrt{3}}a\hat{\mathbf{y}} + z_{11}c\hat{\mathbf{z}} \quad (1c) \quad \text{I V}$$

$$\mathbf{B}_{12} = \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + z_{12}\mathbf{a}_3 = \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2\sqrt{3}}a\hat{\mathbf{y}} + z_{12}c\hat{\mathbf{z}} \quad (1c) \quad \text{I VI}$$

**References:**

- R. N. Kurdyumova and R. V. Baranova, *An electron diffraction study of thin films of cuprous iodide*, Sov. Phys. Crystallogr. **6**, 318–321 (1961).

**Found in:**

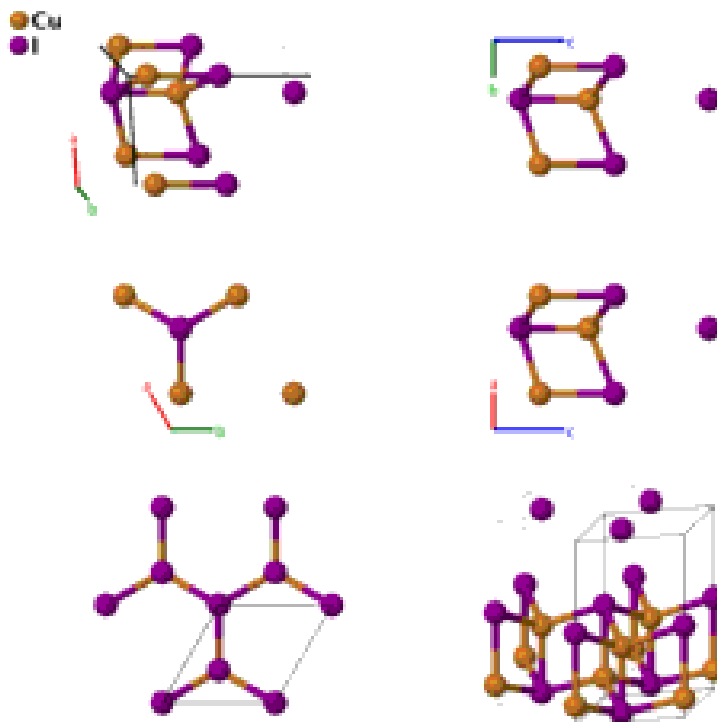
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [912](#)
- POSCAR: pp. [912](#)



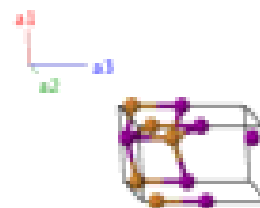
# $\beta$ -CuI Structure: AB\_hP4\_156\_ac\_ac



<b>Prototype</b>	:	$\beta$ -CuI
<b>AFLOW prototype label</b>	:	AB_hP4_156_ac_ac
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP4
<b>Space group number</b>	:	156
<b>Space group symbol</b>	:	$P3m1$
<b>AFLOW prototype command</b>	:	aflow --proto=AB_hP4_156_ac_ac --params=a, c/a, z <sub>1</sub> , z <sub>2</sub> , z <sub>3</sub> , z <sub>4</sub>

## Trigonal Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$= z_1 c \hat{\mathbf{z}}$	(1a)	Cu I
$\mathbf{B}_2$	$= z_2 \mathbf{a}_3$	$= z_2 c \hat{\mathbf{z}}$	(1a)	I I
$\mathbf{B}_3$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(1c)	Cu II
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(1c)	I II

---

**References:**

- T. Sakuma, *Crystal structure of  $\beta$ -CuI*, J. Phys. Soc. Jpn. **57**, 565–569 (1988), [doi:10.1143/JPSJ.57.565](https://doi.org/10.1143/JPSJ.57.565).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

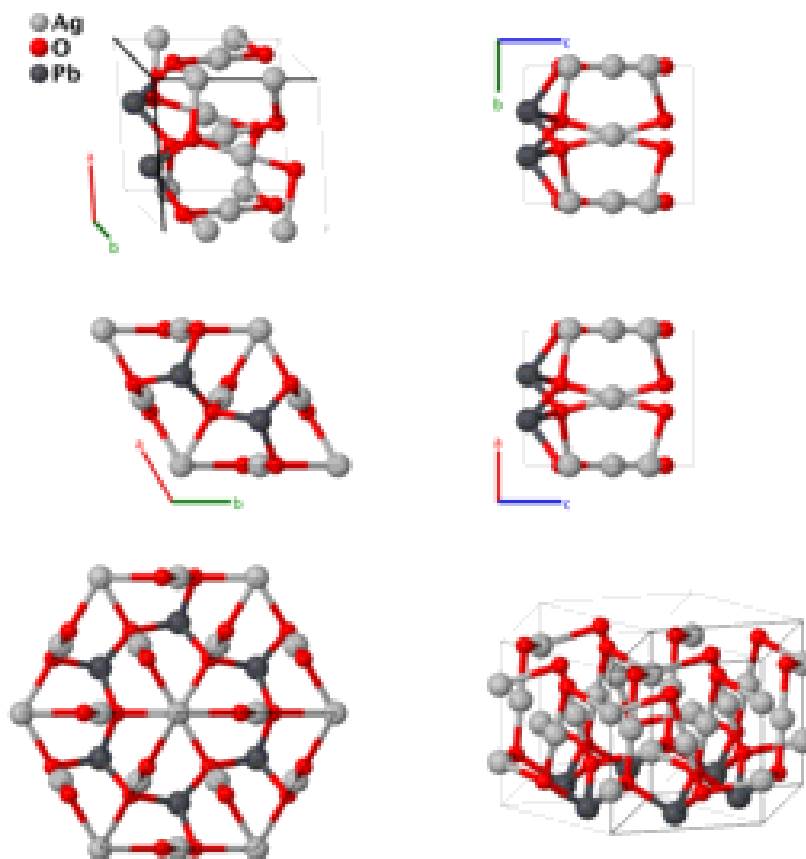
---

**Geometry files:**

- CIF: pp. [912](#)

- POSCAR: pp. [913](#)

# Ag<sub>5</sub>Pb<sub>2</sub>O<sub>6</sub> Structure: A5B6C2\_hP13\_157\_2ac\_2c\_b



<b>Prototype</b>	:	Ag <sub>5</sub> Pb <sub>2</sub> O <sub>6</sub>
<b>AFLOW prototype label</b>	:	A5B6C2_hP13_157_2ac_2c_b
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP13
<b>Space group number</b>	:	157
<b>Space group symbol</b>	:	<i>P</i> 31 <i>m</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A5B6C2_hP13_157_2ac_2c_b --params= <i>a, c/a, z<sub>1</sub>, z<sub>2</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, z<sub>6</sub></i>

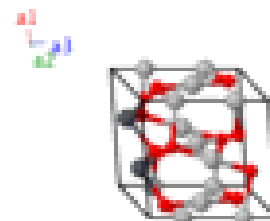
- The original reference (Byström, 1950) lists this structure as Ag<sub>5</sub>Pb<sub>2</sub>O<sub>6</sub>, while (Villars, 1985) lists it as Ag<sub>2</sub>PbO<sub>3</sub>. (Byström, 1950) provides three Wyckoff positions for Ag (1a, 1a, and 3c), while (Villars, 195) only provides two (1a and 3c), giving rise to the stoichiometry discrepancy. While both descriptions yield space group #157, the authors use the structure and coordinates provided by the original reference (Byström, 1950).

**Trigonal Hexagonal primitive vectors:**

$$\mathbf{a}_1 = \frac{1}{2} a \hat{x} - \frac{\sqrt{3}}{2} a \hat{y}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{x} + \frac{\sqrt{3}}{2} a \hat{y}$$

$$\mathbf{a}_3 = c \hat{z}$$



---

**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	=	$z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(1a) Ag I
$\mathbf{B}_2$	=	$z_2 \mathbf{a}_3$	=	$z_2 c \hat{\mathbf{z}}$	(1a) Ag II
$\mathbf{B}_3$	=	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2b) Pb
$\mathbf{B}_4$	=	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2b) Pb
$\mathbf{B}_5$	=	$x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3$	=	$\frac{1}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(3c) Ag III
$\mathbf{B}_6$	=	$x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(3c) Ag III
$\mathbf{B}_7$	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$-x_4 a \hat{\mathbf{x}} + z_4 c \hat{\mathbf{z}}$	(3c) Ag III
$\mathbf{B}_8$	=	$x_5 \mathbf{a}_1 + z_5 \mathbf{a}_3$	=	$\frac{1}{2} x_5 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(3c) O I
$\mathbf{B}_9$	=	$x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\frac{1}{2} x_5 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(3c) O I
$\mathbf{B}_{10}$	=	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$-x_5 a \hat{\mathbf{x}} + z_5 c \hat{\mathbf{z}}$	(3c) O I
$\mathbf{B}_{11}$	=	$x_6 \mathbf{a}_1 + z_6 \mathbf{a}_3$	=	$\frac{1}{2} x_6 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(3c) O II
$\mathbf{B}_{12}$	=	$x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$\frac{1}{2} x_6 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(3c) O II
$\mathbf{B}_{13}$	=	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$-x_6 a \hat{\mathbf{x}} + z_6 c \hat{\mathbf{z}}$	(3c) O II

---

**References:**

- A. Byström and L. Evers, *The Crystal Structures of  $\text{Ag}_2\text{PbO}_2$  and  $\text{Ag}_5\text{Pb}_2\text{O}_6$* , Acta Chem. Scand. **4**, 613–627 (1950), [doi:10.3891/acta.chem.scand.04-0613](https://doi.org/10.3891/acta.chem.scand.04-0613).

**Found in:**

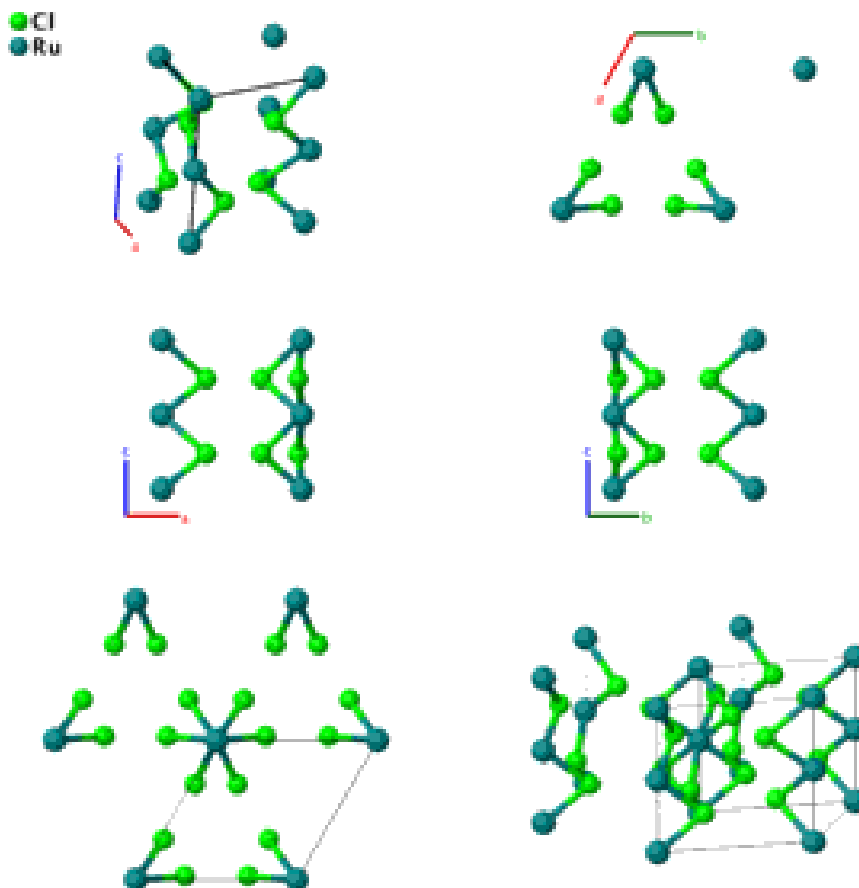
- P. Villars and L. D. Calvert, eds., *Pearson's Handbook of Crystallographic Data for Intermetallic Phases*, vol. 1 (American Society of Metals, Materials Park, Ohio, 1985).

---

**Geometry files:**

- CIF: pp. 913
- POSCAR: pp. 913

# $\beta$ -RuCl<sub>3</sub> Structure: A3B\_hP8\_158\_d\_a

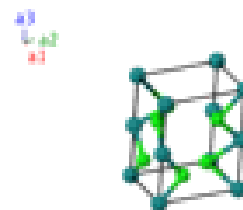


<b>Prototype</b>	:	$\beta$ -RuCl <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B_hP8_158_d_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP8
<b>Space group number</b>	:	158
<b>Space group symbol</b>	:	$P3c1$
<b>AFLOW prototype command</b>	:	aflow --proto=A3B_hP8_158_d_a --params= $a, c/a, z_1, x_2, y_2, z_2$

- Pearson comments that space groups #185, #188, #193, could not be rejected, but this structure is consistent with space group #158. We also provide the structure with space group #185: [β-RuCl<sub>3</sub> \(A3B\\_hP8\\_185\\_c\\_a\) structure](#).

**Trigonal Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{x} - \frac{\sqrt{3}}{2} a \hat{y} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{x} + \frac{\sqrt{3}}{2} a \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$z_1 c \hat{\mathbf{z}}$	(2a)	Ru
$\mathbf{B}_2$	$= \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Ru
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}(x_2 + y_2) a \hat{\mathbf{x}} +$ $\frac{\sqrt{3}}{2}(-x_2 + y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	Cl
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\left(\frac{1}{2}x_2 - y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	Cl
$\mathbf{B}_5$	$= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\left(-x_2 + \frac{1}{2}y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	Cl
$\mathbf{B}_6$	$= -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}(x_2 + y_2) a \hat{\mathbf{x}} +$ $\frac{\sqrt{3}}{2}(-x_2 + y_2) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(6d)	Cl
$\mathbf{B}_7$	$= (-x_2 + y_2) \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$\left(-\frac{1}{2}x_2 + y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(6d)	Cl
$\mathbf{B}_8$	$= x_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$\left(x_2 - \frac{1}{2}y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(6d)	Cl

---

#### References:

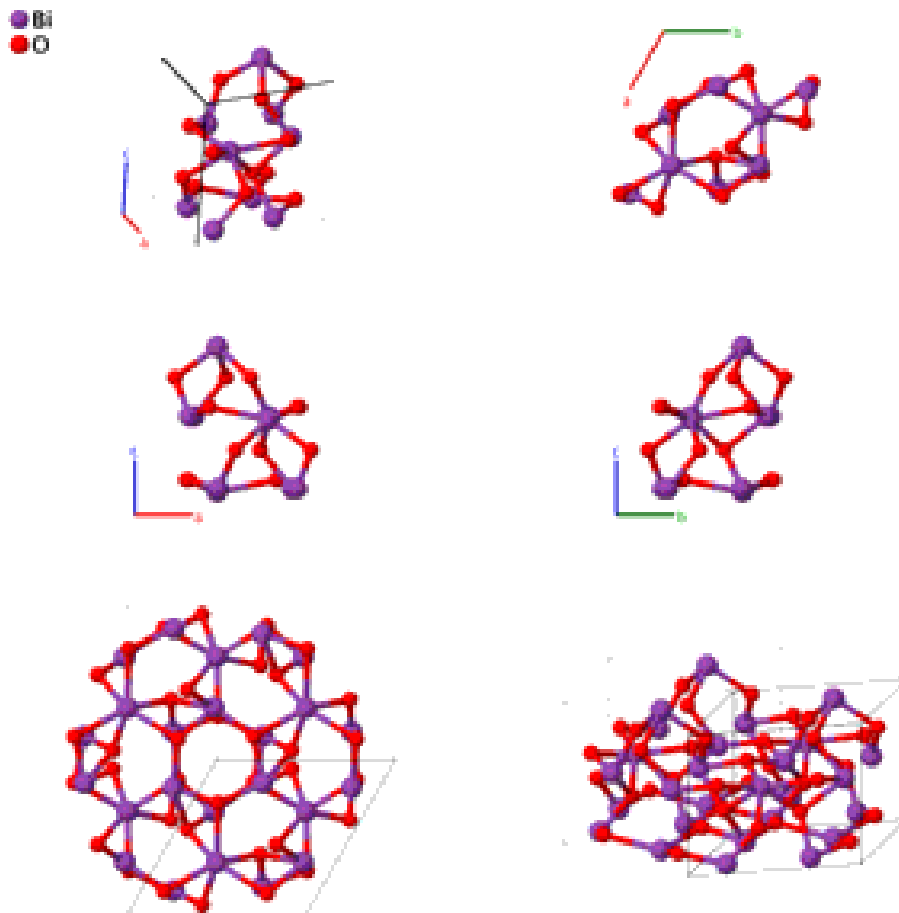
- J. M. Fletcher, W. E. Gardner, A. C. Fox, and G. Topping, *X-Ray, infrared, and magnetic studies of  $\alpha$ - and  $\beta$ -ruthenium trichloride*, J. Chem. Soc. A pp. 1038–1045 (1967), [doi:10.1039/J19670001038](https://doi.org/10.1039/J19670001038).

---

#### Geometry files:

- CIF: pp. 913  
- POSCAR: pp. 913

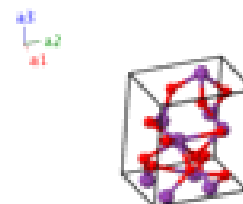
# Bi<sub>2</sub>O<sub>3</sub> (High-pressure) Structure: A2B3\_hP20\_159\_bc\_2c



<b>Prototype</b>	:	Bi <sub>2</sub> O <sub>3</sub>
<b>AFLOW prototype label</b>	:	A2B3_hP20_159_bc_2c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP20
<b>Space group number</b>	:	159
<b>Space group symbol</b>	:	<i>P</i> 31 <i>c</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3_hP20_159_bc_2c --params= <i>a</i> , <i>c/a</i> , <i>z</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>y</i> <sub>2</sub> , <i>z</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub>

## Trigonal Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(2b)	Bi I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2b)	Bi I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} +$ $\frac{\sqrt{3}}{2} (-x_2 + y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(\frac{1}{2} x_2 - y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B}_5$	$= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(-x_2 + \frac{1}{2} y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B}_6$	$= y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_2 - y_2) a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B}_7$	$= (x_2 - y_2) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \left(\frac{1}{2} x_2 - y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B}_8$	$= -x_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \left(-x_2 + \frac{1}{2} y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_2 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} +$ $\frac{\sqrt{3}}{2} (-x_3 + y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_{10}$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(\frac{1}{2} x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_{11}$	$= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(-x_3 + \frac{1}{2} y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_{12}$	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$= \frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_3 - y_3) a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_{13}$	$= (x_3 - y_3) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$= \left(\frac{1}{2} x_3 - y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_{14}$	$= -x_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$= \left(-x_3 + \frac{1}{2} y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_{15}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} +$ $\frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B}_{16}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B}_{17}$	$= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B}_{18}$	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$= \frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_4 - y_4) a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B}_{19}$	$= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$= \left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B}_{20}$	$= -x_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$= \left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(6c)	O II

#### References:

- T. Locherer, D. L. V. K. Prasad, R. Dinnebier, U. Wedig, M. Jansen, G. Garbarino, and T. Hansen, *High-pressure structural evolution of HP-Bi<sub>2</sub>O<sub>3</sub>*, Phys. Rev. B **83**, 214102 (2011), doi:10.1103/PhysRevB.83.214102.

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).



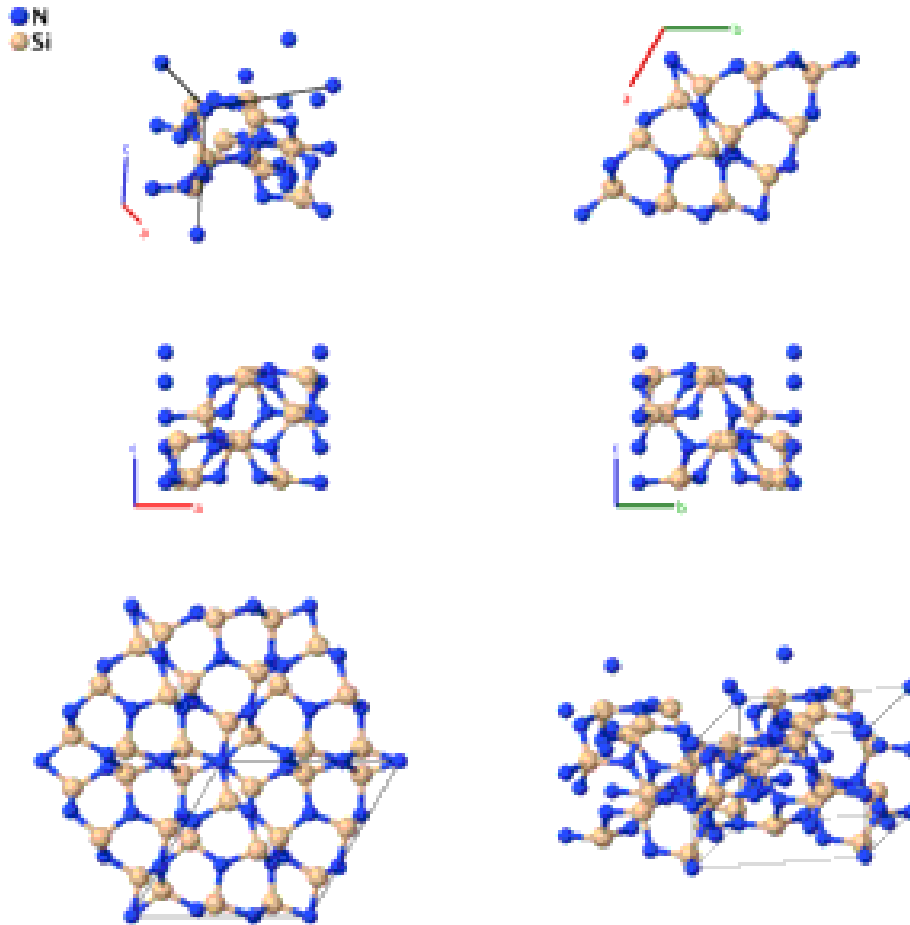
---

**Geometry files:**

- CIF: pp. [914](#)

- POSCAR: pp. [914](#)

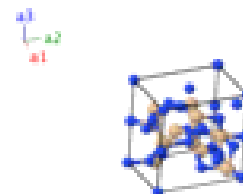
# Nierite ( $\alpha$ -Si<sub>3</sub>N<sub>4</sub>) Structure: A4B3\_hP28\_159\_ab2c\_2c



<b>Prototype</b>	:	$\alpha$ -Si <sub>3</sub> N <sub>4</sub>
<b>AFLOW prototype label</b>	:	A4B3_hP28_159_ab2c_2c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP28
<b>Space group number</b>	:	159
<b>Space group symbol</b>	:	<i>P</i> 31 <i>c</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A4B3_hP28_159_ab2c_2c</code> <code>--params=a, c/a, z1, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6</code>

## Trigonal Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type

$$\begin{aligned}
\mathbf{B}_1 &= z_1 \mathbf{a}_3 &= z_1 c \hat{\mathbf{z}} & (2a) & \text{N I} \\
\mathbf{B}_2 &= \left(\frac{1}{2} + z_1\right) \mathbf{a}_3 &= \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}} & (2a) & \text{N I} \\
\mathbf{B}_3 &= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (2b) & \text{N II} \\
\mathbf{B}_4 &= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (2b) & \text{N II} \\
\mathbf{B}_5 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + & (6c) & \text{N III} \\
&& \frac{\sqrt{3}}{2} (-x_3 + y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & & \\
\mathbf{B}_6 &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \left(\frac{1}{2} x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (6c) & \text{N III} \\
\mathbf{B}_7 &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \left(-x_3 + \frac{1}{2} y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (6c) & \text{N III} \\
\mathbf{B}_8 &= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_3 - y_3) a \hat{\mathbf{y}} + & (6c) & \text{N III} \\
&& \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_9 &= (x_3 - y_3) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} x_3 - y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + & (6c) & \text{N III} \\
&& \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{10} &= -x_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(-x_3 + \frac{1}{2} y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + & (6c) & \text{N III} \\
&& \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{11} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + & (6c) & \text{N IV} \\
&& \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & & \\
\mathbf{B}_{12} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (6c) & \text{N IV} \\
\mathbf{B}_{13} &= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (6c) & \text{N IV} \\
\mathbf{B}_{14} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_4 - y_4) a \hat{\mathbf{y}} + & (6c) & \text{N IV} \\
&& \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{15} &= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + & (6c) & \text{N IV} \\
&& \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{16} &= -x_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + & (6c) & \text{N IV} \\
&& \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{17} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + & (6c) & \text{Si I} \\
&& \frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & & \\
\mathbf{B}_{18} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \left(\frac{1}{2} x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (6c) & \text{Si I} \\
\mathbf{B}_{19} &= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \left(-x_5 + \frac{1}{2} y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (6c) & \text{Si I} \\
\mathbf{B}_{20} &= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_5 - y_5) a \hat{\mathbf{y}} + & (6c) & \text{Si I} \\
&& \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{21} &= (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \left(\frac{1}{2} x_5 - y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + & (6c) & \text{Si I} \\
&& \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{22} &= -x_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \left(-x_5 + \frac{1}{2} y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} + & (6c) & \text{Si I} \\
&& \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{23} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \frac{1}{2} (x_6 + y_6) a \hat{\mathbf{x}} + & (6c) & \text{Si II} \\
&& \frac{\sqrt{3}}{2} (-x_6 + y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & & \\
\mathbf{B}_{24} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \left(\frac{1}{2} x_6 - y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6c) & \text{Si II} \\
\mathbf{B}_{25} &= (-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \left(-x_6 + \frac{1}{2} y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6c) & \text{Si II} \\
\mathbf{B}_{26} &= y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 &= \frac{1}{2} (x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_6 - y_6) a \hat{\mathbf{y}} + & (6c) & \text{Si II} \\
&& \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} & &
\end{aligned}$$

$$\mathbf{B}_{27} = (x_6 - y_6) \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \left(\frac{1}{2}x_6 - y_6\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_6a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right)c \hat{\mathbf{z}} \quad (6c) \quad \text{Si II}$$

$$\mathbf{B}_{28} = -x_6 \mathbf{a}_1 + (-x_6 + y_6) \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \left(-x_6 + \frac{1}{2}y_6\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_6a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right)c \hat{\mathbf{z}} \quad (6c) \quad \text{Si II}$$

**References:**

- D. Hardie and K. H. Jack, *Crystal structures of silicon nitride*, Nature **180**, 332–333 (1957), doi:doi:10.1038/180332a0.

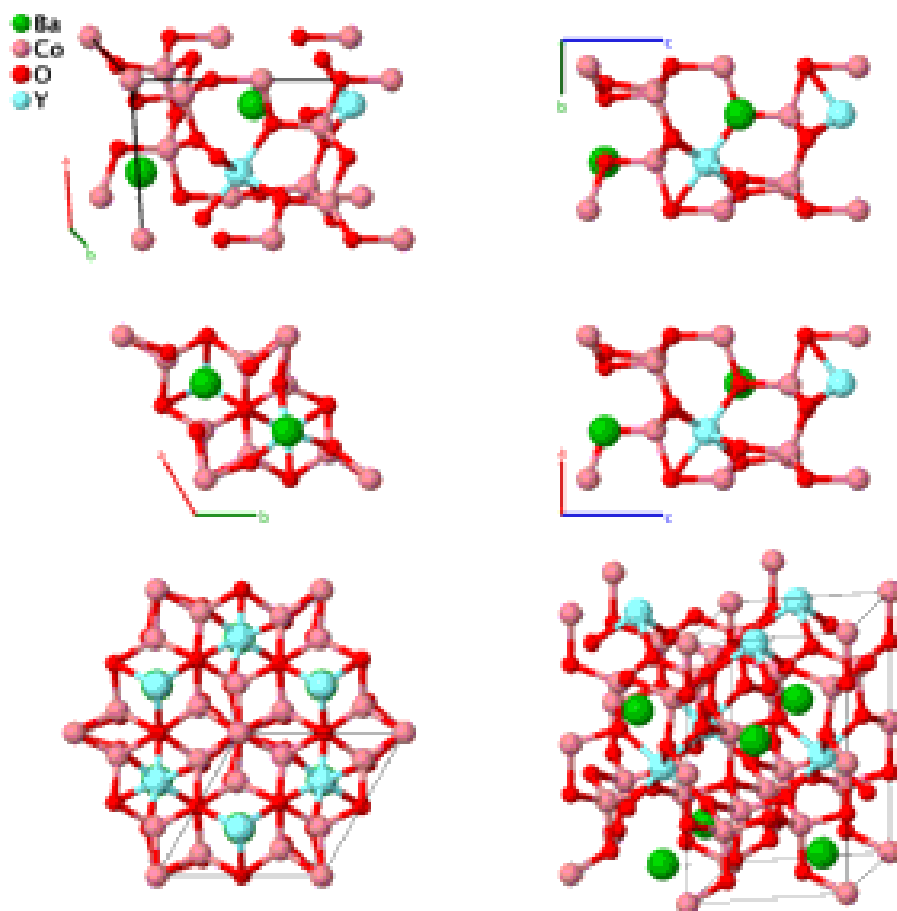
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [914](#)  
 - POSCAR: pp. [914](#)

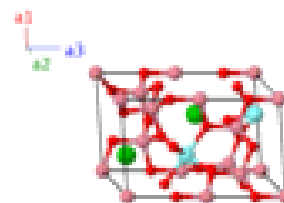
# YbBaCo<sub>4</sub>O<sub>7</sub> Structure: AB4C7D\_hP26\_159\_b\_ac\_a2c\_b



**Prototype** : YbBaCo<sub>4</sub>O<sub>7</sub>  
**AFLOW prototype label** : AB4C7D\_hP26\_159\_b\_ac\_a2c\_b  
**Strukturbericht designation** : None  
**Pearson symbol** : hP26  
**Space group number** : 159  
**Space group symbol** : *P31c*  
**AFLOW prototype command** : `aflow --proto=AB4C7D_hP26_159_b_ac_a2c_b`  
                                   `--params=a, c/a, z1, z2, z3, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7`

**Trigonal Hexagonal primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$z_1 c \hat{\mathbf{z}}$	(2a)	Co I

$$\begin{aligned}
\mathbf{B}_2 &= \left(\frac{1}{2} + z_1\right) \mathbf{a}_3 &= \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}} & (2a) & \text{Co I} \\
\mathbf{B}_3 &= z_2 \mathbf{a}_3 &= z_2 c \hat{\mathbf{z}} & (2a) & \text{O I} \\
\mathbf{B}_4 &= \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (2a) & \text{O I} \\
\mathbf{B}_5 &= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (2b) & \text{Ba} \\
\mathbf{B}_6 &= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (2b) & \text{Ba} \\
\mathbf{B}_7 &= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (2b) & \text{Y} \\
\mathbf{B}_8 &= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (2b) & \text{Y} \\
\mathbf{B}_9 &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + & (6c) & \text{Co II} \\
&& \frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & & \\
\mathbf{B}_{10} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \left(\frac{1}{2} x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (6c) & \text{Co II} \\
\mathbf{B}_{11} &= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \left(-x_5 + \frac{1}{2} y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (6c) & \text{Co II} \\
\mathbf{B}_{12} &= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_5 - y_5) a \hat{\mathbf{y}} + & (6c) & \text{Co II} \\
&& \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{13} &= (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \left(\frac{1}{2} x_5 - y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + & (6c) & \text{Co II} \\
&& \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{14} &= -x_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 &= \left(-x_5 + \frac{1}{2} y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} + & (6c) & \text{Co II} \\
&& \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{15} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \frac{1}{2} (x_6 + y_6) a \hat{\mathbf{x}} + & (6c) & \text{O II} \\
&& \frac{\sqrt{3}}{2} (-x_6 + y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & & \\
\mathbf{B}_{16} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \left(\frac{1}{2} x_6 - y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6c) & \text{O II} \\
\mathbf{B}_{17} &= (-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \left(-x_6 + \frac{1}{2} y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6c) & \text{O II} \\
\mathbf{B}_{18} &= y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 &= \frac{1}{2} (x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_6 - y_6) a \hat{\mathbf{y}} + & (6c) & \text{O II} \\
&& \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{19} &= (x_6 - y_6) \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 &= \left(\frac{1}{2} x_6 - y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + & (6c) & \text{O II} \\
&& \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{20} &= -x_6 \mathbf{a}_1 + (-x_6 + y_6) \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 &= \left(-x_6 + \frac{1}{2} y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_6 a \hat{\mathbf{y}} + & (6c) & \text{O II} \\
&& \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{21} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= \frac{1}{2} (x_7 + y_7) a \hat{\mathbf{x}} + & (6c) & \text{O III} \\
&& \frac{\sqrt{3}}{2} (-x_7 + y_7) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & & \\
\mathbf{B}_{22} &= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= \left(\frac{1}{2} x_7 - y_7\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (6c) & \text{O III} \\
\mathbf{B}_{23} &= (-x_7 + y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= \left(-x_7 + \frac{1}{2} y_7\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (6c) & \text{O III} \\
\mathbf{B}_{24} &= y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3 &= \frac{1}{2} (x_7 + y_7) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_7 - y_7) a \hat{\mathbf{y}} + & (6c) & \text{O III} \\
&& \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{25} &= (x_7 - y_7) \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3 &= \left(\frac{1}{2} x_7 - y_7\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_7 a \hat{\mathbf{y}} + & (6c) & \text{O III} \\
&& \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{26} &= -x_7 \mathbf{a}_1 + (-x_7 + y_7) \mathbf{a}_2 + \left(\frac{1}{2} + z_7\right) \mathbf{a}_3 &= \left(-x_7 + \frac{1}{2} y_7\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_7 a \hat{\mathbf{y}} + & (6c) & \text{O III} \\
&& \left(\frac{1}{2} + z_7\right) c \hat{\mathbf{z}} & &
\end{aligned}$$

## References:

- A. Huq, J. F. Mitchell, H. Zheng, L. C. Chapon, P. G. Radaelli, K. S. Knight, and P. W. Stephens, *Structural and magnetic*

*properties of the Kagomé antiferromagnet YbBaCo<sub>4</sub>O<sub>7</sub>*, J. Solid State Chem. **179**, 1136–1145 (2006),  
[doi:10.1016/j.jssc.2006.01.010](https://doi.org/10.1016/j.jssc.2006.01.010).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

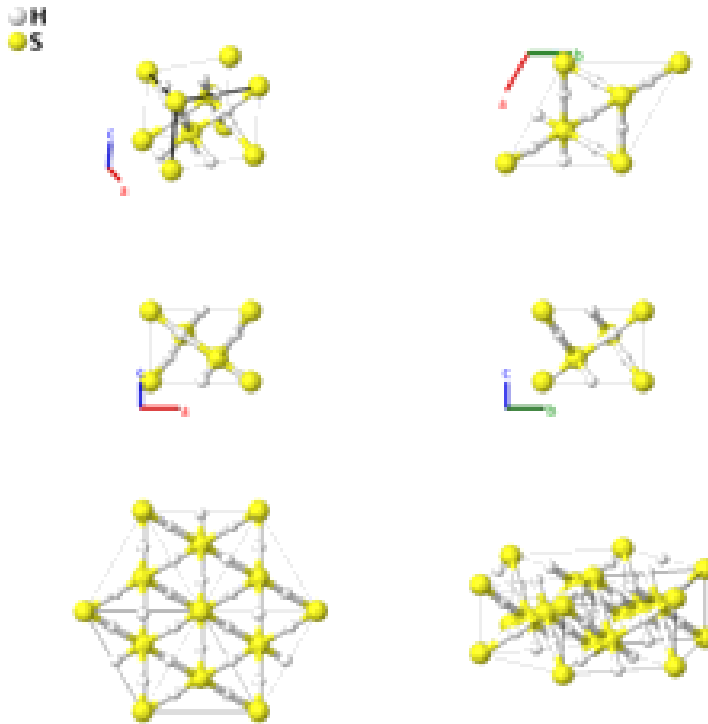
---

**Geometry files:**

- CIF: pp. [915](#)

- POSCAR: pp. [915](#)

# H<sub>3</sub>S (130 GPa) Structure: A3B\_hR4\_160\_b\_a

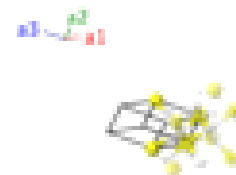


<b>Prototype</b>	:	H <sub>3</sub> S
<b>AFLOW prototype label</b>	:	A3B_hR4_160_b_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hR4
<b>Space group number</b>	:	160
<b>Space group symbol</b>	:	<i>R3m</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A3B_hR4_160_b_a [--hex] --params=a, c/a, x<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub></code>

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H<sub>3</sub>S for pressures between 90 and 150 GPa. When  $c/a \rightarrow \sqrt{8}$ ,  $x_2 \rightarrow 1/2$  and  $z_2 \rightarrow 0$  this structure continuously evolves into the cubic [200 GPa H<sub>3</sub>S Structure](#). The data presented here was computed at 130 GPa.

## Rhombohedral primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type



$$\mathbf{B}_1 = x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3 = x_1 c \hat{\mathbf{z}} \quad (1a) \quad \text{S}$$

$$\mathbf{B}_2 = x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 = \frac{1}{2} (x_2 - z_2) a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} (x_2 - z_2) a \hat{\mathbf{y}} + \left(\frac{2}{3}x_2 + \frac{1}{3}z_2\right) c \hat{\mathbf{z}} \quad (3b) \quad \text{H}$$

$$\mathbf{B}_3 = z_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3 = \frac{1}{2} (-x_2 + z_2) a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} (x_2 - z_2) a \hat{\mathbf{y}} + \left(\frac{2}{3}x_2 + \frac{1}{3}z_2\right) c \hat{\mathbf{z}} \quad (3b) \quad \text{H}$$

$$\mathbf{B}_4 = x_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 + x_2 \mathbf{a}_3 = \frac{1}{\sqrt{3}} (-x_2 + z_2) a \hat{\mathbf{y}} + \left(\frac{2}{3}x_2 + \frac{1}{3}z_2\right) c \hat{\mathbf{z}} \quad (3b) \quad \text{H}$$

### References:

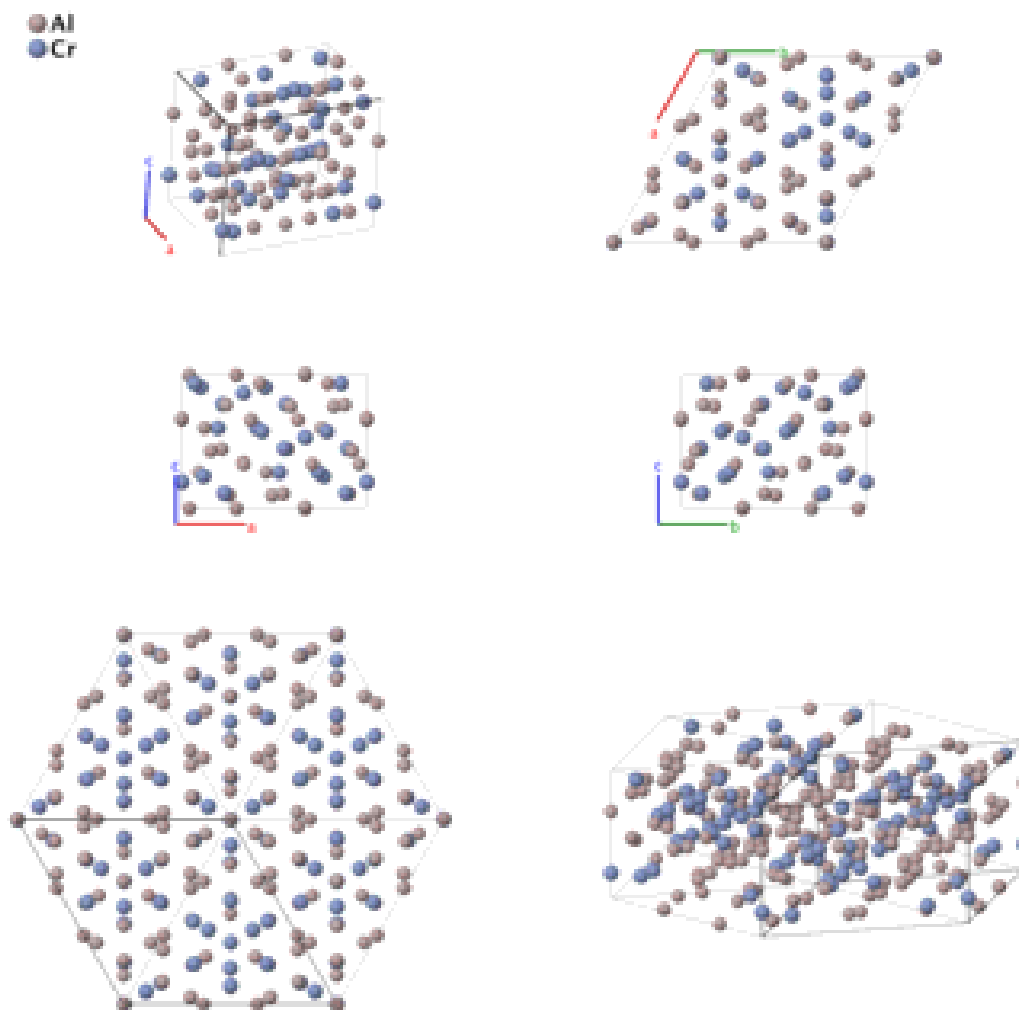
- D. Duan, Y. Liu, F. Tian, D. Li, X. Huang, Z. Zhao, H. Yu, B. Liu, W. Tian, and T. Cui, *Pressure-induced metallization of dense (H<sub>2</sub>S)<sub>2</sub>H<sub>2</sub> with high-T<sub>c</sub> superconductivity*, *Sci. Rep.* **4**, 6968 (2014), [doi:10.1038/srep06968](https://doi.org/10.1038/srep06968).

### Geometry files:

- CIF: pp. [915](#)

- POSCAR: pp. [916](#)

# Al<sub>8</sub>Cr<sub>5</sub> (*D*8<sub>10</sub>) Structure: A8B5\_hR26\_160\_a3bc\_a3b

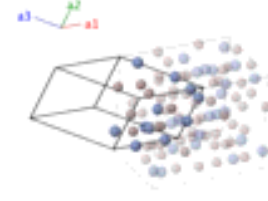


<b>Prototype</b>	:	Al <sub>8</sub> Cr <sub>5</sub>
<b>AFLOW prototype label</b>	:	A8B5_hR26_160_a3bc_a3b
<b>Strukturbericht designation</b>	:	<i>D</i> 8 <sub>10</sub>
<b>Pearson symbol</b>	:	hR26
<b>Space group number</b>	:	160
<b>Space group symbol</b>	:	<i>R</i> 3 <i>m</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A8B5_hR26_160_a3bc_a3b [--hex]</code> <code>--params=<i>a, c/a, x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>, y<sub>9</sub>, z<sub>9</sub></i></code>

- (Bradley, 1937) notes that the positions here are very close to the positions of the atoms in the  $\gamma$ -brass (Cu<sub>5</sub>Zn<sub>8</sub>, *D*8<sub>2</sub>) structure.

## Rhombohedral primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2\sqrt{3}}a\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2\sqrt{3}}a\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3 =$	$x_1 c \hat{\mathbf{z}}$	(1a)	Al I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3 =$	$x_2 c \hat{\mathbf{z}}$	(1a)	Cr I
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 =$	$\frac{1}{2}(x_3 - z_3)a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}(x_3 - z_3)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_3 + \frac{1}{3}z_3\right)c\hat{\mathbf{z}}$	(3b)	Al II
$\mathbf{B}_4$	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3 =$	$\frac{1}{2}(-x_3 + z_3)a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}(x_3 - z_3)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_3 + \frac{1}{3}z_3\right)c\hat{\mathbf{z}}$	(3b)	Al II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3 =$	$\frac{1}{\sqrt{3}}(-x_3 + z_3)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_3 + \frac{1}{3}z_3\right)c\hat{\mathbf{z}}$	(3b)	Al II
$\mathbf{B}_6$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 =$	$\frac{1}{2}(x_4 - z_4)a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}(x_4 - z_4)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_4 + \frac{1}{3}z_4\right)c\hat{\mathbf{z}}$	(3b)	Al III
$\mathbf{B}_7$	$= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 =$	$\frac{1}{2}(-x_4 + z_4)a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}(x_4 - z_4)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_4 + \frac{1}{3}z_4\right)c\hat{\mathbf{z}}$	(3b)	Al III
$\mathbf{B}_8$	$= x_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 =$	$\frac{1}{\sqrt{3}}(-x_4 + z_4)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_4 + \frac{1}{3}z_4\right)c\hat{\mathbf{z}}$	(3b)	Al III
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 =$	$\frac{1}{2}(x_5 - z_5)a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}(x_5 - z_5)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_5 + \frac{1}{3}z_5\right)c\hat{\mathbf{z}}$	(3b)	Al IV
$\mathbf{B}_{10}$	$= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3 =$	$\frac{1}{2}(-x_5 + z_5)a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}(x_5 - z_5)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_5 + \frac{1}{3}z_5\right)c\hat{\mathbf{z}}$	(3b)	Al IV
$\mathbf{B}_{11}$	$= x_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3 =$	$\frac{1}{\sqrt{3}}(-x_5 + z_5)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_5 + \frac{1}{3}z_5\right)c\hat{\mathbf{z}}$	(3b)	Al IV
$\mathbf{B}_{12}$	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 =$	$\frac{1}{2}(x_6 - z_6)a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}(x_6 - z_6)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_6 + \frac{1}{3}z_6\right)c\hat{\mathbf{z}}$	(3b)	Cr II
$\mathbf{B}_{13}$	$= z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3 =$	$\frac{1}{2}(-x_6 + z_6)a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}(x_6 - z_6)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_6 + \frac{1}{3}z_6\right)c\hat{\mathbf{z}}$	(3b)	Cr II
$\mathbf{B}_{14}$	$= x_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3 =$	$\frac{1}{\sqrt{3}}(-x_6 + z_6)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_6 + \frac{1}{3}z_6\right)c\hat{\mathbf{z}}$	(3b)	Cr II
$\mathbf{B}_{15}$	$= x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 =$	$\frac{1}{2}(x_7 - z_7)a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}(x_7 - z_7)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_7 + \frac{1}{3}z_7\right)c\hat{\mathbf{z}}$	(3b)	Cr III
$\mathbf{B}_{16}$	$= z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3 =$	$\frac{1}{2}(-x_7 + z_7)a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}(x_7 - z_7)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_7 + \frac{1}{3}z_7\right)c\hat{\mathbf{z}}$	(3b)	Cr III
$\mathbf{B}_{17}$	$= x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3 =$	$\frac{1}{\sqrt{3}}(-x_7 + z_7)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_7 + \frac{1}{3}z_7\right)c\hat{\mathbf{z}}$	(3b)	Cr III
$\mathbf{B}_{18}$	$= x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 =$	$\frac{1}{2}(x_8 - z_8)a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}(x_8 - z_8)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_8 + \frac{1}{3}z_8\right)c\hat{\mathbf{z}}$	(3b)	Cr IV
$\mathbf{B}_{19}$	$= z_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3 =$	$\frac{1}{2}(-x_8 + z_8)a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}(x_8 - z_8)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_8 + \frac{1}{3}z_8\right)c\hat{\mathbf{z}}$	(3b)	Cr IV
$\mathbf{B}_{20}$	$= x_8 \mathbf{a}_1 + z_8 \mathbf{a}_2 + x_8 \mathbf{a}_3 =$	$\frac{1}{\sqrt{3}}(-x_8 + z_8)a\hat{\mathbf{y}} + \left(\frac{2}{3}x_8 + \frac{1}{3}z_8\right)c\hat{\mathbf{z}}$	(3b)	Cr IV
$\mathbf{B}_{21}$	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 =$	$\frac{1}{2}(x_9 - z_9)a\hat{\mathbf{x}} + \left(-\frac{1}{2\sqrt{3}}x_9 + \frac{1}{\sqrt{3}}y_9 - \frac{1}{2\sqrt{3}}z_9\right)a\hat{\mathbf{y}} + \frac{1}{3}(x_9 + y_9 + z_9)c\hat{\mathbf{z}}$	(6c)	Al V

$$\mathbf{B}_{22} = z_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + y_9 \mathbf{a}_3 = \frac{1}{2}(-y_9 + z_9) a \hat{\mathbf{x}} + \left( \frac{1}{\sqrt{3}} x_9 - \frac{1}{2\sqrt{3}} y_9 - \frac{1}{2\sqrt{3}} z_9 \right) a \hat{\mathbf{y}} + \frac{1}{3}(x_9 + y_9 + z_9) c \hat{\mathbf{z}} \quad (6c) \quad \text{Al V}$$

$$\mathbf{B}_{23} = y_9 \mathbf{a}_1 + z_9 \mathbf{a}_2 + x_9 \mathbf{a}_3 = \frac{1}{2}(-x_9 + y_9) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_9 - \frac{1}{2\sqrt{3}} y_9 + \frac{1}{\sqrt{3}} z_9 \right) a \hat{\mathbf{y}} + \frac{1}{3}(x_9 + y_9 + z_9) c \hat{\mathbf{z}} \quad (6c) \quad \text{Al V}$$

$$\mathbf{B}_{24} = z_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + x_9 \mathbf{a}_3 = \frac{1}{2}(-x_9 + z_9) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_9 + \frac{1}{\sqrt{3}} y_9 - \frac{1}{2\sqrt{3}} z_9 \right) a \hat{\mathbf{y}} + \frac{1}{3}(x_9 + y_9 + z_9) c \hat{\mathbf{z}} \quad (6c) \quad \text{Al V}$$

$$\mathbf{B}_{25} = y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = \frac{1}{2}(y_9 - z_9) a \hat{\mathbf{x}} + \left( \frac{1}{\sqrt{3}} x_9 - \frac{1}{2\sqrt{3}} y_9 - \frac{1}{2\sqrt{3}} z_9 \right) a \hat{\mathbf{y}} + \frac{1}{3}(x_9 + y_9 + z_9) c \hat{\mathbf{z}} \quad (6c) \quad \text{Al V}$$

$$\mathbf{B}_{26} = x_9 \mathbf{a}_1 + z_9 \mathbf{a}_2 + y_9 \mathbf{a}_3 = \frac{1}{2}(x_9 - y_9) a \hat{\mathbf{x}} + \left( -\frac{1}{2\sqrt{3}} x_9 - \frac{1}{2\sqrt{3}} y_9 + \frac{1}{\sqrt{3}} z_9 \right) a \hat{\mathbf{y}} + \frac{1}{3}(x_9 + y_9 + z_9) c \hat{\mathbf{z}} \quad (6c) \quad \text{Al V}$$

### References:

- A. J. Bradley and S. S. Lu, *The Crystal Structures of Cr<sub>2</sub>Al and Cr<sub>5</sub>Al<sub>8</sub>*, *Z. Kristallogr.* **96**, 20–37 (1937), [doi:10.1524/zkri.1937.96.1.20](https://doi.org/10.1524/zkri.1937.96.1.20).

### Found in:

- S. Grazulis, *Crystal Data* (2014). Crystallography-online.com.

### Geometry files:

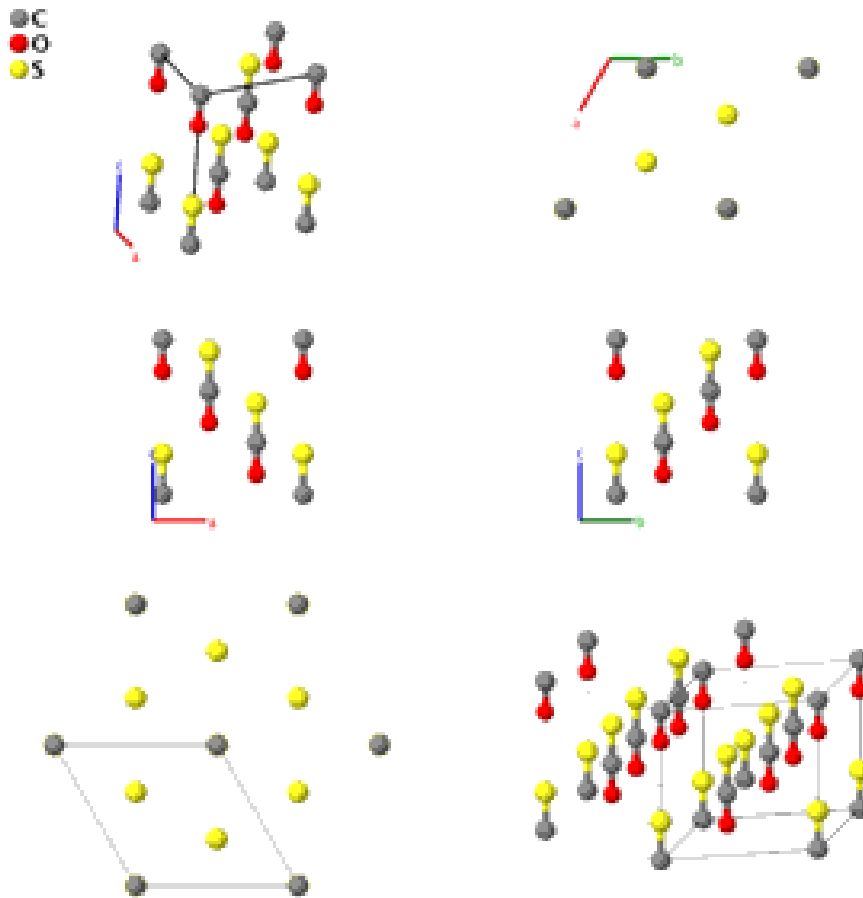
- CIF: pp. [916](#)

- POSCAR: pp. [916](#)

# Carbonyl Sulphide (COS, $F0_2$ ) Structure:

ABC\_hR3\_160\_a\_a\_a

---



<b>Prototype</b>	:	COS
<b>AFLOW prototype label</b>	:	ABC_hR3_160_a_a_a
<b>Strukturbericht designation</b>	:	$F0_2$
<b>Pearson symbol</b>	:	hR3
<b>Space group number</b>	:	160
<b>Space group symbol</b>	:	$R3m$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=ABC_hR3_160_a_a_a [--hex] --params=<math>a, c/a, x_1, x_2, x_3</math></code>

---

- (Overell, 1982) does not give the Wyckoff positions directly. They are inferred from the C-O and C-S bond lengths. The experimental data was obtained at 90 K.

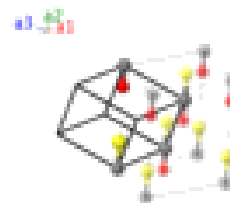
---

**Rhombohedral primitive vectors:**

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = -\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}}$$



---

**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$x_1 c \hat{\mathbf{z}}$	$(1a)$	C
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$x_2 c \hat{\mathbf{z}}$	$(1a)$	O
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$x_3 c \hat{\mathbf{z}}$	$(1a)$	S

---

**References:**

- J. S. W. Overell, G. S. Pawley, and B. M. Powell, *Powder refinement of carbonyl sulphide*, Acta Crystallogr. Sect. B Struct. Sci. **38**, 1121–1123 (1982), [doi:10.1107/S0567740882005111](https://doi.org/10.1107/S0567740882005111).

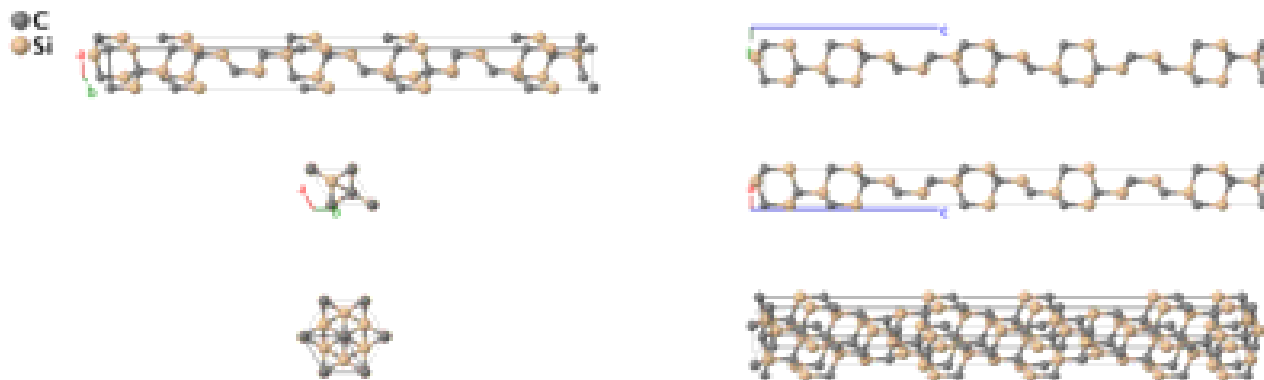
---

**Geometry files:**

- CIF: pp. [916](#)

- POSCAR: pp. [917](#)

# Moissanite-15R (SiC, *B7*) Structure: AB\_hR10\_160\_5a\_5a

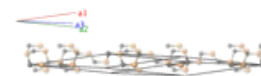


<b>Prototype</b>	:	SiC
<b>AFLOW prototype label</b>	:	AB_hR10_160_5a_5a
<b>Strukturbericht designation</b>	:	<i>B7</i>
<b>Pearson symbol</b>	:	hR10
<b>Space group number</b>	:	160
<b>Space group symbol</b>	:	<i>R3m</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB_hR10_160_5a_5a [--hex]</code> <code>--params=a, c/a, x1, x2, x3, x4, x5, x6, x7, x8, x9, x10</code>

- (Ewald, 1931) and (Thibault, 1944) both call this structure “Type I  $\alpha$ -silicon carbide.”
- The atomic positions are not well determined. We follow (Thibolt, 1944) and assume that the (0001) planes of carbon atoms are equally spaced, and that each carbon atom has a silicon atom at a distance of  $c/20$  along the  $\hat{z}$  axis.

## Rhombohedral primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{x} - \frac{1}{2\sqrt{3}} a \hat{y} + \frac{1}{3} c \hat{z} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}} a \hat{y} + \frac{1}{3} c \hat{z} \\ \mathbf{a}_3 &= -\frac{1}{2} a \hat{x} - \frac{1}{2\sqrt{3}} a \hat{y} + \frac{1}{3} c \hat{z}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$x_1 c \hat{z}$	(1a)	C I
$\mathbf{B}_2$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$x_2 c \hat{z}$	(1a)	C II
$\mathbf{B}_3$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$x_3 c \hat{z}$	(1a)	C III
$\mathbf{B}_4$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$x_4 c \hat{z}$	(1a)	C IV
$\mathbf{B}_5$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$x_5 c \hat{z}$	(1a)	C V
$\mathbf{B}_6$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$x_6 c \hat{z}$	(1a)	Si I
$\mathbf{B}_7$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$x_7 c \hat{z}$	(1a)	Si II

$\mathbf{B}_8$	=	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	=	$x_8 c \hat{\mathbf{z}}$	(1a)	Si III
$\mathbf{B}_9$	=	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	=	$x_9 c \hat{\mathbf{z}}$	(1a)	Si IV
$\mathbf{B}_{10}$	=	$x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	=	$x_{10} c \hat{\mathbf{z}}$	(1a)	Si V

**References:**

- N. W. Thibault, *Morphological and Structural Crystallography and Optical Properties of Silicon Carbide (SiC) Part II: Structural Crystallography and Optical Properties*, Am. Mineral. **29**, 327–362 (1944).
- P. P. Ewald and K. Herrman, eds., *Strukturbericht 1913-1928*, vol. I (Akademische Verlagsgesellschaft M. B. H., 1931).

**Found in:**

- G. L. Harris, ed., *Properties of Silicon Carbide* (INSPEC, London, 1995).

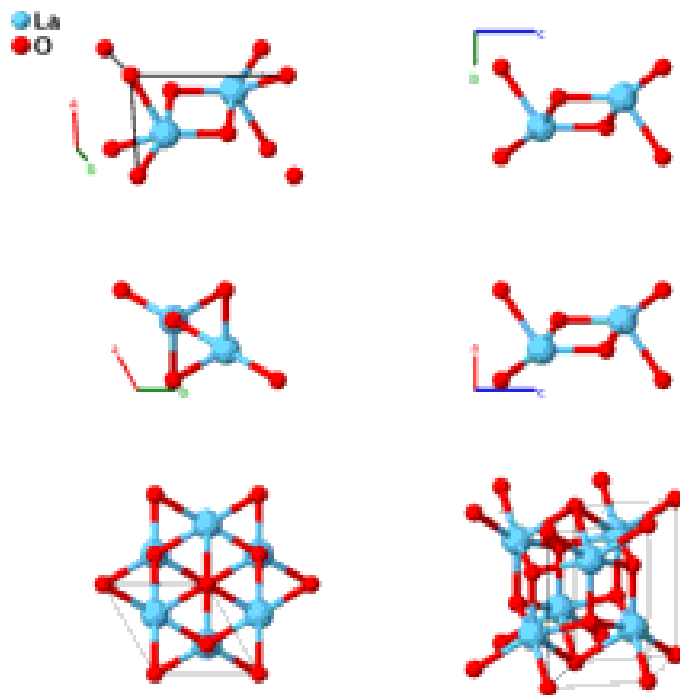
**Geometry files:**

- CIF: pp. [917](#)
- POSCAR: pp. [917](#)



# La<sub>2</sub>O<sub>3</sub> (*D*5<sub>2</sub>) Structure: A2B3\_hP5\_164\_d\_ad

---



<b>Prototype</b>	:	La <sub>2</sub> O <sub>3</sub>
<b>AFLOW prototype label</b>	:	A2B3_hP5_164_d_ad
<b>Strukturbericht designation</b>	:	<i>D</i> 5 <sub>2</sub>
<b>Pearson symbol</b>	:	hP5
<b>Space group number</b>	:	164
<b>Space group symbol</b>	:	<i>P</i> $\bar{3}$ <i>m</i> 1
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A2B3_hP5_164_d_ad --params=a, c/a, z<sub>2</sub>, z<sub>3</sub></code>

---

## Other compounds with this structure:

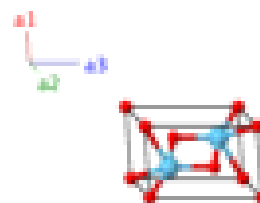
- Ac<sub>2</sub>O<sub>3</sub>, Ce<sub>2</sub>O<sub>3</sub>, Nd<sub>2</sub>O<sub>3</sub>, Pr<sub>2</sub>O<sub>3</sub>, Th<sub>2</sub>N<sub>3</sub>, U<sub>2</sub>N<sub>3</sub>,  $\alpha$ -Bi<sub>2</sub>Mg<sub>3</sub>,  $\alpha$ -Sb<sub>2</sub>Mg<sub>3</sub>

- This structure has proved rather controversial. (Zachariasen 1926, 1929) originally proposed that the crystal structure of La<sub>2</sub>O<sub>3</sub> and other lanthanide series oxides belong to trigonal space group *P*321 #150. This was immediately criticized by (Pauling, 1928), who suggested the trigonal space group (*P* $\bar{3}$ *m*1 #164). This was confirmed by (Koehler, 1953).
- Much later, (Aldebert, 1979) stated that the structure was hexagonal, space group *P*6<sub>3</sub>/*mmc* #194. This would represent a doubling of the *P* $\bar{3}$ *m*1 unit cell in the *z*-direction. However, they give structural parameters, used by us and by (Villars, 1991, 2016), which have a density consistent with the *P* $\bar{3}$ *m*1 structure, and are in reasonable agreement with lattice parameters given in (Pearson, 1958) and (Koehler, 1953). We agree with (Villars, 1991, 2016) that these are close to the correct values for the structure.
- This structure is very similar to Al<sub>3</sub>Ni<sub>2</sub> (*D*5<sub>13</sub>, A3B2\_hP5\_164\_ad\_d). We follow (Pearson, 1958) and assign the intermetallics as *D*5<sub>13</sub>, keeping *D*5<sub>2</sub> for oxides and related compounds.

---

**Trigonal Hexagonal primitive vectors:**

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



---

**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	O I
$\mathbf{B}_2$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2d)	La
$\mathbf{B}_3$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(2d)	La
$\mathbf{B}_4$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2d)	O II
$\mathbf{B}_5$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(2d)	O II

---

**References:**

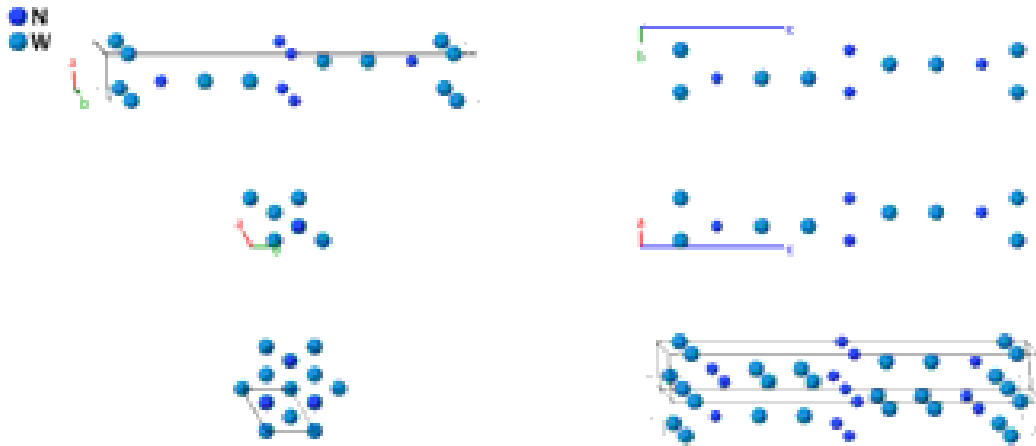
- P. Aldebert and J. P. Traverse, *Etude par diffraction neutronique des structures de haute temperature de  $\text{La}_2\text{O}_3$  et  $\text{Nd}_2\text{O}_3$* , Mater. Res. Bull. **14**, 303–323 (1979), doi:10.1016/0025-5408(79)90095-3.
- W. Zachariasen, *Die Kristallstruktur der  $\hat{I}\hat{S}$ -Modifikation von den Sesquioxiden der seltenen Erdmetalle. ( $\text{La}_2\text{O}_3$ ,  $\text{Ce}_2\text{O}_3$ ,  $\text{Pr}_2\text{O}_3$ ,  $\text{Nd}_2\text{O}_3$ )*, Z. Phys. Chem. **123**, 134 (1926), doi:10.1515/zpch-1926-12309.
- W. H. Zachariasen, *Kürzere Originalmitteilungen und Notizen*, Z. Kristallogr. **70**, 187–188 (1929), doi:10.1524/zkri.1929.70.1.187.
- L. Pauling, *The Crystal Structure of the A-Modification of the Rare Earth Sesquioxides*, Z. Kristallogr. **69**, 415 (1928), doi:10.1524/zkri.1929.69.1.415.
- W. C. Koehler and E. O. Wollan, *Neutron-diffraction study of the structure of the A-form of the rare earth sesquioxides*, Acta Cryst. **6**, 741–742 (1953), doi:10.1107/S0365110X53002076.
- P. Villars, ed., *PAULING FILE in: Inorganic Solid Phases* (SpringerMaterials (online database), Heidelberg, 2016).
- W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

---

**Geometry files:**

- CIF: pp. 917
- POSCAR: pp. 918

# $\delta_H^{\text{II}}$ -NW<sub>2</sub> Structure: AB2\_hP9\_164\_bd\_c2d

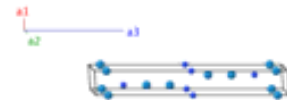


<b>Prototype</b>	:	$\delta_H^{\text{II}}$ -NW <sub>2</sub>
<b>AFLOW prototype label</b>	:	AB2_hP9_164_bd_c2d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP9
<b>Space group number</b>	:	164
<b>Space group symbol</b>	:	$P\bar{3}m1$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB2_hP9_164_bd_c2d</code> <code>--params=a, c/a, z2, z3, z4, z5</code>

- Khitrova and Pinkser put this structure in space group  $P\bar{3}$  (#147), but the Wyckoff positions used are identical with space group  $P\bar{3}m1$  (#164), so we assign this to the higher symmetry space group.

## Trigonal Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} c \hat{\mathbf{z}}$	(1b)	N I
$\mathbf{B}_2$	$= z_2 \mathbf{a}_3$	$= z_2 c \hat{\mathbf{z}}$	(2c)	W I
$\mathbf{B}_3$	$= -z_2 \mathbf{a}_3$	$= -z_2 c \hat{\mathbf{z}}$	(2c)	W I
$\mathbf{B}_4$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2d)	N II
$\mathbf{B}_5$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(2d)	N II
$\mathbf{B}_6$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(2d)	W II
$\mathbf{B}_7$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(2d)	W II

$$\mathbf{B}_8 = \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} \quad (2d) \quad \text{W III}$$

$$\mathbf{B}_9 = \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_5 \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} \quad (2d) \quad \text{W III}$$

---

**References:**

- V. I. Khitrova and Z. G. Pinkser, *Chemical Crystallography of Tungsten Nitrides and of Some Other Interstitial Phases*, Sov. Phys. Crystallogr. **6**, 712–719 (1962).

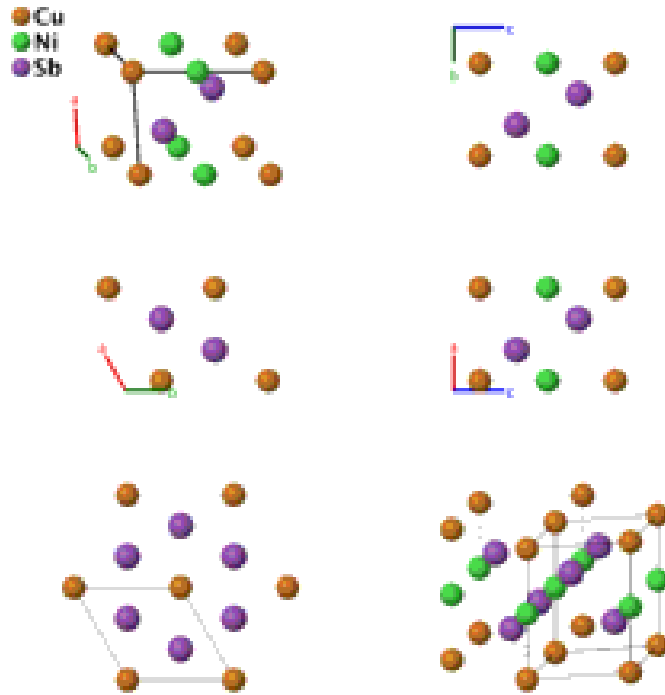
---

**Geometry files:**

- CIF: pp. [918](#)

- POSCAR: pp. [918](#)

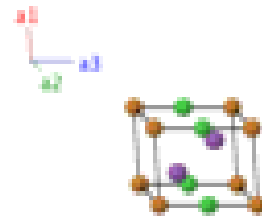
# CuNiSb<sub>2</sub> Structure: ABC2\_hP4\_164\_a\_b\_d



**Prototype** : CuNiSb<sub>2</sub>  
**AFLOW prototype label** : ABC2\_hP4\_164\_a\_b\_d  
**Strukturbericht designation** : None  
**Pearson symbol** : hP4  
**Space group number** : 164  
**Space group symbol** :  $P\bar{3}m1$   
**AFLOW prototype command** : aflow --proto=ABC2\_hP4\_164\_a\_b\_d  
 --params=a, c/a, z<sub>3</sub>

**Trigonal Hexagonal primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Cu
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} c \hat{\mathbf{z}}$	(1b)	Ni
$\mathbf{B}_3$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2d)	Sb
$\mathbf{B}_4$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(2d)	Sb

---

**References:**

- R. L. Kift, *Intermetallic Compounds by Reductive Annealing*, Ph.D. thesis, University of Hull (2010).

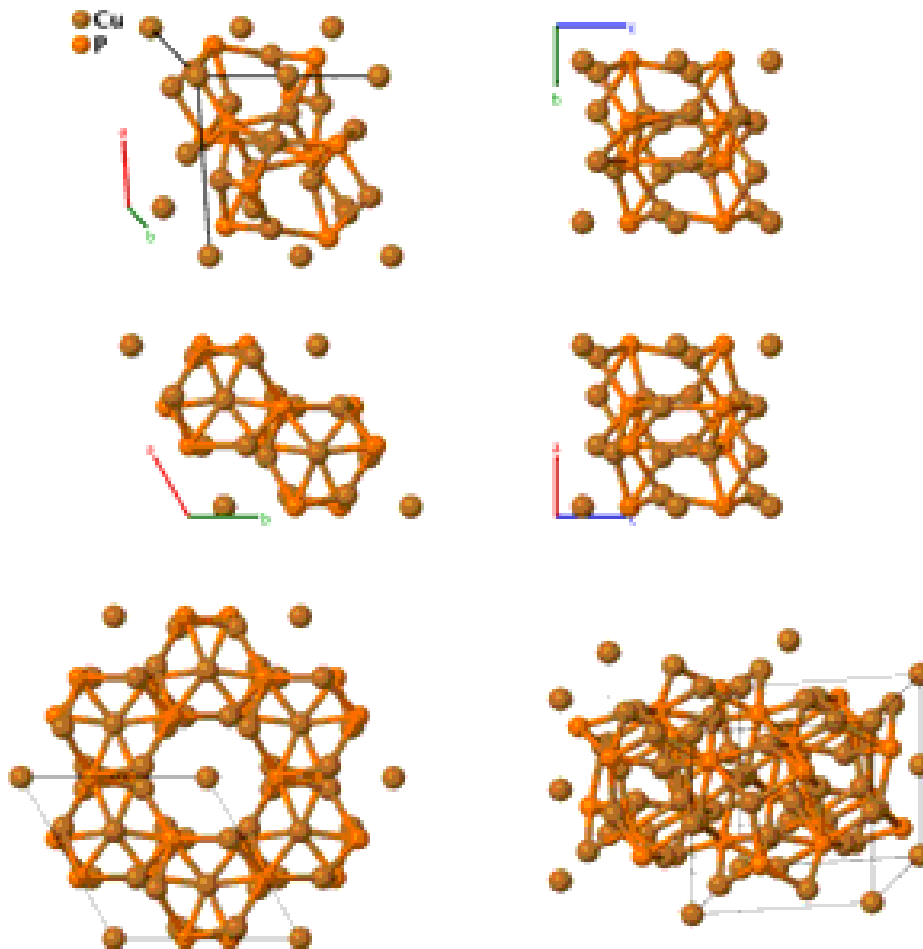
---

**Geometry files:**

- CIF: pp. [918](#)
- POSCAR: pp. [919](#)

# Cu<sub>3</sub>P (*D*0<sub>21</sub>) Structure: A3B\_hP24\_165\_bdg\_f

---



<b>Prototype</b>	:	Cu <sub>3</sub> P
<b>AFLOW prototype label</b>	:	A3B_hP24_165_bdg_f
<b>Strukturbericht designation</b>	:	<i>D</i> 0 <sub>21</sub>
<b>Pearson symbol</b>	:	hP24
<b>Space group number</b>	:	165
<b>Space group symbol</b>	:	<i>P</i> $\bar{3}c1$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A3B_hP24_165_bdg_f --params=a, c/a, z2, x3, x4, y4, z4</code>

---

## Other compounds with this structure:

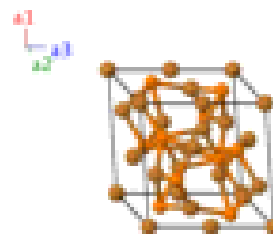
- Cu<sub>3</sub>As, CeF<sub>3</sub>, LaF<sub>3</sub>

- 
- Range and Hafner (Range, 1993) and Olofsson (Olofsson, 1972) argue that several compounds which were previously identified as having this structure actually take on the Cu<sub>3</sub>P structure, space group *P*6<sub>3</sub>*cm*, [A3B\\_hP24\\_185\\_ab2c\\_c](#). These structures include Cu<sub>3</sub>P, Na<sub>3</sub>As, AuMg<sub>3</sub>, Ir<sub>3</sub> and Mg<sub>3</sub>Pt.
  - The *D*1<sub>21</sub> structure is crystallographically equivalent to the H<sub>3</sub>Ho structure, [A3B\\_hP24\\_165\\_adg\\_f](#). We have not found any evidence in the literature showing that either the hydride structure or the fluoride structures mentioned above should be in any other space group.

- We were unable to obtain the original reference, so we use the crystallographic information presented in the American Mineralogist Crystal Structure Database (Downs, 2003). The original version of *Pearson's Handbook* (Pearson, 1958) states that the lattice constants for this structure should be slightly smaller.
- $\text{Cu}_3\text{P}$  (pp. 602) and  $\text{Na}_3\text{As}$  (pp. 607) have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (--params) specified in their corresponding CIF files.

### Trigonal Hexagonal primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



### Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2b)	Cu I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2b)	Cu I
$\mathbf{B}_3$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4d)	Cu II
$\mathbf{B}_4$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(4d)	Cu II
$\mathbf{B}_5$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(4d)	Cu II
$\mathbf{B}_6$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4d)	Cu II
$\mathbf{B}_7$	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6f)	P
$\mathbf{B}_8$	$x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6f)	P
$\mathbf{B}_9$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-x_3 a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6f)	P
$\mathbf{B}_{10}$	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$-\frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6f)	P
$\mathbf{B}_{11}$	$-x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-\frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6f)	P
$\mathbf{B}_{12}$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$x_3 a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6f)	P
$\mathbf{B}_{13}$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B}_{14}$	$-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$\left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B}_{15}$	$(-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$\left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B}_{16}$	$y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_4 - y_4) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B}_{17}$	$(x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$\left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B}_{18}$	$-x_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$\left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B}_{19}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$-\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_4 - y_4) a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(12g)	Cu III



$$\mathbf{B}_{20} = y_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3 = \left(-\frac{1}{2}x_4 + y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} \quad (12g) \quad \text{Cu III}$$

$$\mathbf{B}_{21} = (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = \left(x_4 - \frac{1}{2}y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} \quad (12g) \quad \text{Cu III}$$

$$\mathbf{B}_{22} = -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = -\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} \quad (12g) \quad \text{Cu III}$$

$$\mathbf{B}_{23} = (-x_4 + y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_4 + y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} \quad (12g) \quad \text{Cu III}$$

$$\mathbf{B}_{24} = x_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(x_4 - \frac{1}{2}y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} \quad (12g) \quad \text{Cu III}$$

### References:

- B. Steenberg, *The Crystal Structure of Cu<sub>3</sub>As and Cu<sub>3</sub>P*, Ark. Kem. Mineral. Geol. **A12**, 1–15 (1938).

### Found in:

- W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

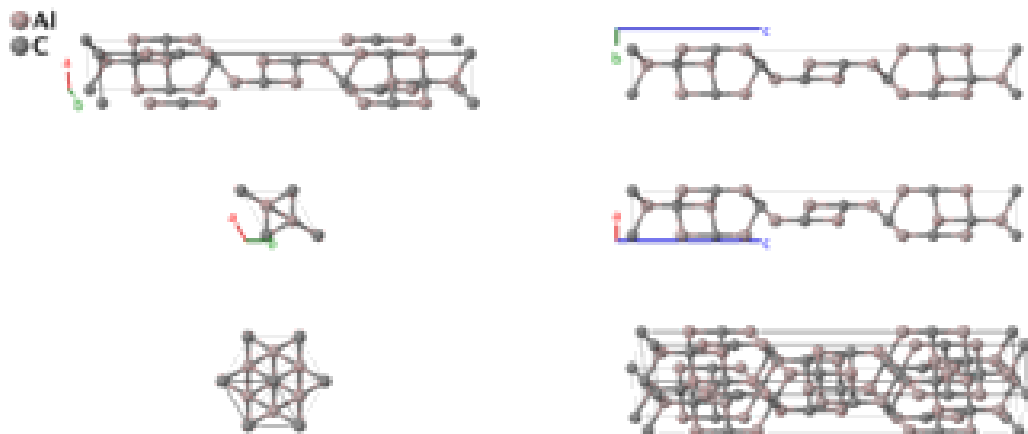
- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

### Geometry files:

- CIF: pp. [919](#)

- POSCAR: pp. [919](#)

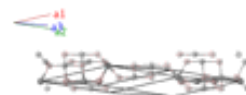
# Al<sub>4</sub>C<sub>3</sub> (*D*7<sub>1</sub>) Structure: A4B3\_hR7\_166\_2c\_ac



<b>Prototype</b>	:	Al <sub>4</sub> C <sub>3</sub>
<b>AFLOW prototype label</b>	:	A4B3_hR7_166_2c_ac
<b>Strukturbericht designation</b>	:	<i>D</i> 7 <sub>1</sub>
<b>Pearson symbol</b>	:	hR7
<b>Space group number</b>	:	166
<b>Space group symbol</b>	:	$R\bar{3}m$
<b>AFLOW prototype command</b>	:	aflow --proto=A4B3_hR7_166_2c_ac [--hex] --params= <i>a, c/a, x<sub>2</sub>, x<sub>3</sub>, x<sub>4</sub></i>

## Rhombohedral primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= 0 <b>a</b> <sub>1</sub> + 0 <b>a</b> <sub>2</sub> + 0 <b>a</b> <sub>3</sub>	= 0 <b>x</b> + 0 <b>y</b> + 0 <b>z</b>	(1a)	C I
<b>B<sub>2</sub></b>	= <i>x</i> <sub>2</sub> <b>a</b> <sub>1</sub> + <i>x</i> <sub>2</sub> <b>a</b> <sub>2</sub> + <i>x</i> <sub>2</sub> <b>a</b> <sub>3</sub>	= <i>x</i> <sub>2</sub> <b>c</b> <b>z</b>	(2c)	Al I
<b>B<sub>3</sub></b>	= - <i>x</i> <sub>2</sub> <b>a</b> <sub>1</sub> - <i>x</i> <sub>2</sub> <b>a</b> <sub>2</sub> - <i>x</i> <sub>2</sub> <b>a</b> <sub>3</sub>	= - <i>x</i> <sub>2</sub> <b>c</b> <b>z</b>	(2c)	Al I
<b>B<sub>4</sub></b>	= <i>x</i> <sub>3</sub> <b>a</b> <sub>1</sub> + <i>x</i> <sub>3</sub> <b>a</b> <sub>2</sub> + <i>x</i> <sub>3</sub> <b>a</b> <sub>3</sub>	= <i>x</i> <sub>3</sub> <b>c</b> <b>z</b>	(2c)	Al II
<b>B<sub>5</sub></b>	= - <i>x</i> <sub>3</sub> <b>a</b> <sub>1</sub> - <i>x</i> <sub>3</sub> <b>a</b> <sub>2</sub> - <i>x</i> <sub>3</sub> <b>a</b> <sub>3</sub>	= - <i>x</i> <sub>3</sub> <b>c</b> <b>z</b>	(2c)	Al II
<b>B<sub>6</sub></b>	= <i>x</i> <sub>4</sub> <b>a</b> <sub>1</sub> + <i>x</i> <sub>4</sub> <b>a</b> <sub>2</sub> + <i>x</i> <sub>4</sub> <b>a</b> <sub>3</sub>	= <i>x</i> <sub>4</sub> <b>c</b> <b>z</b>	(2c)	C II
<b>B<sub>7</sub></b>	= - <i>x</i> <sub>4</sub> <b>a</b> <sub>1</sub> - <i>x</i> <sub>4</sub> <b>a</b> <sub>2</sub> - <i>x</i> <sub>4</sub> <b>a</b> <sub>3</sub>	= - <i>x</i> <sub>4</sub> <b>c</b> <b>z</b>	(2c)	C II

## References:

- T. M. Gesing and W. Jeitschko, *The Crystal Structure and Chemical Properties of U<sub>2</sub>Al<sub>3</sub>C<sub>4</sub> and Structure Refinement of Al<sub>4</sub>C<sub>3</sub>*, Z. Naturforsch. B **50**, 196–200 (1995), doi:10.1515/znB-1995-0206.

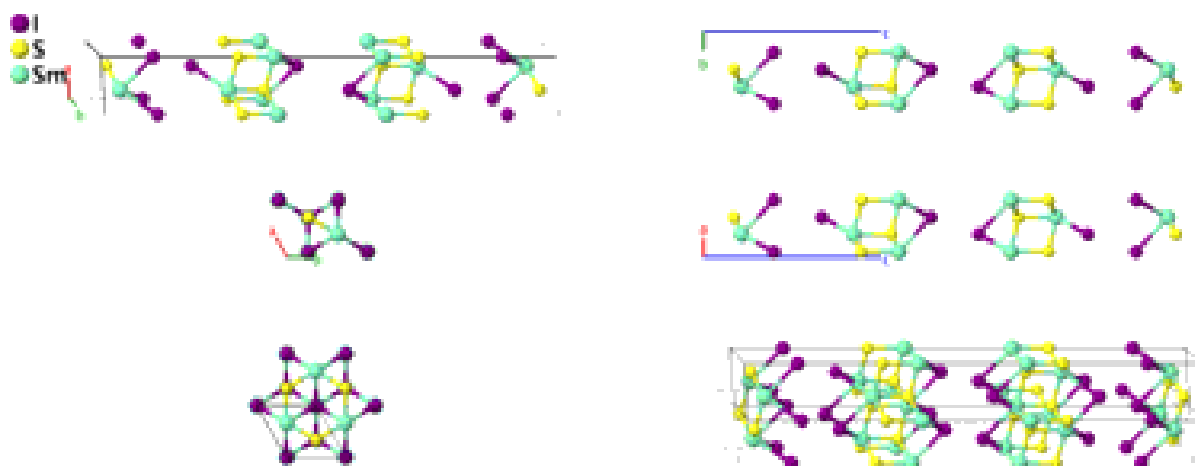
---

**Geometry files:**

- CIF: pp. [919](#)

- POSCAR: pp. [920](#)

# SmSI Structure: ABC\_hR6\_166\_c\_c\_c



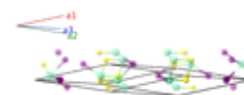
<b>Prototype</b>	:	SmSI
<b>AFLOW prototype label</b>	:	ABC_hR6_166_c_c_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hR6
<b>Space group number</b>	:	166
<b>Space group symbol</b>	:	$R\bar{3}m$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=ABC_hR6_166_c_c_c [--hex] --params=a, c/a, x1, x2, x3</code>

## Other compounds with this structure:

- $\beta$ -CeSI, PrSI, NdSI, and the superconducting alkali metal intercalates  $\beta$ -MNX ( $M = \text{Zr, Hf}; X = \text{Cl, Br, I}$ ).
- Although this has the same crystallographic structure as the C12 structure, the layering is substantially different.

## Rhombohedral primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$x_1 c \hat{\mathbf{z}}$	(2c)	I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-x_1 c \hat{\mathbf{z}}$	(2c)	I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$x_2 c \hat{\mathbf{z}}$	(2c)	S
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-x_2 c \hat{\mathbf{z}}$	(2c)	S
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$x_3 c \hat{\mathbf{z}}$	(2c)	Sm
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-x_3 c \hat{\mathbf{z}}$	(2c)	Sm

---

**References:**

- H. P. Beck and C. Strobel, *Zur Hochdruckpolymorphie der Seltenerdsulfidiodide LnSI*, Z. Anorg. Allg. Chem. **535**, 222–239 (1986), doi:[10.1002/zaac.19865350427](https://doi.org/10.1002/zaac.19865350427).

**Found in:**

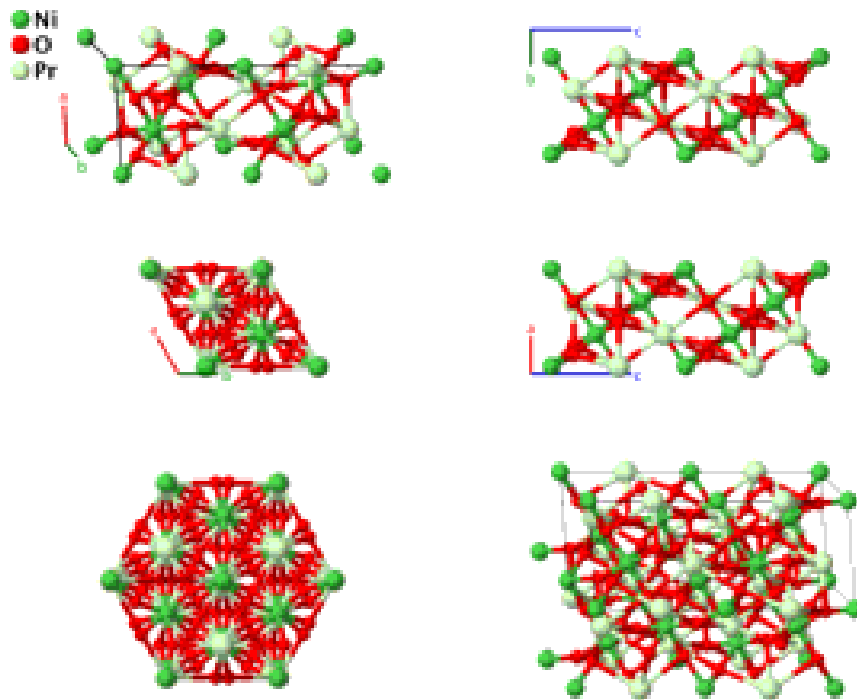
- A. M. Fogg, J. S. O. Evens, and D. O'Hare, *Crystal structure of  $\beta$ -MNX ( $M = \text{Zr, Hf}$ ;  $X = \text{Cl, Br}$ )*, Chem. Comm. **0**, 2269–2270 (1998), doi:[10.1039/A806415F](https://doi.org/10.1039/A806415F).

---

**Geometry files:**

- CIF: pp. [920](#)
- POSCAR: pp. [920](#)

# PrNiO<sub>3</sub> Structure: AB3C\_hR10\_167\_b\_e\_a



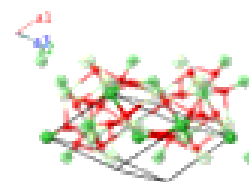
<b>Prototype</b>	:	PrNiO <sub>3</sub>
<b>AFLOW prototype label</b>	:	AB3C_hR10_167_b_e_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hR10
<b>Space group number</b>	:	167
<b>Space group symbol</b>	:	$R\bar{3}c$
<b>AFLOW prototype command</b>	:	aflow --proto=AB3C_hR10_167_b_e_a [--hex] --params=a, c/a, x <sub>3</sub>

## Other compounds with this structure:

- LaNiO<sub>3</sub>
- This structure has the same crystal structure and occupies the same Wyckoff positions as [Calcite \(CaCO<sub>3</sub> Strukturbericht G0<sub>1</sub>, ABC3\\_hR10\\_167\\_a\\_b\\_e\)](#), but  $c/a$  and  $x_3$  are different enough to warrant calling this a new structure. This is the high-temperature form of PrNiO<sub>3</sub>, and we present the data collected at 500° C. Below 500° C this compound transforms to the [orthorhombic perovskite structure \(AB3C\\_oP20\\_62\\_c\\_cd\\_a\)](#).

## Rhombohedral primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates		Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$		(2a)	Pr
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \hat{\mathbf{z}}$		(2a)	Pr
$\mathbf{B}_3$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$		(2b)	Ni
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$		(2b)	Ni
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\left(-\frac{1}{8} + \frac{1}{2}x_3\right) a \hat{\mathbf{x}} + \left(\frac{\sqrt{3}}{8} - \frac{\sqrt{3}}{2}x_3\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$		(6e)	O
$\mathbf{B}_6$	$= \frac{1}{4} \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_3$	$=$	$\left(-\frac{1}{8} + \frac{1}{2}x_3\right) a \hat{\mathbf{x}} + \left(-\frac{\sqrt{3}}{8} + \frac{\sqrt{3}}{2}x_3\right) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$		(6e)	O
$\mathbf{B}_7$	$= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$\left(\frac{1}{4} - x_3\right) a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$		(6e)	O
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a \left(\frac{1}{2}x_3 + \frac{3}{8}\right) \hat{\mathbf{x}} + \left(\frac{1}{8\sqrt{3}} + \frac{\sqrt{3}}{2}x_3\right) a \hat{\mathbf{y}} + \frac{5}{12} c \hat{\mathbf{z}}$		(6e)	O
$\mathbf{B}_9$	$= \frac{3}{4} \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{8} - \frac{1}{2}x_3\right) a \hat{\mathbf{x}} - a \left(\frac{\sqrt{3}}{2}x_3 + \frac{5}{8\sqrt{3}}\right) \hat{\mathbf{y}} + \frac{5}{12} c \hat{\mathbf{z}}$		(6e)	O
$\mathbf{B}_{10}$	$= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\left(\frac{1}{4} + x_3\right) a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{5}{12} c \hat{\mathbf{z}}$		(6e)	O

---

### References:

- T. C. Huang, W. Parrish, H. Toraya, P. Lacorre, and J. B. Torrance, *High-Temperature Crystal Structures of Orthorhombic and Rhombohedral PrNiO<sub>3</sub>*, Mater. Res. Bull. **25**, 1091–1098 (1990), doi:10.1016/0025-5408(90)90138-R.

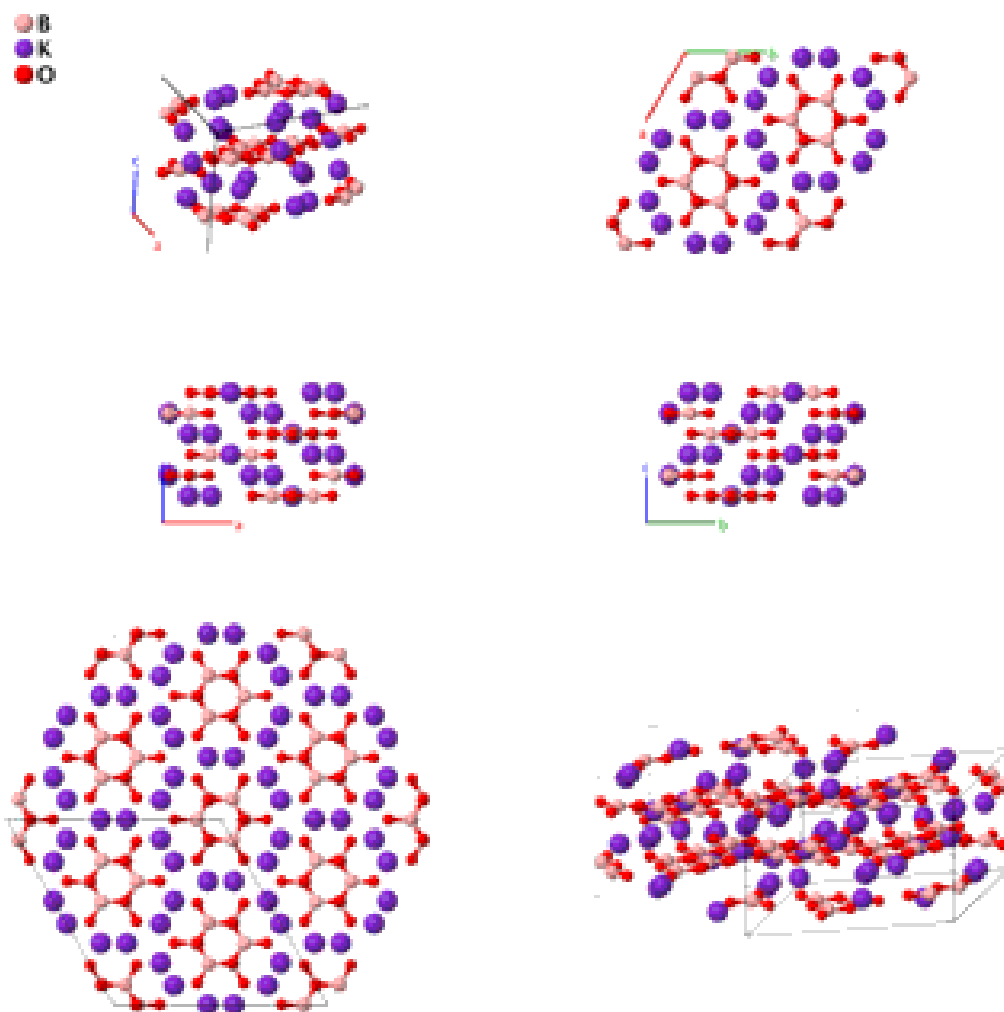
---

### Geometry files:

- CIF: pp. [920](#)  
- POSCAR: pp. [921](#)

# KBO<sub>2</sub> (*F*5<sub>13</sub>) Structure: ABC2\_hR24\_167\_e\_e\_2e

---



<b>Prototype</b>	:	KBO <sub>2</sub>
<b>AFLOW prototype label</b>	:	ABC2_hR24_167_e_e_2e
<b>Strukturbericht designation</b>	:	<i>F</i> 5 <sub>13</sub>
<b>Pearson symbol</b>	:	hR24
<b>Space group number</b>	:	167
<b>Space group symbol</b>	:	$R\bar{3}c$
<b>AFLOW prototype command</b>	:	aflow --proto=ABC2_hR24_167_e_e_2e [--hex] --params= <i>a</i> , <i>c/a</i> , <i>x</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>x</i> <sub>4</sub>

---

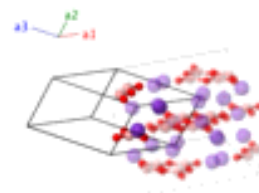
## Other compounds with this structure:

- NaBO<sub>2</sub>, NaBS<sub>2</sub>



## Rhombohedral primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + \left(\frac{1}{2} - x_1\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\left(-\frac{1}{8} + \frac{1}{2}x_1\right) a \hat{\mathbf{x}} + \left(\frac{\sqrt{3}}{8} - \frac{\sqrt{3}}{2}x_1\right) a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	B
$\mathbf{B}_2$	$\frac{1}{4} \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{1}{2} - x_1\right) \mathbf{a}_3$	$\left(-\frac{1}{8} + \frac{1}{2}x_1\right) a \hat{\mathbf{x}} + \left(-\frac{\sqrt{3}}{8} + \frac{\sqrt{3}}{2}x_1\right) a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	B
$\mathbf{B}_3$	$\left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_1 \mathbf{a}_3$	$\left(\frac{1}{4} - x_1\right) a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	B
$\mathbf{B}_4$	$-x_1 \mathbf{a}_1 + \left(\frac{1}{2} + x_1\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-a\left(\frac{1}{2}x_1 + \frac{3}{8}\right) \hat{\mathbf{x}} + \left(\frac{1}{8\sqrt{3}} + \frac{\sqrt{3}}{2}x_1\right) a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	B
$\mathbf{B}_5$	$\frac{3}{4} \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{1}{2} + x_1\right) \mathbf{a}_3$	$\left(\frac{1}{8} - \frac{1}{2}x_1\right) a \hat{\mathbf{x}} - a\left(\frac{\sqrt{3}}{2}x_1 + \frac{5}{8\sqrt{3}}\right) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	B
$\mathbf{B}_6$	$\left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - x_1 \mathbf{a}_3$	$\left(\frac{1}{4} + x_1\right) a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	B
$\mathbf{B}_7$	$x_2 \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\left(-\frac{1}{8} + \frac{1}{2}x_2\right) a \hat{\mathbf{x}} + \left(\frac{\sqrt{3}}{8} - \frac{\sqrt{3}}{2}x_2\right) a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	K
$\mathbf{B}_8$	$\frac{1}{4} \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_3$	$\left(-\frac{1}{8} + \frac{1}{2}x_2\right) a \hat{\mathbf{x}} + \left(-\frac{\sqrt{3}}{8} + \frac{\sqrt{3}}{2}x_2\right) a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	K
$\mathbf{B}_9$	$\left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_2 \mathbf{a}_3$	$\left(\frac{1}{4} - x_2\right) a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	K
$\mathbf{B}_{10}$	$-x_2 \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-a\left(\frac{1}{2}x_2 + \frac{3}{8}\right) \hat{\mathbf{x}} + \left(\frac{1}{8\sqrt{3}} + \frac{\sqrt{3}}{2}x_2\right) a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	K
$\mathbf{B}_{11}$	$\frac{3}{4} \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_3$	$\left(\frac{1}{8} - \frac{1}{2}x_2\right) a \hat{\mathbf{x}} - a\left(\frac{\sqrt{3}}{2}x_2 + \frac{5}{8\sqrt{3}}\right) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	K
$\mathbf{B}_{12}$	$\left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - x_2 \mathbf{a}_3$	$\left(\frac{1}{4} + x_2\right) a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	K
$\mathbf{B}_{13}$	$x_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\left(-\frac{1}{8} + \frac{1}{2}x_3\right) a \hat{\mathbf{x}} + \left(\frac{\sqrt{3}}{8} - \frac{\sqrt{3}}{2}x_3\right) a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B}_{14}$	$\frac{1}{4} \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_3$	$\left(-\frac{1}{8} + \frac{1}{2}x_3\right) a \hat{\mathbf{x}} + \left(-\frac{\sqrt{3}}{8} + \frac{\sqrt{3}}{2}x_3\right) a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B}_{15}$	$\left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_3 \mathbf{a}_3$	$\left(\frac{1}{4} - x_3\right) a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B}_{16}$	$-x_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-a\left(\frac{1}{2}x_3 + \frac{3}{8}\right) \hat{\mathbf{x}} + \left(\frac{1}{8\sqrt{3}} + \frac{\sqrt{3}}{2}x_3\right) a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B}_{17}$	$\frac{3}{4} \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_3$	$\left(\frac{1}{8} - \frac{1}{2}x_3\right) a \hat{\mathbf{x}} - a\left(\frac{\sqrt{3}}{2}x_3 + \frac{5}{8\sqrt{3}}\right) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B}_{18}$	$\left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - x_3 \mathbf{a}_3$	$\left(\frac{1}{4} + x_3\right) a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B}_{19}$	$x_4 \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\left(-\frac{1}{8} + \frac{1}{2}x_4\right) a \hat{\mathbf{x}} + \left(\frac{\sqrt{3}}{8} - \frac{\sqrt{3}}{2}x_4\right) a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B}_{20}$	$\frac{1}{4} \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_3$	$\left(-\frac{1}{8} + \frac{1}{2}x_4\right) a \hat{\mathbf{x}} + \left(-\frac{\sqrt{3}}{8} + \frac{\sqrt{3}}{2}x_4\right) a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B}_{21}$	$\left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_4 \mathbf{a}_3$	$\left(\frac{1}{4} - x_4\right) a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B}_{22}$	$-x_4 \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-a\left(\frac{1}{2}x_4 + \frac{3}{8}\right) \hat{\mathbf{x}} + \left(\frac{1}{8\sqrt{3}} + \frac{\sqrt{3}}{2}x_4\right) a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B}_{23}$	$\frac{3}{4} \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_3$	$\left(\frac{1}{8} - \frac{1}{2}x_4\right) a \hat{\mathbf{x}} - a\left(\frac{\sqrt{3}}{2}x_4 + \frac{5}{8\sqrt{3}}\right) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B}_{24}$	$\left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - x_4 \mathbf{a}_3$	$\left(\frac{1}{4} + x_4\right) a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	O II

## References:

- W. Schneider and G. B. Carpenter, *Bond lengths and thermal parameters of potassium metaborate,  $K_3B_3O_6$* , Acta Crystallogr. Sect. B Struct. Sci. **26**, 1189–1191 (1970), doi:10.1107/S0567740870003849.

**Found in:**

- P. Villars, K. Cenzual, J. Daams, R. Gladyshevskii, O. Shcherban, V. Dubensky, N. Melnichenko-Koblyuk, O. Pavlyuk, I. Savvysyuk, S. Stoyko, and L. Sysa, *Landolt-Börnstein - Group III Condensed Matter (Numerical Data and Functional Relationships in Science and Technology)* (Springer, Berlin, Heidelberg, 2007), vol. 43A5, chap. KBO2 in Structure Types. Part 5: Space Groups (173) P63 - (166) R-3m.

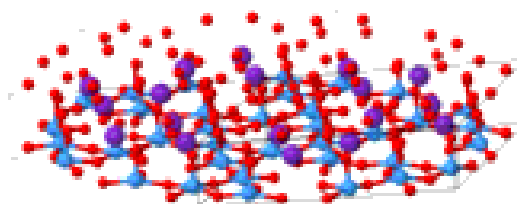
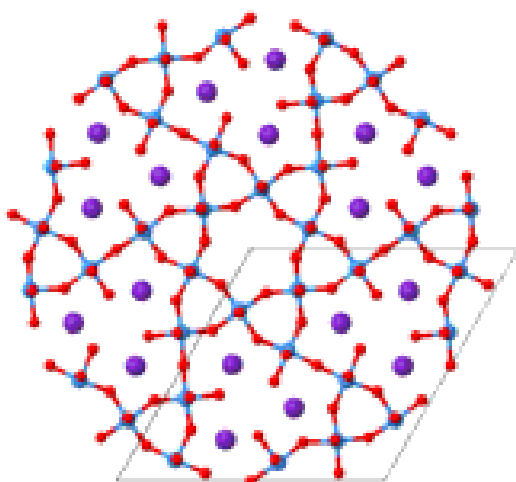
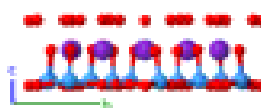
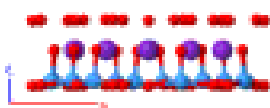
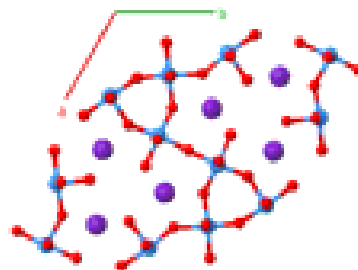
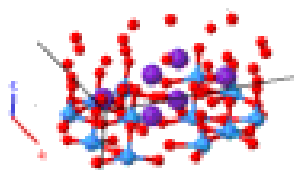
---

**Geometry files:**

- CIF: pp. [921](#)
- POSCAR: pp. [921](#)

# K<sub>2</sub>Ta<sub>4</sub>O<sub>9</sub>F<sub>4</sub> Structure: A2B13C4\_hP57\_168\_d\_c6d\_2d

● K  
● O  
● Ta

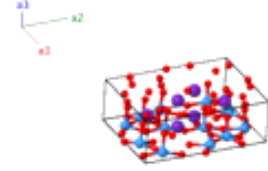


<b>Prototype</b>	:	K <sub>2</sub> Ta <sub>4</sub> O <sub>9</sub> F <sub>4</sub>
<b>AFLOW prototype label</b>	:	A2B13C4_hP57_168_d_c6d_2d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP57
<b>Space group number</b>	:	168
<b>Space group symbol</b>	:	<i>P</i> 6
<b>AFLOW prototype command</b>	:	<pre> aflow --proto=A2B13C4_hP57_168_d_c6d_2d --params=a, c/a, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10                     </pre>

- The O sites are partially occupied with the following concentration 0.692O + 0.308F.

## Hexagonal primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1 + z_1 \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(3c)	O I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(3c)	O I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + z_1 c \hat{\mathbf{z}}$	(3c)	O I
$\mathbf{B}_4$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_2 + y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	K
$\mathbf{B}_5$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(\frac{1}{2} x_2 - y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	K
$\mathbf{B}_6$	$= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(-x_2 + \frac{1}{2} y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	K
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= -\frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_2 - y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	K
$\mathbf{B}_8$	$= y_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(-\frac{1}{2} x_2 + y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	K
$\mathbf{B}_9$	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(x_2 - \frac{1}{2} y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	K
$\mathbf{B}_{10}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_3 + y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6d)	O II
$\mathbf{B}_{11}$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(\frac{1}{2} x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6d)	O II
$\mathbf{B}_{12}$	$= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(-x_3 + \frac{1}{2} y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6d)	O II
$\mathbf{B}_{13}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= -\frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_3 - y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6d)	O II
$\mathbf{B}_{14}$	$= y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(-\frac{1}{2} x_3 + y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6d)	O II
$\mathbf{B}_{15}$	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(x_3 - \frac{1}{2} y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6d)	O II
$\mathbf{B}_{16}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6d)	O III
$\mathbf{B}_{17}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6d)	O III
$\mathbf{B}_{18}$	$= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6d)	O III
$\mathbf{B}_{19}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= -\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_4 - y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6d)	O III
$\mathbf{B}_{20}$	$= y_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \left(-\frac{1}{2} x_4 + y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6d)	O III
$\mathbf{B}_{21}$	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \left(x_4 - \frac{1}{2} y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6d)	O III
$\mathbf{B}_{22}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= \frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(6d)	O IV
$\mathbf{B}_{23}$	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= \left(\frac{1}{2} x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(6d)	O IV
$\mathbf{B}_{24}$	$= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= \left(-x_5 + \frac{1}{2} y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(6d)	O IV
$\mathbf{B}_{25}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= -\frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_5 - y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(6d)	O IV

$$\begin{aligned}
\mathbf{B}_{26} &= y_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 = \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (6d) & \text{O IV} \\
\mathbf{B}_{27} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (6d) & \text{O IV} \\
\mathbf{B}_{28} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \frac{1}{2}(x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_6 + y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6d) & \text{O V} \\
\mathbf{B}_{29} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3 = \left(\frac{1}{2}x_6 - y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6d) & \text{O V} \\
\mathbf{B}_{30} &= (-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \left(-x_6 + \frac{1}{2}y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6d) & \text{O V} \\
\mathbf{B}_{31} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = -\frac{1}{2}(x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_6 - y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6d) & \text{O V} \\
\mathbf{B}_{32} &= y_6 \mathbf{a}_1 + (-x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3 = \left(-\frac{1}{2}x_6 + y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6d) & \text{O V} \\
\mathbf{B}_{33} &= (x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \left(x_6 - \frac{1}{2}y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6d) & \text{O V} \\
\mathbf{B}_{34} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = \frac{1}{2}(x_7 + y_7) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_7 + y_7) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (6d) & \text{O VI} \\
\mathbf{B}_{35} &= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3 = \left(\frac{1}{2}x_7 - y_7\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (6d) & \text{O VI} \\
\mathbf{B}_{36} &= (-x_7 + y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = \left(-x_7 + \frac{1}{2}y_7\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (6d) & \text{O VI} \\
\mathbf{B}_{37} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = -\frac{1}{2}(x_7 + y_7) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_7 - y_7) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (6d) & \text{O VI} \\
\mathbf{B}_{38} &= y_7 \mathbf{a}_1 + (-x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3 = \left(-\frac{1}{2}x_7 + y_7\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (6d) & \text{O VI} \\
\mathbf{B}_{39} &= (x_7 - y_7) \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = \left(x_7 - \frac{1}{2}y_7\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_7 a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (6d) & \text{O VI} \\
\mathbf{B}_{40} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = \frac{1}{2}(x_8 + y_8) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_8 + y_8) a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} & (6d) & \text{O VII} \\
\mathbf{B}_{41} &= -y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3 = \left(\frac{1}{2}x_8 - y_8\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} & (6d) & \text{O VII} \\
\mathbf{B}_{42} &= (-x_8 + y_8) \mathbf{a}_1 - x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = \left(-x_8 + \frac{1}{2}y_8\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} & (6d) & \text{O VII} \\
\mathbf{B}_{43} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = -\frac{1}{2}(x_8 + y_8) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_8 - y_8) a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} & (6d) & \text{O VII} \\
\mathbf{B}_{44} &= y_8 \mathbf{a}_1 + (-x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3 = \left(-\frac{1}{2}x_8 + y_8\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} & (6d) & \text{O VII} \\
\mathbf{B}_{45} &= (x_8 - y_8) \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = \left(x_8 - \frac{1}{2}y_8\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_8 a \hat{\mathbf{y}} + z_8 c \hat{\mathbf{z}} & (6d) & \text{O VII} \\
\mathbf{B}_{46} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = \frac{1}{2}(x_9 + y_9) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_9 + y_9) a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}} & (6d) & \text{Ta I} \\
\mathbf{B}_{47} &= -y_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3 = \left(\frac{1}{2}x_9 - y_9\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}} & (6d) & \text{Ta I} \\
\mathbf{B}_{48} &= (-x_9 + y_9) \mathbf{a}_1 - x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = \left(-x_9 + \frac{1}{2}y_9\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}} & (6d) & \text{Ta I} \\
\mathbf{B}_{49} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = -\frac{1}{2}(x_9 + y_9) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_9 - y_9) a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}} & (6d) & \text{Ta I} \\
\mathbf{B}_{50} &= y_9 \mathbf{a}_1 + (-x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3 = \left(-\frac{1}{2}x_9 + y_9\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}} & (6d) & \text{Ta I} \\
\mathbf{B}_{51} &= (x_9 - y_9) \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = \left(x_9 - \frac{1}{2}y_9\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_9 a \hat{\mathbf{y}} + z_9 c \hat{\mathbf{z}} & (6d) & \text{Ta I} \\
\mathbf{B}_{52} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \frac{1}{2}(x_{10} + y_{10}) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_{10} + y_{10}) a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}} & (6d) & \text{Ta II} \\
\mathbf{B}_{53} &= -y_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \left(\frac{1}{2}x_{10} - y_{10}\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}} & (6d) & \text{Ta II} \\
\mathbf{B}_{54} &= (-x_{10} + y_{10}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \left(-x_{10} + \frac{1}{2}y_{10}\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}} & (6d) & \text{Ta II} \\
\mathbf{B}_{55} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = -\frac{1}{2}(x_{10} + y_{10}) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_{10} - y_{10}) a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}} & (6d) & \text{Ta II} \\
\mathbf{B}_{56} &= y_{10} \mathbf{a}_1 + (-x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \left(-\frac{1}{2}x_{10} + y_{10}\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_{10} a \hat{\mathbf{y}} + z_{10} c \hat{\mathbf{z}} & (6d) & \text{Ta II}
\end{aligned}$$

$$\mathbf{B}_{57} = (x_{10} - y_{10}) \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \left(x_{10} - \frac{1}{2}y_{10}\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_{10}a \hat{\mathbf{y}} + z_{10}c \hat{\mathbf{z}} \quad (6d) \quad \text{Ta II}$$

---

**References:**

- A. Boukhari, J. P. Chaminade, M. Vlasse, and M. Pouchard, *Structure cristalline de l'oxyfluorure de tantale et de potassium*,  $K_2Ta_4F_4O_9$ , Acta Crystallogr. Sect. B Struct. Sci. **35**, 1983–1986 (1979), [doi:10.1107/S056774087900830X](https://doi.org/10.1107/S056774087900830X).

**Found in:**

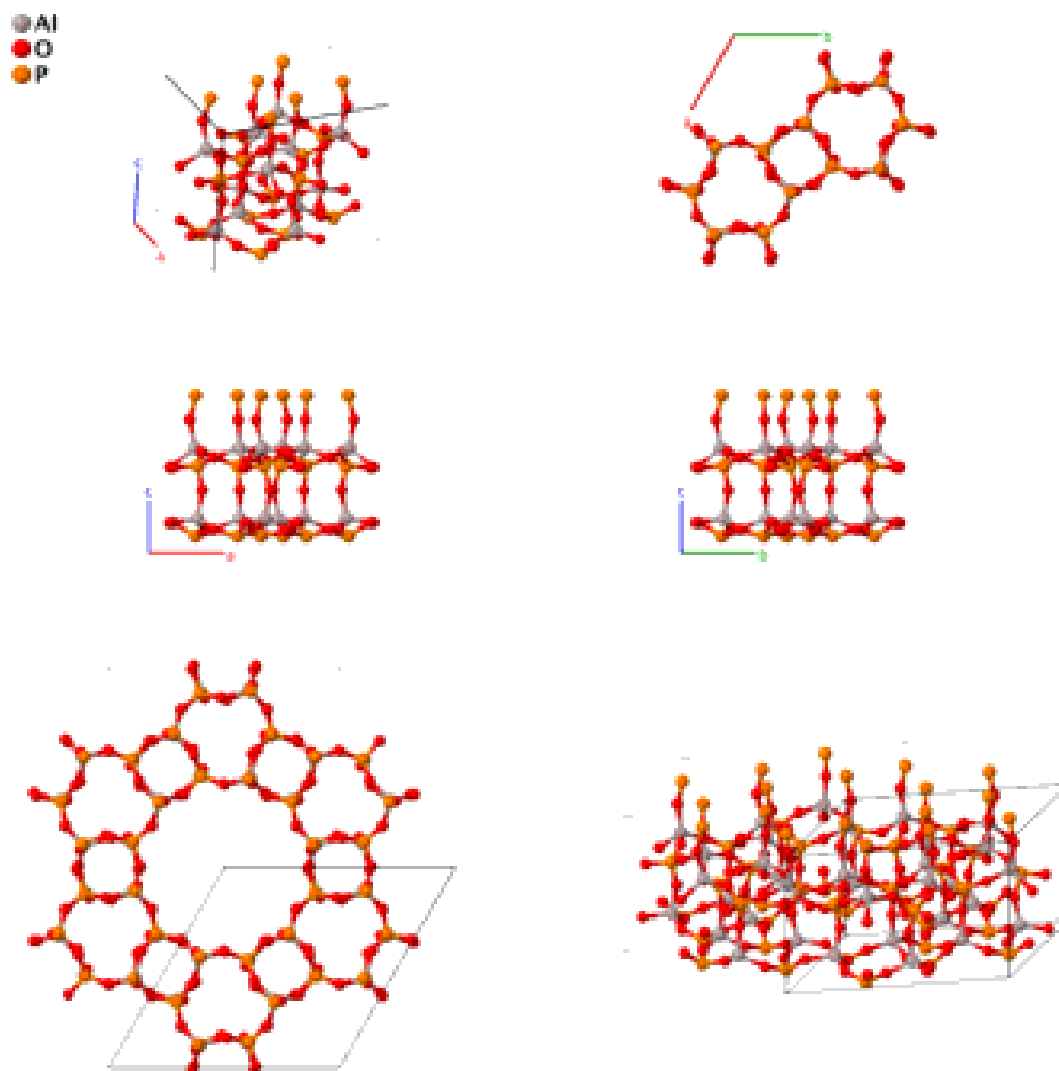
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [922](#)
- POSCAR: pp. [922](#)

# Al[PO<sub>4</sub>] Structure: AB4C\_hP72\_168\_2d\_8d\_2d

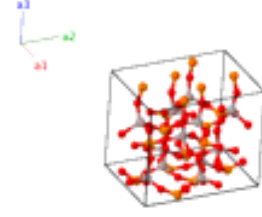


**Prototype** : Al[PO<sub>4</sub>]  
**AFLOW prototype label** : AB4C\_hP72\_168\_2d\_8d\_2d  
**Strukturbericht designation** : None  
**Pearson symbol** : hP72  
**Space group number** : 168  
**Space group symbol** : *P*6  
**AFLOW prototype command** : `aflow --proto=AB4C_hP72_168_2d_8d_2d  
--params=a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12`

- The same compound appears also in a #184 polytype.

## Hexagonal primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{2}(x_1 + y_1) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_1 + y_1) a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(6d)	Al I
$\mathbf{B}_2$	$-y_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \left(\frac{1}{2}x_1 - y_1\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(6d)	Al I
$\mathbf{B}_3$	$(-x_1 + y_1) \mathbf{a}_1 - x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \left(-x_1 + \frac{1}{2}y_1\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(6d)	Al I
$\mathbf{B}_4$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= -\frac{1}{2}(x_1 + y_1) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_1 - y_1) a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(6d)	Al I
$\mathbf{B}_5$	$y_1 \mathbf{a}_1 + (-x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \left(-\frac{1}{2}x_1 + y_1\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(6d)	Al I
$\mathbf{B}_6$	$(x_1 - y_1) \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \left(x_1 - \frac{1}{2}y_1\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(6d)	Al I
$\mathbf{B}_7$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2}(x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_2 + y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	Al II
$\mathbf{B}_8$	$-y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(\frac{1}{2}x_2 - y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	Al II
$\mathbf{B}_9$	$(-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(-x_2 + \frac{1}{2}y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	Al II
$\mathbf{B}_{10}$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= -\frac{1}{2}(x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_2 - y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	Al II
$\mathbf{B}_{11}$	$y_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(-\frac{1}{2}x_2 + y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	Al II
$\mathbf{B}_{12}$	$(x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(x_2 - \frac{1}{2}y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6d)	Al II
$\mathbf{B}_{13}$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6d)	O I
$\mathbf{B}_{14}$	$-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(\frac{1}{2}x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6d)	O I
$\mathbf{B}_{15}$	$(-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(-x_3 + \frac{1}{2}y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6d)	O I
$\mathbf{B}_{16}$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= -\frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6d)	O I
$\mathbf{B}_{17}$	$y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(-\frac{1}{2}x_3 + y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6d)	O I
$\mathbf{B}_{18}$	$(x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \left(x_3 - \frac{1}{2}y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6d)	O I
$\mathbf{B}_{19}$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \frac{1}{2}(x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6d)	O II
$\mathbf{B}_{20}$	$-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \left(\frac{1}{2}x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6d)	O II
$\mathbf{B}_{21}$	$(-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \left(-x_4 + \frac{1}{2}y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6d)	O II
$\mathbf{B}_{22}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= -\frac{1}{2}(x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_4 - y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6d)	O II
$\mathbf{B}_{23}$	$y_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \left(-\frac{1}{2}x_4 + y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6d)	O II
$\mathbf{B}_{24}$	$(x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \left(x_4 - \frac{1}{2}y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6d)	O II





$$\begin{aligned}
\mathbf{B}_{56} &= -y_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \left(\frac{1}{2}x_{10} - y_{10}\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_{10}a \hat{\mathbf{y}} + z_{10}c \hat{\mathbf{z}} & (6d) & \text{O VIII} \\
\mathbf{B}_{57} &= (-x_{10} + y_{10}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \left(-x_{10} + \frac{1}{2}y_{10}\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_{10}a \hat{\mathbf{y}} + z_{10}c \hat{\mathbf{z}} & (6d) & \text{O VIII} \\
\mathbf{B}_{58} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = -\frac{1}{2}(x_{10} + y_{10})a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_{10} - y_{10})a \hat{\mathbf{y}} + z_{10}c \hat{\mathbf{z}} & (6d) & \text{O VIII} \\
\mathbf{B}_{59} &= y_{10} \mathbf{a}_1 + (-x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \left(-\frac{1}{2}x_{10} + y_{10}\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_{10}a \hat{\mathbf{y}} + z_{10}c \hat{\mathbf{z}} & (6d) & \text{O VIII} \\
\mathbf{B}_{60} &= (x_{10} - y_{10}) \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \left(x_{10} - \frac{1}{2}y_{10}\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_{10}a \hat{\mathbf{y}} + z_{10}c \hat{\mathbf{z}} & (6d) & \text{O VIII} \\
\mathbf{B}_{61} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = \frac{1}{2}(x_{11} + y_{11})a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_{11} + y_{11})a \hat{\mathbf{y}} + z_{11}c \hat{\mathbf{z}} & (6d) & \text{P I} \\
\mathbf{B}_{62} &= -y_{11} \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 = \left(\frac{1}{2}x_{11} - y_{11}\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_{11}a \hat{\mathbf{y}} + z_{11}c \hat{\mathbf{z}} & (6d) & \text{P I} \\
\mathbf{B}_{63} &= (-x_{11} + y_{11}) \mathbf{a}_1 - x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = \left(-x_{11} + \frac{1}{2}y_{11}\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_{11}a \hat{\mathbf{y}} + z_{11}c \hat{\mathbf{z}} & (6d) & \text{P I} \\
\mathbf{B}_{64} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = -\frac{1}{2}(x_{11} + y_{11})a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_{11} - y_{11})a \hat{\mathbf{y}} + z_{11}c \hat{\mathbf{z}} & (6d) & \text{P I} \\
\mathbf{B}_{65} &= y_{11} \mathbf{a}_1 + (-x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 = \left(-\frac{1}{2}x_{11} + y_{11}\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_{11}a \hat{\mathbf{y}} + z_{11}c \hat{\mathbf{z}} & (6d) & \text{P I} \\
\mathbf{B}_{66} &= (x_{11} - y_{11}) \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = \left(x_{11} - \frac{1}{2}y_{11}\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_{11}a \hat{\mathbf{y}} + z_{11}c \hat{\mathbf{z}} & (6d) & \text{P I} \\
\mathbf{B}_{67} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \frac{1}{2}(x_{12} + y_{12})a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_{12} + y_{12})a \hat{\mathbf{y}} + z_{12}c \hat{\mathbf{z}} & (6d) & \text{P II} \\
\mathbf{B}_{68} &= -y_{12} \mathbf{a}_1 + (x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \left(\frac{1}{2}x_{12} - y_{12}\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_{12}a \hat{\mathbf{y}} + z_{12}c \hat{\mathbf{z}} & (6d) & \text{P II} \\
\mathbf{B}_{69} &= (-x_{12} + y_{12}) \mathbf{a}_1 - x_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \left(-x_{12} + \frac{1}{2}y_{12}\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_{12}a \hat{\mathbf{y}} + z_{12}c \hat{\mathbf{z}} & (6d) & \text{P II} \\
\mathbf{B}_{70} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = -\frac{1}{2}(x_{12} + y_{12})a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_{12} - y_{12})a \hat{\mathbf{y}} + z_{12}c \hat{\mathbf{z}} & (6d) & \text{P II} \\
\mathbf{B}_{71} &= y_{12} \mathbf{a}_1 + (-x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \left(-\frac{1}{2}x_{12} + y_{12}\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_{12}a \hat{\mathbf{y}} + z_{12}c \hat{\mathbf{z}} & (6d) & \text{P II} \\
\mathbf{B}_{72} &= (x_{12} - y_{12}) \mathbf{a}_1 + x_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \left(x_{12} - \frac{1}{2}y_{12}\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_{12}a \hat{\mathbf{y}} + z_{12}c \hat{\mathbf{z}} & (6d) & \text{P II}
\end{aligned}$$

---

### References:

- J. W. Richardson Jr., J. J. Pluth, and J. V. Smith, *Aluminophosphate number 5: time-of-flight neutron powder diffraction study of calcined powder at 295 K*, Acta Crystallogr. C **43**, 1469–1472 (1987), doi:10.1107/S0108270187091418.

### Found in:

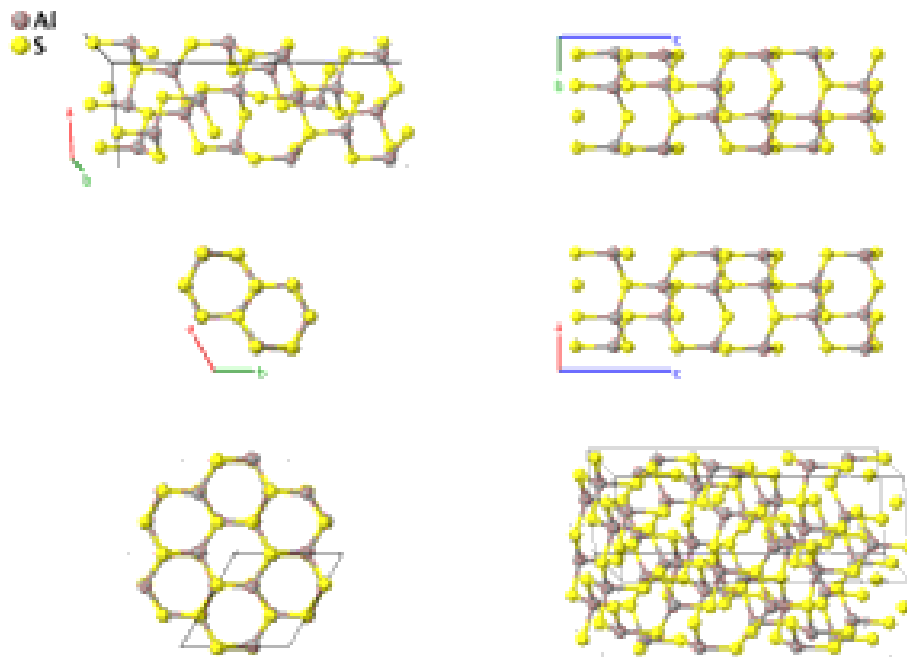
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. [922](#)  
- POSCAR: pp. [923](#)

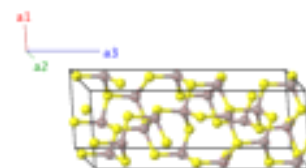
# $\alpha$ -Al<sub>2</sub>S<sub>3</sub> Structure: A2B3\_hP30\_169\_2a\_3a



<b>Prototype</b>	:	$\alpha$ -Al <sub>2</sub> S <sub>3</sub>
<b>AFLOW prototype label</b>	:	A2B3_hP30_169_2a_3a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP30
<b>Space group number</b>	:	169
<b>Space group symbol</b>	:	$P6_1$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3_hP30_169_2a_3a --params= $a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} (x_1 + y_1) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_1 + y_1) a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(6a)	Al I
$\mathbf{B}_2$	$= -y_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + \left(\frac{1}{3} + z_1\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} x_1 - y_1\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_1\right) c \hat{\mathbf{z}}$	(6a)	Al I
$\mathbf{B}_3$	$= (-x_1 + y_1) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{2}{3} + z_1\right) \mathbf{a}_3$	$=$	$\left(-x_1 + \frac{1}{2} y_1\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_1 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_1\right) c \hat{\mathbf{z}}$	(6a)	Al I

$$\begin{aligned}
\mathbf{B}_4 &= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3 = -\frac{1}{2}(x_1 + y_1) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_1 - y_1) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}} & (6a) & \text{Al I} \\
\mathbf{B}_5 &= y_1 \mathbf{a}_1 + (-x_1 + y_1) \mathbf{a}_2 + \left(\frac{5}{6} + z_1\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_1 + y_1\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_1 a \hat{\mathbf{y}} + \left(\frac{5}{6} + z_1\right) c \hat{\mathbf{z}} & (6a) & \text{Al I} \\
\mathbf{B}_6 &= (x_1 - y_1) \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{1}{6} + z_1\right) \mathbf{a}_3 = \left(x_1 - \frac{1}{2}y_1\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_1 a \hat{\mathbf{y}} + \left(\frac{1}{6} + z_1\right) c \hat{\mathbf{z}} & (6a) & \text{Al I} \\
\mathbf{B}_7 &= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 = \frac{1}{2}(x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_2 + y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (6a) & \text{Al II} \\
\mathbf{B}_8 &= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{1}{3} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2}x_2 - y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_2\right) c \hat{\mathbf{z}} & (6a) & \text{Al II} \\
\mathbf{B}_9 &= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{2}{3} + z_2\right) \mathbf{a}_3 = \left(-x_2 + \frac{1}{2}y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_2\right) c \hat{\mathbf{z}} & (6a) & \text{Al II} \\
\mathbf{B}_{10} &= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = -\frac{1}{2}(x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_2 - y_2) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (6a) & \text{Al II} \\
\mathbf{B}_{11} &= y_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + \left(\frac{5}{6} + z_2\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_2 + y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \left(\frac{5}{6} + z_2\right) c \hat{\mathbf{z}} & (6a) & \text{Al II} \\
\mathbf{B}_{12} &= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{6} + z_2\right) \mathbf{a}_3 = \left(x_2 - \frac{1}{2}y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} + \left(\frac{1}{6} + z_2\right) c \hat{\mathbf{z}} & (6a) & \text{Al II} \\
\mathbf{B}_{13} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = \frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{14} &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{1}{3} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2}x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_3\right) c \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{15} &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{2}{3} + z_3\right) \mathbf{a}_3 = \left(-x_3 + \frac{1}{2}y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_3\right) c \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{16} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = -\frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{17} &= y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{5}{6} + z_3\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_3 + y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + \left(\frac{5}{6} + z_3\right) c \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{18} &= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{6} + z_3\right) \mathbf{a}_3 = \left(x_3 - \frac{1}{2}y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + \left(\frac{1}{6} + z_3\right) c \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{19} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = \frac{1}{2}(x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{20} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{1}{3} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2}x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_4\right) c \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{21} &= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{2}{3} + z_4\right) \mathbf{a}_3 = \left(-x_4 + \frac{1}{2}y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_4\right) c \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{22} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = -\frac{1}{2}(x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_4 - y_4) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{23} &= y_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \left(\frac{5}{6} + z_4\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_4 + y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + \left(\frac{5}{6} + z_4\right) c \hat{\mathbf{z}} & (6a) & \text{S II}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{24} &= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{6} + z_4\right) \mathbf{a}_3 = \left(x_4 - \frac{1}{2}y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} + \left(\frac{1}{6} + z_4\right) c \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{25} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{26} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{1}{3} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2}x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_5\right) c \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{27} &= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{2}{3} + z_5\right) \mathbf{a}_3 = \left(-x_5 + \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_5\right) c \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{28} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = -\frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_5 - y_5) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{29} &= y_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \left(\frac{5}{6} + z_5\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{5}{6} + z_5\right) c \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{30} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{6} + z_5\right) \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{1}{6} + z_5\right) c \hat{\mathbf{z}} & (6a) & \text{S III}
\end{aligned}$$

**References:**

- B. Eisenmann, *Crystal structure of  $\alpha$ -dialuminium trisulfide,  $Al_2S_3$* , Z. Kristallogr. **198**, 307–308 (1992).

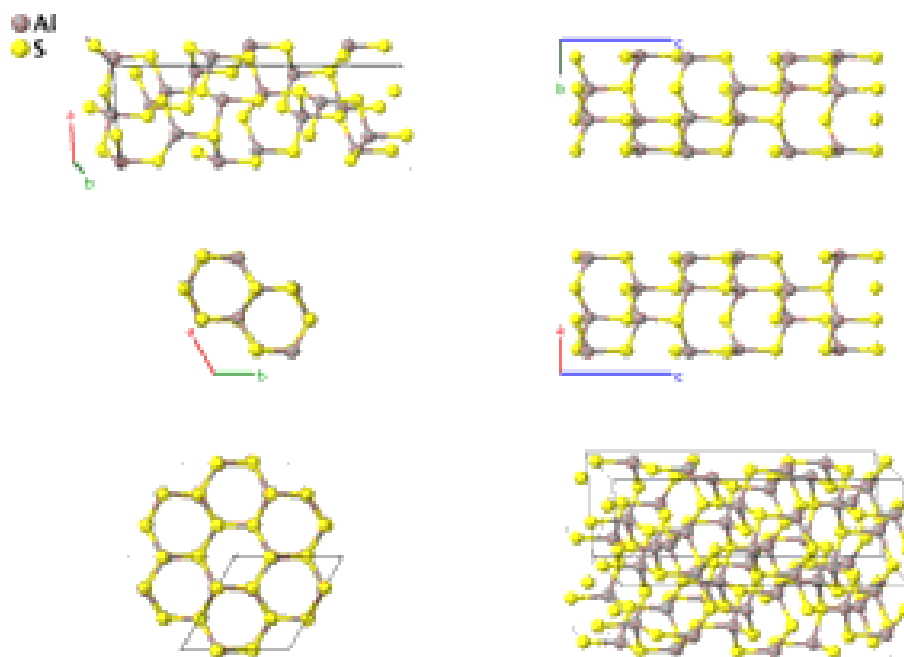
**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

**Geometry files:**

- CIF: pp. [923](#)  
- POSCAR: pp. [924](#)

# Al<sub>2</sub>S<sub>3</sub> Structure: A2B3\_hP30\_170\_2a\_3a



<b>Prototype</b>	:	Al <sub>2</sub> S <sub>3</sub>
<b>AFLOW prototype label</b>	:	A2B3_hP30_170_2a_3a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP30
<b>Space group number</b>	:	170
<b>Space group symbol</b>	:	<i>P</i> 6 <sub>5</sub>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3_hP30_170_2a_3a --params= <i>a</i> , <i>c/a</i> , <i>x</i> <sub>1</sub> , <i>y</i> <sub>1</sub> , <i>z</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>y</i> <sub>2</sub> , <i>z</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub>

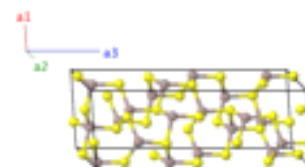
- This structure is the enantiomorph of the [Al<sub>2</sub>S<sub>3</sub> \(A2B3\\_hP30\\_169\\_2a\\_3a\) structure](#), and was generated by reflecting the coordinates of the space group #169 structure through the *z* = 0 plane.

## Hexagonal primitive vectors:

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	= $\frac{1}{2} (x_1 + y_1) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_1 + y_1) a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(6a)	Al I
<b>B<sub>2</sub></b>	= $-y_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + \left(\frac{2}{3} + z_1\right) \mathbf{a}_3$	= $\left(\frac{1}{2} x_1 - y_1\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_1\right) c \hat{\mathbf{z}}$	(6a)	Al I

$$\begin{aligned}
\mathbf{B}_3 &= (-x_1 + y_1) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{1}{3} + z_1\right) \mathbf{a}_3 = \left(-x_1 + \frac{1}{2}y_1\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_1 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_1\right) c \hat{\mathbf{z}} & (6a) & \text{Al I} \\
\mathbf{B}_4 &= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3 = -\frac{1}{2}(x_1 + y_1) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_1 - y_1) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}} & (6a) & \text{Al I} \\
\mathbf{B}_5 &= y_1 \mathbf{a}_1 + (-x_1 + y_1) \mathbf{a}_2 + \left(\frac{1}{6} + z_1\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_1 + y_1\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_1 a \hat{\mathbf{y}} + \left(\frac{1}{6} + z_1\right) c \hat{\mathbf{z}} & (6a) & \text{Al I} \\
\mathbf{B}_6 &= (x_1 - y_1) \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{5}{6} + z_1\right) \mathbf{a}_3 = \left(x_1 - \frac{1}{2}y_1\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_1 a \hat{\mathbf{y}} + \left(\frac{5}{6} + z_1\right) c \hat{\mathbf{z}} & (6a) & \text{Al I} \\
\mathbf{B}_7 &= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 = \frac{1}{2}(x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_2 + y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (6a) & \text{Al II} \\
\mathbf{B}_8 &= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{2}{3} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2}x_2 - y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_2\right) c \hat{\mathbf{z}} & (6a) & \text{Al II} \\
\mathbf{B}_9 &= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{3} + z_2\right) \mathbf{a}_3 = \left(-x_2 + \frac{1}{2}y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_2\right) c \hat{\mathbf{z}} & (6a) & \text{Al II} \\
\mathbf{B}_{10} &= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = -\frac{1}{2}(x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_2 - y_2) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (6a) & \text{Al II} \\
\mathbf{B}_{11} &= y_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + \left(\frac{1}{6} + z_2\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_2 + y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \left(\frac{1}{6} + z_2\right) c \hat{\mathbf{z}} & (6a) & \text{Al II} \\
\mathbf{B}_{12} &= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{5}{6} + z_2\right) \mathbf{a}_3 = \left(x_2 - \frac{1}{2}y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} + \left(\frac{5}{6} + z_2\right) c \hat{\mathbf{z}} & (6a) & \text{Al II} \\
\mathbf{B}_{13} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = \frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{14} &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{2}{3} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2}x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_3\right) c \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{15} &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{3} + z_3\right) \mathbf{a}_3 = \left(-x_3 + \frac{1}{2}y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_3\right) c \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{16} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = -\frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{17} &= y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{1}{6} + z_3\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_3 + y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + \left(\frac{1}{6} + z_3\right) c \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{18} &= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{5}{6} + z_3\right) \mathbf{a}_3 = \left(x_3 - \frac{1}{2}y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + \left(\frac{5}{6} + z_3\right) c \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{19} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = \frac{1}{2}(x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{20} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{2}{3} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2}x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_4\right) c \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{21} &= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{3} + z_4\right) \mathbf{a}_3 = \left(-x_4 + \frac{1}{2}y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_4\right) c \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{22} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = -\frac{1}{2}(x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_4 - y_4) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (6a) & \text{S II}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{23} &= y_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \left(\frac{1}{6} + z_4\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_4 + y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + \left(\frac{1}{6} + z_4\right) c \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{24} &= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{5}{6} + z_4\right) \mathbf{a}_3 = \left(x_4 - \frac{1}{2}y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} + \left(\frac{5}{6} + z_4\right) c \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{25} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{26} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{2}{3} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2}x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_5\right) c \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{27} &= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{3} + z_5\right) \mathbf{a}_3 = \left(-x_5 + \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_5\right) c \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{28} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = -\frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_5 - y_5) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{29} &= y_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \left(\frac{1}{6} + z_5\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{1}{6} + z_5\right) c \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{30} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{5}{6} + z_5\right) \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{5}{6} + z_5\right) c \hat{\mathbf{z}} & (6a) & \text{S III}
\end{aligned}$$

---

#### References:

- B. Eisenmann, *Crystal structure of  $\alpha$ -dialuminium trisulfide,  $Al_2S_3$* , Z. Kristallogr. **198**, 307–308 (1992).

---

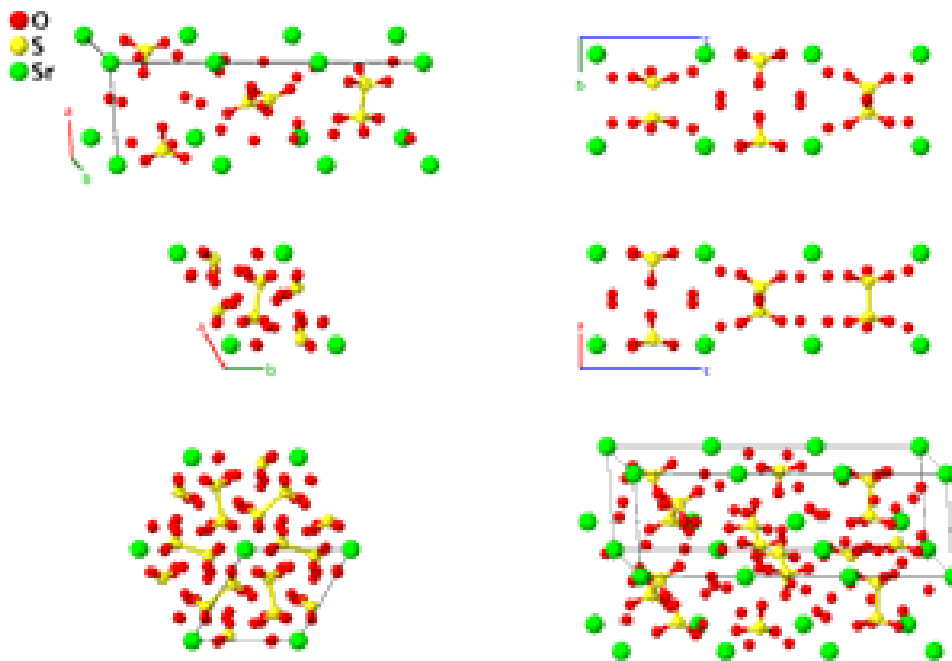
#### Geometry files:

- CIF: pp. [924](#)

- POSCAR: pp. [924](#)



# Sr[S<sub>2</sub>O<sub>6</sub>][H<sub>2</sub>O]<sub>4</sub> Structure: A10B2C\_hP39\_171\_5c\_c\_a

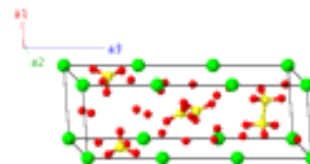


<b>Prototype</b>	:	Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub>
<b>AFLOW prototype label</b>	:	A10B2C_hP39_171_5c_c_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP39
<b>Space group number</b>	:	171
<b>Space group symbol</b>	:	<i>P</i> 6 <sub>2</sub>
<b>AFLOW prototype command</b>	:	aflow --proto=A10B2C_hP39_171_5c_c_a --params= <i>a</i> , <i>c/a</i> , <i>z</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>y</i> <sub>2</sub> , <i>z</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>x</i> <sub>6</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub> , <i>x</i> <sub>7</sub> , <i>y</i> <sub>7</sub> , <i>z</i> <sub>7</sub>

- This structure is the enantiomorph of the [Sr\[S<sub>2</sub>O<sub>6</sub>\]\[H<sub>2</sub>O\]<sub>4</sub> \(A10B2C\\_hP39\\_172\\_5c\\_c\\_a\)](#) structure. Only the non-hydrogen atoms are included in the prototype.

## Hexagonal primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type	
<b>B</b> <sub>1</sub>	=	<i>z</i> <sub>1</sub> <b>a</b> <sub>3</sub>	=	<i>z</i> <sub>1</sub> <i>c</i> <b>z</b> <b>^</b>	(3 <i>a</i> )	Sr
<b>B</b> <sub>2</sub>	=	( $\frac{2}{3} + z_1$ ) <b>a</b> <sub>3</sub>	=	( $\frac{2}{3} + z_1$ ) <i>c</i> <b>z</b> <b>^</b>	(3 <i>a</i> )	Sr
<b>B</b> <sub>3</sub>	=	( $\frac{1}{3} + z_1$ ) <b>a</b> <sub>3</sub>	=	( $\frac{1}{3} + z_1$ ) <i>c</i> <b>z</b> <b>^</b>	(3 <i>a</i> )	Sr

$$\begin{aligned}
\mathbf{B}_4 &= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 = \frac{1}{2}(x_2 + y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_2 + y_2)a \hat{\mathbf{y}} + z_2c \hat{\mathbf{z}} & (6c) & \quad \text{O I} \\
\mathbf{B}_5 &= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{2}{3} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2}x_2 - y_2\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_2\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O I} \\
\mathbf{B}_6 &= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{3} + z_2\right) \mathbf{a}_3 = \left(-x_2 + \frac{1}{2}y_2\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_2\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O I} \\
\mathbf{B}_7 &= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 = -\frac{1}{2}(x_2 + y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_2 - y_2)a \hat{\mathbf{y}} + z_2c \hat{\mathbf{z}} & (6c) & \quad \text{O I} \\
\mathbf{B}_8 &= y_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + \left(\frac{2}{3} + z_2\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_2 + y_2\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_2\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O I} \\
\mathbf{B}_9 &= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{3} + z_2\right) \mathbf{a}_3 = \left(x_2 - \frac{1}{2}y_2\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_2a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_2\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O I} \\
\mathbf{B}_{10} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = \frac{1}{2}(x_3 + y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3)a \hat{\mathbf{y}} + z_3c \hat{\mathbf{z}} & (6c) & \quad \text{O II} \\
\mathbf{B}_{11} &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{2}{3} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2}x_3 - y_3\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_3\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O II} \\
\mathbf{B}_{12} &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{3} + z_3\right) \mathbf{a}_3 = \left(-x_3 + \frac{1}{2}y_3\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_3\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O II} \\
\mathbf{B}_{13} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = -\frac{1}{2}(x_3 + y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3)a \hat{\mathbf{y}} + z_3c \hat{\mathbf{z}} & (6c) & \quad \text{O II} \\
\mathbf{B}_{14} &= y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{2}{3} + z_3\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_3 + y_3\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_3\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O II} \\
\mathbf{B}_{15} &= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{3} + z_3\right) \mathbf{a}_3 = \left(x_3 - \frac{1}{2}y_3\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_3\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O II} \\
\mathbf{B}_{16} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = \frac{1}{2}(x_4 + y_4)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_4 + y_4)a \hat{\mathbf{y}} + z_4c \hat{\mathbf{z}} & (6c) & \quad \text{O III} \\
\mathbf{B}_{17} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{2}{3} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2}x_4 - y_4\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_4\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O III} \\
\mathbf{B}_{18} &= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{3} + z_4\right) \mathbf{a}_3 = \left(-x_4 + \frac{1}{2}y_4\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_4\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O III} \\
\mathbf{B}_{19} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = -\frac{1}{2}(x_4 + y_4)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_4 - y_4)a \hat{\mathbf{y}} + z_4c \hat{\mathbf{z}} & (6c) & \quad \text{O III} \\
\mathbf{B}_{20} &= y_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \left(\frac{2}{3} + z_4\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_4 + y_4\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_4a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_4\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O III} \\
\mathbf{B}_{21} &= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{3} + z_4\right) \mathbf{a}_3 = \left(x_4 - \frac{1}{2}y_4\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_4a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_4\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O III} \\
\mathbf{B}_{22} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \frac{1}{2}(x_5 + y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5)a \hat{\mathbf{y}} + z_5c \hat{\mathbf{z}} & (6c) & \quad \text{O IV} \\
\mathbf{B}_{23} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{2}{3} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2}x_5 - y_5\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_5\right)c \hat{\mathbf{z}} & (6c) & \quad \text{O IV}
\end{aligned}$$

$$\begin{aligned} \mathbf{B}_{24} &= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{3} + z_5\right) \mathbf{a}_3 = \left(-x_5 + \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_5\right) c \hat{\mathbf{z}} & (6c) & \text{O IV} \\ \mathbf{B}_{25} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = -\frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_5 - y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (6c) & \text{O IV} \\ \mathbf{B}_{26} &= y_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \left(\frac{2}{3} + z_5\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_5\right) c \hat{\mathbf{z}} & (6c) & \text{O IV} \\ \mathbf{B}_{27} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{3} + z_5\right) \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_5\right) c \hat{\mathbf{z}} & (6c) & \text{O IV} \\ \mathbf{B}_{28} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \frac{1}{2}(x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_6 + y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6c) & \text{O V} \\ \mathbf{B}_{29} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \left(\frac{2}{3} + z_6\right) \mathbf{a}_3 = \left(\frac{1}{2}x_6 - y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_6 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_6\right) c \hat{\mathbf{z}} & (6c) & \text{O V} \\ \mathbf{B}_{30} &= (-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(\frac{1}{3} + z_6\right) \mathbf{a}_3 = \left(-x_6 + \frac{1}{2}y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_6 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_6\right) c \hat{\mathbf{z}} & (6c) & \text{O V} \\ \mathbf{B}_{31} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = -\frac{1}{2}(x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_6 - y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6c) & \text{O V} \\ \mathbf{B}_{32} &= y_6 \mathbf{a}_1 + (-x_6 + y_6) \mathbf{a}_2 + \left(\frac{2}{3} + z_6\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_6 + y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_6 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_6\right) c \hat{\mathbf{z}} & (6c) & \text{O V} \\ \mathbf{B}_{33} &= (x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(\frac{1}{3} + z_6\right) \mathbf{a}_3 = \left(x_6 - \frac{1}{2}y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_6 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_6\right) c \hat{\mathbf{z}} & (6c) & \text{O V} \\ \mathbf{B}_{34} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = \frac{1}{2}(x_7 + y_7) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_7 + y_7) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (6c) & \text{S} \\ \mathbf{B}_{35} &= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \left(\frac{2}{3} + z_7\right) \mathbf{a}_3 = \left(\frac{1}{2}x_7 - y_7\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_7 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_7\right) c \hat{\mathbf{z}} & (6c) & \text{S} \\ \mathbf{B}_{36} &= (-x_7 + y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(\frac{1}{3} + z_7\right) \mathbf{a}_3 = \left(-x_7 + \frac{1}{2}y_7\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_7 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_7\right) c \hat{\mathbf{z}} & (6c) & \text{S} \\ \mathbf{B}_{37} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = -\frac{1}{2}(x_7 + y_7) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_7 - y_7) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (6c) & \text{S} \\ \mathbf{B}_{38} &= y_7 \mathbf{a}_1 + (-x_7 + y_7) \mathbf{a}_2 + \left(\frac{2}{3} + z_7\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_7 + y_7\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_7 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_7\right) c \hat{\mathbf{z}} & (6c) & \text{S} \\ \mathbf{B}_{39} &= (x_7 - y_7) \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(\frac{1}{3} + z_7\right) \mathbf{a}_3 = \left(x_7 - \frac{1}{2}y_7\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_7 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_7\right) c \hat{\mathbf{z}} & (6c) & \text{S} \end{aligned}$$

#### References:

- R. N. Hargreaves and E. Stanley, *The structure of strontium dithionate tetrahydrate*, *Zeitschrift für Kristallographie - Crystalline Materials* **135**, 399–407 (1972), doi:10.1524/zkri.1972.135.5-6.399.

#### Found in:

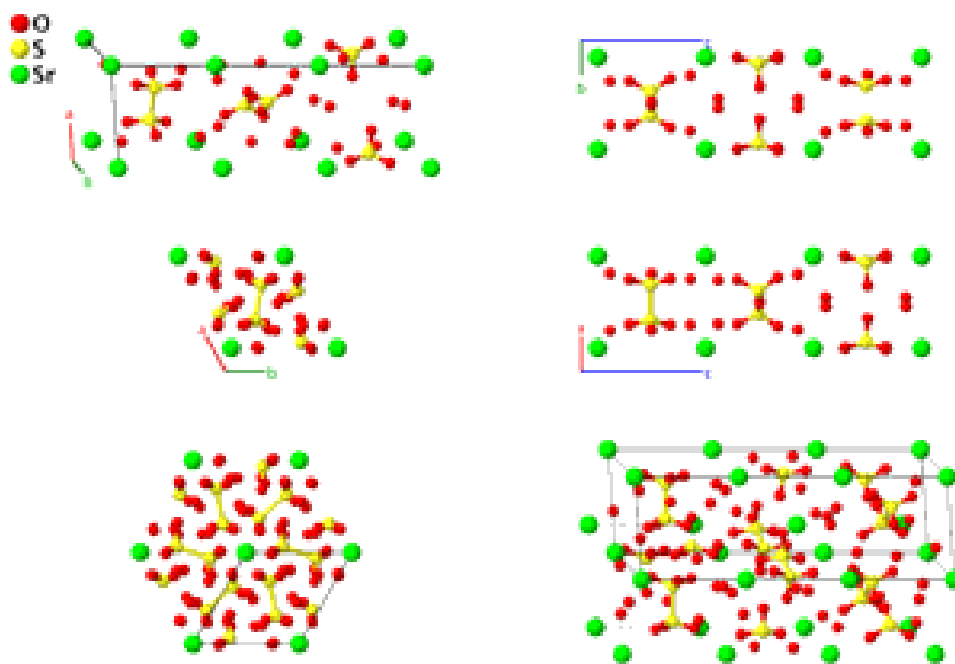
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

#### Geometry files:

- CIF: pp. 924

- POSCAR: pp. [925](#)

# Sr[S<sub>2</sub>O<sub>6</sub>][H<sub>2</sub>O]<sub>4</sub> Structure: A10B2C\_hP39\_172\_5c\_c\_a

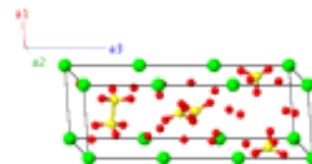


<b>Prototype</b>	:	Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub>
<b>AFLOW prototype label</b>	:	A10B2C_hP39_172_5c_c_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP39
<b>Space group number</b>	:	172
<b>Space group symbol</b>	:	<i>P</i> 6 <sub>4</sub>
<b>AFLOW prototype command</b>	:	aflow --proto=A10B2C_hP39_172_5c_c_a --params= <i>a</i> , <i>c/a</i> , <i>z</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>y</i> <sub>2</sub> , <i>z</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>x</i> <sub>6</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub> , <i>x</i> <sub>7</sub> , <i>y</i> <sub>7</sub> , <i>z</i> <sub>7</sub>

- This structure is the enantiomorph of the [Sr\[S<sub>2</sub>O<sub>6</sub>\]\[H<sub>2</sub>O\]<sub>4</sub> \(A10B2C\\_hP39\\_171\\_5c\\_c\\_a\)](#) structure, and was generated by reflecting the coordinates of the space group #171 structure through the *z* = 0 plane. Only the non-hydrogen atoms are included in the prototype.

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub> =	<i>z</i> <sub>1</sub> <b>a</b> <sub>3</sub>	=	<i>z</i> <sub>1</sub> <i>c</i> <b>z</b> <sup>^</sup>	(3 <i>a</i> )	Sr
<b>B</b> <sub>2</sub> =	( $\frac{1}{3} + z_1$ ) <b>a</b> <sub>3</sub>	=	( $\frac{1}{3} + z_1$ ) <i>c</i> <b>z</b> <sup>^</sup>	(3 <i>a</i> )	Sr
<b>B</b> <sub>3</sub> =	( $\frac{2}{3} + z_1$ ) <b>a</b> <sub>3</sub>	=	( $\frac{2}{3} + z_1$ ) <i>c</i> <b>z</b> <sup>^</sup>	(3 <i>a</i> )	Sr

$$\begin{aligned}
\mathbf{B}_4 &= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 = \frac{1}{2}(x_2 + y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_2 + y_2)a \hat{\mathbf{y}} + z_2c \hat{\mathbf{z}} & (6c) & \text{O I} \\
\mathbf{B}_5 &= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{1}{3} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2}x_2 - y_2\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_2\right)c \hat{\mathbf{z}} & (6c) & \text{O I} \\
\mathbf{B}_6 &= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{2}{3} + z_2\right) \mathbf{a}_3 = \left(-x_2 + \frac{1}{2}y_2\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_2\right)c \hat{\mathbf{z}} & (6c) & \text{O I} \\
\mathbf{B}_7 &= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 = -\frac{1}{2}(x_2 + y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_2 - y_2)a \hat{\mathbf{y}} + z_2c \hat{\mathbf{z}} & (6c) & \text{O I} \\
\mathbf{B}_8 &= y_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + \left(\frac{1}{3} + z_2\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_2 + y_2\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_2\right)c \hat{\mathbf{z}} & (6c) & \text{O I} \\
\mathbf{B}_9 &= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{2}{3} + z_2\right) \mathbf{a}_3 = \left(x_2 - \frac{1}{2}y_2\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_2a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_2\right)c \hat{\mathbf{z}} & (6c) & \text{O I} \\
\mathbf{B}_{10} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = \frac{1}{2}(x_3 + y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3)a \hat{\mathbf{y}} + z_3c \hat{\mathbf{z}} & (6c) & \text{O II} \\
\mathbf{B}_{11} &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{1}{3} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2}x_3 - y_3\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_3\right)c \hat{\mathbf{z}} & (6c) & \text{O II} \\
\mathbf{B}_{12} &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{2}{3} + z_3\right) \mathbf{a}_3 = \left(-x_3 + \frac{1}{2}y_3\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_3\right)c \hat{\mathbf{z}} & (6c) & \text{O II} \\
\mathbf{B}_{13} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = -\frac{1}{2}(x_3 + y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3)a \hat{\mathbf{y}} + z_3c \hat{\mathbf{z}} & (6c) & \text{O II} \\
\mathbf{B}_{14} &= y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{1}{3} + z_3\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_3 + y_3\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_3\right)c \hat{\mathbf{z}} & (6c) & \text{O II} \\
\mathbf{B}_{15} &= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{2}{3} + z_3\right) \mathbf{a}_3 = \left(x_3 - \frac{1}{2}y_3\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_3\right)c \hat{\mathbf{z}} & (6c) & \text{O II} \\
\mathbf{B}_{16} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = \frac{1}{2}(x_4 + y_4)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_4 + y_4)a \hat{\mathbf{y}} + z_4c \hat{\mathbf{z}} & (6c) & \text{O III} \\
\mathbf{B}_{17} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{1}{3} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2}x_4 - y_4\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_4\right)c \hat{\mathbf{z}} & (6c) & \text{O III} \\
\mathbf{B}_{18} &= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{2}{3} + z_4\right) \mathbf{a}_3 = \left(-x_4 + \frac{1}{2}y_4\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_4\right)c \hat{\mathbf{z}} & (6c) & \text{O III} \\
\mathbf{B}_{19} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = -\frac{1}{2}(x_4 + y_4)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_4 - y_4)a \hat{\mathbf{y}} + z_4c \hat{\mathbf{z}} & (6c) & \text{O III} \\
\mathbf{B}_{20} &= y_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \left(\frac{1}{3} + z_4\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_4 + y_4\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_4a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_4\right)c \hat{\mathbf{z}} & (6c) & \text{O III} \\
\mathbf{B}_{21} &= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{2}{3} + z_4\right) \mathbf{a}_3 = \left(x_4 - \frac{1}{2}y_4\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_4a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_4\right)c \hat{\mathbf{z}} & (6c) & \text{O III} \\
\mathbf{B}_{22} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \frac{1}{2}(x_5 + y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5)a \hat{\mathbf{y}} + z_5c \hat{\mathbf{z}} & (6c) & \text{O IV} \\
\mathbf{B}_{23} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{1}{3} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2}x_5 - y_5\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_5\right)c \hat{\mathbf{z}} & (6c) & \text{O IV}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{24} &= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{2}{3} + z_5\right) \mathbf{a}_3 = \left(-x_5 + \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_5\right) c \hat{\mathbf{z}} & (6c) & \text{O IV} \\
\mathbf{B}_{25} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = -\frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_5 - y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (6c) & \text{O IV} \\
\mathbf{B}_{26} &= y_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \left(\frac{1}{3} + z_5\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_5\right) c \hat{\mathbf{z}} & (6c) & \text{O IV} \\
\mathbf{B}_{27} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{2}{3} + z_5\right) \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_5\right) c \hat{\mathbf{z}} & (6c) & \text{O IV} \\
\mathbf{B}_{28} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \frac{1}{2}(x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_6 + y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6c) & \text{O V} \\
\mathbf{B}_{29} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \left(\frac{1}{3} + z_6\right) \mathbf{a}_3 = \left(\frac{1}{2}x_6 - y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_6 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_6\right) c \hat{\mathbf{z}} & (6c) & \text{O V} \\
\mathbf{B}_{30} &= (-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(\frac{2}{3} + z_6\right) \mathbf{a}_3 = \left(-x_6 + \frac{1}{2}y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_6 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_6\right) c \hat{\mathbf{z}} & (6c) & \text{O V} \\
\mathbf{B}_{31} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = -\frac{1}{2}(x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_6 - y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (6c) & \text{O V} \\
\mathbf{B}_{32} &= y_6 \mathbf{a}_1 + (-x_6 + y_6) \mathbf{a}_2 + \left(\frac{1}{3} + z_6\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_6 + y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_6 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_6\right) c \hat{\mathbf{z}} & (6c) & \text{O V} \\
\mathbf{B}_{33} &= (x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(\frac{2}{3} + z_6\right) \mathbf{a}_3 = \left(x_6 - \frac{1}{2}y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_6 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_6\right) c \hat{\mathbf{z}} & (6c) & \text{O V} \\
\mathbf{B}_{34} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = \frac{1}{2}(x_7 + y_7) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_7 + y_7) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (6c) & \text{S} \\
\mathbf{B}_{35} &= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \left(\frac{1}{3} + z_7\right) \mathbf{a}_3 = \left(\frac{1}{2}x_7 - y_7\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_7 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_7\right) c \hat{\mathbf{z}} & (6c) & \text{S} \\
\mathbf{B}_{36} &= (-x_7 + y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(\frac{2}{3} + z_7\right) \mathbf{a}_3 = \left(-x_7 + \frac{1}{2}y_7\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_7 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_7\right) c \hat{\mathbf{z}} & (6c) & \text{S} \\
\mathbf{B}_{37} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = -\frac{1}{2}(x_7 + y_7) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_7 - y_7) a \hat{\mathbf{y}} + z_7 c \hat{\mathbf{z}} & (6c) & \text{S} \\
\mathbf{B}_{38} &= y_7 \mathbf{a}_1 + (-x_7 + y_7) \mathbf{a}_2 + \left(\frac{1}{3} + z_7\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_7 + y_7\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_7 a \hat{\mathbf{y}} + \left(\frac{1}{3} + z_7\right) c \hat{\mathbf{z}} & (6c) & \text{S} \\
\mathbf{B}_{39} &= (x_7 - y_7) \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(\frac{2}{3} + z_7\right) \mathbf{a}_3 = \left(x_7 - \frac{1}{2}y_7\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_7 a \hat{\mathbf{y}} + \left(\frac{2}{3} + z_7\right) c \hat{\mathbf{z}} & (6c) & \text{S}
\end{aligned}$$

## References:

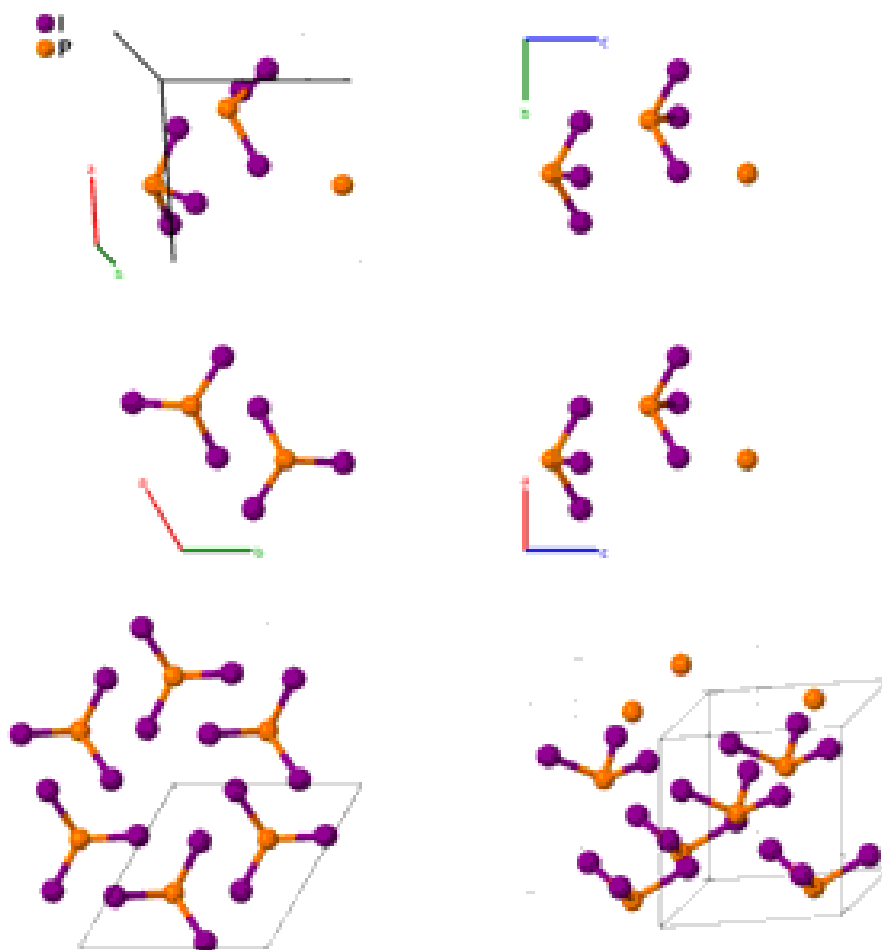
- R. N. Hargreaves and E. Stanley, *The structure of strontium dithionate tetrahydrate*, *Zeitschrift für Kristallographie - Crystalline Materials* **135**, 399–407 (1972), doi:10.1524/zkri.1972.135.5-6.399.

## Geometry files:

- CIF: pp. 925

- POSCAR: pp. 925

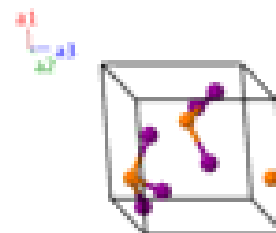
# PI<sub>3</sub> Structure: A3B\_hP8\_173\_c\_b



<b>Prototype</b>	:	PI <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B_hP8_173_c_b
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP8
<b>Space group number</b>	:	173
<b>Space group symbol</b>	:	<i>P</i> 6 <sub>3</sub>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A3B_hP8_173_c_b --params=a, c/a, z1, x2, y2, z2</code>

**Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**



	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(2b)	P
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2b)	P
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} +$ $\frac{\sqrt{3}}{2} (-x_2 + y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6c)	I
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} x_2 - y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6c)	I
$\mathbf{B}_5$	$= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\left(-x_2 + \frac{1}{2} y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6c)	I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$-\frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} +$ $\frac{\sqrt{3}}{2} (x_2 - y_2) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(6c)	I
$\mathbf{B}_7$	$= y_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$\left(-\frac{1}{2} x_2 + y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(6c)	I
$\mathbf{B}_8$	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$\left(x_2 - \frac{1}{2} y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_2 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(6c)	I

---

#### References:

- E. T. Lance, J. M. Haschke, and D. R. Peacor, *Crystal and molecular structure of phosphorus triiodide*, Inorg. Chem. **15**, 780–781 (1976), doi:10.1021/ic50158a007.

#### Found in:

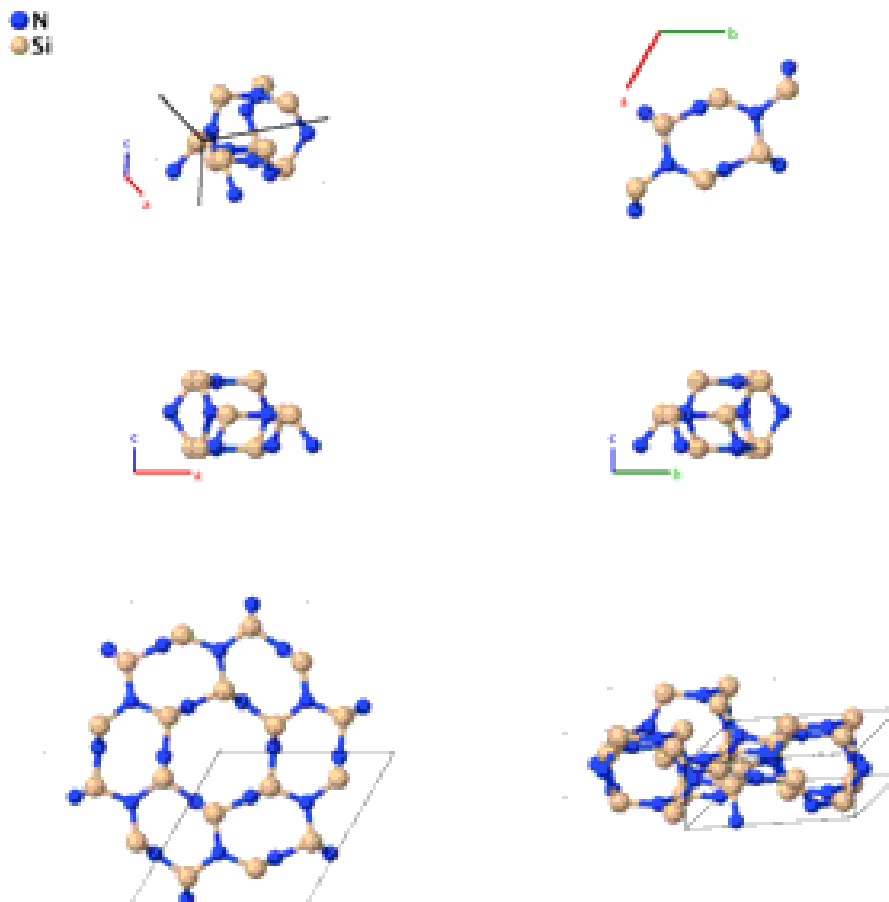
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 925  
- POSCAR: pp. 926

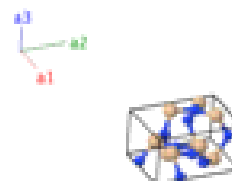
# $\beta$ -Si<sub>3</sub>N<sub>4</sub> Structure: A4B3\_hP14\_173\_bc\_c



<b>Prototype</b>	:	$\beta$ -Si <sub>3</sub> N <sub>4</sub>
<b>AFLOW prototype label</b>	:	A4B3_hP14_173_bc_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP14
<b>Space group number</b>	:	173
<b>Space group symbol</b>	:	$P6_3$
<b>AFLOW prototype command</b>	:	aflow --proto=A4B3_hP14_173_bc_c --params=a, c/a, z <sub>1</sub> , x <sub>2</sub> , y <sub>2</sub> , z <sub>2</sub> , x <sub>3</sub> , y <sub>3</sub> , z <sub>3</sub>

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type

$$\begin{aligned}
\mathbf{B}_1 &= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_1 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}} & (2b) & \text{N I} \\
\mathbf{B}_2 &= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}} & (2b) & \text{N I} \\
\mathbf{B}_3 &= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 &= \frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} + & (6c) & \text{N II} \\
& & \frac{\sqrt{3}}{2} (-x_2 + y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & & \\
\mathbf{B}_4 &= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3 &= \left(\frac{1}{2} x_2 - y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (6c) & \text{N II} \\
\mathbf{B}_5 &= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3 &= \left(-x_2 + \frac{1}{2} y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}} & (6c) & \text{N II} \\
\mathbf{B}_6 &= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= -\frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} + & (6c) & \text{N II} \\
& & \frac{\sqrt{3}}{2} (x_2 - y_2) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_7 &= y_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(-\frac{1}{2} x_2 + y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + & (6c) & \text{N II} \\
& & \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_8 &= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \left(x_2 - \frac{1}{2} y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_2 a \hat{\mathbf{y}} + & (6c) & \text{N II} \\
& & \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + & (6c) & \text{Si} \\
& & \frac{\sqrt{3}}{2} (-x_3 + y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & & \\
\mathbf{B}_{10} &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \left(\frac{1}{2} x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (6c) & \text{Si} \\
\mathbf{B}_{11} &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \left(-x_3 + \frac{1}{2} y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (6c) & \text{Si} \\
\mathbf{B}_{12} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= -\frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + & (6c) & \text{Si} \\
& & \frac{\sqrt{3}}{2} (x_3 - y_3) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{13} &= y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(-\frac{1}{2} x_3 + y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + & (6c) & \text{Si} \\
& & \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & & \\
\mathbf{B}_{14} &= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= \left(x_3 - \frac{1}{2} y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + & (6c) & \text{Si} \\
& & \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & &
\end{aligned}$$

---

#### References:

- W. D. Forgeng and B. F. Decker, *Nitrides of silicon*, T. Am. I. Min. Met. Eng. **212**, 343–348 (1958).

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

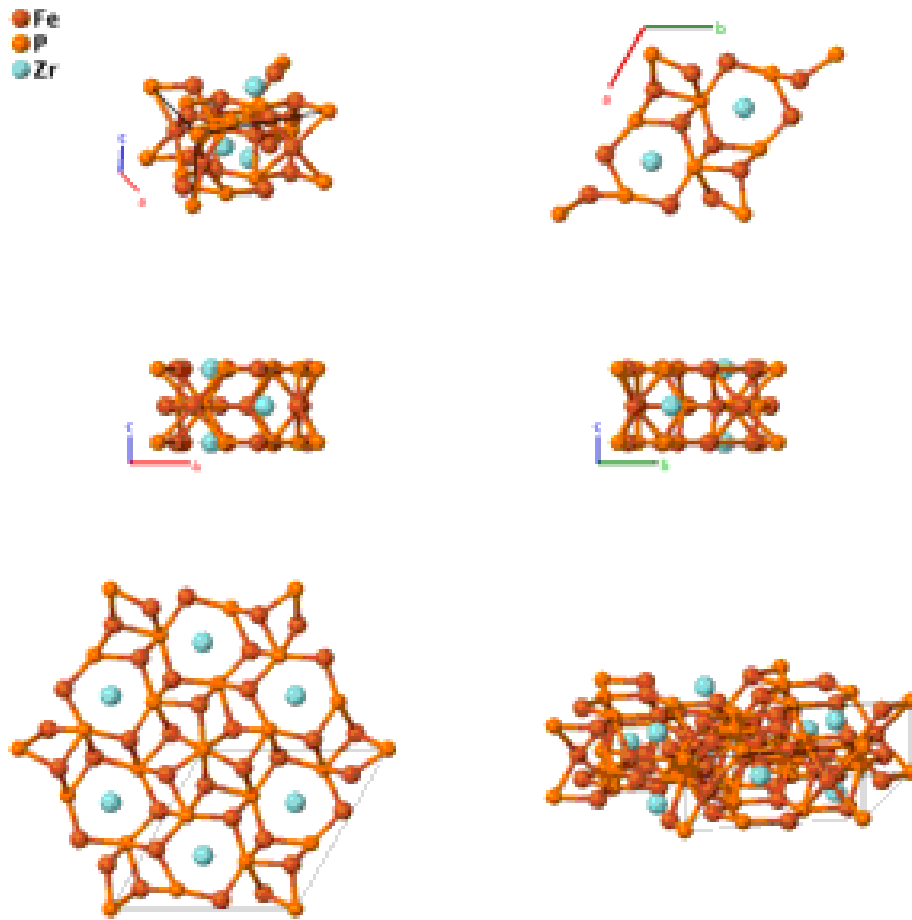
---

#### Geometry files:

- CIF: pp. [926](#)

- POSCAR: pp. [926](#)

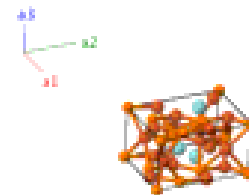
# Fe<sub>12</sub>Zr<sub>2</sub>P<sub>7</sub> Structure: A12B7C2\_hP21\_174\_2j2k\_ajk\_cf



<b>Prototype</b>	:	Fe <sub>12</sub> Zr <sub>2</sub> P <sub>7</sub>
<b>AFLOW prototype label</b>	:	A12B7C2_hP21_174_2j2k_ajk_cf
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP21
<b>Space group number</b>	:	174
<b>Space group symbol</b>	:	$P\bar{6}$
<b>AFLOW prototype command</b>	:	aflow --proto=A12B7C2_hP21_174_2j2k_ajk_cf --params=a, c/a, x <sub>4</sub> , y <sub>4</sub> , x <sub>5</sub> , y <sub>5</sub> , x <sub>6</sub> , y <sub>6</sub> , x <sub>7</sub> , y <sub>7</sub> , x <sub>8</sub> , y <sub>8</sub> , x <sub>9</sub> , y <sub>9</sub>

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type

$$\begin{aligned}
\mathbf{B}_1 &= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3 &= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}} & (1a) & \text{P I} \\
\mathbf{B}_2 &= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} & (1c) & \text{Zr I} \\
\mathbf{B}_3 &= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (1f) & \text{Zr II} \\
\mathbf{B}_4 &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 &= \frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} & (3j) & \text{Fe I} \\
\mathbf{B}_5 &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 &= \left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} & (3j) & \text{Fe I} \\
\mathbf{B}_6 &= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 &= \left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} & (3j) & \text{Fe I} \\
\mathbf{B}_7 &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 &= \frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}} & (3j) & \text{Fe II} \\
\mathbf{B}_8 &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 &= \left(\frac{1}{2} x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} & (3j) & \text{Fe II} \\
\mathbf{B}_9 &= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 &= \left(-x_5 + \frac{1}{2} y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} & (3j) & \text{Fe II} \\
\mathbf{B}_{10} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 &= \frac{1}{2} (x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_6 + y_6) a \hat{\mathbf{y}} & (3j) & \text{P II} \\
\mathbf{B}_{11} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 &= \left(\frac{1}{2} x_6 - y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} & (3j) & \text{P II} \\
\mathbf{B}_{12} &= (-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 &= \left(-x_6 + \frac{1}{2} y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_6 a \hat{\mathbf{y}} & (3j) & \text{P II} \\
\mathbf{B}_{13} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \frac{1}{2} (x_7 + y_7) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_7 + y_7) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (3k) & \text{Fe III} \\
\mathbf{B}_{14} &= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} x_7 - y_7\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_7 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (3k) & \text{Fe III} \\
\mathbf{B}_{15} &= (-x_7 + y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(-x_7 + \frac{1}{2} y_7\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_7 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (3k) & \text{Fe III} \\
\mathbf{B}_{16} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \frac{1}{2} (x_8 + y_8) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_8 + y_8) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (3k) & \text{Fe IV} \\
\mathbf{B}_{17} &= -y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} x_8 - y_8\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_8 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (3k) & \text{Fe IV} \\
\mathbf{B}_{18} &= (-x_8 + y_8) \mathbf{a}_1 - x_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(-x_8 + \frac{1}{2} y_8\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_8 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (3k) & \text{Fe IV} \\
\mathbf{B}_{19} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \frac{1}{2} (x_9 + y_9) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_9 + y_9) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (3k) & \text{P III} \\
\mathbf{B}_{20} &= -y_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} x_9 - y_9\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_9 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (3k) & \text{P III} \\
\mathbf{B}_{21} &= (-x_9 + y_9) \mathbf{a}_1 - x_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(-x_9 + \frac{1}{2} y_9\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_9 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (3k) & \text{P III}
\end{aligned}$$

## References:

- E. Ganglberger, *Die Kristallstruktur von Fe<sub>12</sub>Zr<sub>2</sub>P<sub>7</sub>*, *Monatsh. Chem.* **99**, 557–565 (1968), [doi:10.1007/BF00901204](https://doi.org/10.1007/BF00901204).

## Found in:

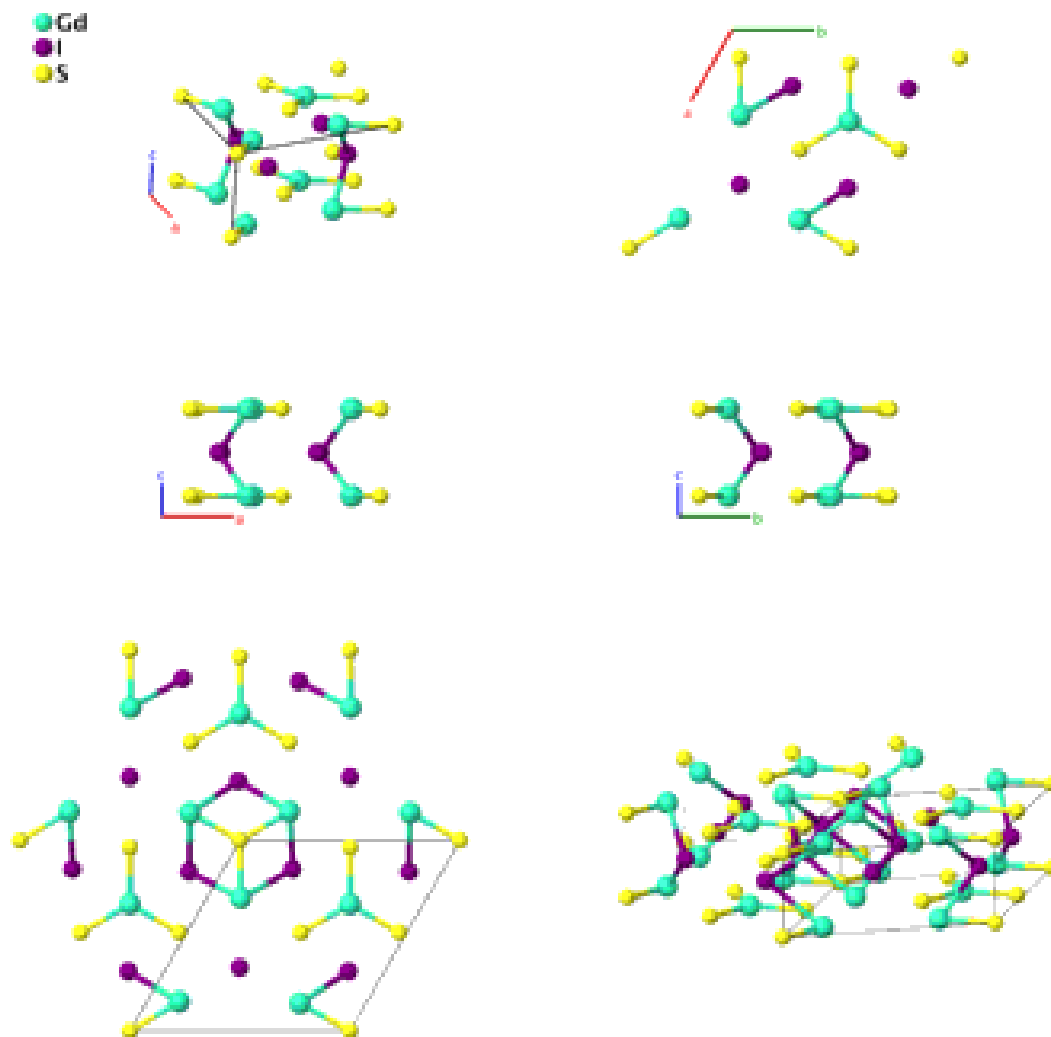
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

## Geometry files:

- CIF: pp. [926](#)

- POSCAR: pp. [927](#)

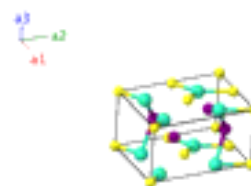
# GdSI Structure: ABC\_hP12\_174\_cj\_fk\_aj



<b>Prototype</b>	:	GdSI
<b>AFLOW prototype label</b>	:	ABC_hP12_174_cj_fk_aj
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP12
<b>Space group number</b>	:	174
<b>Space group symbol</b>	:	$P\bar{6}$
<b>AFLOW prototype command</b>	:	aflow --proto=ABC_hP12_174_cj_fk_aj --params= $a, c/a, x_4, y_4, x_5, y_5, x_6, y_6$

**Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type	
<b>B</b> <sub>1</sub>	=	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	S I
<b>B</b> <sub>2</sub>	=	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}}$	(1c)	Gd I
<b>B</b> <sub>3</sub>	=	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(1f)	II
<b>B</b> <sub>4</sub>	=	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	=	$\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}}$	(3j)	Gd II
<b>B</b> <sub>5</sub>	=	$-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2$	=	$(\frac{1}{2} x_4 - y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}}$	(3j)	Gd II
<b>B</b> <sub>6</sub>	=	$(-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2$	=	$(-x_4 + \frac{1}{2} y_4) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}}$	(3j)	Gd II
<b>B</b> <sub>7</sub>	=	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	=	$\frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}}$	(3j)	S II
<b>B</b> <sub>8</sub>	=	$-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2$	=	$(\frac{1}{2} x_5 - y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}}$	(3j)	S II
<b>B</b> <sub>9</sub>	=	$(-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2$	=	$(-x_5 + \frac{1}{2} y_5) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}}$	(3j)	S II
<b>B</b> <sub>10</sub>	=	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} (x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_6 + y_6) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(3k)	I II
<b>B</b> <sub>11</sub>	=	$-y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$(\frac{1}{2} x_6 - y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(3k)	I II
<b>B</b> <sub>12</sub>	=	$(-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$(-x_6 + \frac{1}{2} y_6) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_6 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(3k)	I II

---

#### References:

- C. Dagron and F. Thevet, *Répartition des types cristallins dans la série des iodosulfures et fluorosulfures des éléments des terres rares et d'yttrium*, C. R. Hebd. Séances Acad. Sci. C **268**, 1867–1869 (1969).

#### Found in:

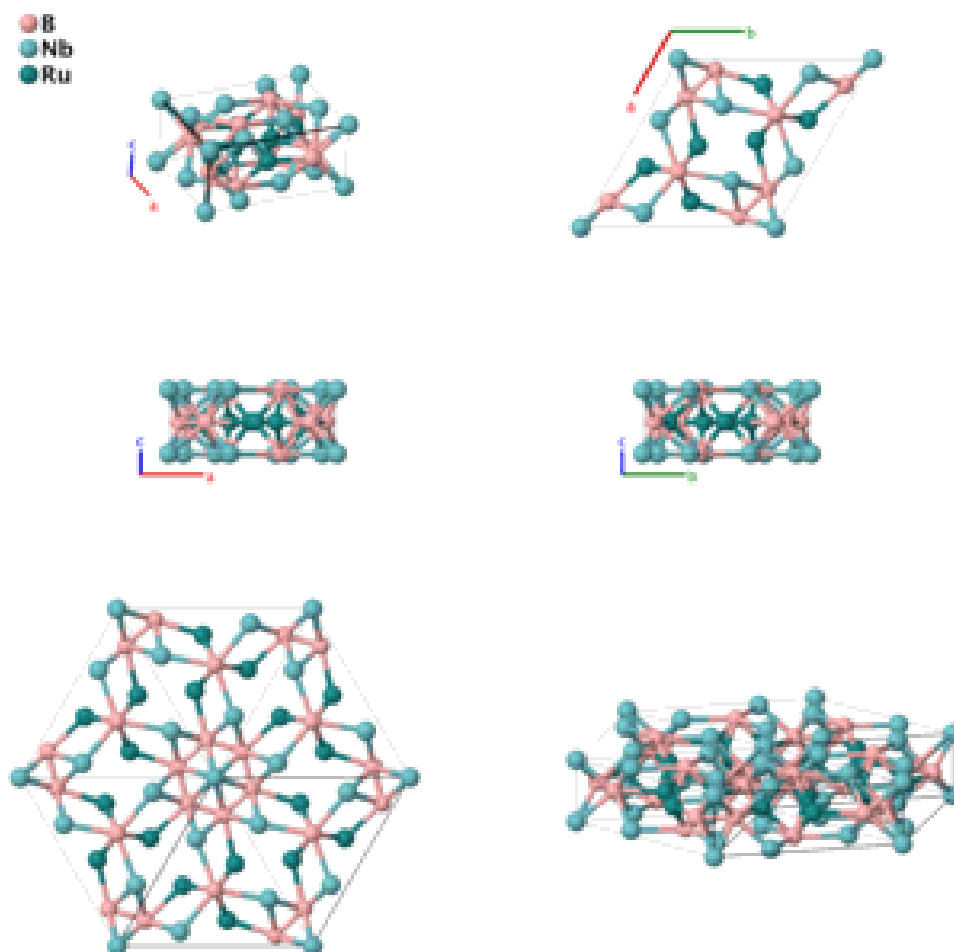
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [927](#)
- POSCAR: pp. [927](#)

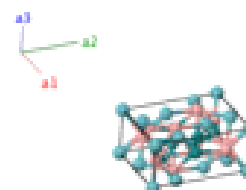
# Nb<sub>7</sub>Ru<sub>6</sub>B<sub>8</sub> Structure: A8B7C6\_hP21\_175\_ck\_aj\_k



<b>Prototype</b>	:	Nb <sub>7</sub> Ru <sub>6</sub> B <sub>8</sub>
<b>AFLOW prototype label</b>	:	A8B7C6_hP21_175_ck_aj_k
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP21
<b>Space group number</b>	:	175
<b>Space group symbol</b>	:	<i>P6/m</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A8B7C6_hP21_175_ck_aj_k --params= <i>a, c/a, x<sub>3</sub>, y<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub></i>

**Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**



	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Nb I
$\mathbf{B}_2$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}}$	(2c)	B I
$\mathbf{B}_3$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}}$	(2c)	B I
$\mathbf{B}_4$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$\frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_3 + y_3) a \hat{\mathbf{y}}$	(6j)	Nb II
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2$	$=$	$(\frac{1}{2} x_3 - y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}}$	(6j)	Nb II
$\mathbf{B}_6$	$= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$(-x_3 + \frac{1}{2} y_3) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}}$	(6j)	Nb II
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-\frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_3 - y_3) a \hat{\mathbf{y}}$	(6j)	Nb II
$\mathbf{B}_8$	$= y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2$	$=$	$(-\frac{1}{2} x_3 + y_3) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}}$	(6j)	Nb II
$\mathbf{B}_9$	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$(x_3 - \frac{1}{2} y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}}$	(6j)	Nb II
$\mathbf{B}_{10}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6k)	B II
$\mathbf{B}_{11}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$(\frac{1}{2} x_4 - y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6k)	B II
$\mathbf{B}_{12}$	$= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$(-x_4 + \frac{1}{2} y_4) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6k)	B II
$\mathbf{B}_{13}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_4 - y_4) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6k)	B II
$\mathbf{B}_{14}$	$= y_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$(-\frac{1}{2} x_4 + y_4) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6k)	B II
$\mathbf{B}_{15}$	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$(x_4 - \frac{1}{2} y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6k)	B II
$\mathbf{B}_{16}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6k)	Ru
$\mathbf{B}_{17}$	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$(\frac{1}{2} x_5 - y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6k)	Ru
$\mathbf{B}_{18}$	$= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$(-x_5 + \frac{1}{2} y_5) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6k)	Ru
$\mathbf{B}_{19}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_5 - y_5) a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6k)	Ru
$\mathbf{B}_{20}$	$= y_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$(-\frac{1}{2} x_5 + y_5) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6k)	Ru
$\mathbf{B}_{21}$	$= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$(x_5 - \frac{1}{2} y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6k)	Ru

## References:

- Q. Zheng, M. Kohout, R. Gumeniuk, N. Abramchuk, H. Borrmann, Y. Prots, U. Burkhardt, W. Schnelle, L. Akselrud, H. Gu, A. Leithe-Jasper, and Y. Grin, *TM<sub>7</sub> TM'<sub>6</sub>B<sub>8</sub> (TM = Ta, Nb; TM' = Ru, Rh, Ir): New Compounds with [B<sub>6</sub>] Ring Polyanions*, Inorg. Chem. **51**, 7472–7483 (2012), doi:10.1021/ic201978n.

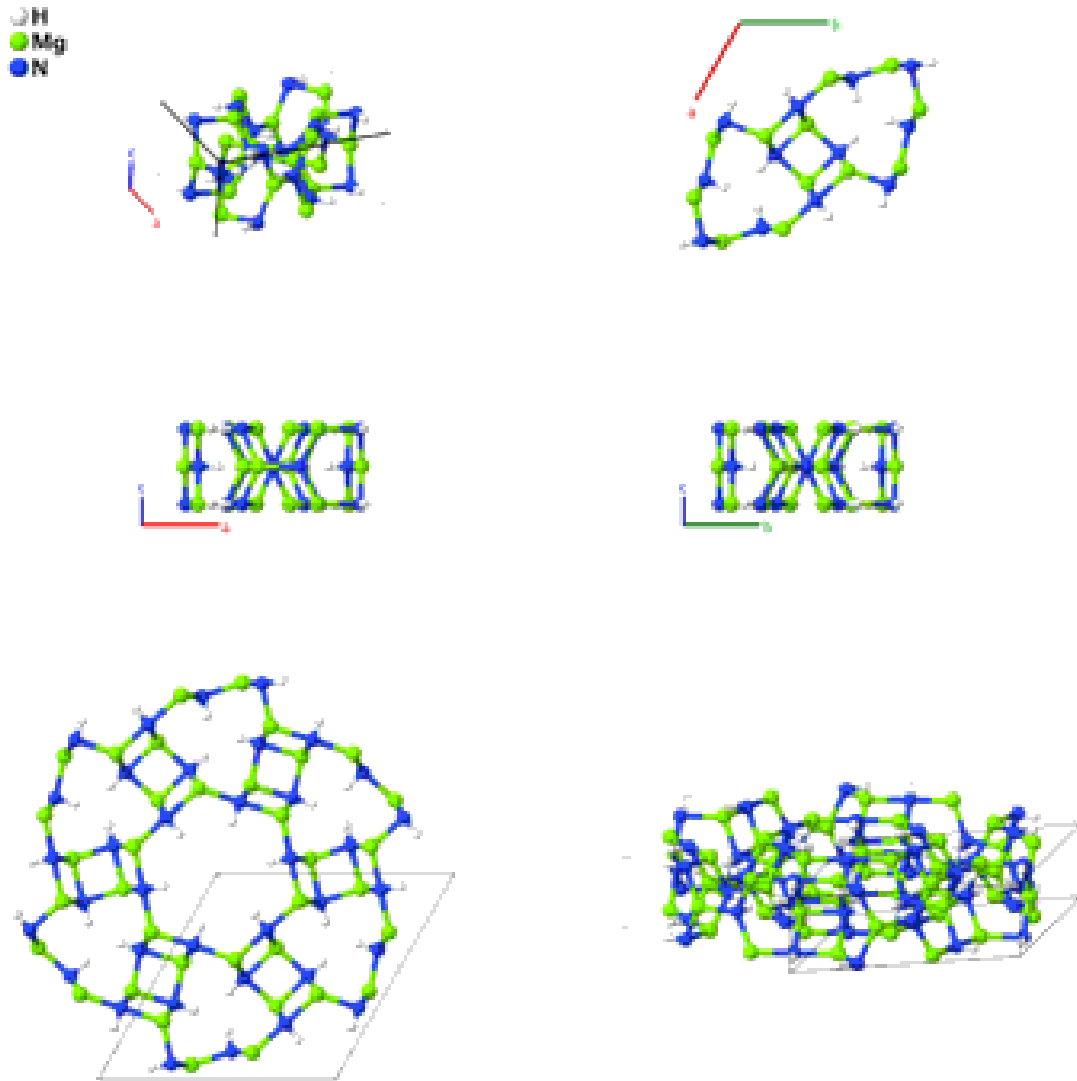
## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

## Geometry files:

- CIF: pp. 927  
 - POSCAR: pp. 928

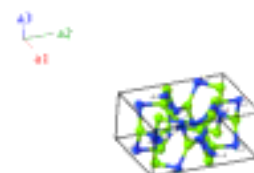
# Mg[NH] Structure: ABC\_hP36\_175\_jk\_jk\_jk



<b>Prototype</b>	:	Mg[NH]
<b>AFLOW prototype label</b>	:	ABC_hP36_175_jk_jk_jk
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP36
<b>Space group number</b>	:	175
<b>Space group symbol</b>	:	$P6/m$
<b>AFLOW prototype command</b>	:	aflow --proto=ABC_hP36_175_jk_jk_jk --params= $a, c/a, x_1, y_1, x_2, y_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6$

**Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates		Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	=	$\frac{1}{2}(x_1 + y_1)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_1 + y_1)a \hat{\mathbf{y}}$	(6j)		H I
<b>B</b> <sub>2</sub>	= $-y_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2$	=	$(\frac{1}{2}x_1 - y_1)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_1a \hat{\mathbf{y}}$	(6j)		H I
<b>B</b> <sub>3</sub>	= $(-x_1 + y_1) \mathbf{a}_1 - x_1 \mathbf{a}_2$	=	$(-x_1 + \frac{1}{2}y_1)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_1a \hat{\mathbf{y}}$	(6j)		H I
<b>B</b> <sub>4</sub>	= $-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	=	$-\frac{1}{2}(x_1 + y_1)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_1 - y_1)a \hat{\mathbf{y}}$	(6j)		H I
<b>B</b> <sub>5</sub>	= $y_1 \mathbf{a}_1 + (-x_1 + y_1) \mathbf{a}_2$	=	$(-\frac{1}{2}x_1 + y_1)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_1a \hat{\mathbf{y}}$	(6j)		H I
<b>B</b> <sub>6</sub>	= $(x_1 - y_1) \mathbf{a}_1 + x_1 \mathbf{a}_2$	=	$(x_1 - \frac{1}{2}y_1)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_1a \hat{\mathbf{y}}$	(6j)		H I
<b>B</b> <sub>7</sub>	= $x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	=	$\frac{1}{2}(x_2 + y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_2 + y_2)a \hat{\mathbf{y}}$	(6j)		Mg I
<b>B</b> <sub>8</sub>	= $-y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2$	=	$(\frac{1}{2}x_2 - y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}}$	(6j)		Mg I
<b>B</b> <sub>9</sub>	= $(-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2$	=	$(-x_2 + \frac{1}{2}y_2)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2a \hat{\mathbf{y}}$	(6j)		Mg I
<b>B</b> <sub>10</sub>	= $-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	=	$-\frac{1}{2}(x_2 + y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_2 - y_2)a \hat{\mathbf{y}}$	(6j)		Mg I
<b>B</b> <sub>11</sub>	= $y_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2$	=	$(-\frac{1}{2}x_2 + y_2)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}}$	(6j)		Mg I
<b>B</b> <sub>12</sub>	= $(x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2$	=	$(x_2 - \frac{1}{2}y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_2a \hat{\mathbf{y}}$	(6j)		Mg I
<b>B</b> <sub>13</sub>	= $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	=	$\frac{1}{2}(x_3 + y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3)a \hat{\mathbf{y}}$	(6j)		N I
<b>B</b> <sub>14</sub>	= $-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2$	=	$(\frac{1}{2}x_3 - y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}}$	(6j)		N I
<b>B</b> <sub>15</sub>	= $(-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2$	=	$(-x_3 + \frac{1}{2}y_3)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3a \hat{\mathbf{y}}$	(6j)		N I
<b>B</b> <sub>16</sub>	= $-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	=	$-\frac{1}{2}(x_3 + y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3)a \hat{\mathbf{y}}$	(6j)		N I
<b>B</b> <sub>17</sub>	= $y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2$	=	$(-\frac{1}{2}x_3 + y_3)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}}$	(6j)		N I
<b>B</b> <sub>18</sub>	= $(x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2$	=	$(x_3 - \frac{1}{2}y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3a \hat{\mathbf{y}}$	(6j)		N I
<b>B</b> <sub>19</sub>	= $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}(x_4 + y_4)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_4 + y_4)a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		H II
<b>B</b> <sub>20</sub>	= $-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$(\frac{1}{2}x_4 - y_4)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		H II
<b>B</b> <sub>21</sub>	= $(-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$(-x_4 + \frac{1}{2}y_4)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		H II
<b>B</b> <sub>22</sub>	= $-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-\frac{1}{2}(x_4 + y_4)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_4 - y_4)a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		H II
<b>B</b> <sub>23</sub>	= $y_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$(-\frac{1}{2}x_4 + y_4)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_4a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		H II
<b>B</b> <sub>24</sub>	= $(x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$(x_4 - \frac{1}{2}y_4)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_4a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		H II
<b>B</b> <sub>25</sub>	= $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}(x_5 + y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5)a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		Mg II
<b>B</b> <sub>26</sub>	= $-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$(\frac{1}{2}x_5 - y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		Mg II
<b>B</b> <sub>27</sub>	= $(-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$(-x_5 + \frac{1}{2}y_5)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		Mg II
<b>B</b> <sub>28</sub>	= $-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-\frac{1}{2}(x_5 + y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_5 - y_5)a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		Mg II
<b>B</b> <sub>29</sub>	= $y_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$(-\frac{1}{2}x_5 + y_5)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		Mg II
<b>B</b> <sub>30</sub>	= $(x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$(x_5 - \frac{1}{2}y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		Mg II
<b>B</b> <sub>31</sub>	= $x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}(x_6 + y_6)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_6 + y_6)a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		N II
<b>B</b> <sub>32</sub>	= $-y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$(\frac{1}{2}x_6 - y_6)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_6a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		N II
<b>B</b> <sub>33</sub>	= $(-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$(-x_6 + \frac{1}{2}y_6)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_6a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		N II
<b>B</b> <sub>34</sub>	= $-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-\frac{1}{2}(x_6 + y_6)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_6 - y_6)a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)		N II

$$\mathbf{B}_{35} = y_6 \mathbf{a}_1 + (-x_6 + y_6) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = \left(-\frac{1}{2}x_6 + y_6\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_6a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \quad (6k) \quad \text{N II}$$

$$\mathbf{B}_{36} = (x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = \left(x_6 - \frac{1}{2}y_6\right)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_6a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \quad (6k) \quad \text{N II}$$

---

**References:**

- F. Dolci, E. Napolitano, E. Weidner, S. Enzo, P. Moretto, M. Brunelli, T. Hansen, M. Fichtner, and W. Lohstroh, *Magnesium imide: synthesis and structure determination of an unconventional alkaline earth imide from decomposition of magnesium amide*, *Inorg. Chem.* **50**, 1116–1122 (2010), [doi:10.1021/ic1023778](https://doi.org/10.1021/ic1023778).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

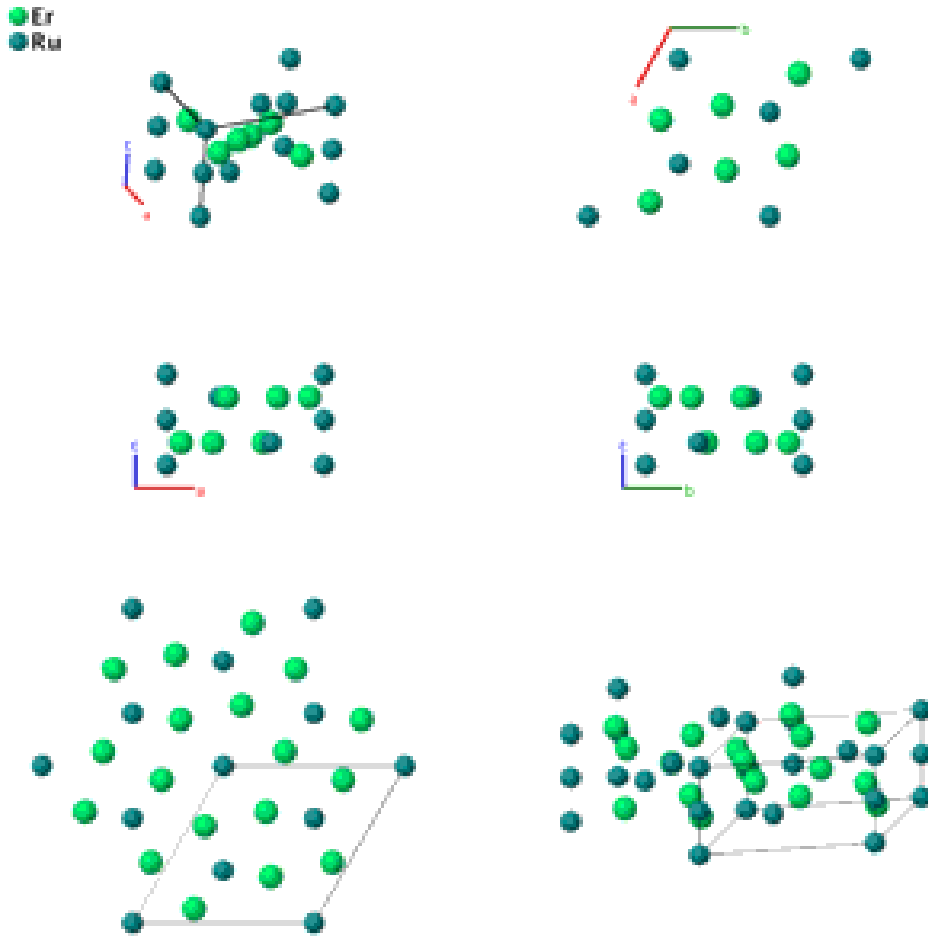
---

**Geometry files:**

- CIF: pp. [928](#)

- POSCAR: pp. [928](#)

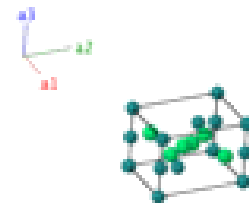
# Er<sub>3</sub>Ru<sub>2</sub> Structure: A3B2\_hP10\_176\_h\_bd



<b>Prototype</b>	:	Er <sub>3</sub> Ru <sub>2</sub>
<b>AFLOW prototype label</b>	:	A3B2_hP10_176_h_bd
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP10
<b>Space group number</b>	:	176
<b>Space group symbol</b>	:	$P6_3/m$
<b>AFLOW prototype command</b>	:	aflow --proto=A3B2_hP10_176_h_bd --params=a, c/a, x <sub>3</sub> , y <sub>3</sub>

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	=	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2b) Ru I
<b>B</b> <sub>2</sub>	=	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} c \hat{\mathbf{z}}$	(2b) Ru I
<b>B</b> <sub>3</sub>	=	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2d) Ru II
<b>B</b> <sub>4</sub>	=	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2d) Ru II
<b>B</b> <sub>5</sub>	=	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_3 + y_3) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h) Er
<b>B</b> <sub>6</sub>	=	$-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\left(\frac{1}{2} x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h) Er
<b>B</b> <sub>7</sub>	=	$(-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\left(-x_3 + \frac{1}{2} y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h) Er
<b>B</b> <sub>8</sub>	=	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-\frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_3 - y_3) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h) Er
<b>B</b> <sub>9</sub>	=	$y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\left(-\frac{1}{2} x_3 + y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h) Er
<b>B</b> <sub>10</sub>	=	$(x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\left(x_3 - \frac{1}{2} y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h) Er

---

#### References:

- A. Palenzona, *The phase diagram of the Er-Ru system*, J. Less-Common Met. **159**, L21–L23 (1990), [doi:10.1016/0022-5088\(90\)90169-K](https://doi.org/10.1016/0022-5088(90)90169-K).

#### Found in:

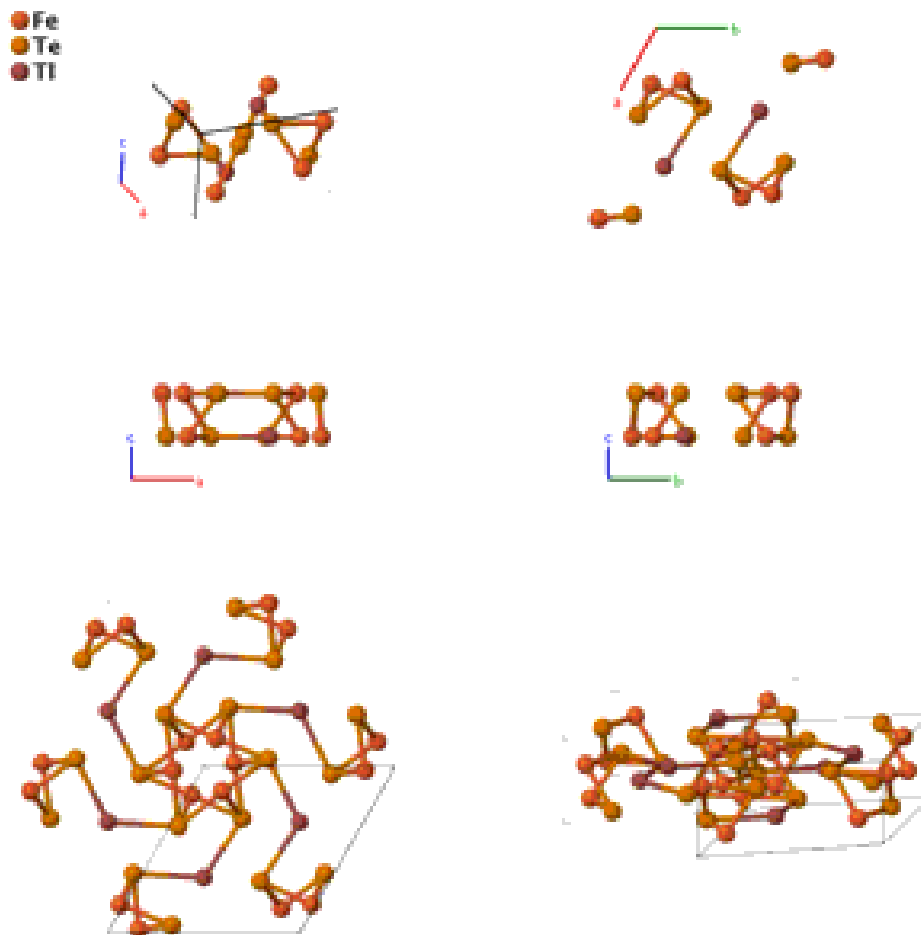
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. 929  
- POSCAR: pp. 929

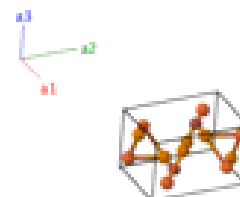
# Fe<sub>3</sub>Te<sub>3</sub>Tl Structure: A3B3C\_hP14\_176\_h\_h\_d



<b>Prototype</b>	:	Fe <sub>3</sub> Te <sub>3</sub> Tl
<b>AFLOW prototype label</b>	:	A3B3C_hP14_176_h_h_d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP14
<b>Space group number</b>	:	176
<b>Space group symbol</b>	:	<i>P</i> 6 <sub>3</sub> / <i>m</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3B3C_hP14_176_h_h_d --params= <i>a</i> , <i>c/a</i> , <i>x</i> <sub>2</sub> , <i>y</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>y</i> <sub>3</sub>

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2d)	Tl
$\mathbf{B}_2$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2d)	Tl
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}(x_2 + y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_2 + y_2)a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Fe
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$(\frac{1}{2}x_2 - y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Fe
$\mathbf{B}_5$	$= (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$(-x_2 + \frac{1}{2}y_2)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Fe
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}(x_2 + y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_2 - y_2)a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Fe
$\mathbf{B}_7$	$= y_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$(-\frac{1}{2}x_2 + y_2)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Fe
$\mathbf{B}_8$	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$(x_2 - \frac{1}{2}y_2)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_2a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Fe
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}(x_3 + y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3)a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Te
$\mathbf{B}_{10}$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$(\frac{1}{2}x_3 - y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Te
$\mathbf{B}_{11}$	$= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$(-x_3 + \frac{1}{2}y_3)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Te
$\mathbf{B}_{12}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}(x_3 + y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3)a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Te
$\mathbf{B}_{13}$	$= y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$(-\frac{1}{2}x_3 + y_3)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Te
$\mathbf{B}_{14}$	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$(x_3 - \frac{1}{2}y_3)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Te

---

#### References:

- K. Klepp and H. Boller, *Crystal Structures of Thallium-Iron Chalcogenides*, Acta Crystallogr. Sect. A **34**, S160–S161 (1978).

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

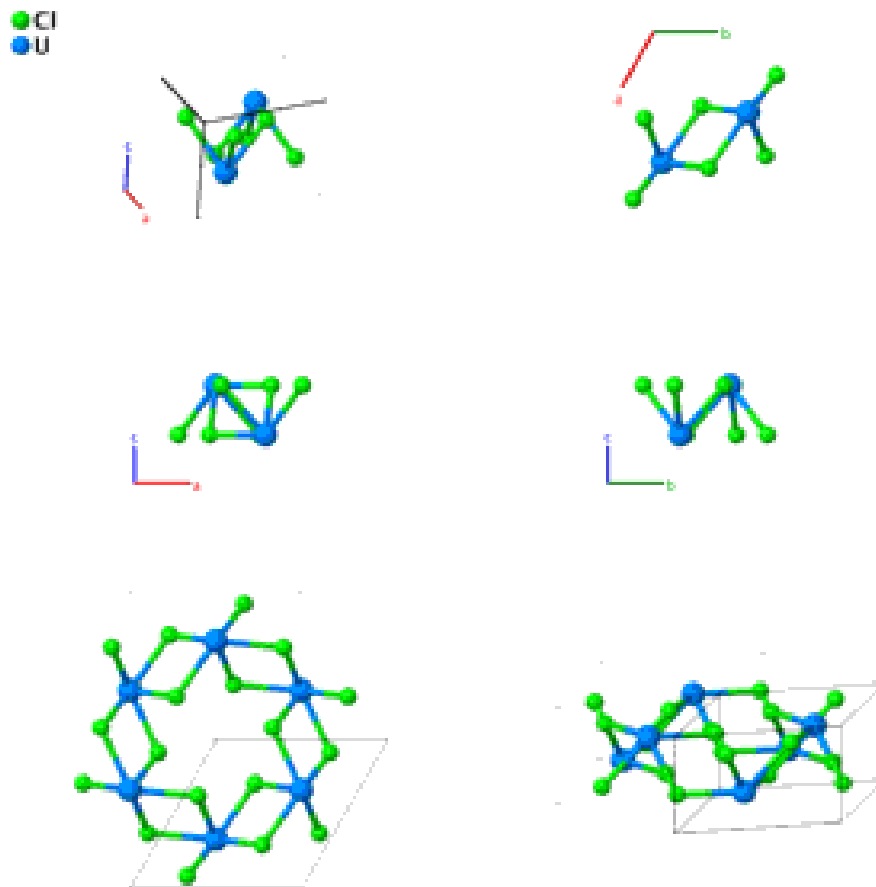
---

#### Geometry files:

- CIF: pp. [929](#)
- POSCAR: pp. [929](#)



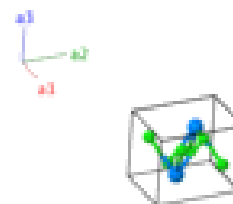
# UCl<sub>3</sub> Structure: A3B\_hP8\_176\_h\_d



<b>Prototype</b>	: UCl <sub>3</sub>
<b>AFLOW prototype label</b>	: A3B_hP8_176_h_d
<b>Strukturbericht designation</b>	: None
<b>Pearson symbol</b>	: hP8
<b>Space group number</b>	: 176
<b>Space group symbol</b>	: $P6_3/m$
<b>AFLOW prototype command</b>	: <code>aflow --proto=A3B_hP8_176_h_d</code> <code>--params=a, c/a, x<sub>2</sub>, y<sub>2</sub></code>

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type

$$\mathbf{B}_1 = \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} \quad (2d) \quad \text{U}$$

$$\mathbf{B}_2 = \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} \quad (2d) \quad \text{U}$$

$$\mathbf{B}_3 = x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 = \frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_2 + y_2) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} \quad (6h) \quad \text{Cl}$$

$$\mathbf{B}_4 = -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 = \left(\frac{1}{2} x_2 - y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} \quad (6h) \quad \text{Cl}$$

$$\mathbf{B}_5 = (-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 = \left(-x_2 + \frac{1}{2} y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} \quad (6h) \quad \text{Cl}$$

$$\mathbf{B}_6 = -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 = -\frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_2 - y_2) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} \quad (6h) \quad \text{Cl}$$

$$\mathbf{B}_7 = y_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 = \left(-\frac{1}{2} x_2 + y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} \quad (6h) \quad \text{Cl}$$

$$\mathbf{B}_8 = (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 = \left(x_2 - \frac{1}{2} y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} \quad (6h) \quad \text{Cl}$$

### References:

- W. H. Zachariasen, *Crystal chemical studies of the 5f-series of elements. I. New structure types*, Acta Cryst. **1**, 265–268 (1948), doi:10.1107/S0365110X48000703.

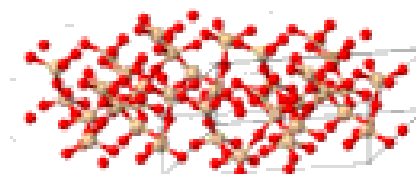
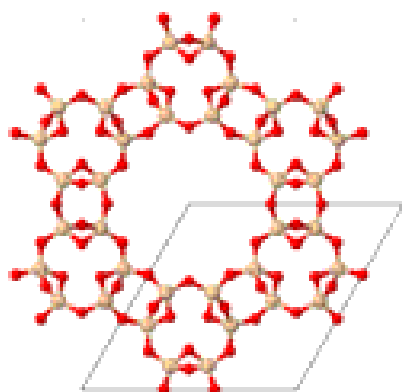
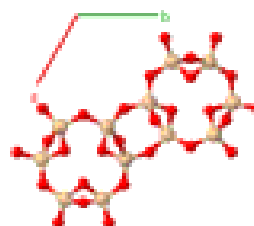
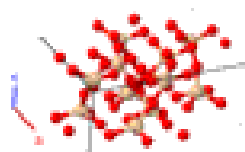
### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

### Geometry files:

- CIF: pp. 930
- POSCAR: pp. 930

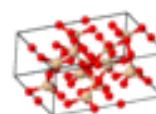
# SiO<sub>2</sub> Structure: A2B\_hP36\_177\_j2lm\_n



<b>Prototype</b>	:	SiO <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_hP36_177_j2lm_n
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP36
<b>Space group number</b>	:	177
<b>Space group symbol</b>	:	<i>P</i> 622
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_hP36_177_j2lm_n --params= <i>a</i> , <i>c/a</i> , <i>x</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub>

**Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1$	$=$	$\frac{1}{2}x_1a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_1a \hat{\mathbf{y}}$	(6j)	O I
$\mathbf{B}_2$	$= x_1 \mathbf{a}_2$	$=$	$\frac{1}{2}x_1a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_1a \hat{\mathbf{y}}$	(6j)	O I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-x_1a \hat{\mathbf{x}}$	(6j)	O I
$\mathbf{B}_4$	$= -x_1 \mathbf{a}_1$	$=$	$-\frac{1}{2}x_1a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_1a \hat{\mathbf{y}}$	(6j)	O I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_2$	$=$	$-\frac{1}{2}x_1a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_1a \hat{\mathbf{y}}$	(6j)	O I
$\mathbf{B}_6$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$x_1a \hat{\mathbf{x}}$	(6j)	O I
$\mathbf{B}_7$	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-\sqrt{3}x_2a \hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B}_8$	$= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2$	$=$	$\frac{3}{2}x_2a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B}_9$	$= -2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-\frac{3}{2}x_2a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B}_{10}$	$= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$\sqrt{3}x_2a \hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B}_{11}$	$= -x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2$	$=$	$-\frac{3}{2}x_2a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B}_{12}$	$= 2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$\frac{3}{2}x_2a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B}_{13}$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-\sqrt{3}x_3a \hat{\mathbf{y}}$	(6l)	O III
$\mathbf{B}_{14}$	$= x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2$	$=$	$\frac{3}{2}x_3a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}}$	(6l)	O III
$\mathbf{B}_{15}$	$= -2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-\frac{3}{2}x_3a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}}$	(6l)	O III
$\mathbf{B}_{16}$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$\sqrt{3}x_3a \hat{\mathbf{y}}$	(6l)	O III
$\mathbf{B}_{17}$	$= -x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2$	$=$	$-\frac{3}{2}x_3a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}}$	(6l)	O III
$\mathbf{B}_{18}$	$= 2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$\frac{3}{2}x_3a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}}$	(6l)	O III
$\mathbf{B}_{19}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\sqrt{3}x_4a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6m)	O IV
$\mathbf{B}_{20}$	$= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{2}x_4a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6m)	O IV
$\mathbf{B}_{21}$	$= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{3}{2}x_4a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6m)	O IV
$\mathbf{B}_{22}$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\sqrt{3}x_4a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6m)	O IV
$\mathbf{B}_{23}$	$= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{3}{2}x_4a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_4a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6m)	O IV
$\mathbf{B}_{24}$	$= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{2}x_4a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_4a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6m)	O IV
$\mathbf{B}_{25}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}(x_5 + y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5)a \hat{\mathbf{y}} + z_5c \hat{\mathbf{z}}$	(12n)	Si
$\mathbf{B}_{26}$	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(\frac{1}{2}x_5 - y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5a \hat{\mathbf{y}} + z_5c \hat{\mathbf{z}}$	(12n)	Si
$\mathbf{B}_{27}$	$= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(-x_5 + \frac{1}{2}y_5)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5a \hat{\mathbf{y}} + z_5c \hat{\mathbf{z}}$	(12n)	Si
$\mathbf{B}_{28}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}(x_5 + y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_5 - y_5)a \hat{\mathbf{y}} + z_5c \hat{\mathbf{z}}$	(12n)	Si
$\mathbf{B}_{29}$	$= y_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(-\frac{1}{2}x_5 + y_5)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5a \hat{\mathbf{y}} + z_5c \hat{\mathbf{z}}$	(12n)	Si
$\mathbf{B}_{30}$	$= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(x_5 - \frac{1}{2}y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5a \hat{\mathbf{y}} + z_5c \hat{\mathbf{z}}$	(12n)	Si
$\mathbf{B}_{31}$	$= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}(x_5 + y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_5 - y_5)a \hat{\mathbf{y}} - z_5c \hat{\mathbf{z}}$	(12n)	Si
$\mathbf{B}_{32}$	$= (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$(\frac{1}{2}x_5 - y_5)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5a \hat{\mathbf{y}} - z_5c \hat{\mathbf{z}}$	(12n)	Si
$\mathbf{B}_{33}$	$= -x_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$(-x_5 + \frac{1}{2}y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5a \hat{\mathbf{y}} - z_5c \hat{\mathbf{z}}$	(12n)	Si
$\mathbf{B}_{34}$	$= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}(x_5 + y_5)a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5)a \hat{\mathbf{y}} - z_5c \hat{\mathbf{z}}$	(12n)	Si

$$\mathbf{B}_{35} = (-x_5 + y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} \quad (12n) \quad \text{Si}$$

$$\mathbf{B}_{36} = x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} \quad (12n) \quad \text{Si}$$

---

**References:**

- M. D. Foster, O. Delgado Friedrichs, R. G. Bell, and F. A. Almeida Paz and J. Klinowski, *Chemical Evaluation of Hypothetical Uninodal Zeolites*, J. Am. Chem. Soc. **126**, 9769–9775 (2004), doi:10.1021/ja037334j.

**Found in:**

- ICSD, *Inorganic Crystal Structure Database*. ID 170519.

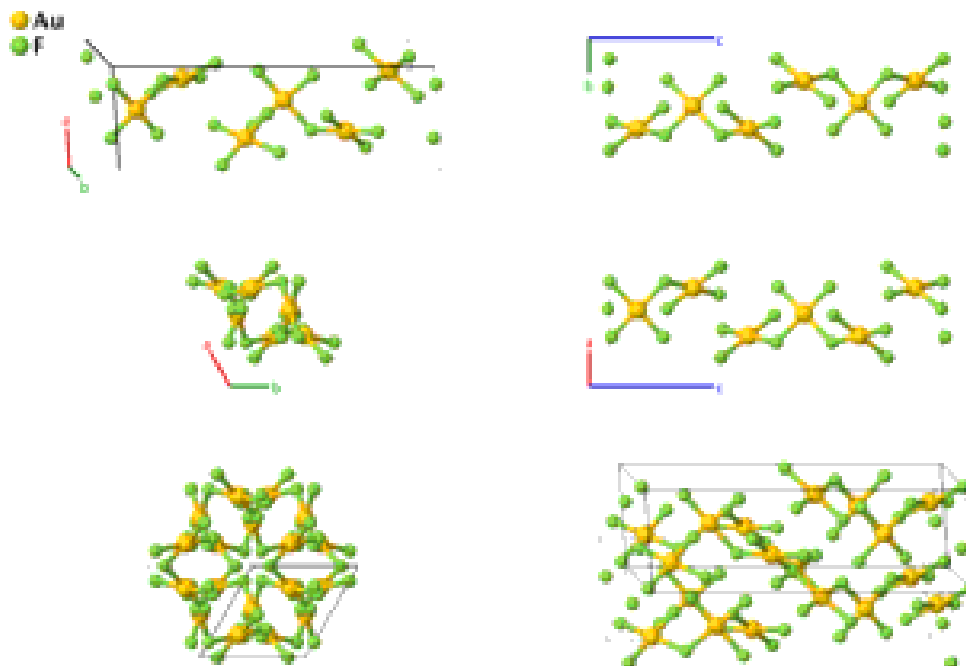
---

**Geometry files:**

- CIF: pp. 930

- POSCAR: pp. 930

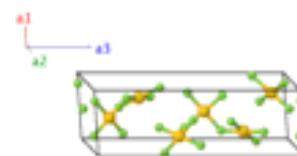
# AuF<sub>3</sub> Structure: AB3\_hP24\_178\_b\_ac



<b>Prototype</b>	:	AuF <sub>3</sub>
<b>AFLOW prototype label</b>	:	AB3_hP24_178_b_ac
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP24
<b>Space group number</b>	:	178
<b>Space group symbol</b>	:	<i>P</i> 6 <sub>1</sub> 22
<b>AFLOW prototype command</b>	:	aflow --proto=AB3_hP24_178_b_ac --params= <i>a, c/a, x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub></i>

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $x_1 \mathbf{a}_1$	= $\frac{1}{2} x_1 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}}$	(6a)	FI
<b>B</b> <sub>2</sub>	= $x_1 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	= $\frac{1}{2} x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}}$	(6a)	FI
<b>B</b> <sub>3</sub>	= $-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	= $-x_1 a \hat{\mathbf{x}} + \frac{2}{3} c \hat{\mathbf{z}}$	(6a)	FI
<b>B</b> <sub>4</sub>	= $-x_1 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	= $-\frac{1}{2} x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6a)	FI
<b>B</b> <sub>5</sub>	= $-x_1 \mathbf{a}_2 + \frac{5}{6} \mathbf{a}_3$	= $-\frac{1}{2} x_1 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{5}{6} c \hat{\mathbf{z}}$	(6a)	FI
<b>B</b> <sub>6</sub>	= $x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{6} \mathbf{a}_3$	= $x_1 a \hat{\mathbf{x}} + \frac{1}{6} c \hat{\mathbf{z}}$	(6a)	FI

$$\begin{aligned}
\mathbf{B}_7 &= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{3}{2}x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(6b) & \text{Au} \\
\mathbf{B}_8 &= -2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{7}{12} \mathbf{a}_3 &= -\frac{3}{2}x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \frac{7}{12}c \hat{\mathbf{z}} &(6b) & \text{Au} \\
\mathbf{B}_9 &= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{11}{12} \mathbf{a}_3 &= -\sqrt{3}x_2 a \hat{\mathbf{y}} + \frac{11}{12}c \hat{\mathbf{z}} &(6b) & \text{Au} \\
\mathbf{B}_{10} &= -x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -\frac{3}{2}x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(6b) & \text{Au} \\
\mathbf{B}_{11} &= 2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{12} \mathbf{a}_3 &= \frac{3}{2}x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \frac{1}{12}c \hat{\mathbf{z}} &(6b) & \text{Au} \\
\mathbf{B}_{12} &= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{5}{12} \mathbf{a}_3 &= \sqrt{3}x_2 a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}} &(6b) & \text{Au} \\
\mathbf{B}_{13} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + &(12c) & \text{F II} \\
&&& \frac{\sqrt{3}}{2}(-x_3 + y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} \\
\mathbf{B}_{14} &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{1}{3} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2}x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{1}{3} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{15} &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{2}{3} + z_3\right) \mathbf{a}_3 &= \left(-x_3 + \frac{1}{2}y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{2}{3} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{16} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= -\frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + &(12c) & \text{F II} \\
&&& \frac{\sqrt{3}}{2}(x_3 - y_3) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{17} &= y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{5}{6} + z_3\right) \mathbf{a}_3 &= \left(-\frac{1}{2}x_3 + y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{5}{6} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{18} &= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{6} + z_3\right) \mathbf{a}_3 &= \left(x_3 - \frac{1}{2}y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{1}{6} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{19} &= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{3} - z_3\right) \mathbf{a}_3 &= \frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3) a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{1}{3} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{20} &= (x_3 - y_3) \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= \left(\frac{1}{2}x_3 - y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} &(12c) & \text{F II} \\
\mathbf{B}_{21} &= -x_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{2}{3} - z_3\right) \mathbf{a}_3 &= \left(-x_3 + \frac{1}{2}y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{2}{3} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{22} &= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{5}{6} - z_3\right) \mathbf{a}_3 &= -\frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + &(12c) & \text{F II} \\
&&& \frac{\sqrt{3}}{2}(-x_3 + y_3) a \hat{\mathbf{y}} + \left(\frac{5}{6} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{23} &= (-x_3 + y_3) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= \left(-\frac{1}{2}x_3 + y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{24} &= x_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{1}{6} - z_3\right) \mathbf{a}_3 &= \left(x_3 - \frac{1}{2}y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{1}{6} - z_3\right) c \hat{\mathbf{z}}
\end{aligned}$$

### References:

- L. B. Asprey, F. H. Kruse, K. H. Jack, and R. Maitland, *Preparation and properties of crystalline gold trifluoride*, Inorg. Chem. **3**, 602–604 (1964), doi:10.1021/jc50014a037.

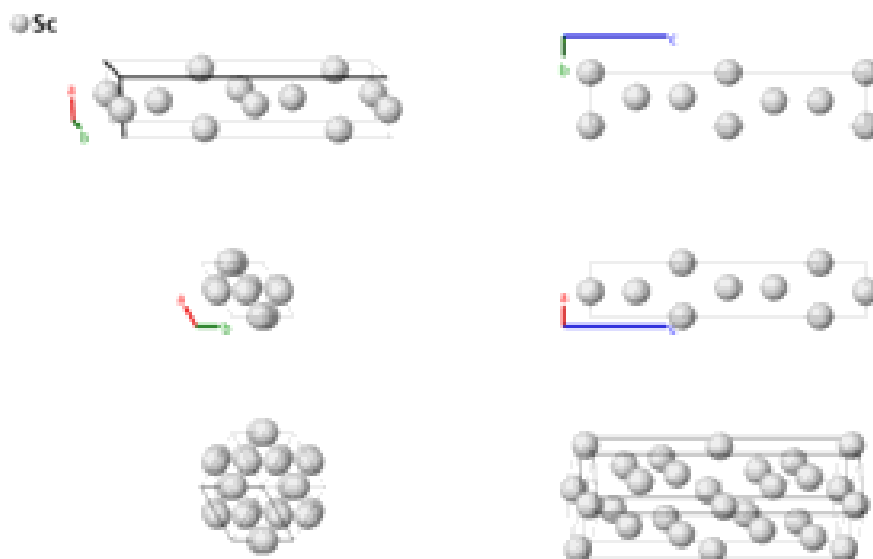
### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

### Geometry files:

- CIF: pp. 930  
- POSCAR: pp. 931

# Sc-V (High-pressure) Structure: A\_hP6\_178\_a



<b>Prototype</b>	:	Sc
<b>AFLOW prototype label</b>	:	A_hP6_178_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP6
<b>Space group number</b>	:	178
<b>Space group symbol</b>	:	$P6_122$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A_hP6_178_a --params=a, c/a, x1</code>

- This high pressure phase of scandium becomes stable at 240 GPa. We use the experimental data at 242 GPa and 297 K. This chiral structure could also have been presented in the enantiomorphic space group  $P6_522$  (#179).

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1$	$= \frac{1}{2} x_1 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}}$	(6a)	Sc
$\mathbf{B}_2$	$= x_1 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$= \frac{1}{2} x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{1}{3} c \hat{\mathbf{z}}$	(6a)	Sc
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}} + \frac{2}{3} c \hat{\mathbf{z}}$	(6a)	Sc
$\mathbf{B}_4$	$= -x_1 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$= -\frac{1}{2} x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6a)	Sc
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_2 + \frac{5}{6} \mathbf{a}_3$	$= -\frac{1}{2} x_1 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{5}{6} c \hat{\mathbf{z}}$	(6a)	Sc
$\mathbf{B}_6$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{6} \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + \frac{1}{6} c \hat{\mathbf{z}}$	(6a)	Sc



---

**References:**

- Y. Akahama, H. Fujihisa, and H. Kawamura, *New Helical Chain Structure for Scandium at 240 GPa*, Phys. Rev. Lett. **94**, 195503 (2005), doi:[10.1103/PhysRevLett.94.195503](https://doi.org/10.1103/PhysRevLett.94.195503).

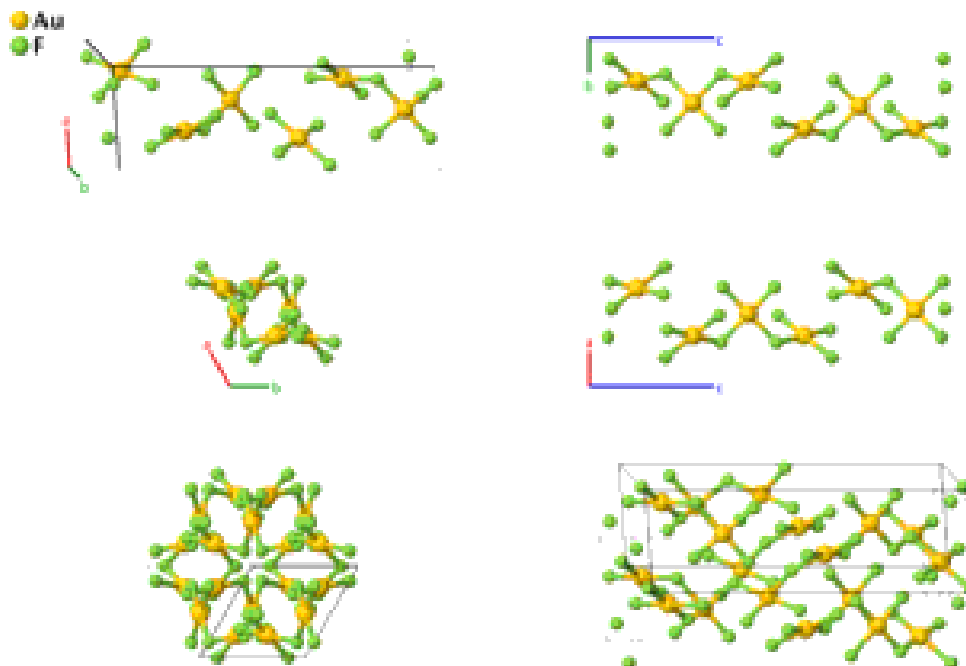
---

**Geometry files:**

- CIF: pp. [931](#)

- POSCAR: pp. [931](#)

# AuF<sub>3</sub> Structure: AB3\_hP24\_179\_b\_ac

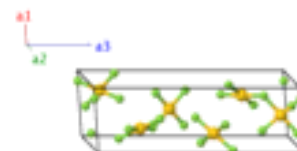


<b>Prototype</b>	:	AuF <sub>3</sub>
<b>AFLOW prototype label</b>	:	AB3_hP24_179_b_ac
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP24
<b>Space group number</b>	:	179
<b>Space group symbol</b>	:	<i>P</i> 6 <sub>5</sub> 22
<b>AFLOW prototype command</b>	:	aflow --proto=AB3_hP24_179_b_ac --params= <i>a, c/a, x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub></i>

- This structure is the enantiomorph of the [AuF<sub>3</sub> \(AB3\\_hP24\\_178\\_b\\_ac\) structure](#), and was generated by reflecting the coordinates of the space group #178 structure through the  $z = 0$  plane.

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1$	$=$	$\frac{1}{2} x_1 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}}$	(6a)	F I
$\mathbf{B}_2$	$= x_1 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{1}{2} x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{2}{3} c \hat{\mathbf{z}}$	(6a)	F I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$-x_1 a \hat{\mathbf{x}} + \frac{1}{3} c \hat{\mathbf{z}}$	(6a)	F I

$$\begin{aligned}
\mathbf{B}_4 &= -x_1 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3 &= -\frac{1}{2}x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_1 a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(6a) & \text{F I} \\
\mathbf{B}_5 &= -x_1 \mathbf{a}_2 + \frac{1}{6} \mathbf{a}_3 &= -\frac{1}{2}x_1 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_1 a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}} &(6a) & \text{F I} \\
\mathbf{B}_6 &= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{5}{6} \mathbf{a}_3 &= x_1 a \hat{\mathbf{x}} + \frac{5}{6}c \hat{\mathbf{z}} &(6a) & \text{F I} \\
\mathbf{B}_7 &= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{3}{2}x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(6b) & \text{Au} \\
\mathbf{B}_8 &= -2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{5}{12} \mathbf{a}_3 &= -\frac{3}{2}x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}} &(6b) & \text{Au} \\
\mathbf{B}_9 &= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{12} \mathbf{a}_3 &= -\sqrt{3}x_2 a \hat{\mathbf{y}} + \frac{1}{12}c \hat{\mathbf{z}} &(6b) & \text{Au} \\
\mathbf{B}_{10} &= -x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -\frac{3}{2}x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(6b) & \text{Au} \\
\mathbf{B}_{11} &= 2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{11}{12} \mathbf{a}_3 &= \frac{3}{2}x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \frac{11}{12}c \hat{\mathbf{z}} &(6b) & \text{Au} \\
\mathbf{B}_{12} &= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{7}{12} \mathbf{a}_3 &= \sqrt{3}x_2 a \hat{\mathbf{y}} + \frac{7}{12}c \hat{\mathbf{z}} &(6b) & \text{Au} \\
\mathbf{B}_{13} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= \frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + &(12c) & \text{F II} \\
&&& \frac{\sqrt{3}}{2}(-x_3 + y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} \\
\mathbf{B}_{14} &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{2}{3} + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{2}x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{2}{3} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{15} &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{3} + z_3\right) \mathbf{a}_3 &= \left(-x_3 + \frac{1}{2}y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{1}{3} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{16} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 &= -\frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + &(12c) & \text{F II} \\
&&& \frac{\sqrt{3}}{2}(x_3 - y_3) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{17} &= y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{1}{6} + z_3\right) \mathbf{a}_3 &= \left(-\frac{1}{2}x_3 + y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{1}{6} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{18} &= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{5}{6} + z_3\right) \mathbf{a}_3 &= \left(x_3 - \frac{1}{2}y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{5}{6} + z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{19} &= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{2}{3} - z_3\right) \mathbf{a}_3 &= \frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3) a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{2}{3} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{20} &= (x_3 - y_3) \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= \left(\frac{1}{2}x_3 - y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}} &(12c) & \text{F II} \\
\mathbf{B}_{21} &= -x_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{1}{3} - z_3\right) \mathbf{a}_3 &= \left(-x_3 + \frac{1}{2}y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{1}{3} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{22} &= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{6} - z_3\right) \mathbf{a}_3 &= -\frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + &(12c) & \text{F II} \\
&&& \frac{\sqrt{3}}{2}(-x_3 + y_3) a \hat{\mathbf{y}} + \left(\frac{1}{6} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{23} &= (-x_3 + y_3) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 &= \left(-\frac{1}{2}x_3 + y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{1}{2} - z_3\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{24} &= x_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{5}{6} - z_3\right) \mathbf{a}_3 &= \left(x_3 - \frac{1}{2}y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + &(12c) & \text{F II} \\
&&& \left(\frac{5}{6} - z_3\right) c \hat{\mathbf{z}}
\end{aligned}$$

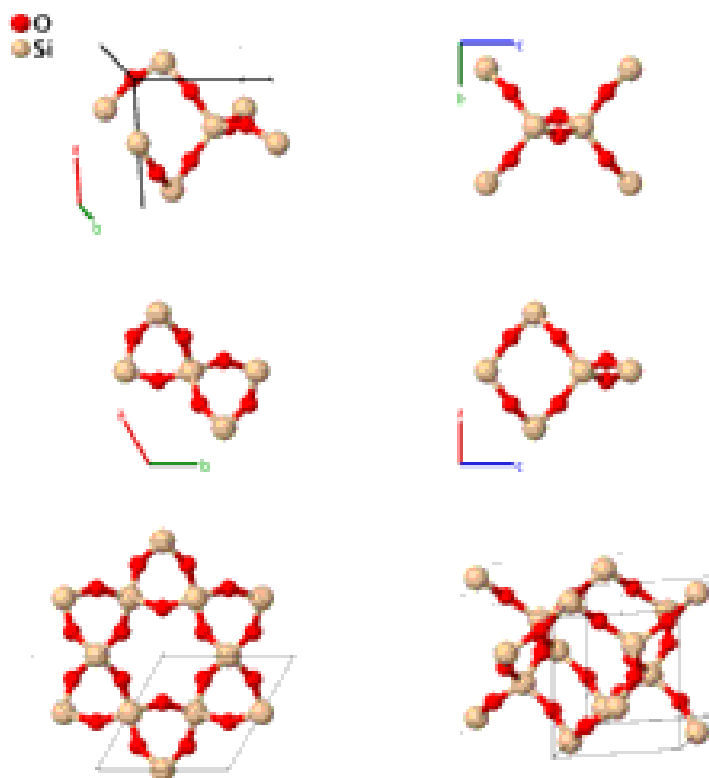
## References:

- L. B. Asprey, F. H. Kruse, K. H. Jack, and R. Maitland, *Preparation and properties of crystalline gold trifluoride*, Inorg. Chem. **3**, 602–604 (1964), doi:10.1021/ic50014a037.

## Geometry files:

- CIF: pp. 931  
- POSCAR: pp. 932

# $\beta$ -SiO<sub>2</sub> Structure: A2B\_hP9\_181\_j\_c

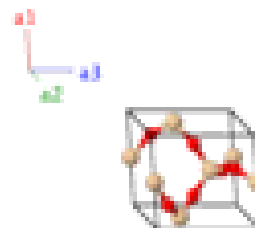


<b>Prototype</b>	:	$\beta$ -SiO <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_hP9_181_j_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP9
<b>Space group number</b>	:	181
<b>Space group symbol</b>	:	$P6_422$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_hP9_181_j_c --params=a, c/a, x <sub>2</sub>

- This structure is the enantiomorph of the  $\beta$ -Quartz (A2B\_hP9\_180\_j\_c) structure, and was generated by reflecting the coordinates of the space group #180 structure through the  $z = 0$  plane.

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= $\frac{1}{2} \mathbf{a}_1$	=	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(3c)	Si
<b>B<sub>2</sub></b>	= $\frac{1}{2} \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3c)	Si
<b>B<sub>3</sub></b>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3c)	Si
<b>B<sub>4</sub></b>	= $x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{3}{2}x_2a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6j)	O
<b>B<sub>5</sub></b>	= $-2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{5}{6} \mathbf{a}_3$	=	$-\frac{3}{2}x_2a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \frac{5}{6}c \hat{\mathbf{z}}$	(6j)	O
<b>B<sub>6</sub></b>	= $x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{6} \mathbf{a}_3$	=	$-\sqrt{3}x_2a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(6j)	O
<b>B<sub>7</sub></b>	= $-x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-\frac{3}{2}x_2a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6j)	O
<b>B<sub>8</sub></b>	= $2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{5}{6} \mathbf{a}_3$	=	$\frac{3}{2}x_2a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \frac{5}{6}c \hat{\mathbf{z}}$	(6j)	O
<b>B<sub>9</sub></b>	= $-x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{6} \mathbf{a}_3$	=	$\sqrt{3}x_2a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(6j)	O

---

### References:

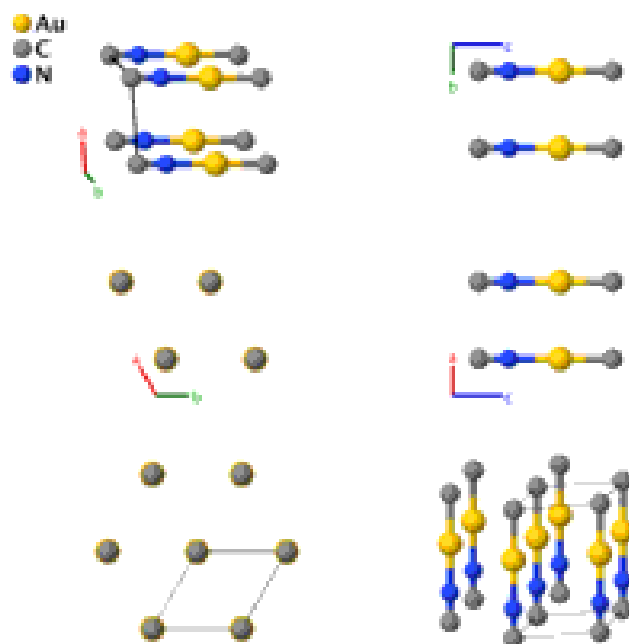
- A. F. Wright and M. S. Lehmann, *The Structure of Quartz at 25 and 590° C Determined by Neutron Diffraction*, J. Solid State Chem. **36**, 371–380 (1981), doi:10.1016/0022-4596(81)90449-7.

---

### Geometry files:

- CIF: pp. [932](#)  
- POSCAR: pp. [932](#)

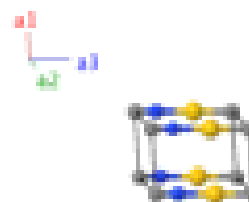
# AuCN Structure: ABC\_hP3\_183\_a\_a\_a



<b>Prototype</b>	:	AuCN
<b>AFLOW prototype label</b>	:	ABC_hP3_183_a_a_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP3
<b>Space group number</b>	:	183
<b>Space group symbol</b>	:	$P6mm$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=ABC_hP3_183_a_a_a --params=a, c/a, z1, z2, z3</code>

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$z_1 c \hat{\mathbf{z}}$	(1a)	Au
$\mathbf{B}_2$	$= z_2 \mathbf{a}_3$	$=$	$z_2 c \hat{\mathbf{z}}$	(1a)	C
$\mathbf{B}_3$	$= z_3 \mathbf{a}_3$	$=$	$z_3 c \hat{\mathbf{z}}$	(1a)	N

## References:

- S. J. Hibble, A. C. Hannon, and S. M. Cheyne, *Structure of AuCN determined from total neutron diffraction*, *Inorg. Chem.* **42**, 4724–4730 (2003), [doi:10.1021/ic0342043](https://doi.org/10.1021/ic0342043).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

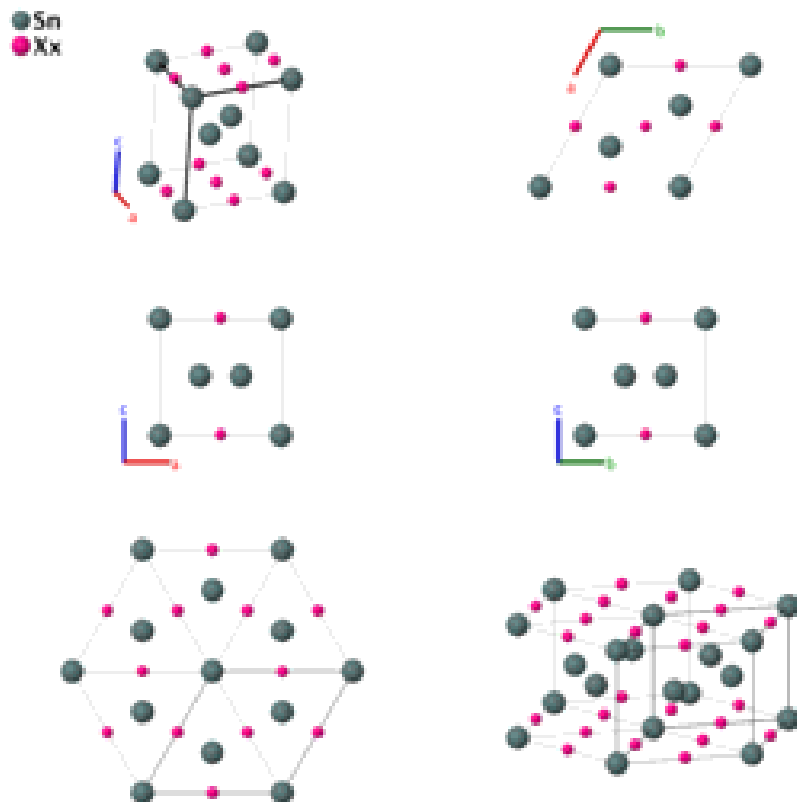
---

**Geometry files:**

- CIF: pp. [932](#)

- POSCAR: pp. [933](#)

# CrFe<sub>3</sub>NiSn<sub>5</sub> Structure: AB\_hP6\_183\_c\_ab

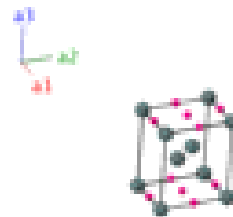


<b>Prototype</b>	:	CrFe <sub>3</sub> NiSn <sub>5</sub>
<b>AFLOW prototype label</b>	:	AB_hP6_183_c_ab
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP6
<b>Space group number</b>	:	183
<b>Space group symbol</b>	:	<i>P6mm</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB_hP6_183_c_ab</code> <code>--params=a, c/a, z1, z2, z3</code>

- Here, the M sites are mixed occupation 0.6Fe+0.2Cr+0.2Ni The Jmol image does not distinguish between the different M labels and is represented by the "Xx" atoms.

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:



	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	=	$z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(1a) Sn I
$\mathbf{B}_2$	=	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2b) Sn II
$\mathbf{B}_3$	=	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(2b) Sn II
$\mathbf{B}_4$	=	$\frac{1}{2} \mathbf{a}_1 + z_3 \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(3c) M
$\mathbf{B}_5$	=	$\frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(3c) M
$\mathbf{B}_6$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + z_3 c \hat{\mathbf{z}}$	(3c) M

**References:**

- J. Huang, L. Zeng, and Z. Sun, *X-ray powder diffraction data and Rietveld refinement of CrFe<sub>3</sub>NiSn<sub>5</sub>*, Powder Diffraction **19**, 372–374 (2004), [doi:10.1154/1.1763153](https://doi.org/10.1154/1.1763153).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

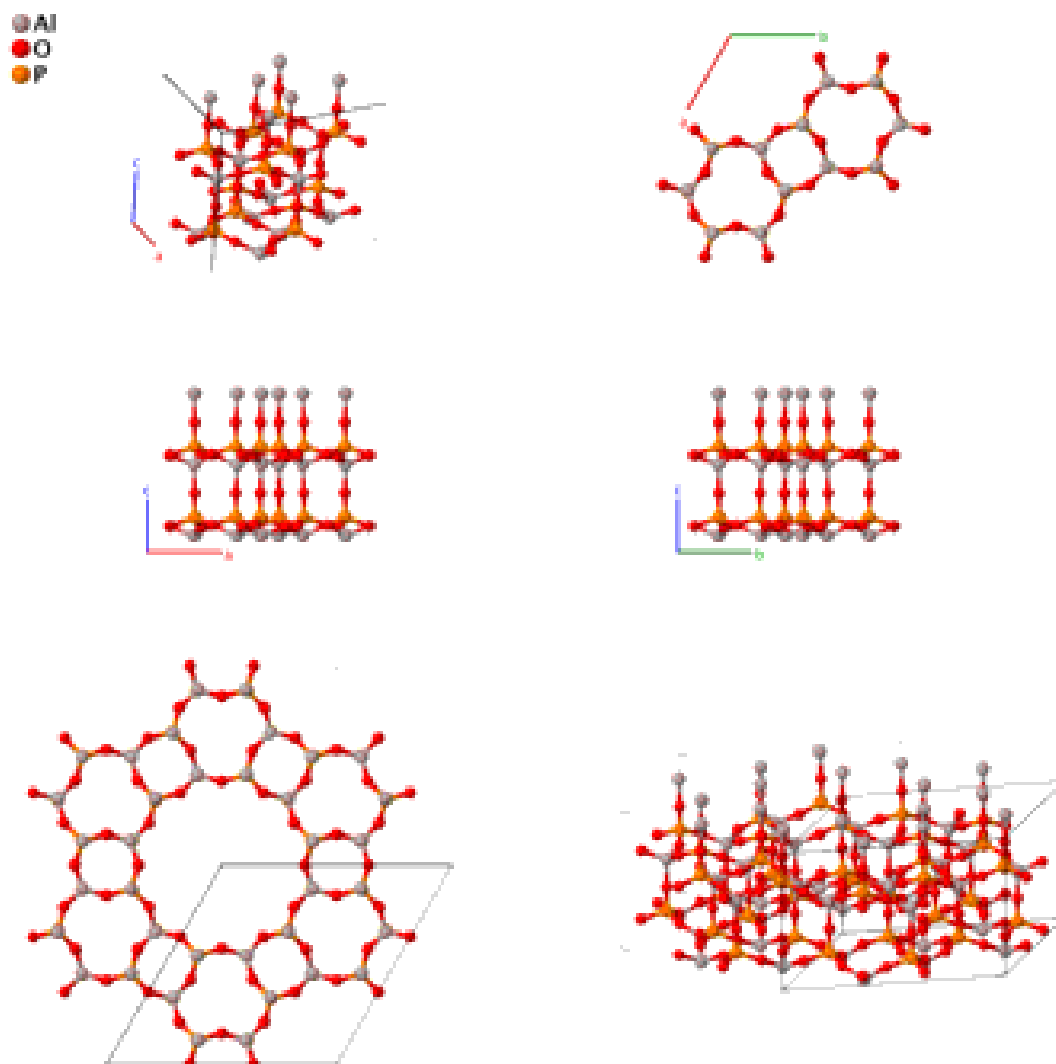
**Geometry files:**

- CIF: pp. [933](#)  
 - POSCAR: pp. [933](#)

# Al[PO<sub>4</sub>] (Framework type AFI) Structure:

AB4C\_hP72\_184\_d\_4d\_d

---

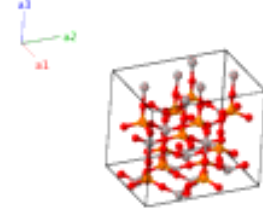


<b>Prototype</b>	:	Al[PO <sub>4</sub> ]
<b>AFLOW prototype label</b>	:	AB4C_hP72_184_d_4d_d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP72
<b>Space group number</b>	:	184
<b>Space group symbol</b>	:	<i>P6cc</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB4C_hP72_184_d_4d_d --params=a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6</code>

- 
- This is the structure of AlPO<sub>4</sub>-5, which has the zeolite framework designation AFI.

## Hexagonal primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{2} (x_1 + y_1) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_1 + y_1) a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(12d)	Al
$\mathbf{B}_2$	$-y_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \left(\frac{1}{2} x_1 - y_1\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(12d)	Al
$\mathbf{B}_3$	$(-x_1 + y_1) \mathbf{a}_1 - x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \left(-x_1 + \frac{1}{2} y_1\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(12d)	Al
$\mathbf{B}_4$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= -\frac{1}{2} (x_1 + y_1) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_1 - y_1) a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(12d)	Al
$\mathbf{B}_5$	$y_1 \mathbf{a}_1 + (-x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \left(-\frac{1}{2} x_1 + y_1\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(12d)	Al
$\mathbf{B}_6$	$(x_1 - y_1) \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \left(x_1 - \frac{1}{2} y_1\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_1 a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	(12d)	Al
$\mathbf{B}_7$	$-y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= -\frac{1}{2} (x_1 + y_1) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_1 + y_1) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(12d)	Al
$\mathbf{B}_8$	$(-x_1 + y_1) \mathbf{a}_1 + y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \left(-\frac{1}{2} x_1 + y_1\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(12d)	Al
$\mathbf{B}_9$	$x_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \left(x_1 - \frac{1}{2} y_1\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(12d)	Al
$\mathbf{B}_{10}$	$y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \frac{1}{2} (x_1 + y_1) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_1 - y_1) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(12d)	Al
$\mathbf{B}_{11}$	$(x_1 - y_1) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} x_1 - y_1\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(12d)	Al
$\mathbf{B}_{12}$	$-x_1 \mathbf{a}_1 + (-x_1 + y_1) \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \left(-x_1 + \frac{1}{2} y_1\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(12d)	Al
$\mathbf{B}_{13}$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_2 + y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B}_{14}$	$-y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(\frac{1}{2} x_2 - y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B}_{15}$	$(-x_2 + y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(-x_2 + \frac{1}{2} y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B}_{16}$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= -\frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_2 - y_2) a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B}_{17}$	$y_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(-\frac{1}{2} x_2 + y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B}_{18}$	$(x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \left(x_2 - \frac{1}{2} y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B}_{19}$	$-y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= -\frac{1}{2} (x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_2 + y_2) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(12d)	O I

$$\begin{aligned}
\mathbf{B}_{20} &= (-x_2 + y_2) \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_2 + y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (12d) & \text{O I} \\
\mathbf{B}_{21} &= x_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \left(x_2 - \frac{1}{2}y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (12d) & \text{O I} \\
\mathbf{B}_{22} &= y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \frac{1}{2}(x_2 + y_2) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_2 - y_2) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (12d) & \text{O I} \\
\mathbf{B}_{23} &= (x_2 - y_2) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \left(\frac{1}{2}x_2 - y_2\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (12d) & \text{O I} \\
\mathbf{B}_{24} &= -x_2 \mathbf{a}_1 + (-x_2 + y_2) \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 = \left(-x_2 + \frac{1}{2}y_2\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} & (12d) & \text{O I} \\
\mathbf{B}_{25} &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = \frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (12d) & \text{O II} \\
\mathbf{B}_{26} &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3 = \left(\frac{1}{2}x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (12d) & \text{O II} \\
\mathbf{B}_{27} &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = \left(-x_3 + \frac{1}{2}y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (12d) & \text{O II} \\
\mathbf{B}_{28} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = -\frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3) a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (12d) & \text{O II} \\
\mathbf{B}_{29} &= y_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3 = \left(-\frac{1}{2}x_3 + y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (12d) & \text{O II} \\
\mathbf{B}_{30} &= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = \left(x_3 - \frac{1}{2}y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}} & (12d) & \text{O II} \\
\mathbf{B}_{31} &= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = -\frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (12d) & \text{O II} \\
\mathbf{B}_{32} &= (-x_3 + y_3) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_3 + y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (12d) & \text{O II} \\
\mathbf{B}_{33} &= x_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(x_3 - \frac{1}{2}y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (12d) & \text{O II} \\
\mathbf{B}_{34} &= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \frac{1}{2}(x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (12d) & \text{O II} \\
\mathbf{B}_{35} &= (x_3 - y_3) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2}x_3 - y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (12d) & \text{O II} \\
\mathbf{B}_{36} &= -x_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(-x_3 + \frac{1}{2}y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}} & (12d) & \text{O II} \\
\mathbf{B}_{37} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = \frac{1}{2}(x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (12d) & \text{O III} \\
\mathbf{B}_{38} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 = \left(\frac{1}{2}x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (12d) & \text{O III} \\
\mathbf{B}_{39} &= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = \left(-x_4 + \frac{1}{2}y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (12d) & \text{O III} \\
\mathbf{B}_{40} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = -\frac{1}{2}(x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_4 - y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (12d) & \text{O III} \\
\mathbf{B}_{41} &= y_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 = \left(-\frac{1}{2}x_4 + y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (12d) & \text{O III} \\
\mathbf{B}_{42} &= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = \left(x_4 - \frac{1}{2}y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} & (12d) & \text{O III} \\
\mathbf{B}_{43} &= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = -\frac{1}{2}(x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_4 + y_4) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (12d) & \text{O III}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{44} &= (-x_4 + y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_4 + y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (12d) & \text{O III} \\
\mathbf{B}_{45} &= x_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(x_4 - \frac{1}{2}y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (12d) & \text{O III} \\
\mathbf{B}_{46} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \frac{1}{2}(x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_4 - y_4) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (12d) & \text{O III} \\
\mathbf{B}_{47} &= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2}x_4 - y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (12d) & \text{O III} \\
\mathbf{B}_{48} &= -x_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 = \left(-x_4 + \frac{1}{2}y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} & (12d) & \text{O III} \\
\mathbf{B}_{49} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (12d) & \text{O IV} \\
\mathbf{B}_{50} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 = \left(\frac{1}{2}x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (12d) & \text{O IV} \\
\mathbf{B}_{51} &= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \left(-x_5 + \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (12d) & \text{O IV} \\
\mathbf{B}_{52} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = -\frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_5 - y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (12d) & \text{O IV} \\
\mathbf{B}_{53} &= y_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 = \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (12d) & \text{O IV} \\
\mathbf{B}_{54} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} & (12d) & \text{O IV} \\
\mathbf{B}_{55} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = -\frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (12d) & \text{O IV} \\
\mathbf{B}_{56} &= (-x_5 + y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (12d) & \text{O IV} \\
\mathbf{B}_{57} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (12d) & \text{O IV} \\
\mathbf{B}_{58} &= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_5 - y_5) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (12d) & \text{O IV} \\
\mathbf{B}_{59} &= (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2}x_5 - y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (12d) & \text{O IV} \\
\mathbf{B}_{60} &= -x_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(-x_5 + \frac{1}{2}y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (12d) & \text{O IV} \\
\mathbf{B}_{61} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \frac{1}{2}(x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_6 + y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (12d) & \text{P} \\
\mathbf{B}_{62} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3 = \left(\frac{1}{2}x_6 - y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (12d) & \text{P} \\
\mathbf{B}_{63} &= (-x_6 + y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \left(-x_6 + \frac{1}{2}y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (12d) & \text{P} \\
\mathbf{B}_{64} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = -\frac{1}{2}(x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_6 - y_6) a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (12d) & \text{P} \\
\mathbf{B}_{65} &= y_6 \mathbf{a}_1 + (-x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3 = \left(-\frac{1}{2}x_6 + y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (12d) & \text{P} \\
\mathbf{B}_{66} &= (x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \left(x_6 - \frac{1}{2}y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}} & (12d) & \text{P} \\
\mathbf{B}_{67} &= -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = -\frac{1}{2}(x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_6 + y_6) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} & (12d) & \text{P}
\end{aligned}$$

$$\mathbf{B}_{68} = (-x_6 + y_6) \mathbf{a}_1 + y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_6 + y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} \quad (12d) \quad \text{P}$$

$$\mathbf{B}_{69} = x_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \left(x_6 - \frac{1}{2}y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} \quad (12d) \quad \text{P}$$

$$\mathbf{B}_{70} = y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \frac{1}{2}(x_6 + y_6) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_6 - y_6) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} \quad (12d) \quad \text{P}$$

$$\mathbf{B}_{71} = (x_6 - y_6) \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \left(\frac{1}{2}x_6 - y_6\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} \quad (12d) \quad \text{P}$$

$$\mathbf{B}_{72} = -x_6 \mathbf{a}_1 + (-x_6 + y_6) \mathbf{a}_2 + \left(\frac{1}{2} + z_6\right) \mathbf{a}_3 = \left(-x_6 + \frac{1}{2}y_6\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_6 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) c \hat{\mathbf{z}} \quad (12d) \quad \text{P}$$

### References:

- G. J. Klap, H. van Koningsveld, H. Graafsma, and A. M. M. Schreurs, *Absolute configuration and domain structure of AlPO<sub>4</sub>-5 studied by single crystal X-ray diffraction*, *Microporous Mesoporous Mater.* **38**, 403–412 (2000), [doi:10.1016/S1387-1811\(00\)00161-X](https://doi.org/10.1016/S1387-1811(00)00161-X).

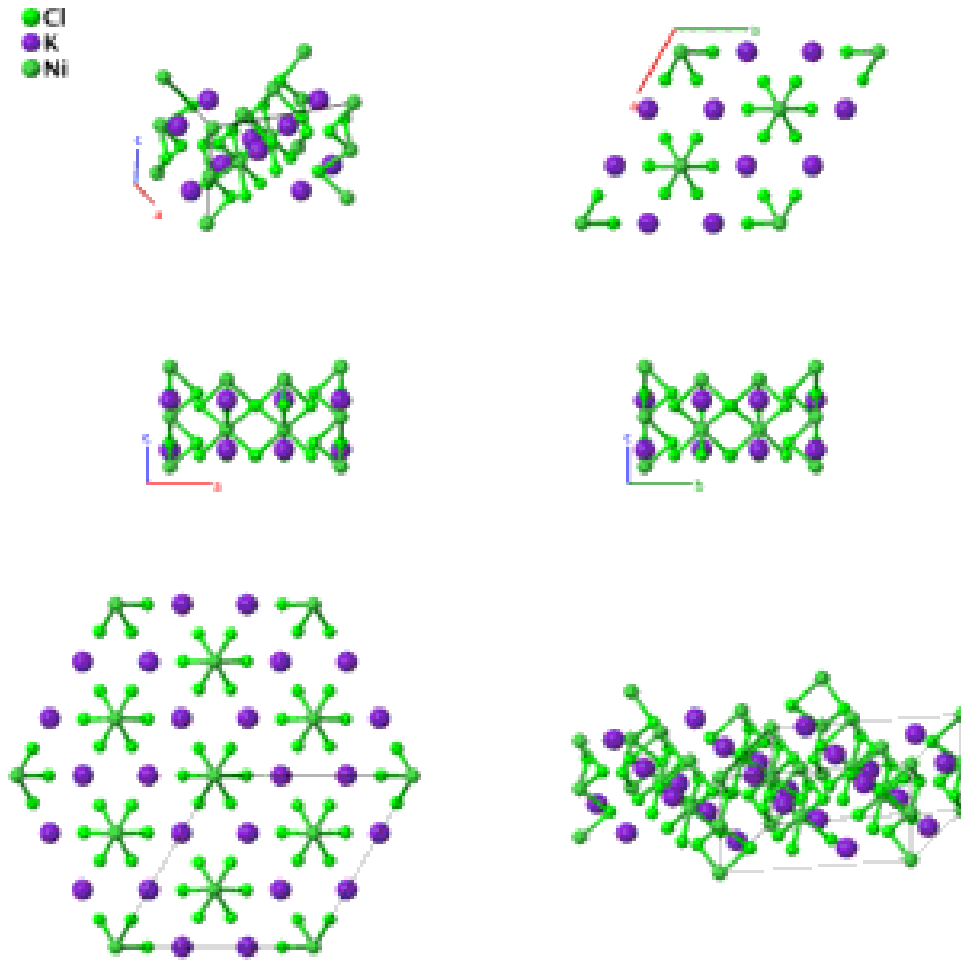
### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

### Geometry files:

- CIF: pp. [933](#)  
 - POSCAR: pp. [934](#)

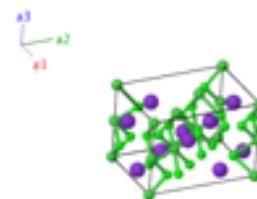
# KNiCl<sub>3</sub> (Room-temperature) Structure: A3BC\_hP30\_185\_cd\_c\_ab



<b>Prototype</b>	:	KNiCl <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3BC_hP30_185_cd_c_ab
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP30
<b>Space group number</b>	:	185
<b>Space group symbol</b>	:	<i>P6<sub>3</sub>cm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3BC_hP30_185_cd_c_ab --params= <i>a, c/a, z<sub>1</sub>, z<sub>2</sub>, x<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub></i>

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$z_1 c \hat{\mathbf{z}}$	(2a)	Ni I
$\mathbf{B}_2$	$= \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Ni I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4b)	Ni II
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4b)	Ni II
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4b)	Ni II
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4b)	Ni II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_8$	$= x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + z_3 c \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$-\frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$-\frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_{12}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6c)	K
$\mathbf{B}_{14}$	$= x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6c)	K
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + z_4 c \hat{\mathbf{z}}$	(6c)	K
$\mathbf{B}_{16}$	$= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$-\frac{1}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(6c)	K
$\mathbf{B}_{17}$	$= -x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$-\frac{1}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(6c)	K
$\mathbf{B}_{18}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(6c)	K
$\mathbf{B}_{19}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} +$ $\frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{20}$	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{21}$	$= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\left(-x_5 + \frac{1}{2} y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{22}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$-\frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} +$ $\frac{\sqrt{3}}{2} (x_5 - y_5) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{23}$	$= y_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$\left(-\frac{1}{2} x_5 + y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{24}$	$= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$\left(x_5 - \frac{1}{2} y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{25}$	$= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$-\frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} +$ $\frac{\sqrt{3}}{2} (-x_5 + y_5) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{26}$	$= (-x_5 + y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$\left(-\frac{1}{2} x_5 + y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{27}$	$= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$\left(x_5 - \frac{1}{2} y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_5 a \hat{\mathbf{y}} +$ $\left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{28}$	$= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} (x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_5 - y_5) a \hat{\mathbf{y}} +$ $z_5 c \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{29}$	$= (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} x_5 - y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(12d)	Cl II



$$\mathbf{B}_{30} = -x_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 = \left(-x_5 + \frac{1}{2}y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}} \quad (12d) \quad \text{CI II}$$

---

**References:**

- D. Visser, G. C. Verschoor, and D. J. W. IJdo, *The structure of KNiCl<sub>3</sub> at room temperature*, Acta Crystallogr. Sect. B Struct. Sci. **36**, 28–34 (1980), doi:[10.1107/S0567740880002385](https://doi.org/10.1107/S0567740880002385).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

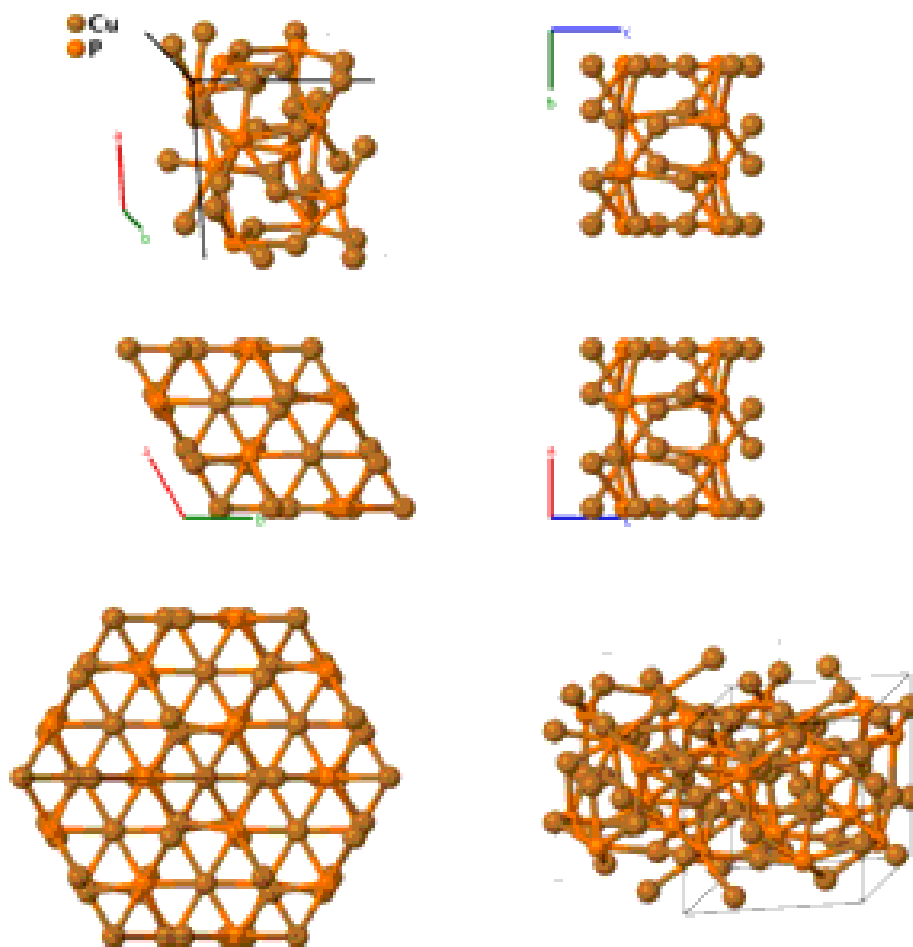
---

**Geometry files:**

- CIF: pp. [934](#)
- POSCAR: pp. [934](#)

# Cu<sub>3</sub>P Structure: A3B\_hP24\_185\_ab2c\_c

---



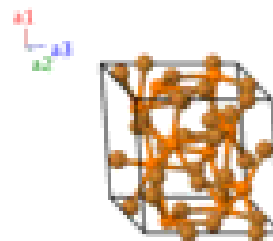
<b>Prototype</b>	:	Cu <sub>3</sub> P
<b>AFLOW prototype label</b>	:	A3B_hP24_185_ab2c_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP24
<b>Space group number</b>	:	185
<b>Space group symbol</b>	:	$P6_3cm$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A3B_hP24_185_ab2c_c --params=a, c/a, z1, z2, x3, z3, x4, z4, x5, z5</code>

---

- Olofsson (Olofsson, 1972) argues that this is the correct structure for Cu<sub>3</sub>P rather than the structure which was originally identified as *Strukturbericht* D0<sub>21</sub>, space group  $P\bar{3}c1$ , [A3B\\_hP24\\_165\\_bdg\\_f](#).
- Hafner and Range (Hafner, 1994) state that this is also the correct structure for AsNa<sub>3</sub>, rather than *Strukturbericht* D0<sub>18</sub>, space group  $P6_3/mmc$ , [AB3\\_hP8\\_194\\_c\\_bf](#).
- Finally, AuMg<sub>3</sub>, IrMg<sub>3</sub> and Mg<sub>3</sub>Pt, which have been described by both the D0<sub>18</sub> and D0<sub>21</sub> structures, are also claimed to actually be in this structure (Range, 1993).

## Hexagonal primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$= z_1 c \hat{\mathbf{z}}$	(2a)	Cu I
$\mathbf{B}_2$	$= \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Cu I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4b)	Cu II
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4b)	Cu II
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4b)	Cu II
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4b)	Cu II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_3$	$= \frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6c)	Cu III
$\mathbf{B}_8$	$= x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6c)	Cu III
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= -x_3 a \hat{\mathbf{x}} + z_3 c \hat{\mathbf{z}}$	(6c)	Cu III
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$= -\frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(6c)	Cu III
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$= -\frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(6c)	Cu III
$\mathbf{B}_{12}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(6c)	Cu III
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3$	$= \frac{1}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6c)	Cu IV
$\mathbf{B}_{14}$	$= x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \frac{1}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6c)	Cu IV
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= -x_4 a \hat{\mathbf{x}} + z_4 c \hat{\mathbf{z}}$	(6c)	Cu IV
$\mathbf{B}_{16}$	$= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$= -\frac{1}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(6c)	Cu IV
$\mathbf{B}_{17}$	$= -x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$= -\frac{1}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(6c)	Cu IV
$\mathbf{B}_{18}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$= x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(6c)	Cu IV
$\mathbf{B}_{19}$	$= x_5 \mathbf{a}_1 + z_5 \mathbf{a}_3$	$= \frac{1}{2} x_5 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(6c)	P
$\mathbf{B}_{20}$	$= x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= \frac{1}{2} x_5 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(6c)	P
$\mathbf{B}_{21}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= -x_5 a \hat{\mathbf{x}} + z_5 c \hat{\mathbf{z}}$	(6c)	P
$\mathbf{B}_{22}$	$= -x_5 \mathbf{a}_1 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$= -\frac{1}{2} x_5 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(6c)	P
$\mathbf{B}_{23}$	$= -x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$= -\frac{1}{2} x_5 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(6c)	P
$\mathbf{B}_{24}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$= x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(6c)	P

## References:

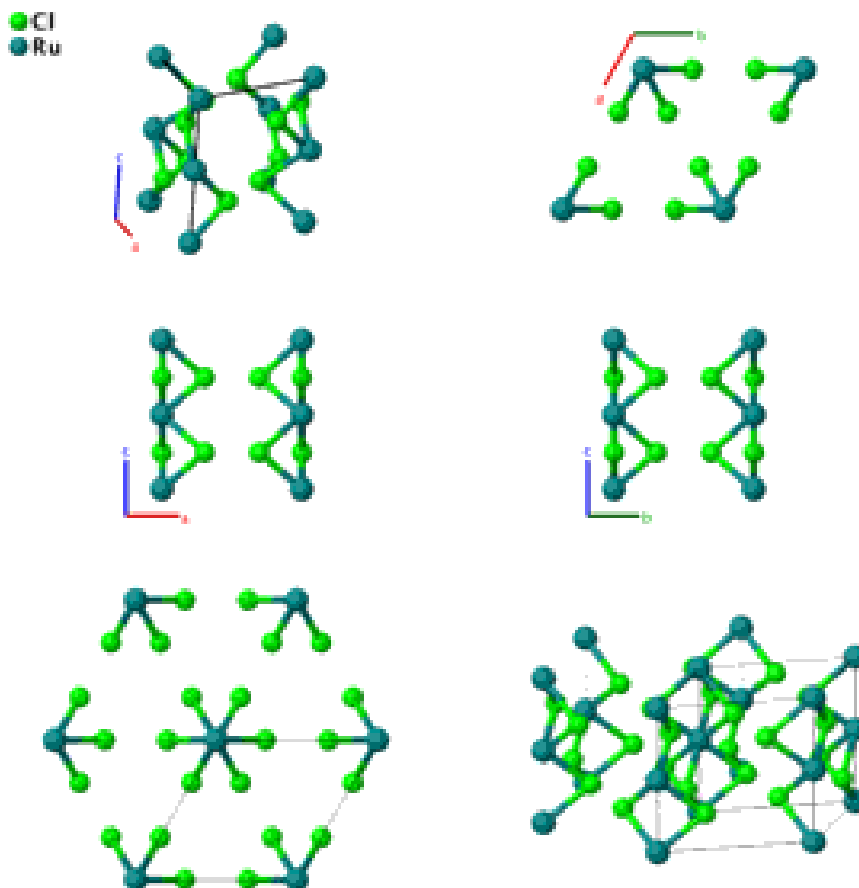
- O. Olofsson, *The Crystal Structure of Cu<sub>3</sub>P*, Acta Chem. Scand. **26**, 2777–2787 (1972),  
doi:10.3891/acta.chem.scand.26-2771.

- P. Hafner and K.-J. Range, *Na<sub>3</sub>As revisited: high-pressure synthesis of single crystals and structure refinement*, J. Alloys Compd. **216**, 7–10 (1994), [doi:10.1016/0925-8388\(94\)91033-2](https://doi.org/10.1016/0925-8388(94)91033-2).
  - K.-J. Range and P. Hafner, *Structure refinement of AuMg<sub>3</sub>, IrMg<sub>3</sub> and IrMg<sub>2.8</sub>*, J. Alloys Compd. **191**, L5–L7 (1993), [doi:10.1016/0925-8388\(93\)90053-P](https://doi.org/10.1016/0925-8388(93)90053-P).
- 

**Geometry files:**

- CIF: pp. [935](#)
- POSCAR: pp. [935](#)

# $\beta$ -RuCl<sub>3</sub> Structure: A3B\_hP8\_185\_c\_a

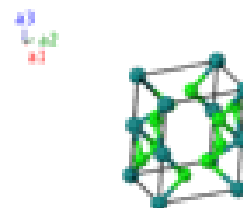


<b>Prototype</b>	:	$\beta$ -RuCl <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B_hP8_185_c_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP8
<b>Space group number</b>	:	185
<b>Space group symbol</b>	:	$P6_3cm$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A3B_hP8_185_c_a --params=a, c/a, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub></code>

- Pearson comments that space groups #158, #188, #193, could not be rejected, but this structure is consistent with space group #185. We also provide the structure with space group #158: [β-RuCl<sub>3</sub> \(A3B\\_hP8\\_158\\_d\\_a\) structure](#).

**Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{x} - \frac{\sqrt{3}}{2} a \hat{y} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{x} + \frac{\sqrt{3}}{2} a \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	=	Cartesian Coordinates		Wyckoff Position	Atom Type
$\mathbf{B}_1$	=	$z_1 \mathbf{a}_3$	=	$z_1 c \hat{\mathbf{z}}$	(2a)	Ru
$\mathbf{B}_2$	=	$\left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	=	$\left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Ru
$\mathbf{B}_3$	=	$x_2 \mathbf{a}_1 + z_2 \mathbf{a}_3$	=	$\frac{1}{2} x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6c)	Cl
$\mathbf{B}_4$	=	$x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2} x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(6c)	Cl
$\mathbf{B}_5$	=	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$-x_2 a \hat{\mathbf{x}} + z_2 c \hat{\mathbf{z}}$	(6c)	Cl
$\mathbf{B}_6$	=	$-x_2 \mathbf{a}_1 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	=	$-\frac{1}{2} x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(6c)	Cl
$\mathbf{B}_7$	=	$-x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	=	$-\frac{1}{2} x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(6c)	Cl
$\mathbf{B}_8$	=	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	=	$x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(6c)	Cl

---

#### References:

- J. M. Fletcher, W. E. Gardner, A. C. Fox, and G. Topping, *X-Ray, infrared, and magnetic studies of  $\alpha$ - and  $\beta$ -ruthenium trichloride*, J. Chem. Soc. A pp. 1038–1045 (1967), doi:10.1039/J19670001038.

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

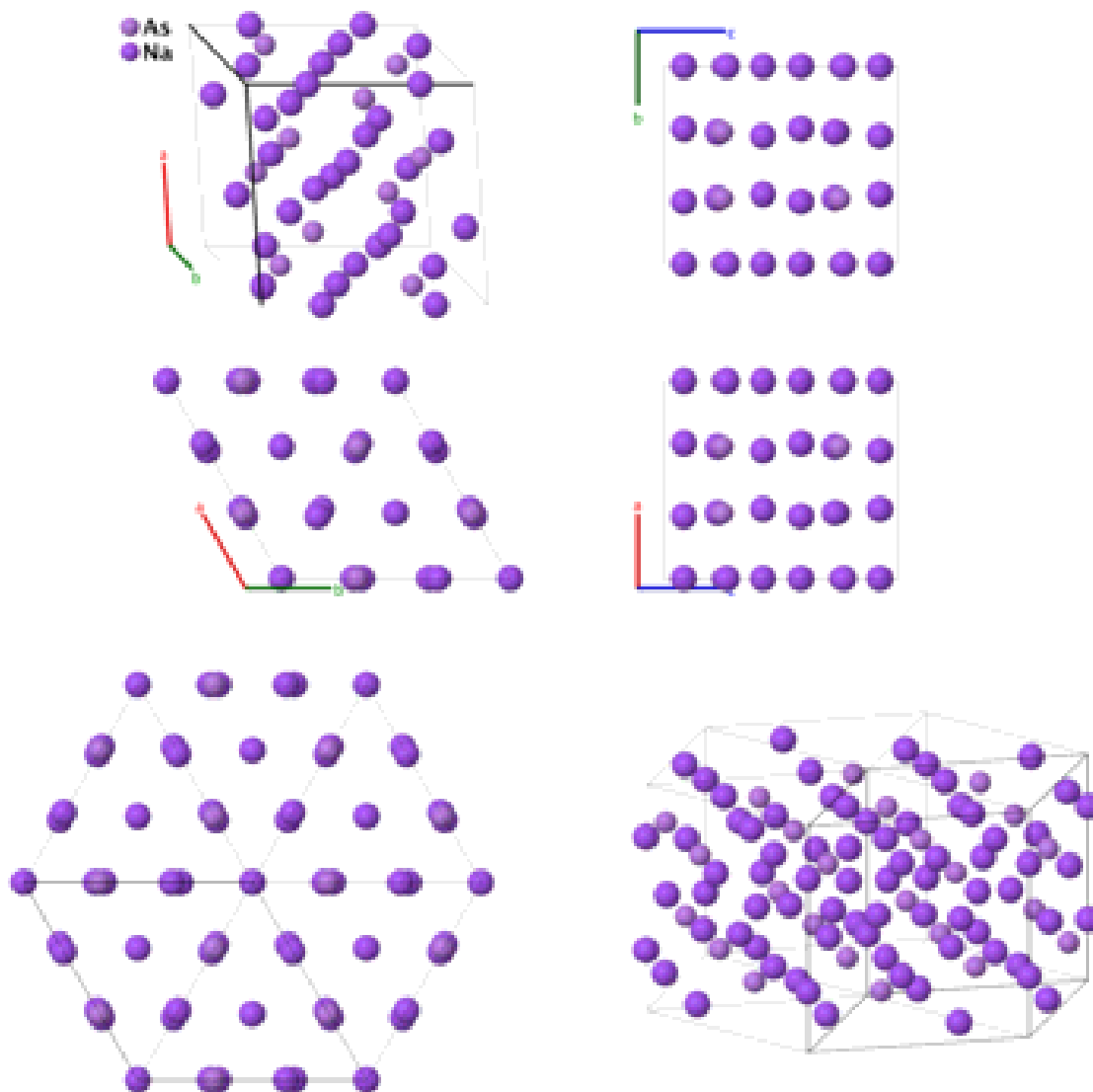
---

#### Geometry files:

- CIF: pp. 935  
- POSCAR: pp. 935

# Na<sub>3</sub>As Structure: AB3\_hP24\_185\_c\_ab2c

---



<b>Prototype</b>	:	Na <sub>3</sub> As
<b>AFLOW prototype label</b>	:	AB3_hP24_185_c_ab2c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP24
<b>Space group number</b>	:	185
<b>Space group symbol</b>	:	<i>P</i> 6 <sub>3</sub> <i>cm</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=AB3_hP24_185_c_ab2c</code> <code>--params=<i>a, c/a, z</i><sub>1, z</sub><sub>2, x</sub><sub>3, z</sub><sub>3, x</sub><sub>4, z</sub><sub>4, x</sub><sub>5, z</sub><sub>5</sub></code>

---

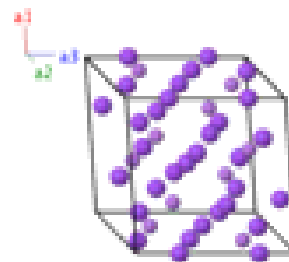
## Other compounds with the structure:

- Cu<sub>3</sub>P

- 
- The authors state that this is a correction of the *D*0<sub>18</sub> Na<sub>3</sub>As structure. Cu<sub>3</sub>P (pp. 602) and Na<sub>3</sub>As (pp. 607) have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

## Hexagonal primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$= z_1 c \hat{\mathbf{z}}$	(2a)	Na I
$\mathbf{B}_2$	$= \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	(2a)	Na I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_3$	$= \frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6c)	As
$\mathbf{B}_8$	$= x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(6c)	As
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= -x_3 a \hat{\mathbf{x}} + z_3 c \hat{\mathbf{z}}$	(6c)	As
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$= -\frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(6c)	As
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$= -\frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(6c)	As
$\mathbf{B}_{12}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	(6c)	As
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3$	$= \frac{1}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6c)	Na III
$\mathbf{B}_{14}$	$= x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= \frac{1}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(6c)	Na III
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= -x_4 a \hat{\mathbf{x}} + z_4 c \hat{\mathbf{z}}$	(6c)	Na III
$\mathbf{B}_{16}$	$= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$= -\frac{1}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(6c)	Na III
$\mathbf{B}_{17}$	$= -x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$= -\frac{1}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(6c)	Na III
$\mathbf{B}_{18}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$= x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(6c)	Na III
$\mathbf{B}_{19}$	$= x_5 \mathbf{a}_1 + z_5 \mathbf{a}_3$	$= \frac{1}{2} x_5 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(6c)	Na IV
$\mathbf{B}_{20}$	$= x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= \frac{1}{2} x_5 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(6c)	Na IV
$\mathbf{B}_{21}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= -x_5 a \hat{\mathbf{x}} + z_5 c \hat{\mathbf{z}}$	(6c)	Na IV
$\mathbf{B}_{22}$	$= -x_5 \mathbf{a}_1 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$= -\frac{1}{2} x_5 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(6c)	Na IV
$\mathbf{B}_{23}$	$= -x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$= -\frac{1}{2} x_5 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(6c)	Na IV
$\mathbf{B}_{24}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$= x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(6c)	Na IV

## References:

- P. Hafner and K.-J. Range, *Na<sub>3</sub>As revisited: high-pressure synthesis of single crystals and structure refinement*, J. Alloys Compd. **216**, 7–10 (1994), doi:10.1016/0925-8388(94)91033-2.



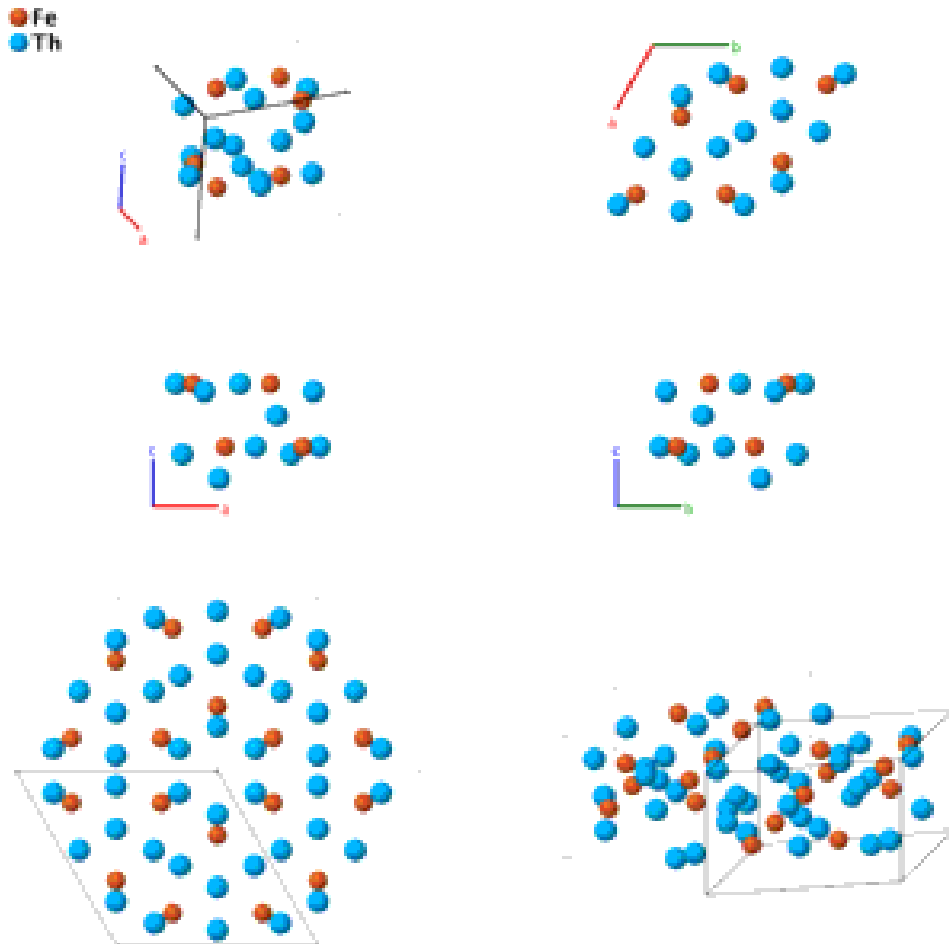
---

**Geometry files:**

- CIF: pp. [936](#)

- POSCAR: pp. [936](#)

# Fe<sub>3</sub>Th<sub>7</sub> (*D*10<sub>2</sub>) Structure: A3B7\_hP20\_186\_c\_b2c



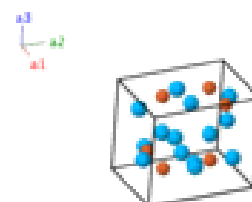
<b>Prototype</b>	:	Fe <sub>3</sub> Th <sub>7</sub>
<b>AFLOW prototype label</b>	:	A3B7_hP20_186_c_b2c
<b>Strukturbericht designation</b>	:	<i>D</i> 10 <sub>2</sub>
<b>Pearson symbol</b>	:	hP20
<b>Space group number</b>	:	186
<b>Space group symbol</b>	:	<i>P</i> 6 <sub>3</sub> <i>m</i> <i>c</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3B7_hP20_186_c_b2c --params= <i>a</i> , <i>c/a</i> , <i>z</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>z</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>z</i> <sub>4</sub>

## Other compounds with this structure:

- Th<sub>7</sub>Co<sub>3</sub>, Th<sub>7</sub>Ni<sub>3</sub>

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



---

**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates		Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_1 c \hat{\mathbf{z}}$	$(2b)$	Th I	
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) c \hat{\mathbf{z}}$	$(2b)$	Th I	
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-\sqrt{3} x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	$(6c)$	Fe	
$\mathbf{B}_4$	$= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{3}{2} x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	$(6c)$	Fe	
$\mathbf{B}_5$	$= -2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-\frac{3}{2} x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	$(6c)$	Fe	
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$\sqrt{3} x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	$(6c)$	Fe	
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$-\frac{3}{2} x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	$(6c)$	Fe	
$\mathbf{B}_8$	$= 2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$\frac{3}{2} x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	$(6c)$	Fe	
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-\sqrt{3} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	$(6c)$	Th II	
$\mathbf{B}_{10}$	$= x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{3}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	$(6c)$	Th II	
$\mathbf{B}_{11}$	$= -2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-\frac{3}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	$(6c)$	Th II	
$\mathbf{B}_{12}$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$\sqrt{3} x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	$(6c)$	Th II	
$\mathbf{B}_{13}$	$= -x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$-\frac{3}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	$(6c)$	Th II	
$\mathbf{B}_{14}$	$= 2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3$	$=$	$\frac{3}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) c \hat{\mathbf{z}}$	$(6c)$	Th II	
$\mathbf{B}_{15}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\sqrt{3} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	$(6c)$	Th III	
$\mathbf{B}_{16}$	$= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{3}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	$(6c)$	Th III	
$\mathbf{B}_{17}$	$= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{3}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	$(6c)$	Th III	
$\mathbf{B}_{18}$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$\sqrt{3} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	$(6c)$	Th III	
$\mathbf{B}_{19}$	$= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$-\frac{3}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	$(6c)$	Th III	
$\mathbf{B}_{20}$	$= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$=$	$\frac{3}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	$(6c)$	Th III	

---

**References:**

- J. V. Florio, N. C. Baenziger, and R. E. Rundle, *Compounds of thorium with transition metals. II. Systems with iron, cobalt and nickel*, *Acta Cryst.* **9**, 367–372 (1956), doi:10.1107/S0365110X5600108X.

**Found in:**

- ICSD, *Inorganic Crystal Structure Database*. ID 401657.

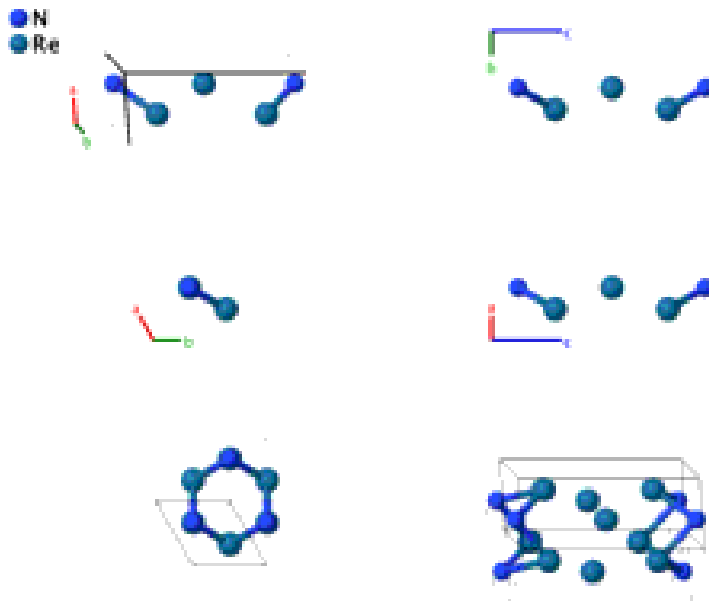
---

**Geometry files:**

- CIF: pp. 936

- POSCAR: pp. 937

# Re<sub>3</sub>N Structure: AB3\_hP4\_187\_e\_fh

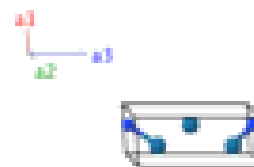


<b>Prototype</b>	:	Re <sub>3</sub> N
<b>AFLOW prototype label</b>	:	AB3_hP4_187_e_fh
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP4
<b>Space group number</b>	:	187
<b>Space group symbol</b>	:	$P\bar{6}m2$
<b>AFLOW prototype command</b>	:	aflow --proto=AB3_hP4_187_e_fh --params=a, c/a, z <sub>3</sub>

- The reference presents both experimental findings and the results of Density Functional Theory calculations. We obtain our data from the density functional theory calculations at equilibrium ( $P = 0$ ), which are consistent with the lattice constants found experimentally.

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}}$	(1e)	N
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(1f)	Re I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(2h)	Re II
$\mathbf{B}_4$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_3 c \hat{\mathbf{z}}$	(2h)	Re II

---

**References:**

- A. Friedrich, B. Winkler, L. Bayarjargal, W. Morgenroth, E. A. Juarez-Arellano, V. Milman, K. Refson, M. Kunz, and K. Chen, *Novel Rhenium Nitrides*, Phys. Rev. Lett. **105**, 085504 (2010), doi:[10.1103/PhysRevLett.105.085504](https://doi.org/10.1103/PhysRevLett.105.085504).

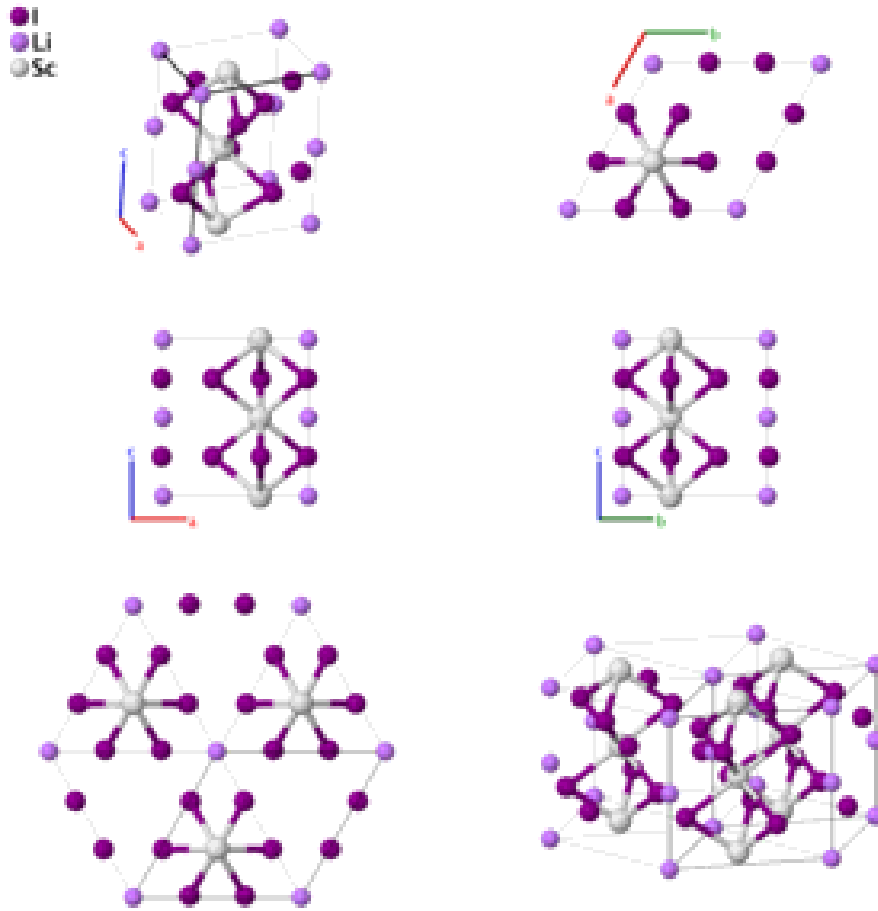
---

**Geometry files:**

- CIF: pp. [937](#)

- POSCAR: pp. [937](#)

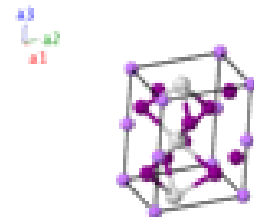
# LiScI<sub>3</sub> Structure: A3BC\_hP10\_188\_k\_a\_e



**Prototype** : LiScI<sub>3</sub>  
**AFLOW prototype label** : A3BC\_hP10\_188\_k\_a\_e  
**Strukturbericht designation** : None  
**Pearson symbol** : hP10  
**Space group number** : 188  
**Space group symbol** :  $P\bar{6}c2$   
**AFLOW prototype command** : `aflow --proto=A3BC_hP10_188_k_a_e`  
`--params=a, c/a, x3, y3`

**Hexagonal primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type

$$\begin{aligned}
\mathbf{B}_1 &= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3 &= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}} && (2a) && \text{Li} \\
\mathbf{B}_2 &= \frac{1}{2} \mathbf{a}_3 &= \frac{1}{2} c \hat{\mathbf{z}} && (2a) && \text{Li} \\
\mathbf{B}_3 &= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} && (2e) && \text{Sc} \\
\mathbf{B}_4 &= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} && (2e) && \text{Sc} \\
\mathbf{B}_5 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_3 + y_3) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} && (6k) && \text{I} \\
\mathbf{B}_6 &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \left(\frac{1}{2} x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} && (6k) && \text{I} \\
\mathbf{B}_7 &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \left(-x_3 + \frac{1}{2} y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} && (6k) && \text{I} \\
\mathbf{B}_8 &= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -\frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_3 + y_3) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} && (6k) && \text{I} \\
\mathbf{B}_9 &= (-x_3 + y_3) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(-\frac{1}{2} x_3 + y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} && (6k) && \text{I} \\
\mathbf{B}_{10} &= x_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(x_3 - \frac{1}{2} y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} && (6k) && \text{I}
\end{aligned}$$

### References:

- A. Lachgar, D. S. Dudis, P. K. Dorhout, and J. D. Corbett, *Synthesis and properties of two novel line phases that contain linear scandium chains, lithium scandium iodide (LiScI<sub>3</sub>) and sodium scandium iodide (Na<sub>0.5</sub>ScI<sub>3</sub>)*, *Inorg. Chem.* **30**, 3321–3326 (1991), [doi:10.1021/ic00017a019](https://doi.org/10.1021/ic00017a019).

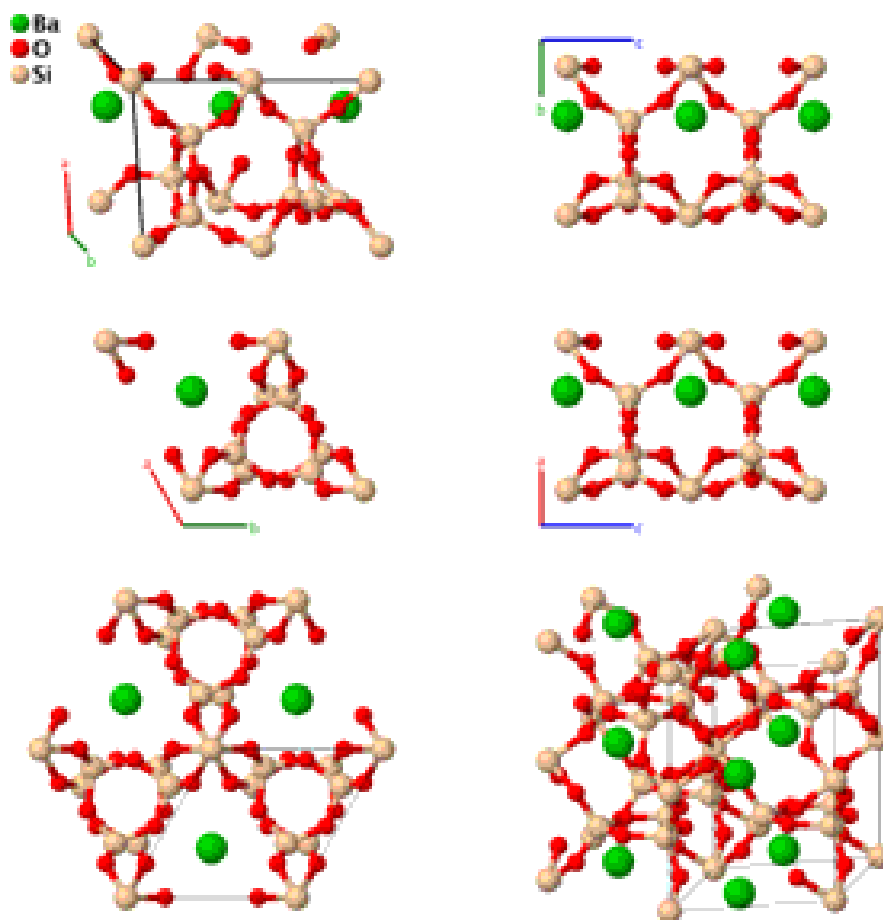
### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

### Geometry files:

- CIF: pp. [937](#)  
- POSCAR: pp. [938](#)

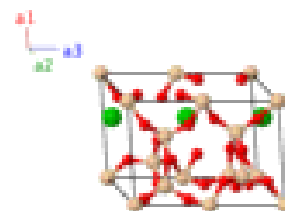
# BaSi<sub>4</sub>O<sub>9</sub> Structure: AB9C4\_hP28\_188\_e\_kl\_ak



**Prototype** : BaSi<sub>4</sub>O<sub>9</sub>  
**AFLOW prototype label** : AB9C4\_hP28\_188\_e\_kl\_ak  
**Strukturbericht designation** : None  
**Pearson symbol** : hP28  
**Space group number** : 188  
**Space group symbol** :  $P\bar{6}c2$   
**AFLOW prototype command** : `aflow --proto=AB9C4_hP28_188_e_kl_ak`  
                                   `--params=a, c/a, x3, y3, x4, y4, x5, y5, z5`

**Hexagonal primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
---------------------	-----------------------	------------------	-----------





$$\mathbf{B}_{28} = x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right)a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5a \hat{\mathbf{y}} - z_5c \hat{\mathbf{z}} \quad (12l) \quad \text{O II}$$

---

**References:**

- L. W. Finger, R. M. Hazen, and B. A. Fursenko, *Refinement of the crystal structure of BaSi<sub>4</sub>O<sub>9</sub> in the benitoite form*, J. Phys. Chem. Solids **56**, 1389–1393 (1995), doi:[10.1016/0022-3697\(95\)00075-5](https://doi.org/10.1016/0022-3697(95)00075-5).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

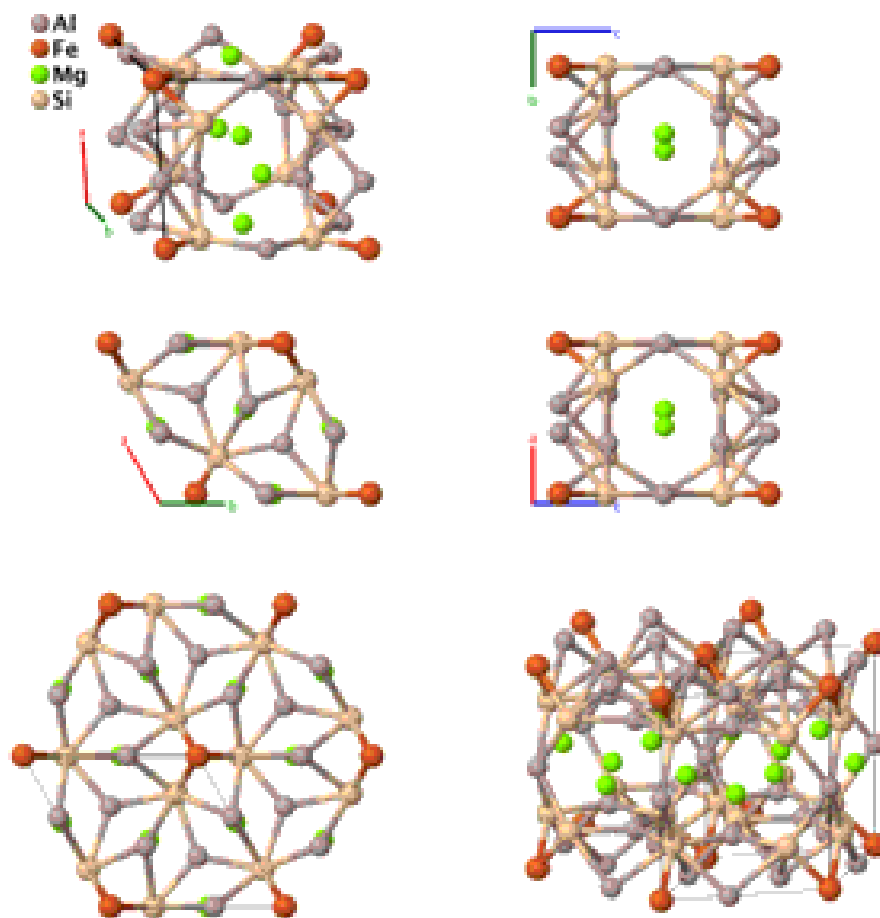
**Geometry files:**

- CIF: pp. [938](#)

- POSCAR: pp. [938](#)

# $\pi$ -FeMg<sub>3</sub>Al<sub>8</sub>Si<sub>6</sub> ( $E9_b$ ) Structure: A8BC3D6\_hP18\_189\_bfh\_a\_g\_i

---



<b>Prototype</b>	:	$\pi$ -FeMg <sub>3</sub> Al <sub>8</sub> Si <sub>6</sub>
<b>AFLOW prototype label</b>	:	A8BC3D6_hP18_189_bfh_a_g_i
<b>Strukturbericht designation</b>	:	$E9_b$
<b>Pearson symbol</b>	:	hP18
<b>Space group number</b>	:	189
<b>Space group symbol</b>	:	$P\bar{6}2m$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A8BC3D6_hP18_189_bfh_a_g_i --params=a, c/a, x<sub>3</sub>, x<sub>4</sub>, z<sub>5</sub>, x<sub>6</sub>, z<sub>6</sub></code>

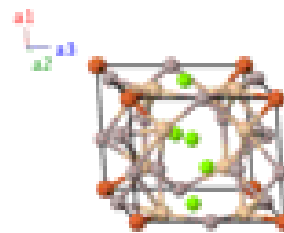
---

- We have been unable to obtain a copy of (Perlitz, 1942), and use the data provided by (Brandes, 1992) and (Foss, 2003). Foss *et al.* argue that the actual composition of this phase should be FeMg<sub>3</sub>Al<sub>9</sub>Si<sub>5</sub>. This requires a reordering of the atomic positions, as described in [A9BC3D5\\_hP18\\_189\\_fi\\_a\\_g\\_bh](#).

---

**Hexagonal primitive vectors:**

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



---

**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Fe
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} c \hat{\mathbf{z}}$	(1b)	Al I
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1$	$= \frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}}$	(3f)	Al II
$\mathbf{B}_4$	$= x_3 \mathbf{a}_2$	$= \frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}}$	(3f)	Al II
$\mathbf{B}_5$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$= -x_3 a \hat{\mathbf{x}}$	(3f)	Al II
$\mathbf{B}_6$	$= x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(3g)	Mg
$\mathbf{B}_7$	$= x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(3g)	Mg
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= -x_4 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(3g)	Mg
$\mathbf{B}_9$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4h)	Al III
$\mathbf{B}_{10}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(4h)	Al III
$\mathbf{B}_{11}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(4h)	Al III
$\mathbf{B}_{12}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4h)	Al III
$\mathbf{B}_{13}$	$= x_6 \mathbf{a}_1 + z_6 \mathbf{a}_3$	$= \frac{1}{2} x_6 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(6i)	Si
$\mathbf{B}_{14}$	$= x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$= \frac{1}{2} x_6 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(6i)	Si
$\mathbf{B}_{15}$	$= -x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$= -x_6 a \hat{\mathbf{x}} + z_6 c \hat{\mathbf{z}}$	(6i)	Si
$\mathbf{B}_{16}$	$= x_6 \mathbf{a}_1 + -z_6 \mathbf{a}_3$	$= \frac{1}{2} x_6 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(6i)	Si
$\mathbf{B}_{17}$	$= x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$= \frac{1}{2} x_6 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(6i)	Si
$\mathbf{B}_{18}$	$= -x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$= -x_6 a \hat{\mathbf{x}} - z_6 c \hat{\mathbf{z}}$	(6i)	Si

---

**References:**

- H. Perltitz and A. Westgren, *The Crystal Structure of  $Al_8Si_6Mg_3Fe$* , Ark. Kem. Mineral. Geol. **15B**, 1–8 (1942).
- E. A. Brandes and G. B. Brook, eds., *Smithells Metals Reference Book* (Butterworth Heinemann, Oxford, Auckland, Boston, Johannesburg, Melbourne, New Delhi, 1992), chap. 6, pp. 6–60, seventh edn.

**Found in:**

- S. Foss, A. Olsen, C. J. Simensen, and J. Tafto, *Determination of the crystal structure of the  $\pi$ -AlFeMgSi phase using symmetry- and site-sensitive electron microscope techniques*, Acta Crystallogr. Sect. B Struct. Sci. **59**, 36–42 (2003), [doi:10.1107/S0108768102022887](https://doi.org/10.1107/S0108768102022887).

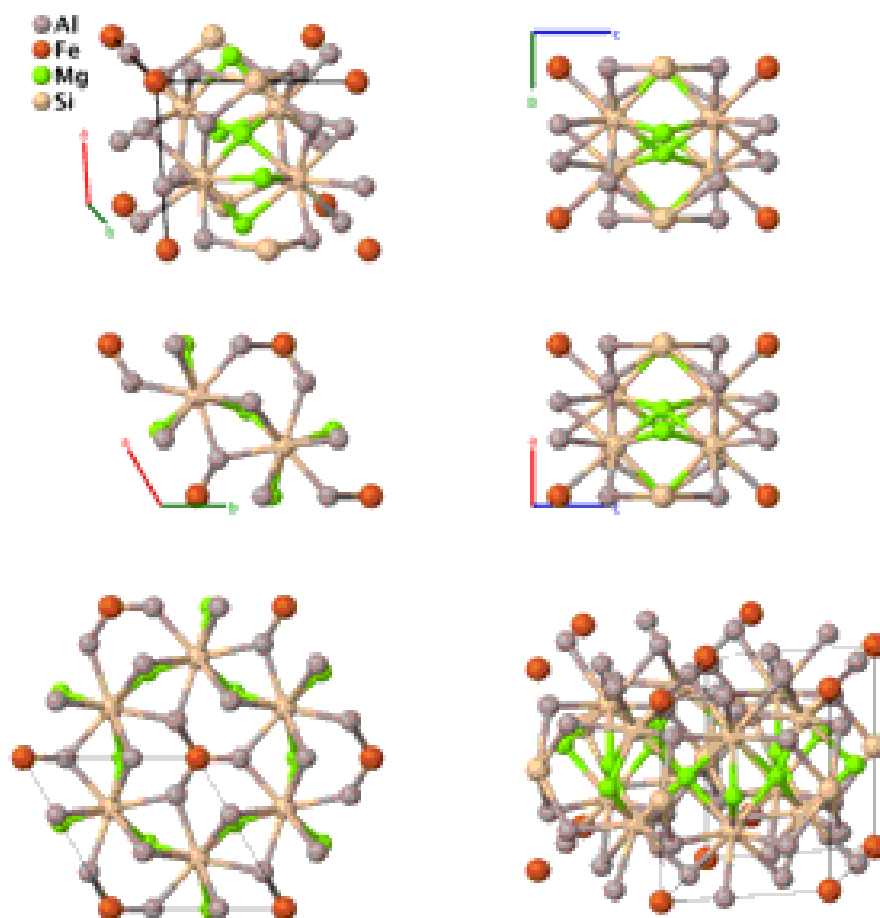
---

**Geometry files:**

- CIF: pp. [938](#)

- POSCAR: pp. [939](#)

# $\pi$ -FeMg<sub>3</sub>Al<sub>9</sub>Si<sub>5</sub> Structure: A9BC3D5\_hP18\_189\_fi\_a\_g\_bh



<b>Prototype</b>	:	$\pi$ -FeMg <sub>3</sub> Al <sub>9</sub> Si <sub>5</sub>
<b>AFLOW prototype label</b>	:	A9BC3D5_hP18_189_fi_a_g_bh
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP18
<b>Space group number</b>	:	189
<b>Space group symbol</b>	:	$P\bar{6}2m$
<b>AFLOW prototype command</b>	:	aflow --proto=A9BC3D5_hP18_189_fi_a_g_bh --params=a, c/a, x <sub>3</sub> , x <sub>4</sub> , z <sub>5</sub> , x <sub>6</sub> , z <sub>6</sub>

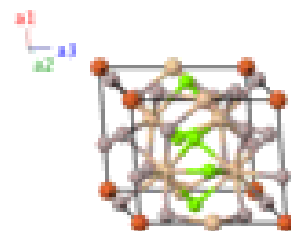
- This is a reanalysis of the  $\pi$ -FeMg<sub>3</sub>Al<sub>8</sub>Si<sub>6</sub> (*E9<sub>b</sub>*) structure. The space group and occupied Wyckoff positions are unchanged, but the ordering, stoichiometry, and atomic positions are different.

**Hexagonal primitive vectors:**

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



---

**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Fe
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(1b)	Si I
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1$	$=$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}}$	(3f)	Al I
$\mathbf{B}_4$	$= x_3 \mathbf{a}_2$	$=$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}}$	(3f)	Al I
$\mathbf{B}_5$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-x_3 a \hat{\mathbf{x}}$	(3f)	Al I
$\mathbf{B}_6$	$= x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(3g)	Mg
$\mathbf{B}_7$	$= x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(3g)	Mg
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(3g)	Mg
$\mathbf{B}_9$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4h)	Si II
$\mathbf{B}_{10}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(4h)	Si II
$\mathbf{B}_{11}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(4h)	Si II
$\mathbf{B}_{12}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(4h)	Si II
$\mathbf{B}_{13}$	$= x_6 \mathbf{a}_1 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} x_6 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(6i)	Al II
$\mathbf{B}_{14}$	$= x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} x_6 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} + z_6 c \hat{\mathbf{z}}$	(6i)	Al II
$\mathbf{B}_{15}$	$= -x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} + z_6 c \hat{\mathbf{z}}$	(6i)	Al II
$\mathbf{B}_{16}$	$= x_6 \mathbf{a}_1 + -z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} x_6 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(6i)	Al II
$\mathbf{B}_{17}$	$= x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} x_6 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_6 a \hat{\mathbf{y}} - z_6 c \hat{\mathbf{z}}$	(6i)	Al II
$\mathbf{B}_{18}$	$= -x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} + -z_6 c \hat{\mathbf{z}}$	(6i)	Al II

---

**References:**

- S. Foss, A. Olsen, C. J. Simensen, and J. Taftø, *Determination of the crystal structure of the  $\pi$ -AlFeMgSi phase using symmetry- and site-sensitive electron microscope techniques*, Acta Crystallogr. Sect. B Struct. Sci. **59**, 36–42 (2003), [doi:10.1107/S0108768102022887](https://doi.org/10.1107/S0108768102022887).

**Found in:**

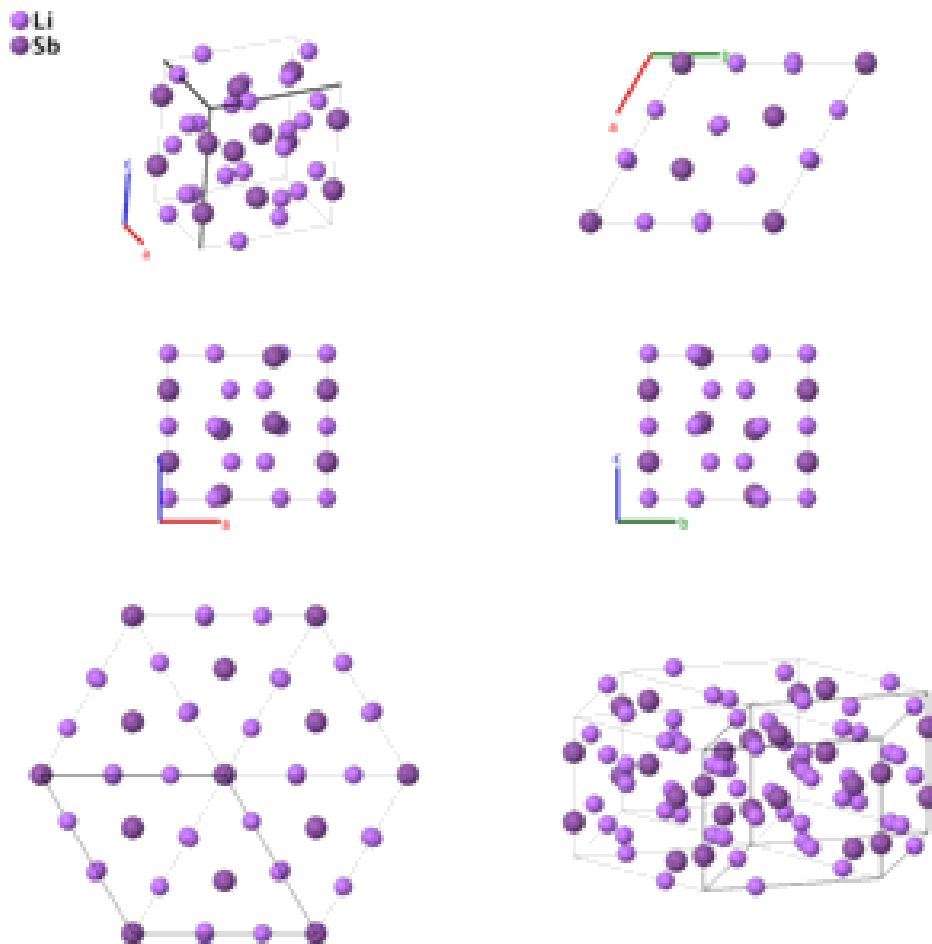
- *The Materials Project*,  $Mg_3Al_9FeSi_5$ , [doi:10.17188/1286117](https://doi.org/10.17188/1286117). ID mp-7062.  
- ICSD, *Inorganic Crystal Structure Database*. ID 96905.

---

**Geometry files:**

- CIF: pp. [939](#)  
- POSCAR: pp. [939](#)

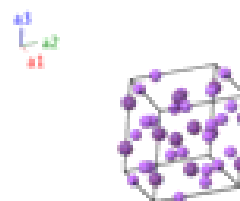
# Li<sub>2</sub>Sb Structure: A2B\_hP18\_190\_gh\_bf



<b>Prototype</b>	:	Li <sub>2</sub> Sb
<b>AFLOW prototype label</b>	:	A2B_hP18_190_gh_bf
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP18
<b>Space group number</b>	:	190
<b>Space group symbol</b>	:	$P\bar{6}2c$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_hP18_190_gh_bf --params= $a, c/a, z_2, x_3, x_4, y_4$

**Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**



	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$	(2b)	Sb I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \hat{\mathbf{z}}$	(2b)	Sb I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4f)	Sb II
$\mathbf{B}_4$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}}$	(4f)	Sb II
$\mathbf{B}_5$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}}$	(4f)	Sb II
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}}$	(4f)	Sb II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1$	$=$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}}$	(6g)	Li I
$\mathbf{B}_8$	$= x_3 \mathbf{a}_2$	$=$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}}$	(6g)	Li I
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-x_3 a \hat{\mathbf{x}}$	(6g)	Li I
$\mathbf{B}_{10}$	$= x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6g)	Li I
$\mathbf{B}_{11}$	$= x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6g)	Li I
$\mathbf{B}_{12}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6g)	Li I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Li II
$\mathbf{B}_{14}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Li II
$\mathbf{B}_{15}$	$= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Li II
$\mathbf{B}_{16}$	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_4 - y_4) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Li II
$\mathbf{B}_{17}$	$= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Li II
$\mathbf{B}_{18}$	$= -x_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Li II

---

#### References:

- W. Müller, *Darstellung und Struktur der Phase Li<sub>2</sub>Sb*, Z. Naturforsch. B **32**, 357–359 (1977).

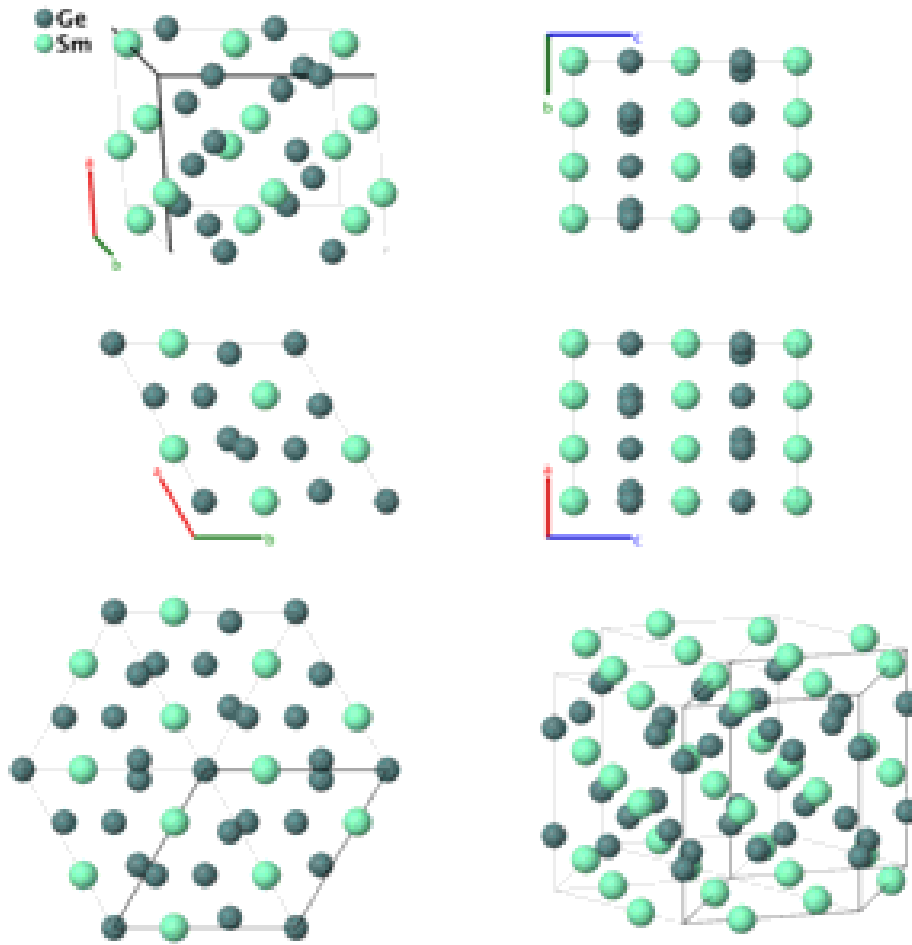
---

#### Geometry files:

- CIF: pp. [939](#)

- POSCAR: pp. [940](#)

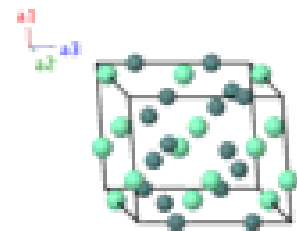
# $\alpha$ -Sm<sub>3</sub>Ge<sub>5</sub> (High-temperature) Structure: A5B3\_hP16\_190\_bdh\_g



<b>Prototype</b>	:	$\alpha$ -Sm <sub>3</sub> Ge <sub>5</sub>
<b>AFLOW prototype label</b>	:	A5B3_hP16_190_bdh_g
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP16
<b>Space group number</b>	:	190
<b>Space group symbol</b>	:	$P\bar{6}2c$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A5B3_hP16_190_bdh_g --params=a, c/a, x3, x4, y4</code>

**Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$	(2b)	Ge I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \hat{\mathbf{z}}$	(2b)	Ge I
$\mathbf{B}_3$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2d)	Ge II
$\mathbf{B}_4$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2d)	Ge II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1$	$=$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}}$	(6g)	Sm
$\mathbf{B}_6$	$= x_3 \mathbf{a}_2$	$=$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}}$	(6g)	Sm
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-x_3 a \hat{\mathbf{x}}$	(6g)	Sm
$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6g)	Sm
$\mathbf{B}_9$	$= x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6g)	Sm
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6g)	Sm
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Ge III
$\mathbf{B}_{12}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$(\frac{1}{2} x_4 - y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Ge III
$\mathbf{B}_{13}$	$= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$(-x_4 + \frac{1}{2} y_4) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Ge III
$\mathbf{B}_{14}$	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_4 - y_4) a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Ge III
$\mathbf{B}_{15}$	$= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$(\frac{1}{2} x_4 - y_4) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Ge III
$\mathbf{B}_{16}$	$= -x_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$(-x_4 + \frac{1}{2} y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Ge III

---

#### References:

- P. H. Tobash, D. Lins, S. Bobev, N. Hur, J. D. Thompson, and J. L. Sarrao, *Vacancy ordering in  $\text{SmGe}_{2-x}$  and  $\text{GdGe}_{2-x}$  ( $x = 0.33$ ): Structure and properties of two  $\text{Sm}_3\text{Ge}_5$  polymorphs and of  $\text{Gd}_3\text{Ge}_5$* , Inorg. Chem. **45**, 7286–7294 (2006), [doi:10.1021/ic060913f](https://doi.org/10.1021/ic060913f).

#### Found in:

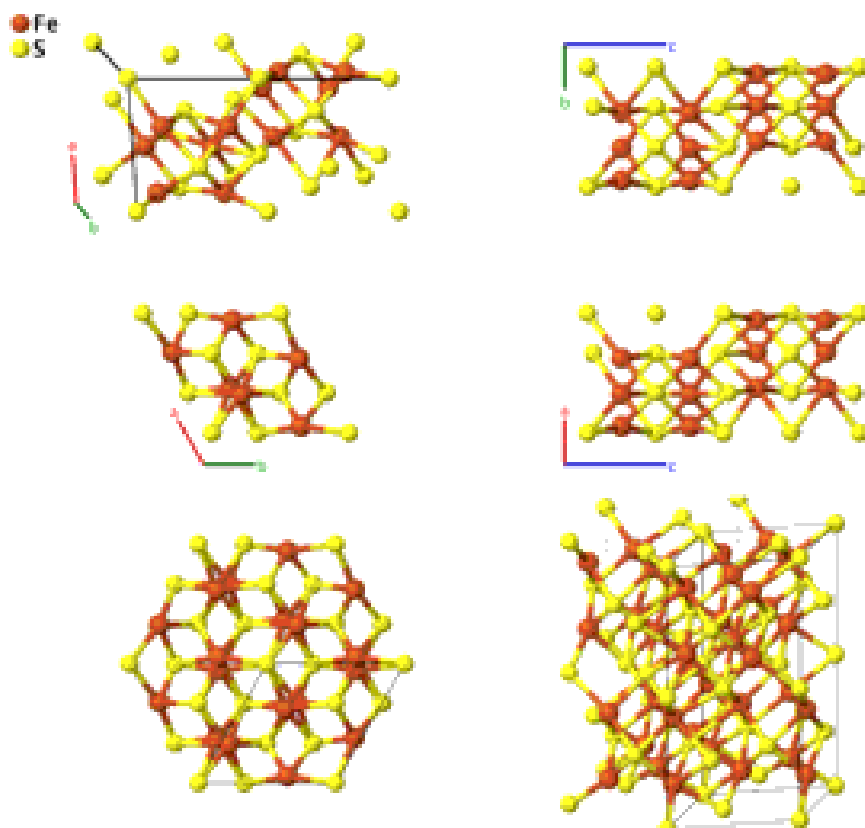
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [940](#)  
- POSCAR: pp. [940](#)

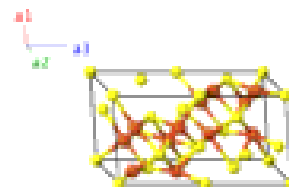
# Troilite (FeS) Structure: AB\_hP24\_190\_i\_afh



<b>Prototype</b>	:	FeS
<b>AFLOW prototype label</b>	:	AB_hP24_190_i_afh
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP24
<b>Space group number</b>	:	190
<b>Space group symbol</b>	:	$P\bar{6}2c$
<b>AFLOW prototype command</b>	:	aflow --proto=AB_hP24_190_i_afh --params= $a, c/a, z_2, x_3, y_3, x_4, y_4, z_4$

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	S I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2a)	S I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + z_2 c \hat{\mathbf{z}}$	(4f)	S II

$$\begin{aligned}
\mathbf{B}_4 &= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) c \hat{\mathbf{z}} && (4f) && \text{S II} \\
\mathbf{B}_5 &= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} - z_2 c \hat{\mathbf{z}} && (4f) && \text{S II} \\
\mathbf{B}_6 &= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) c \hat{\mathbf{z}} && (4f) && \text{S II} \\
\mathbf{B}_7 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + && (6h) && \text{S III} \\
&&& \frac{\sqrt{3}}{2} (-x_3 + y_3) a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} \\
\mathbf{B}_8 &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \left(\frac{1}{2} x_3 - y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} && (6h) && \text{S III} \\
\mathbf{B}_9 &= (-x_3 + y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \left(-x_3 + \frac{1}{2} y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} && (6h) && \text{S III} \\
\mathbf{B}_{10} &= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2} (x_3 + y_3) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_3 - y_3) a \hat{\mathbf{y}} + && (6h) && \text{S III} \\
&&& \frac{3}{4} c \hat{\mathbf{z}} \\
\mathbf{B}_{11} &= (x_3 - y_3) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(\frac{1}{2} x_3 - y_3\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} && (6h) && \text{S III} \\
\mathbf{B}_{12} &= -x_3 \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \left(-x_3 + \frac{1}{2} y_3\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} && (6h) && \text{S III} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + && (12i) && \text{Fe} \\
&&& \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} \\
\mathbf{B}_{14} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (12i) && \text{Fe} \\
\mathbf{B}_{15} &= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= \left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}} && (12i) && \text{Fe} \\
\mathbf{B}_{16} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + && (12i) && \text{Fe} \\
&&& \frac{\sqrt{3}}{2} (-x_4 + y_4) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{17} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + && (12i) && \text{Fe} \\
&&& \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{18} &= (-x_4 + y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3 &= \left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + && (12i) && \text{Fe} \\
&&& \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{19} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_4 - y_4) a \hat{\mathbf{y}} - && (12i) && \text{Fe} \\
&&& z_4 c \hat{\mathbf{z}} \\
\mathbf{B}_{20} &= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (12i) && \text{Fe} \\
\mathbf{B}_{21} &= -x_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}} && (12i) && \text{Fe} \\
\mathbf{B}_{22} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \frac{1}{2} (x_4 + y_4) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} (x_4 - y_4) a \hat{\mathbf{y}} + && (12i) && \text{Fe} \\
&&& \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{23} &= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(\frac{1}{2} x_4 - y_4\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + && (12i) && \text{Fe} \\
&&& \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}} \\
\mathbf{B}_{24} &= -x_4 \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3 &= \left(-x_4 + \frac{1}{2} y_4\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} y_4 a \hat{\mathbf{y}} + && (12i) && \text{Fe} \\
&&& \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}
\end{aligned}$$

## References:

- N. Morimoto, H. Nakazawa, K. Nishigucmi, and M. Tokonami, *Pyrrhotites: Stoichiometric Compounds with Composition  $Fe_{n-1}S_n$  ( $n \geq 8$ )*, Science **168**, 964–966 (1970), doi:10.1126/science.168.3934.964.

## Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

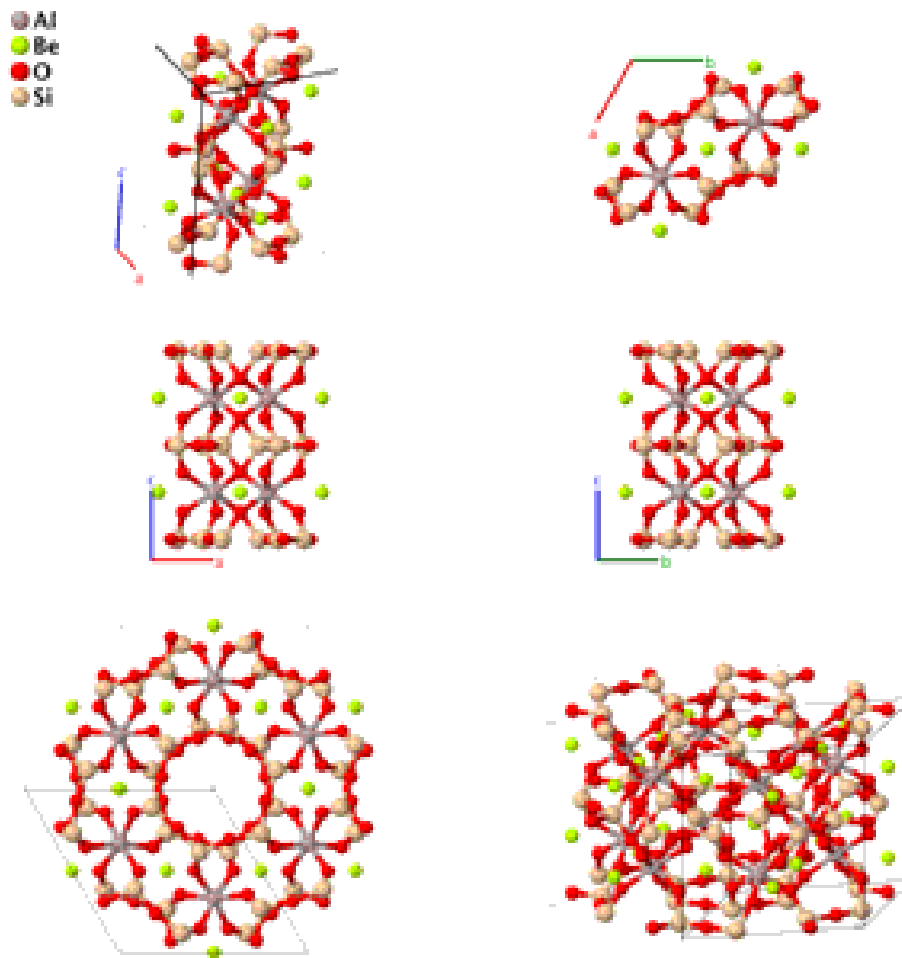
## Geometry files:

- CIF: pp. 940

- POSCAR: pp. [941](#)

# Beryl ( $\text{Be}_3\text{Al}_2\text{Si}_6\text{O}_{18}$ , $G3_1$ ) Structure: A2B3C18D6\_hP58\_192\_c\_f\_lm\_1

---



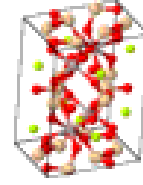
**Prototype** :  $\text{Be}_3\text{Al}_2\text{Si}_6\text{O}_{18}$   
**AFLOW prototype label** : A2B3C18D6\_hP58\_192\_c\_f\_lm\_1  
**Strukturbericht designation** :  $G3_1$   
**Pearson symbol** : hP58  
**Space group number** : 192  
**Space group symbol** :  $P6/mcc$   
**AFLOW prototype command** : `aflow --proto=A2B3C18D6_hP58_192_c_f_lm_1`  
                                   `--params=a, c/a, x3, y3, x4, y4, x5, y5, z5`

---

- (Morosin, 1972) places oxygen atoms on the (2a) Wyckoff site (lattice coordinates  $(0, 0, \pm 1/4)$ ), with an occupation of (0.0991). We follow (Hazen, 1986) and ignore this small contribution to the structure.

## Hexagonal primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4c)	Al
$\mathbf{B}_2$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2\sqrt{3}}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4c)	Al
$\mathbf{B}_3$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2\sqrt{3}}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(4c)	Al
$\mathbf{B}_4$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(4c)	Al
$\mathbf{B}_5$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_3$	$= \frac{1}{4}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6f)	Be
$\mathbf{B}_6$	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$= \frac{1}{4}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6f)	Be
$\mathbf{B}_7$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6f)	Be
$\mathbf{B}_8$	$= \frac{1}{2}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_3$	$= \frac{1}{4}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6f)	Be
$\mathbf{B}_9$	$= \frac{1}{2}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$= \frac{1}{4}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6f)	Be
$\mathbf{B}_{10}$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$= \frac{1}{2}a\hat{\mathbf{x}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6f)	Be
$\mathbf{B}_{11}$	$= x_3\mathbf{a}_1 + y_3\mathbf{a}_2$	$= \frac{1}{2}(x_3 + y_3)a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3)a\hat{\mathbf{y}}$	(12l)	O I
$\mathbf{B}_{12}$	$= -y_3\mathbf{a}_1 + (x_3 - y_3)\mathbf{a}_2$	$= \left(\frac{1}{2}x_3 - y_3\right)a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3a\hat{\mathbf{y}}$	(12l)	O I
$\mathbf{B}_{13}$	$= (-x_3 + y_3)\mathbf{a}_1 - x_3\mathbf{a}_2$	$= \left(-x_3 + \frac{1}{2}y_3\right)a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3a\hat{\mathbf{y}}$	(12l)	O I
$\mathbf{B}_{14}$	$= -x_3\mathbf{a}_1 - y_3\mathbf{a}_2$	$= -\frac{1}{2}(x_3 + y_3)a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3)a\hat{\mathbf{y}}$	(12l)	O I
$\mathbf{B}_{15}$	$= y_3\mathbf{a}_1 + (-x_3 + y_3)\mathbf{a}_2$	$= \left(-\frac{1}{2}x_3 + y_3\right)a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3a\hat{\mathbf{y}}$	(12l)	O I
$\mathbf{B}_{16}$	$= (x_3 - y_3)\mathbf{a}_1 + x_3\mathbf{a}_2$	$= \left(x_3 - \frac{1}{2}y_3\right)a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3a\hat{\mathbf{y}}$	(12l)	O I
$\mathbf{B}_{17}$	$= y_3\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$= \frac{1}{2}(x_3 + y_3)a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_3 - y_3)a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(12l)	O I
$\mathbf{B}_{18}$	$= (x_3 - y_3)\mathbf{a}_1 - y_3\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$= \left(\frac{1}{2}x_3 - y_3\right)a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(12l)	O I
$\mathbf{B}_{19}$	$= -x_3\mathbf{a}_1 + (-x_3 + y_3)\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$= \left(-x_3 + \frac{1}{2}y_3\right)a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_3a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(12l)	O I
$\mathbf{B}_{20}$	$= -y_3\mathbf{a}_1 - x_3\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$= -\frac{1}{2}(x_3 + y_3)a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_3 + y_3)a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(12l)	O I
$\mathbf{B}_{21}$	$= (-x_3 + y_3)\mathbf{a}_1 + y_3\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$= \left(-\frac{1}{2}x_3 + y_3\right)a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(12l)	O I
$\mathbf{B}_{22}$	$= x_3\mathbf{a}_1 + (x_3 - y_3)\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$= \left(x_3 - \frac{1}{2}y_3\right)a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_3a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(12l)	O I
$\mathbf{B}_{23}$	$= x_4\mathbf{a}_1 + y_4\mathbf{a}_2$	$= \frac{1}{2}(x_4 + y_4)a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_4 + y_4)a\hat{\mathbf{y}}$	(12l)	Si
$\mathbf{B}_{24}$	$= -y_4\mathbf{a}_1 + (x_4 - y_4)\mathbf{a}_2$	$= \left(\frac{1}{2}x_4 - y_4\right)a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_4a\hat{\mathbf{y}}$	(12l)	Si
$\mathbf{B}_{25}$	$= (-x_4 + y_4)\mathbf{a}_1 - x_4\mathbf{a}_2$	$= \left(-x_4 + \frac{1}{2}y_4\right)a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_4a\hat{\mathbf{y}}$	(12l)	Si
$\mathbf{B}_{26}$	$= -x_4\mathbf{a}_1 - y_4\mathbf{a}_2$	$= -\frac{1}{2}(x_4 + y_4)a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_4 - y_4)a\hat{\mathbf{y}}$	(12l)	Si
$\mathbf{B}_{27}$	$= y_4\mathbf{a}_1 + (-x_4 + y_4)\mathbf{a}_2$	$= \left(-\frac{1}{2}x_4 + y_4\right)a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_4a\hat{\mathbf{y}}$	(12l)	Si





$$\mathbf{B}_{54} = (-x_5 + y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} \quad (24m) \quad \text{O II}$$

$$\mathbf{B}_{55} = x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} \quad (24m) \quad \text{O II}$$

$$\mathbf{B}_{56} = y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_5 - y_5) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} \quad (24m) \quad \text{O II}$$

$$\mathbf{B}_{57} = (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2}x_5 - y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} \quad (24m) \quad \text{O II}$$

$$\mathbf{B}_{58} = -x_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(-x_5 + \frac{1}{2}y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} \quad (24m) \quad \text{O II}$$

**References:**

- R. M. Hazen, A. Y. Au, and L. W. Finger, *High-pressure crystal chemistry of beryl (Be<sub>3</sub>Al<sub>2</sub>Si<sub>6</sub>O<sub>18</sub>) and euclase (BeAlSi<sub>4</sub>O<sub>4</sub>OH)*, Am. Mineral. **71**, 977–984 (1986).
- B. Morosin, *Structure and Thermal Expansion of Beryl*, Acta Crystallogr. Sect. B Struct. Sci. **28**, 1899–1903 (1972), [doi:10.1107/S0567740872005199](https://doi.org/10.1107/S0567740872005199).

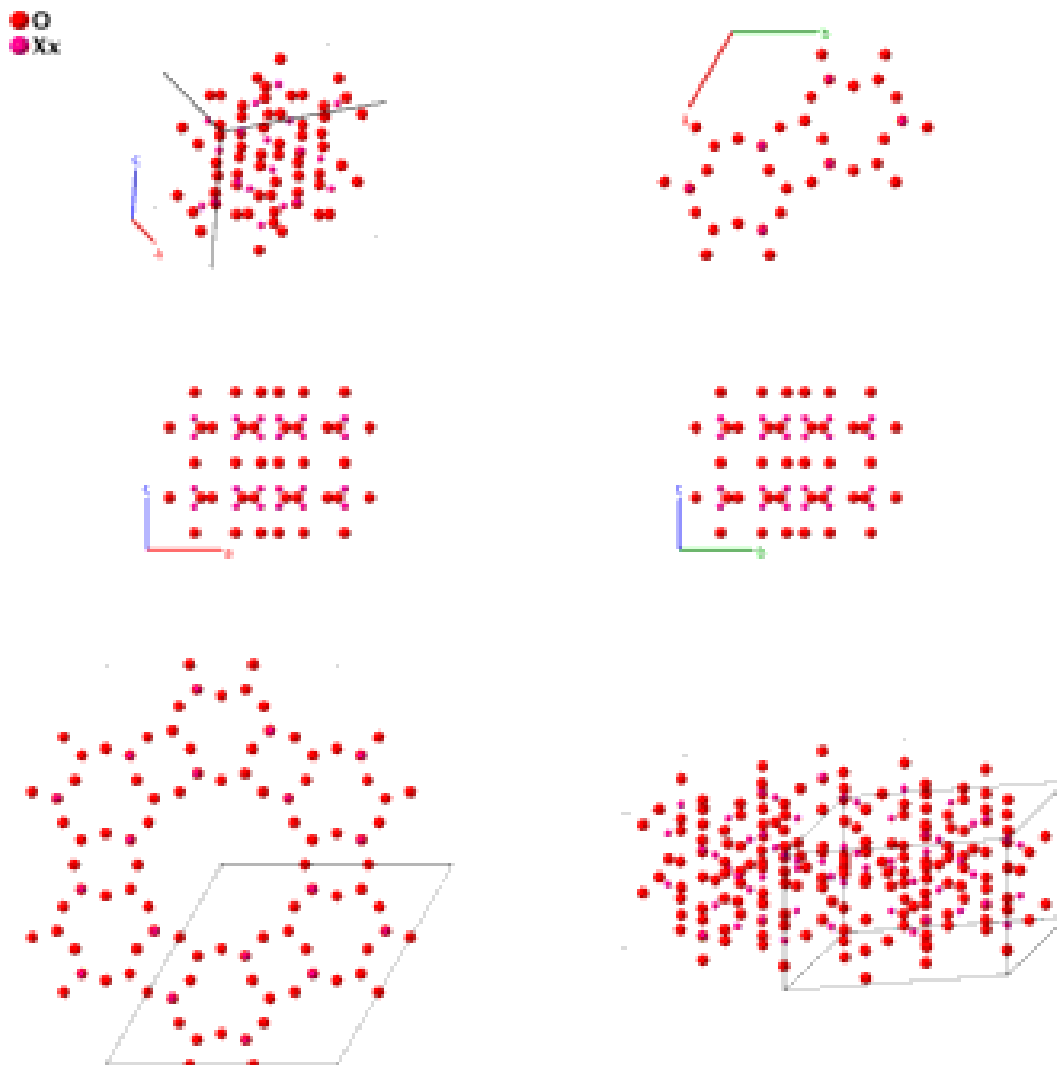
**Found in:**

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

**Geometry files:**

- CIF: pp. [941](#)
- POSCAR: pp. [941](#)

# AlPO<sub>4</sub> Structure: AB2\_hP72\_192\_m\_j2kl

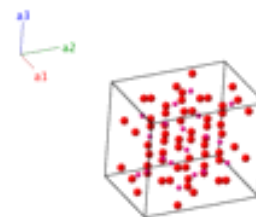


**Prototype** : AlPO<sub>4</sub>  
**AFLOW prototype label** : AB2\_hP72\_192\_m\_j2kl  
**Strukturbericht designation** : None  
**Pearson symbol** : hP72  
**Space group number** : 192  
**Space group symbol** : *P6/mcc*  
**AFLOW prototype command** : `aflow --proto=AB2_hP72_192_m_j2kl`  
`--params=a, c/a, x1, x2, x3, x4, y4, x5, y5, z5`

- Here, the M sites are partially occupied with 0.5Al+0.5P. The Jmol image does not distinguish between the different M labels and is represented by the "Xx" atoms. Polytypes of this compound also appear in a space groups #168 and #184.

## Hexagonal primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$\frac{1}{2} x_1 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12j)	O I
$\mathbf{B}_2$	$x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{1}{2} x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12j)	O I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12j)	O I
$\mathbf{B}_4$	$-x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$-\frac{1}{2} x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12j)	O I
$\mathbf{B}_5$	$-x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-\frac{1}{2} x_1 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12j)	O I
$\mathbf{B}_6$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12j)	O I
$\mathbf{B}_7$	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$-\frac{1}{2} x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(12j)	O I
$\mathbf{B}_8$	$-x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-\frac{1}{2} x_1 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(12j)	O I
$\mathbf{B}_9$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$x_1 a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}}$	(12j)	O I
$\mathbf{B}_{10}$	$x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$\frac{1}{2} x_1 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(12j)	O I
$\mathbf{B}_{11}$	$x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{1}{2} x_1 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_1 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(12j)	O I
$\mathbf{B}_{12}$	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-x_1 a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}}$	(12j)	O I
$\mathbf{B}_{13}$	$x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{3}{2} x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B}_{14}$	$-2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-\frac{3}{2} x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B}_{15}$	$x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-\sqrt{3} x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B}_{16}$	$-x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-\frac{3}{2} x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B}_{17}$	$2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{3}{2} x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B}_{18}$	$-x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\sqrt{3} x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B}_{19}$	$-x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-\frac{3}{2} x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B}_{20}$	$2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{3}{2} x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B}_{21}$	$-x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\sqrt{3} x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B}_{22}$	$x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{3}{2} x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B}_{23}$	$-2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-\frac{3}{2} x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B}_{24}$	$x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-\sqrt{3} x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B}_{25}$	$x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{3}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12k)	O III
$\mathbf{B}_{26}$	$-2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-\frac{3}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12k)	O III
$\mathbf{B}_{27}$	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-\sqrt{3} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12k)	O III
$\mathbf{B}_{28}$	$-x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-\frac{3}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(12k)	O III



$$\begin{aligned}
\mathbf{B}_{59} &= (-x_5 + y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{60} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{61} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = -\frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_5 - y_5) a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{62} &= y_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 = \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{63} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{64} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = \frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5) a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{65} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 = \left(\frac{1}{2}x_5 - y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{66} &= (-x_5 + y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = \left(-x_5 + \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{67} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = -\frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(-x_5 + y_5) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{68} &= (-x_5 + y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(-\frac{1}{2}x_5 + y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{69} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(x_5 - \frac{1}{2}y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{70} &= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \frac{1}{2}(x_5 + y_5) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}(x_5 - y_5) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{71} &= (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2}x_5 - y_5\right) a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (24m) & \text{M} \\
\mathbf{B}_{72} &= -x_5 \mathbf{a}_1 + (-x_5 + y_5) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(-x_5 + \frac{1}{2}y_5\right) a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}} & (24m) & \text{M}
\end{aligned}$$

---

### References:

- J. W. Richardson Jr., J. J. Pluth, and J. V. Smith, *Aluminophosphate number 5: time-of-flight neutron powder diffraction study of calcined powder at 295 K*, Acta Crystallogr. C **43**, 1469–1472 (1987), doi:10.1107/S0108270187091418.

### Found in:

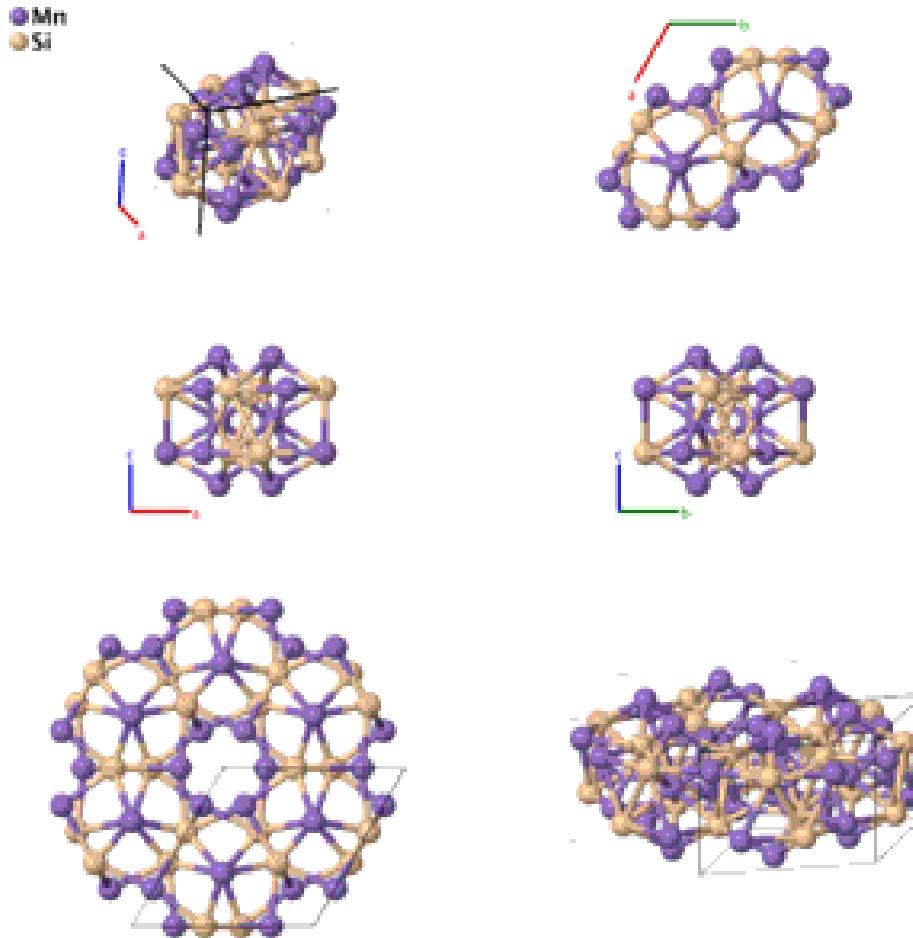
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. 942
- POSCAR: pp. 942

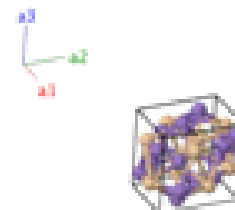
# Mavlyanovite (Mn<sub>5</sub>Si<sub>3</sub>) Structure: A5B3\_hP16\_193\_dg\_g



<b>Prototype</b>	:	Mn <sub>5</sub> Si <sub>3</sub>
<b>AFLOW prototype label</b>	:	A5B3_hP16_193_dg_g
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	hP16
<b>Space group number</b>	:	193
<b>Space group symbol</b>	:	<i>P</i> 6 <sub>3</sub> / <i>mcm</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A5B3_hP16_193_dg_g --params= <i>a, c/a, x<sub>2</sub>, x<sub>3</sub></i>

**Hexagonal primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}a \hat{\mathbf{y}}$	(4d)	Mn I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4d)	Mn I
$\mathbf{B}_3$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}}a \hat{\mathbf{y}}$	(4d)	Mn I
$\mathbf{B}_4$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4d)	Mn I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}x_2a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6g)	Mn II
$\mathbf{B}_6$	$= x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}x_2a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6g)	Mn II
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-x_2a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6g)	Mn II
$\mathbf{B}_8$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}x_2a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6g)	Mn II
$\mathbf{B}_9$	$= -x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}x_2a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_2a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6g)	Mn II
$\mathbf{B}_{10}$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$x_2a \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6g)	Mn II
$\mathbf{B}_{11}$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}x_3a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6g)	Si
$\mathbf{B}_{12}$	$= x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}x_3a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6g)	Si
$\mathbf{B}_{13}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-x_3a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6g)	Si
$\mathbf{B}_{14}$	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}x_3a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6g)	Si
$\mathbf{B}_{15}$	$= -x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}x_3a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}x_3a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6g)	Si
$\mathbf{B}_{16}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$x_3a \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6g)	Si

---

#### References:

- B. Aronsson, *A note on the compositions and crystal structures of MnB<sub>2</sub>, Mn<sub>3</sub>Si, Mn<sub>5</sub>Si<sub>3</sub>, and FeSi<sub>2</sub>*, Acta Chem. Scand. **14**, 1414–1418 (1960), doi:10.3891/acta.chem.scand.14-1414.

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

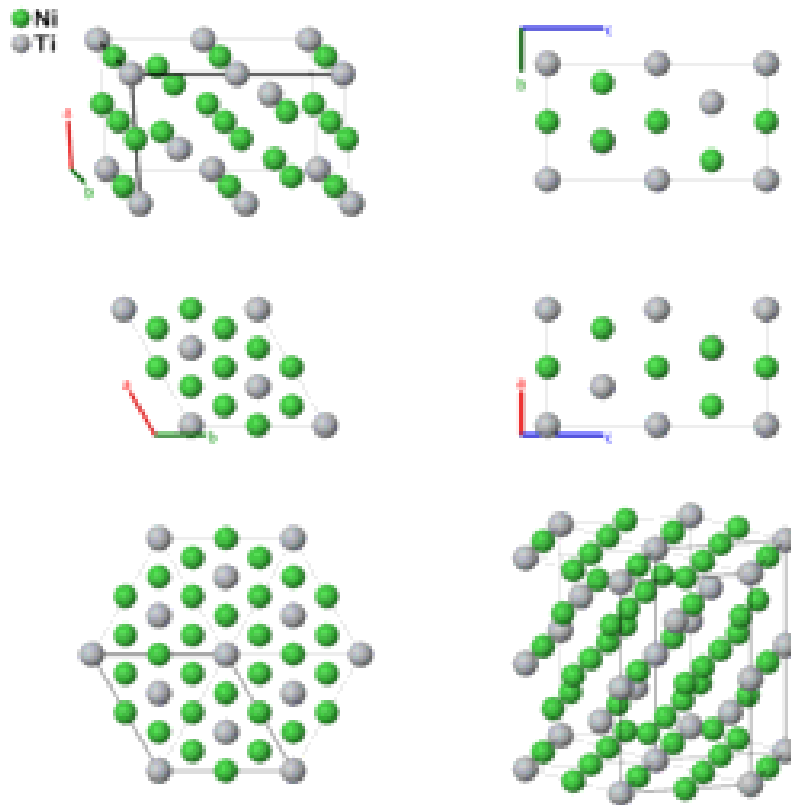
---

#### Geometry files:

- CIF: pp. 943  
- POSCAR: pp. 943



# Ni<sub>3</sub>Ti (*D*0<sub>24</sub>) Structure: A3B\_hP16\_194\_gh\_ac



<b>Prototype</b>	:	Ni <sub>3</sub> Ti
<b>AFLOW prototype label</b>	:	A3B_hP16_194_gh_ac
<b>Strukturbericht designation</b>	:	<i>D</i> 0 <sub>24</sub>
<b>Pearson symbol</b>	:	hP16
<b>Space group number</b>	:	194
<b>Space group symbol</b>	:	<i>P</i> 6 <sub>3</sub> / <i>m</i> <i>m</i> <i>c</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A3B_hP16_194_gh_ac --params= <i>a</i> , <i>c/a</i> , <i>x</i> <sub>4</sub>

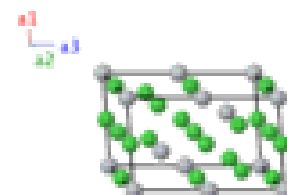
## Other compounds with this structure:

- NpPd<sub>3</sub>, HfPd<sub>3</sub>, TiPd<sub>3</sub>, ZrPd<sub>3</sub>, HfPt<sub>3</sub>, ZrPt<sub>3</sub>

- The internal coordinate  $x_4$  was not determined by any reference we could find. We follow (Villars, 2016) and set  $x_4 = -1/6$ , which places the Nb atoms in line with the Ti atoms in the  $z = 1/4$  and  $z = 3/4$  planes. This is not required by symmetry, and it is likely that the actual value of  $x_4$  will be close, but not equal to  $-1/6$ .

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



---

**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	Ti I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Ti I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2c)	Ti II
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2c)	Ti II
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4} a \hat{\mathbf{y}}$	(6g)	Ni I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4} a \hat{\mathbf{y}}$	(6g)	Ni I
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(6g)	Ni I
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6g)	Ni I
$\mathbf{B}_9$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6g)	Ni I
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(6g)	Ni I
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Ni II
$\mathbf{B}_{12}$	$= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Ni II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3} x_4 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Ni II
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Ni II
$\mathbf{B}_{15}$	$= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Ni II
$\mathbf{B}_{16}$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3} x_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Ni II

---

**References:**

- F. Laves and H. J. Wallbaum, *Die Kristallstruktur von Ni<sub>3</sub>Ti und Si<sub>2</sub>Ti (Zwei neue Typen.)*, Z. Kristallogr. **101**, 78–93 (1939), doi:10.1524/zkri.1939.101.1.78.

- P. Villars, ed., *PAULING FILE in: Inorganic Solid Phases* (SpringerMaterials (online database), Heidelberg, 2016).

---

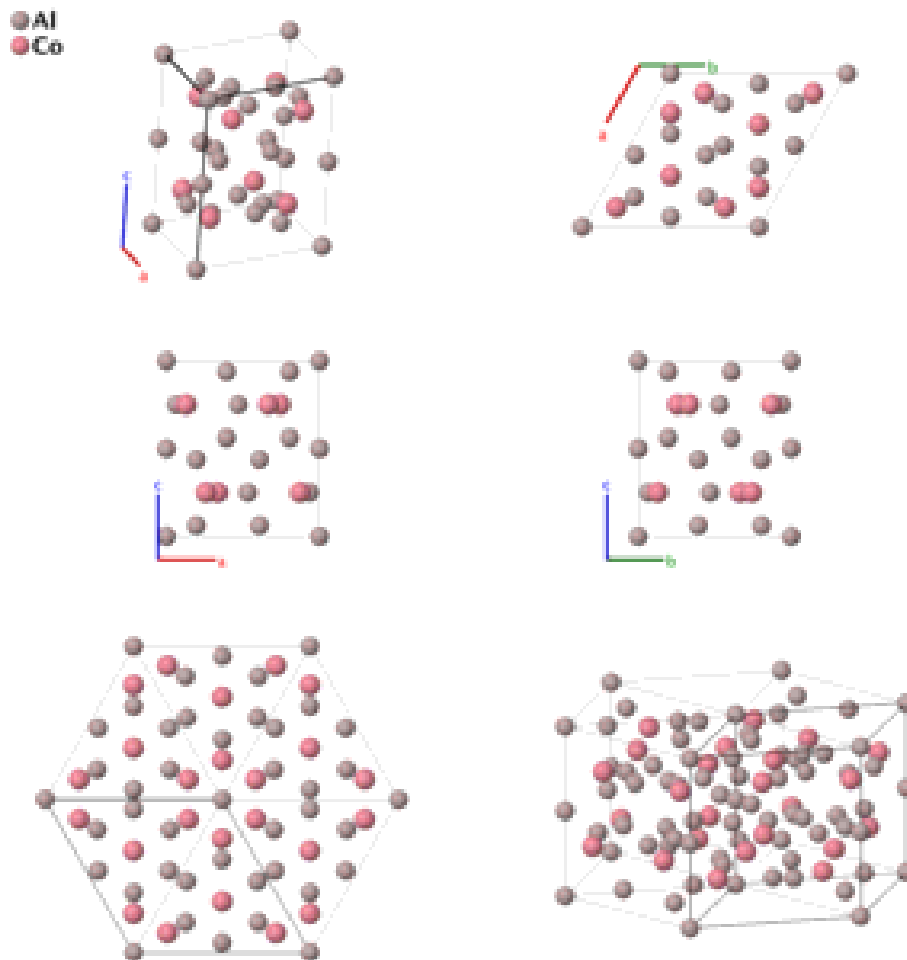
**Geometry files:**

- CIF: pp. 943

- POSCAR: pp. 943

# Co<sub>2</sub>Al<sub>5</sub> (*D*8<sub>11</sub>) Structure: A5B2\_hP28\_194\_ahk\_ch

---



<b>Prototype</b>	:	Co <sub>2</sub> Al <sub>5</sub>
<b>AFLOW prototype label</b>	:	A5B2_hP28_194_ahk_ch
<b>Strukturbericht designation</b>	:	<i>D</i> 8 <sub>11</sub>
<b>Pearson symbol</b>	:	hP28
<b>Space group number</b>	:	194
<b>Space group symbol</b>	:	<i>P</i> 6 <sub>3</sub> / <i>m</i> <i>m</i> <i>c</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A5B2_hP28_194_ahk_ch</code> <code>--params=<i>a, c/a, x<sub>3</sub>, x<sub>4</sub>, x<sub>5</sub>, z<sub>5</sub></i></code>

---

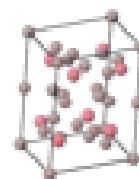
## Other compounds with this structure:

- Rh<sub>2</sub>Mg<sub>5</sub>, Pd<sub>2</sub>Mg<sub>5</sub>

- 
- (Newkirk, 1961) puts the Co I atoms at the (2d) Wyckoff sites. We have shifted the origin by  $1/2c\hat{z}$ , which shifts the Co atoms to the (2c) sites.

## Hexagonal primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2c)	Co I
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2\sqrt{3}} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2c)	Co I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{3}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Al II
$\mathbf{B}_6$	$= -2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= -\frac{3}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Al II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= -\sqrt{3} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Al II
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= -\frac{3}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Al II
$\mathbf{B}_9$	$= 2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{3}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Al II
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \sqrt{3} x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Al II
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{3}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Co II
$\mathbf{B}_{12}$	$= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= -\frac{3}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Co II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= -\sqrt{3} x_4 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Co II
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= -\frac{3}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Co II
$\mathbf{B}_{15}$	$= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{3}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Co II
$\mathbf{B}_{16}$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \sqrt{3} x_4 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Co II
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= \frac{3}{2} x_5 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{18}$	$= -2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= -\frac{3}{2} x_5 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{19}$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= -\sqrt{3} x_5 a \hat{\mathbf{y}} + z_5 c \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{20}$	$= -x_5 \mathbf{a}_1 - 2x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$= -\frac{3}{2} x_5 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{21}$	$= 2x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$= \frac{3}{2} x_5 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{22}$	$= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$= \sqrt{3} x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) c \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{23}$	$= 2x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$= \frac{3}{2} x_5 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{24}$	$= -x_5 \mathbf{a}_1 - 2x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$= -\frac{3}{2} x_5 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{25}$	$= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$= \sqrt{3} x_5 a \hat{\mathbf{y}} - z_5 c \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{26}$	$= -2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3$	$= -\frac{3}{2} x_5 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{27}$	$= x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3$	$= \frac{3}{2} x_5 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{28}$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3$	$= -\sqrt{3} x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) c \hat{\mathbf{z}}$	(12k)	Al III

---

**References:**

- J. B. Newkirk, P. J. Black, and A. Damjanovic, *The refinement of the  $Co_2Al_5$  structures*, Acta Cryst. **14**, 532–533 (1961), [doi:10.1107/S0365110X61001637](https://doi.org/10.1107/S0365110X61001637).

**Found in:**

- L. Westin, *A Palladium-Magnesium Alloy Phase of  $Co_2Al_5$  Type*, Acta Chem. Scand. **22**, 2574–2580 (1968), [doi:10.3891/acta.chem.scand.22-2574](https://doi.org/10.3891/acta.chem.scand.22-2574).

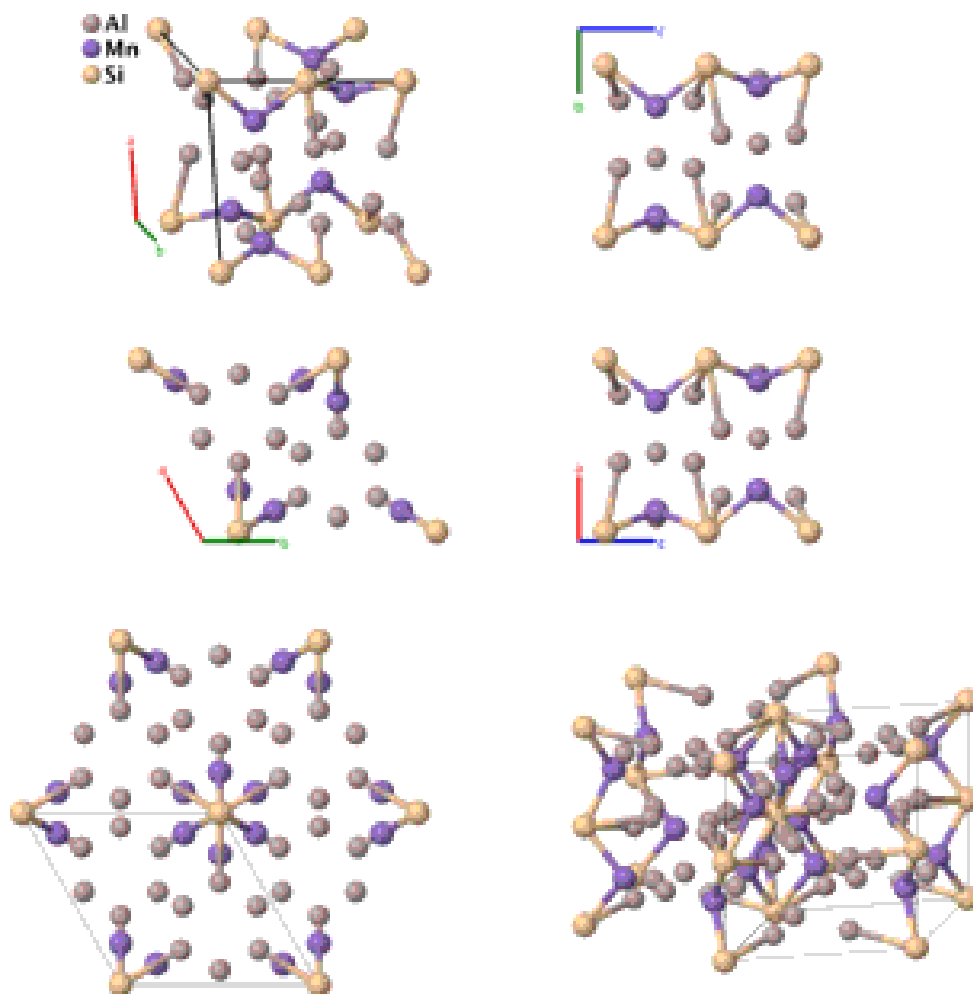
---

**Geometry files:**

- CIF: pp. [944](#)  
- POSCAR: pp. [944](#)

# Al<sub>9</sub>Mn<sub>3</sub>Si (*E9<sub>c</sub>*) Structure: A9B3C\_hP26\_194\_hk\_h\_a

---



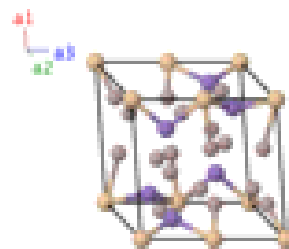
<b>Prototype</b>	:	Al <sub>9</sub> Mn <sub>3</sub> Si
<b>AFLOW prototype label</b>	:	A9B3C_hP26_194_hk_h_a
<b>Strukturbericht designation</b>	:	<i>E9<sub>c</sub></i>
<b>Pearson symbol</b>	:	hP26
<b>Space group number</b>	:	194
<b>Space group symbol</b>	:	<i>P6<sub>3</sub>/mmc</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A9B3C_hP26_194_hk_h_a --params=a, c/a, x<sub>2</sub>, x<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub></code>

---

- (Pearson, 1958) quotes (Pratt, 1951) for this structure, but this paper does not contain useful structural information. Pearson also cites (Robinson, 1952) for this structure, but that reference actually discusses Ni<sub>4</sub>Mn<sub>11</sub>Al<sub>60</sub>. We use the lattice constants given by Pearson, who states that the structure is stabilized by vacancies. Pearson calls this structure  $\beta$ -Al-Mn-Si. The atomic positions are taken from (Brandes, 1992), who give no reference.

## Hexagonal primitive vectors:

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	Si
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_3$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Si
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{3}{2} x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_4$	$-2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-\frac{3}{2} x_2 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-\sqrt{3} x_2 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_6$	$-x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-\frac{3}{2} x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_7$	$2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{3}{2} x_2 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_8$	$-x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\sqrt{3} x_2 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_9$	$x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{3}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Mn
$\mathbf{B}_{10}$	$-2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-\frac{3}{2} x_3 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Mn
$\mathbf{B}_{11}$	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-\sqrt{3} x_3 a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Mn
$\mathbf{B}_{12}$	$-x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-\frac{3}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Mn
$\mathbf{B}_{13}$	$2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\frac{3}{2} x_3 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Mn
$\mathbf{B}_{14}$	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$\sqrt{3} x_3 a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Mn
$\mathbf{B}_{15}$	$x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$\frac{3}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{16}$	$-2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$-\frac{3}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{17}$	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$-\sqrt{3} x_4 a \hat{\mathbf{y}} + z_4 c \hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{18}$	$-x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$-\frac{3}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{19}$	$2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$\frac{3}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{20}$	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} + z_4\right) \mathbf{a}_3$	$\sqrt{3} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) c \hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{21}$	$2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$\frac{3}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{22}$	$-x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$-\frac{3}{2} x_4 a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{23}$	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$\sqrt{3} x_4 a \hat{\mathbf{y}} - z_4 c \hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{24}$	$-2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$-\frac{3}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{25}$	$x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$\frac{3}{2} x_4 a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{26}$	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} - z_4\right) \mathbf{a}_3$	$-\sqrt{3} x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) c \hat{\mathbf{z}}$	(12k)	Al II

## References:

- K. Robinson, *LXXIII. The unit cell and Brillouin Zones of Ni<sub>4</sub>Mn<sub>11</sub>Al<sub>60</sub> and belated compounds*, *Philos. Mag.* **43**, 775–782 (1952), doi:[10.1080/14786440708520993](https://doi.org/10.1080/14786440708520993).
- J. N. Pratt and G. V. Raynor, *The intermetallic compounds in the alloys of aluminium and silicon with chromium, manganese, iron, cobalt and nickel*, *J. Inst. Met.* **79**, 211 (1951).

**Found in:**

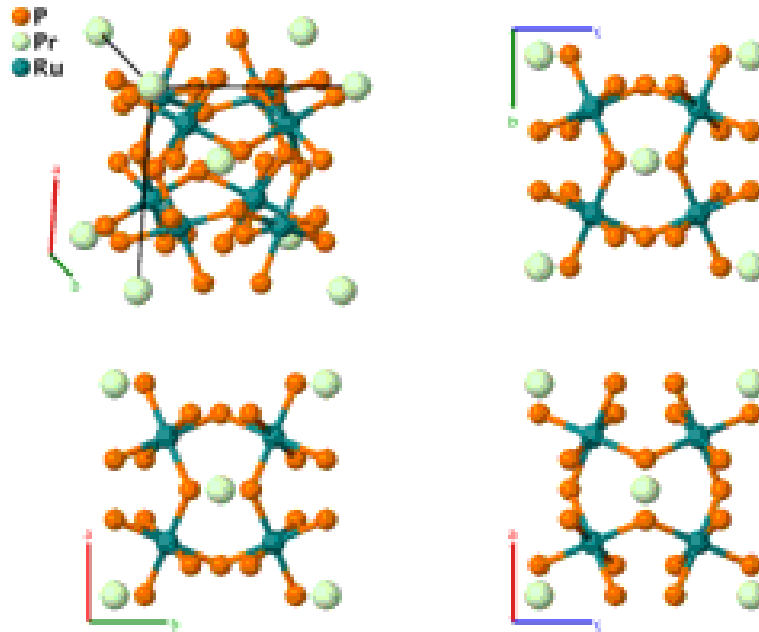
- W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.
  - E. A. Brandes and G. B. Brook, eds., *Smithells Metals Reference Book* (Butterworth Heinemann, Oxford, Auckland, Boston, Johannesburg, Melbourne, New Delhi, 1992), chap. 6, pp. 6–60, seventh edn.
- 

**Geometry files:**

- CIF: pp. [944](#)
- POSCAR: pp. [945](#)



# PrRu<sub>4</sub>P<sub>12</sub> Structure: A12BC4\_cP34\_195\_2j\_ab\_2e



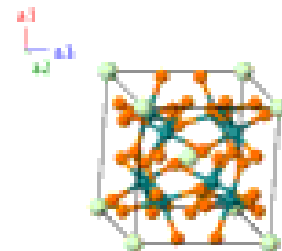
**Prototype** : PrRu<sub>4</sub>P<sub>12</sub>  
**AFLOW prototype label** : A12BC4\_cP34\_195\_2j\_ab\_2e  
**Strukturbericht designation** : None  
**Pearson symbol** : cP34  
**Space group number** : 195  
**Space group symbol** : *P*23  
**AFLOW prototype command** : aflow --proto=A12BC4\_cP34\_195\_2j\_ab\_2e  
 --params=*a*, *x*<sub>3</sub>, *x*<sub>4</sub>, *x*<sub>5</sub>, *y*<sub>5</sub>, *z*<sub>5</sub>, *x*<sub>6</sub>, *y*<sub>6</sub>, *z*<sub>6</sub>

Simple Cubic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Pr I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(1b)	Pr II
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}}$	(4e)	Ru I
$\mathbf{B}_4$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$= -x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}}$	(4e)	Ru I

$\mathbf{B}_5$	$=$	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}}$	(4e)	Ru I
$\mathbf{B}_6$	$=$	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}}$	(4e)	Ru I
$\mathbf{B}_7$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}}$	(4e)	Ru II
$\mathbf{B}_8$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}}$	(4e)	Ru II
$\mathbf{B}_9$	$=$	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}}$	(4e)	Ru II
$\mathbf{B}_{10}$	$=$	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}}$	(4e)	Ru II
$\mathbf{B}_{11}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 a \hat{\mathbf{z}}$	(12j)	PI
$\mathbf{B}_{12}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 a \hat{\mathbf{z}}$	(12j)	PI
$\mathbf{B}_{13}$	$=$	$-x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}}$	(12j)	PI
$\mathbf{B}_{14}$	$=$	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}}$	(12j)	PI
$\mathbf{B}_{15}$	$=$	$z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$z_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + y_5 a \hat{\mathbf{z}}$	(12j)	PI
$\mathbf{B}_{16}$	$=$	$z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$z_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}}$	(12j)	PI
$\mathbf{B}_{17}$	$=$	$-z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$-z_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + y_5 a \hat{\mathbf{z}}$	(12j)	PI
$\mathbf{B}_{18}$	$=$	$-z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-z_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}}$	(12j)	PI
$\mathbf{B}_{19}$	$=$	$y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} + z_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(12j)	PI
$\mathbf{B}_{20}$	$=$	$-y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} + z_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(12j)	PI
$\mathbf{B}_{21}$	$=$	$y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} - z_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(12j)	PI
$\mathbf{B}_{22}$	$=$	$-y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} - z_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(12j)	PI
$\mathbf{B}_{23}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 a \hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B}_{24}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + z_6 a \hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B}_{25}$	$=$	$-x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} - z_6 a \hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B}_{26}$	$=$	$x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} - z_6 a \hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B}_{27}$	$=$	$z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$z_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + y_6 a \hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B}_{28}$	$=$	$z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$z_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} - y_6 a \hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B}_{29}$	$=$	$-z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$-z_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + y_6 a \hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B}_{30}$	$=$	$-z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$-z_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} - y_6 a \hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B}_{31}$	$=$	$y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{x}} + z_6 a \hat{\mathbf{y}} + x_6 a \hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B}_{32}$	$=$	$-y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{x}} + z_6 a \hat{\mathbf{y}} - x_6 a \hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B}_{33}$	$=$	$y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{x}} - z_6 a \hat{\mathbf{y}} - x_6 a \hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B}_{34}$	$=$	$-y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{x}} - z_6 a \hat{\mathbf{y}} + x_6 a \hat{\mathbf{z}}$	(12j)	P II

## References:

- C. H. Lee, H. Matsuhata, H. Yamaguchi, C. Sekine, K. Kihou, and I. Shirovani, *A study of the crystal structure at low temperature in the metal–insulator transition compound PrRu<sub>4</sub>P<sub>12</sub>*, *J. Magn. Magn. Mater.* **272**, 426–427 (2004), [doi:10.1016/j.jmmm.2003.12.433](https://doi.org/10.1016/j.jmmm.2003.12.433).
- H. T. Stokes and D. M. Hatch, *FINDSYM: Program for identifying the space group symmetry of a crystal*, *J. Appl. Crystallogr.* **38**, 237–238 (2005), [doi:10.1107/S0021889804031528](https://doi.org/10.1107/S0021889804031528).
- D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy, and S. Curtarolo, *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*, *Acta Crystallogr. Sect. A* **74**,

184–203 (2018), doi:[10.1107/S2053273318003066](https://doi.org/10.1107/S2053273318003066).

- A. L. Spek, *Single-crystal structure validation with the program PLATON*, *J. Appl. Crystallogr.* **36**, 7–13 (2003), doi:[10.1107/S0021889802022112](https://doi.org/10.1107/S0021889802022112).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

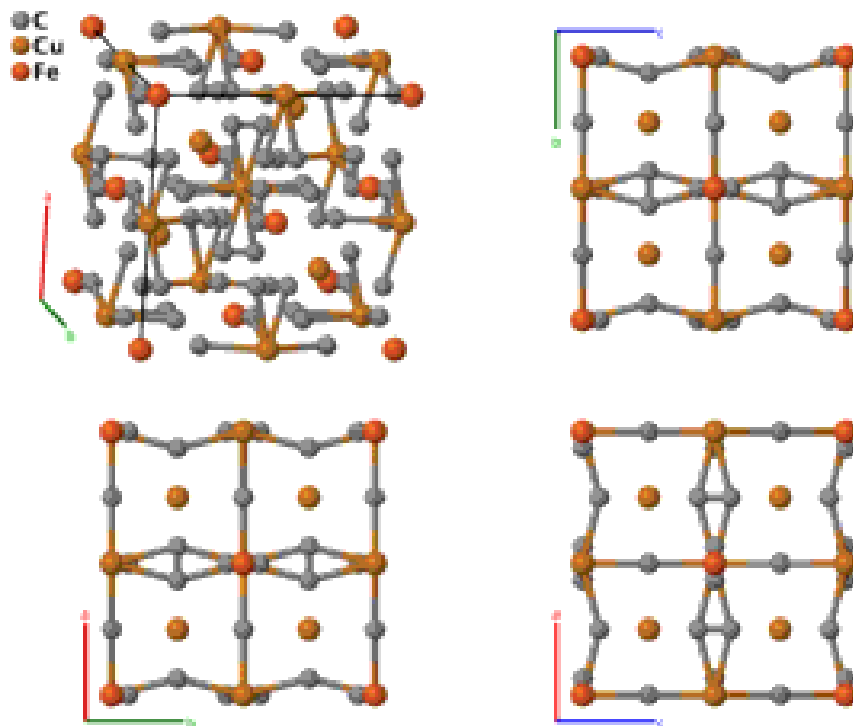
---

**Geometry files:**

- CIF: pp. [945](#)

- POSCAR: pp. [945](#)

# Cu<sub>2</sub>Fe[CN]<sub>6</sub> Structure: A12B2C\_cF60\_196\_h\_bc\_a



<b>Prototype</b>	:	Cu <sub>2</sub> Fe[CN] <sub>6</sub>
<b>AFLOW prototype label</b>	:	A12B2C_cF60_196_h_bc_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cF60
<b>Space group number</b>	:	196
<b>Space group symbol</b>	:	<i>F</i> 23
<b>AFLOW prototype command</b>	:	aflow --proto=A12B2C_cF60_196_h_bc_a --params= <i>a</i> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub>

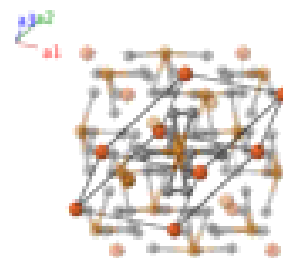
- The C sites are partially occupied with 0.5C + 0.5N.

## Face-centered Cubic primitive vectors:

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(4 <i>a</i> )	Fe

$$\begin{aligned}
\mathbf{B}_2 &= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} &(4b) & \text{Cu I} \\
\mathbf{B}_3 &= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}} &(4c) & \text{Cu II} \\
\mathbf{B}_4 &= (-x_4 + y_4 + z_4) \mathbf{a}_1 + (x_4 - y_4 + z_4) \mathbf{a}_2 + &= x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 a \hat{\mathbf{z}} &(48h) & \text{C} \\
&\quad (x_4 + y_4 - z_4) \mathbf{a}_3 \\
\mathbf{B}_5 &= (x_4 - y_4 + z_4) \mathbf{a}_1 + (-x_4 + y_4 + z_4) \mathbf{a}_2 + &= -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + z_4 a \hat{\mathbf{z}} &(48h) & \text{C} \\
&\quad (-x_4 - y_4 - z_4) \mathbf{a}_3 \\
\mathbf{B}_6 &= (x_4 + y_4 - z_4) \mathbf{a}_1 + (-x_4 - y_4 - z_4) \mathbf{a}_2 + &= -x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} - z_4 a \hat{\mathbf{z}} &(48h) & \text{C} \\
&\quad (-x_4 + y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_7 &= (-x_4 - y_4 - z_4) \mathbf{a}_1 + (x_4 + y_4 - z_4) \mathbf{a}_2 + &= x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} - z_4 a \hat{\mathbf{z}} &(48h) & \text{C} \\
&\quad (x_4 - y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_8 &= (x_4 + y_4 - z_4) \mathbf{a}_1 + (-x_4 + y_4 + z_4) \mathbf{a}_2 + &= z_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + y_4 a \hat{\mathbf{z}} &(48h) & \text{C} \\
&\quad (x_4 - y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_9 &= (-x_4 - y_4 - z_4) \mathbf{a}_1 + (x_4 - y_4 + z_4) \mathbf{a}_2 + &= z_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - y_4 a \hat{\mathbf{z}} &(48h) & \text{C} \\
&\quad (-x_4 + y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{10} &= (-x_4 + y_4 + z_4) \mathbf{a}_1 + (x_4 + y_4 - z_4) \mathbf{a}_2 + &= -z_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + y_4 a \hat{\mathbf{z}} &(48h) & \text{C} \\
&\quad (-x_4 - y_4 - z_4) \mathbf{a}_3 \\
\mathbf{B}_{11} &= (x_4 - y_4 + z_4) \mathbf{a}_1 + (-x_4 - y_4 - z_4) \mathbf{a}_2 + &= -z_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - y_4 a \hat{\mathbf{z}} &(48h) & \text{C} \\
&\quad (x_4 + y_4 - z_4) \mathbf{a}_3 \\
\mathbf{B}_{12} &= (x_4 - y_4 + z_4) \mathbf{a}_1 + (x_4 + y_4 - z_4) \mathbf{a}_2 + &= y_4 a \hat{\mathbf{x}} + z_4 a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}} &(48h) & \text{C} \\
&\quad (-x_4 + y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{13} &= (-x_4 + y_4 + z_4) \mathbf{a}_1 + (-x_4 - y_4 - z_4) \mathbf{a}_2 + &= -y_4 a \hat{\mathbf{x}} + z_4 a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}} &(48h) & \text{C} \\
&\quad (x_4 - y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{14} &= (-x_4 - y_4 - z_4) \mathbf{a}_1 + (-x_4 + y_4 + z_4) \mathbf{a}_2 + &= y_4 a \hat{\mathbf{x}} - z_4 a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}} &(48h) & \text{C} \\
&\quad (x_4 + y_4 - z_4) \mathbf{a}_3 \\
\mathbf{B}_{15} &= (x_4 + y_4 - z_4) \mathbf{a}_1 + (x_4 - y_4 + z_4) \mathbf{a}_2 + &= -y_4 a \hat{\mathbf{x}} - z_4 a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}} &(48h) & \text{C} \\
&\quad (-x_4 - y_4 - z_4) \mathbf{a}_3
\end{aligned}$$

---

#### References:

- R. Rigamonti, *Structure of Cupriferrocyanides I. Copper Ferrocyanide and Potassium Copper Ferrocyanide*, Gazz. Chim. Ital. **67**, 137–146 (1937).

#### Found in:

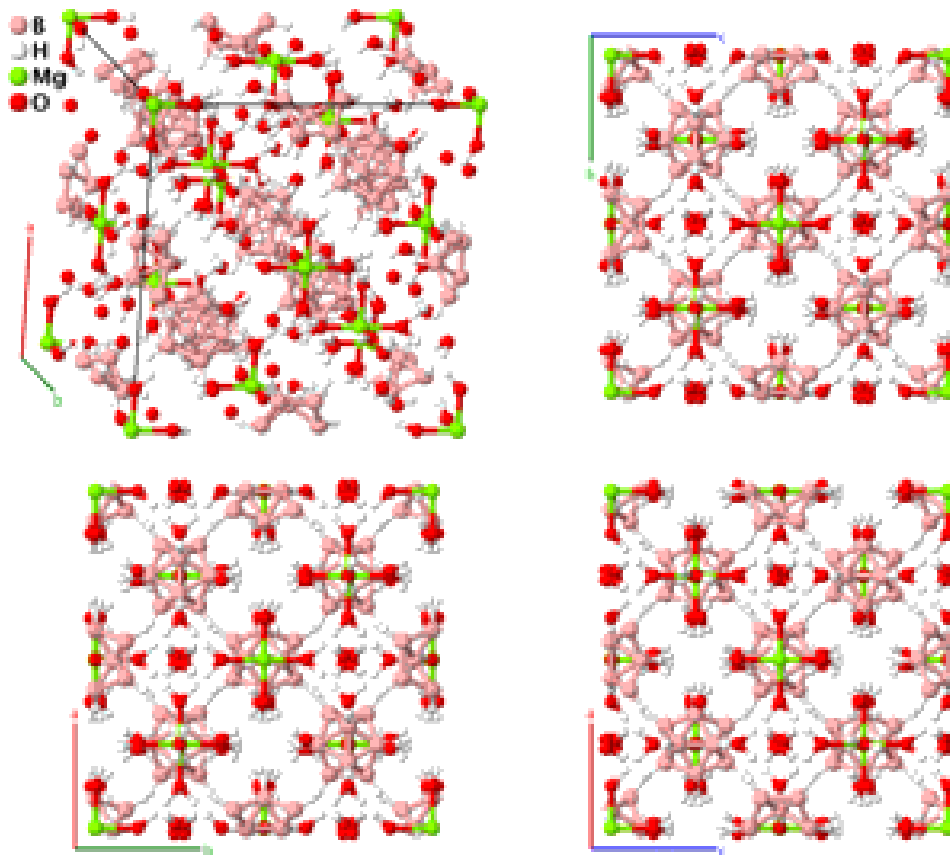
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [945](#)  
- POSCAR: pp. [946](#)

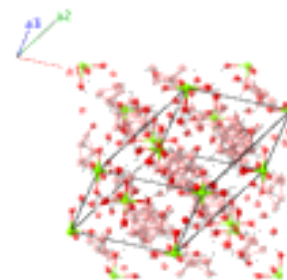
# MgB<sub>12</sub>H<sub>12</sub>[H<sub>2</sub>O]<sub>12</sub> Structure: A12B36CD12\_cF488\_196\_2h\_6h\_ac\_fgh



<b>Prototype</b>	:	MgB <sub>12</sub> H <sub>12</sub> [H <sub>2</sub> O] <sub>12</sub>
<b>AFLOW prototype label</b>	:	A12B36CD12_cF488_196_2h_6h_ac_fgh
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cF488
<b>Space group number</b>	:	196
<b>Space group symbol</b>	:	<i>F</i> 23
<b>AFLOW prototype command</b>	:	aflow --proto=A12B36CD12_cF488_196_2h_6h_ac_fgh --params= <i>a</i> , <i>x</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>x</i> <sub>6</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub> , <i>x</i> <sub>7</sub> , <i>y</i> <sub>7</sub> , <i>z</i> <sub>7</sub> , <i>x</i> <sub>8</sub> , <i>y</i> <sub>8</sub> , <i>z</i> <sub>8</sub> , <i>x</i> <sub>9</sub> , <i>y</i> <sub>9</sub> , <i>z</i> <sub>9</sub> , <i>x</i> <sub>10</sub> , <i>y</i> <sub>10</sub> , <i>z</i> <sub>10</sub> , <i>x</i> <sub>11</sub> , <i>y</i> <sub>11</sub> , <i>z</i> <sub>11</sub> , <i>x</i> <sub>12</sub> , <i>y</i> <sub>12</sub> , <i>z</i> <sub>12</sub> , <i>x</i> <sub>13</sub> , <i>y</i> <sub>13</sub> , <i>z</i> <sub>13</sub>

**Face-centered Cubic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(4a)	Mg I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4c)	Mg II
$\mathbf{B}_3$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}}$	(24f)	O I
$\mathbf{B}_4$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}}$	(24f)	O I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{y}}$	(24f)	O I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{y}}$	(24f)	O I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{z}}$	(24f)	O I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{z}}$	(24f)	O I
$\mathbf{B}_9$	$= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B}_{10}$	$= x_4 \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B}_{12}$	$= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B}_{14}$	$= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B}_{15}$	$= (-x_5 + y_5 + z_5) \mathbf{a}_1 + (x_5 - y_5 + z_5) \mathbf{a}_2 + (x_5 + y_5 - z_5) \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 a \hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B}_{16}$	$= (x_5 - y_5 + z_5) \mathbf{a}_1 + (-x_5 + y_5 + z_5) \mathbf{a}_2 + (-x_5 - y_5 - z_5) \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + z_5 a \hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B}_{17}$	$= (x_5 + y_5 - z_5) \mathbf{a}_1 + (-x_5 - y_5 - z_5) \mathbf{a}_2 + (-x_5 + y_5 + z_5) \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B}_{18}$	$= (-x_5 - y_5 - z_5) \mathbf{a}_1 + (x_5 + y_5 - z_5) \mathbf{a}_2 + (x_5 - y_5 + z_5) \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B}_{19}$	$= (x_5 + y_5 - z_5) \mathbf{a}_1 + (-x_5 + y_5 + z_5) \mathbf{a}_2 + (x_5 - y_5 + z_5) \mathbf{a}_3$	$=$	$z_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + y_5 a \hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B}_{20}$	$= (-x_5 - y_5 - z_5) \mathbf{a}_1 + (x_5 - y_5 + z_5) \mathbf{a}_2 + (-x_5 + y_5 + z_5) \mathbf{a}_3$	$=$	$z_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B}_{21}$	$= (-x_5 + y_5 + z_5) \mathbf{a}_1 + (x_5 + y_5 - z_5) \mathbf{a}_2 + (-x_5 - y_5 - z_5) \mathbf{a}_3$	$=$	$-z_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + y_5 a \hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B}_{22}$	$= (x_5 - y_5 + z_5) \mathbf{a}_1 + (-x_5 - y_5 - z_5) \mathbf{a}_2 + (x_5 + y_5 - z_5) \mathbf{a}_3$	$=$	$-z_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B}_{23}$	$= (x_5 - y_5 + z_5) \mathbf{a}_1 + (x_5 + y_5 - z_5) \mathbf{a}_2 + (-x_5 + y_5 + z_5) \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} + z_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B}_{24}$	$= (-x_5 + y_5 + z_5) \mathbf{a}_1 + (-x_5 - y_5 - z_5) \mathbf{a}_2 + (x_5 - y_5 + z_5) \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} + z_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B}_{25}$	$= (-x_5 - y_5 - z_5) \mathbf{a}_1 + (-x_5 + y_5 + z_5) \mathbf{a}_2 + (x_5 + y_5 - z_5) \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} - z_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B}_{26}$	$= (x_5 + y_5 - z_5) \mathbf{a}_1 + (x_5 - y_5 + z_5) \mathbf{a}_2 + (-x_5 - y_5 - z_5) \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} - z_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B}_{27}$	$= (-x_6 + y_6 + z_6) \mathbf{a}_1 + (x_6 - y_6 + z_6) \mathbf{a}_2 + (x_6 + y_6 - z_6) \mathbf{a}_3$	$=$	$x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 a \hat{\mathbf{z}}$	(48h)	B II
$\mathbf{B}_{28}$	$= (x_6 - y_6 + z_6) \mathbf{a}_1 + (-x_6 + y_6 + z_6) \mathbf{a}_2 + (-x_6 - y_6 - z_6) \mathbf{a}_3$	$=$	$-x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + z_6 a \hat{\mathbf{z}}$	(48h)	B II

$$\begin{aligned}
\mathbf{B}_{29} &= (x_6 + y_6 - z_6) \mathbf{a}_1 + (-x_6 - y_6 - z_6) \mathbf{a}_2 + (-x_6 + y_6 + z_6) \mathbf{a}_3 &= -x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} - z_6 a \hat{\mathbf{z}} &(48h) & \text{B II} \\
\mathbf{B}_{30} &= (-x_6 - y_6 - z_6) \mathbf{a}_1 + (x_6 + y_6 - z_6) \mathbf{a}_2 + (x_6 - y_6 + z_6) \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} - z_6 a \hat{\mathbf{z}} &(48h) & \text{B II} \\
\mathbf{B}_{31} &= (x_6 + y_6 - z_6) \mathbf{a}_1 + (-x_6 + y_6 + z_6) \mathbf{a}_2 + (x_6 - y_6 + z_6) \mathbf{a}_3 &= z_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + y_6 a \hat{\mathbf{z}} &(48h) & \text{B II} \\
\mathbf{B}_{32} &= (-x_6 - y_6 - z_6) \mathbf{a}_1 + (x_6 - y_6 + z_6) \mathbf{a}_2 + (-x_6 + y_6 + z_6) \mathbf{a}_3 &= z_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} - y_6 a \hat{\mathbf{z}} &(48h) & \text{B II} \\
\mathbf{B}_{33} &= (-x_6 + y_6 + z_6) \mathbf{a}_1 + (x_6 + y_6 - z_6) \mathbf{a}_2 + (-x_6 - y_6 - z_6) \mathbf{a}_3 &= -z_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + y_6 a \hat{\mathbf{z}} &(48h) & \text{B II} \\
\mathbf{B}_{34} &= (x_6 - y_6 + z_6) \mathbf{a}_1 + (-x_6 - y_6 - z_6) \mathbf{a}_2 + (x_6 + y_6 - z_6) \mathbf{a}_3 &= -z_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} - y_6 a \hat{\mathbf{z}} &(48h) & \text{B II} \\
\mathbf{B}_{35} &= (x_6 - y_6 + z_6) \mathbf{a}_1 + (x_6 + y_6 - z_6) \mathbf{a}_2 + (-x_6 + y_6 + z_6) \mathbf{a}_3 &= y_6 a \hat{\mathbf{x}} + z_6 a \hat{\mathbf{y}} + x_6 a \hat{\mathbf{z}} &(48h) & \text{B II} \\
\mathbf{B}_{36} &= (-x_6 + y_6 + z_6) \mathbf{a}_1 + (-x_6 - y_6 - z_6) \mathbf{a}_2 + (x_6 - y_6 + z_6) \mathbf{a}_3 &= -y_6 a \hat{\mathbf{x}} + z_6 a \hat{\mathbf{y}} - x_6 a \hat{\mathbf{z}} &(48h) & \text{B II} \\
\mathbf{B}_{37} &= (-x_6 - y_6 - z_6) \mathbf{a}_1 + (-x_6 + y_6 + z_6) \mathbf{a}_2 + (x_6 + y_6 - z_6) \mathbf{a}_3 &= y_6 a \hat{\mathbf{x}} - z_6 a \hat{\mathbf{y}} - x_6 a \hat{\mathbf{z}} &(48h) & \text{B II} \\
\mathbf{B}_{38} &= (x_6 + y_6 - z_6) \mathbf{a}_1 + (x_6 - y_6 + z_6) \mathbf{a}_2 + (-x_6 - y_6 - z_6) \mathbf{a}_3 &= -y_6 a \hat{\mathbf{x}} - z_6 a \hat{\mathbf{y}} + x_6 a \hat{\mathbf{z}} &(48h) & \text{B II} \\
\mathbf{B}_{39} &= (-x_7 + y_7 + z_7) \mathbf{a}_1 + (x_7 - y_7 + z_7) \mathbf{a}_2 + (x_7 + y_7 - z_7) \mathbf{a}_3 &= x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + z_7 a \hat{\mathbf{z}} &(48h) & \text{H I} \\
\mathbf{B}_{40} &= (x_7 - y_7 + z_7) \mathbf{a}_1 + (-x_7 + y_7 + z_7) \mathbf{a}_2 + (-x_7 - y_7 - z_7) \mathbf{a}_3 &= -x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + z_7 a \hat{\mathbf{z}} &(48h) & \text{H I} \\
\mathbf{B}_{41} &= (x_7 + y_7 - z_7) \mathbf{a}_1 + (-x_7 - y_7 - z_7) \mathbf{a}_2 + (-x_7 + y_7 + z_7) \mathbf{a}_3 &= -x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} - z_7 a \hat{\mathbf{z}} &(48h) & \text{H I} \\
\mathbf{B}_{42} &= (-x_7 - y_7 - z_7) \mathbf{a}_1 + (x_7 + y_7 - z_7) \mathbf{a}_2 + (x_7 - y_7 + z_7) \mathbf{a}_3 &= x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} - z_7 a \hat{\mathbf{z}} &(48h) & \text{H I} \\
\mathbf{B}_{43} &= (x_7 + y_7 - z_7) \mathbf{a}_1 + (-x_7 + y_7 + z_7) \mathbf{a}_2 + (x_7 - y_7 + z_7) \mathbf{a}_3 &= z_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + y_7 a \hat{\mathbf{z}} &(48h) & \text{H I} \\
\mathbf{B}_{44} &= (-x_7 - y_7 - z_7) \mathbf{a}_1 + (x_7 - y_7 + z_7) \mathbf{a}_2 + (-x_7 + y_7 + z_7) \mathbf{a}_3 &= z_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} - y_7 a \hat{\mathbf{z}} &(48h) & \text{H I} \\
\mathbf{B}_{45} &= (-x_7 + y_7 + z_7) \mathbf{a}_1 + (x_7 + y_7 - z_7) \mathbf{a}_2 + (-x_7 - y_7 - z_7) \mathbf{a}_3 &= -z_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + y_7 a \hat{\mathbf{z}} &(48h) & \text{H I} \\
\mathbf{B}_{46} &= (x_7 - y_7 + z_7) \mathbf{a}_1 + (-x_7 - y_7 - z_7) \mathbf{a}_2 + (x_7 + y_7 - z_7) \mathbf{a}_3 &= -z_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} - y_7 a \hat{\mathbf{z}} &(48h) & \text{H I} \\
\mathbf{B}_{47} &= (x_7 - y_7 + z_7) \mathbf{a}_1 + (x_7 + y_7 - z_7) \mathbf{a}_2 + (-x_7 + y_7 + z_7) \mathbf{a}_3 &= y_7 a \hat{\mathbf{x}} + z_7 a \hat{\mathbf{y}} + x_7 a \hat{\mathbf{z}} &(48h) & \text{H I} \\
\mathbf{B}_{48} &= (-x_7 + y_7 + z_7) \mathbf{a}_1 + (-x_7 - y_7 - z_7) \mathbf{a}_2 + (x_7 - y_7 + z_7) \mathbf{a}_3 &= -y_7 a \hat{\mathbf{x}} + z_7 a \hat{\mathbf{y}} - x_7 a \hat{\mathbf{z}} &(48h) & \text{H I} \\
\mathbf{B}_{49} &= (-x_7 - y_7 - z_7) \mathbf{a}_1 + (-x_7 + y_7 + z_7) \mathbf{a}_2 + (x_7 + y_7 - z_7) \mathbf{a}_3 &= y_7 a \hat{\mathbf{x}} - z_7 a \hat{\mathbf{y}} - x_7 a \hat{\mathbf{z}} &(48h) & \text{H I} \\
\mathbf{B}_{50} &= (x_7 + y_7 - z_7) \mathbf{a}_1 + (x_7 - y_7 + z_7) \mathbf{a}_2 + (-x_7 - y_7 - z_7) \mathbf{a}_3 &= -y_7 a \hat{\mathbf{x}} - z_7 a \hat{\mathbf{y}} + x_7 a \hat{\mathbf{z}} &(48h) & \text{H I} \\
\mathbf{B}_{51} &= (-x_8 + y_8 + z_8) \mathbf{a}_1 + (x_8 - y_8 + z_8) \mathbf{a}_2 + (x_8 + y_8 - z_8) \mathbf{a}_3 &= x_8 a \hat{\mathbf{x}} + y_8 a \hat{\mathbf{y}} + z_8 a \hat{\mathbf{z}} &(48h) & \text{H II} \\
\mathbf{B}_{52} &= (x_8 - y_8 + z_8) \mathbf{a}_1 + (-x_8 + y_8 + z_8) \mathbf{a}_2 + (-x_8 - y_8 - z_8) \mathbf{a}_3 &= -x_8 a \hat{\mathbf{x}} - y_8 a \hat{\mathbf{y}} + z_8 a \hat{\mathbf{z}} &(48h) & \text{H II}
\end{aligned}$$



$$\begin{aligned}
\mathbf{B}_{53} &= (x_8 + y_8 - z_8) \mathbf{a}_1 + (-x_8 - y_8 - z_8) \mathbf{a}_2 + (-x_8 + y_8 + z_8) \mathbf{a}_3 &= -x_8 a \hat{\mathbf{x}} + y_8 a \hat{\mathbf{y}} - z_8 a \hat{\mathbf{z}} &(48h) & \text{H II} \\
\mathbf{B}_{54} &= (-x_8 - y_8 - z_8) \mathbf{a}_1 + (x_8 + y_8 - z_8) \mathbf{a}_2 + (x_8 - y_8 + z_8) \mathbf{a}_3 &= x_8 a \hat{\mathbf{x}} - y_8 a \hat{\mathbf{y}} - z_8 a \hat{\mathbf{z}} &(48h) & \text{H II} \\
\mathbf{B}_{55} &= (x_8 + y_8 - z_8) \mathbf{a}_1 + (-x_8 + y_8 + z_8) \mathbf{a}_2 + (x_8 - y_8 + z_8) \mathbf{a}_3 &= z_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} + y_8 a \hat{\mathbf{z}} &(48h) & \text{H II} \\
\mathbf{B}_{56} &= (-x_8 - y_8 - z_8) \mathbf{a}_1 + (x_8 - y_8 + z_8) \mathbf{a}_2 + (-x_8 + y_8 + z_8) \mathbf{a}_3 &= z_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} - y_8 a \hat{\mathbf{z}} &(48h) & \text{H II} \\
\mathbf{B}_{57} &= (-x_8 + y_8 + z_8) \mathbf{a}_1 + (x_8 + y_8 - z_8) \mathbf{a}_2 + (-x_8 - y_8 - z_8) \mathbf{a}_3 &= -z_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} + y_8 a \hat{\mathbf{z}} &(48h) & \text{H II} \\
\mathbf{B}_{58} &= (x_8 - y_8 + z_8) \mathbf{a}_1 + (-x_8 - y_8 - z_8) \mathbf{a}_2 + (x_8 + y_8 - z_8) \mathbf{a}_3 &= -z_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} - y_8 a \hat{\mathbf{z}} &(48h) & \text{H II} \\
\mathbf{B}_{59} &= (x_8 - y_8 + z_8) \mathbf{a}_1 + (x_8 + y_8 - z_8) \mathbf{a}_2 + (-x_8 + y_8 + z_8) \mathbf{a}_3 &= y_8 a \hat{\mathbf{x}} + z_8 a \hat{\mathbf{y}} + x_8 a \hat{\mathbf{z}} &(48h) & \text{H II} \\
\mathbf{B}_{60} &= (-x_8 + y_8 + z_8) \mathbf{a}_1 + (-x_8 - y_8 - z_8) \mathbf{a}_2 + (x_8 - y_8 + z_8) \mathbf{a}_3 &= -y_8 a \hat{\mathbf{x}} + z_8 a \hat{\mathbf{y}} - x_8 a \hat{\mathbf{z}} &(48h) & \text{H II} \\
\mathbf{B}_{61} &= (-x_8 - y_8 - z_8) \mathbf{a}_1 + (-x_8 + y_8 + z_8) \mathbf{a}_2 + (x_8 + y_8 - z_8) \mathbf{a}_3 &= y_8 a \hat{\mathbf{x}} - z_8 a \hat{\mathbf{y}} - x_8 a \hat{\mathbf{z}} &(48h) & \text{H II} \\
\mathbf{B}_{62} &= (x_8 + y_8 - z_8) \mathbf{a}_1 + (x_8 - y_8 + z_8) \mathbf{a}_2 + (-x_8 - y_8 - z_8) \mathbf{a}_3 &= -y_8 a \hat{\mathbf{x}} - z_8 a \hat{\mathbf{y}} + x_8 a \hat{\mathbf{z}} &(48h) & \text{H II} \\
\mathbf{B}_{63} &= (-x_9 + y_9 + z_9) \mathbf{a}_1 + (x_9 - y_9 + z_9) \mathbf{a}_2 + (x_9 + y_9 - z_9) \mathbf{a}_3 &= x_9 a \hat{\mathbf{x}} + y_9 a \hat{\mathbf{y}} + z_9 a \hat{\mathbf{z}} &(48h) & \text{H III} \\
\mathbf{B}_{64} &= (x_9 - y_9 + z_9) \mathbf{a}_1 + (-x_9 + y_9 + z_9) \mathbf{a}_2 + (-x_9 - y_9 - z_9) \mathbf{a}_3 &= -x_9 a \hat{\mathbf{x}} - y_9 a \hat{\mathbf{y}} + z_9 a \hat{\mathbf{z}} &(48h) & \text{H III} \\
\mathbf{B}_{65} &= (x_9 + y_9 - z_9) \mathbf{a}_1 + (-x_9 - y_9 - z_9) \mathbf{a}_2 + (-x_9 + y_9 + z_9) \mathbf{a}_3 &= -x_9 a \hat{\mathbf{x}} + y_9 a \hat{\mathbf{y}} - z_9 a \hat{\mathbf{z}} &(48h) & \text{H III} \\
\mathbf{B}_{66} &= (-x_9 - y_9 - z_9) \mathbf{a}_1 + (x_9 + y_9 - z_9) \mathbf{a}_2 + (x_9 - y_9 + z_9) \mathbf{a}_3 &= x_9 a \hat{\mathbf{x}} - y_9 a \hat{\mathbf{y}} - z_9 a \hat{\mathbf{z}} &(48h) & \text{H III} \\
\mathbf{B}_{67} &= (x_9 + y_9 - z_9) \mathbf{a}_1 + (-x_9 + y_9 + z_9) \mathbf{a}_2 + (x_9 - y_9 + z_9) \mathbf{a}_3 &= z_9 a \hat{\mathbf{x}} + x_9 a \hat{\mathbf{y}} + y_9 a \hat{\mathbf{z}} &(48h) & \text{H III} \\
\mathbf{B}_{68} &= (-x_9 - y_9 - z_9) \mathbf{a}_1 + (x_9 - y_9 + z_9) \mathbf{a}_2 + (-x_9 + y_9 + z_9) \mathbf{a}_3 &= z_9 a \hat{\mathbf{x}} - x_9 a \hat{\mathbf{y}} - y_9 a \hat{\mathbf{z}} &(48h) & \text{H III} \\
\mathbf{B}_{69} &= (-x_9 + y_9 + z_9) \mathbf{a}_1 + (x_9 + y_9 - z_9) \mathbf{a}_2 + (-x_9 - y_9 - z_9) \mathbf{a}_3 &= -z_9 a \hat{\mathbf{x}} - x_9 a \hat{\mathbf{y}} + y_9 a \hat{\mathbf{z}} &(48h) & \text{H III} \\
\mathbf{B}_{70} &= (x_9 - y_9 + z_9) \mathbf{a}_1 + (-x_9 - y_9 - z_9) \mathbf{a}_2 + (x_9 + y_9 - z_9) \mathbf{a}_3 &= -z_9 a \hat{\mathbf{x}} + x_9 a \hat{\mathbf{y}} - y_9 a \hat{\mathbf{z}} &(48h) & \text{H III} \\
\mathbf{B}_{71} &= (x_9 - y_9 + z_9) \mathbf{a}_1 + (x_9 + y_9 - z_9) \mathbf{a}_2 + (-x_9 + y_9 + z_9) \mathbf{a}_3 &= y_9 a \hat{\mathbf{x}} + z_9 a \hat{\mathbf{y}} + x_9 a \hat{\mathbf{z}} &(48h) & \text{H III} \\
\mathbf{B}_{72} &= (-x_9 + y_9 + z_9) \mathbf{a}_1 + (-x_9 - y_9 - z_9) \mathbf{a}_2 + (x_9 - y_9 + z_9) \mathbf{a}_3 &= -y_9 a \hat{\mathbf{x}} + z_9 a \hat{\mathbf{y}} - x_9 a \hat{\mathbf{z}} &(48h) & \text{H III} \\
\mathbf{B}_{73} &= (-x_9 - y_9 - z_9) \mathbf{a}_1 + (-x_9 + y_9 + z_9) \mathbf{a}_2 + (x_9 + y_9 - z_9) \mathbf{a}_3 &= y_9 a \hat{\mathbf{x}} - z_9 a \hat{\mathbf{y}} - x_9 a \hat{\mathbf{z}} &(48h) & \text{H III} \\
\mathbf{B}_{74} &= (x_9 + y_9 - z_9) \mathbf{a}_1 + (x_9 - y_9 + z_9) \mathbf{a}_2 + (-x_9 - y_9 - z_9) \mathbf{a}_3 &= -y_9 a \hat{\mathbf{x}} - z_9 a \hat{\mathbf{y}} + x_9 a \hat{\mathbf{z}} &(48h) & \text{H III} \\
\mathbf{B}_{75} &= (-x_{10} + y_{10} + z_{10}) \mathbf{a}_1 + (x_{10} - y_{10} + z_{10}) \mathbf{a}_2 + (x_{10} + y_{10} - z_{10}) \mathbf{a}_3 &= x_{10} a \hat{\mathbf{x}} + y_{10} a \hat{\mathbf{y}} + z_{10} a \hat{\mathbf{z}} &(48h) & \text{H IV} \\
\mathbf{B}_{76} &= (x_{10} - y_{10} + z_{10}) \mathbf{a}_1 + (-x_{10} + y_{10} + z_{10}) \mathbf{a}_2 + (-x_{10} - y_{10} - z_{10}) \mathbf{a}_3 &= -x_{10} a \hat{\mathbf{x}} - y_{10} a \hat{\mathbf{y}} + z_{10} a \hat{\mathbf{z}} &(48h) & \text{H IV}
\end{aligned}$$





---

**References:**

- I. Tiritiris and T. Schleid, *Synthesis, Crystal Structure, and Thermal Decomposition of  $Mg(H_2O)_6[B_{12}H_{12}] \times 6H_2O$* , ChemInform **35** (2004), doi:[10.1002/chin.200425008](https://doi.org/10.1002/chin.200425008).

**Found in:**

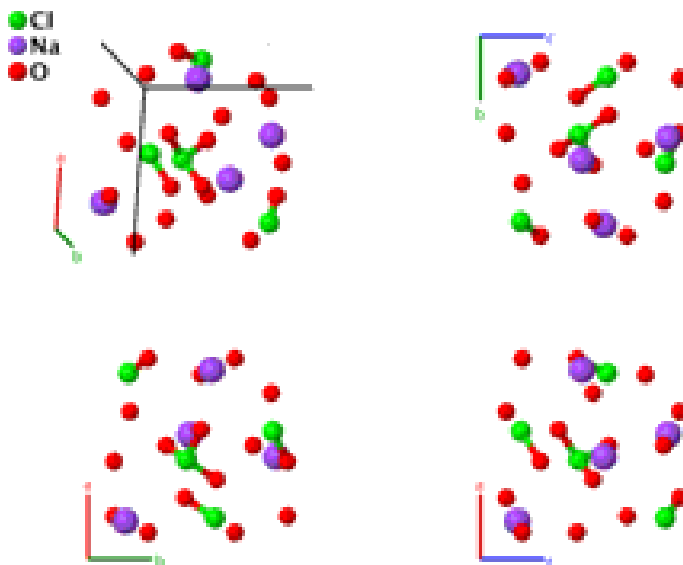
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

**Geometry files:**

- CIF: pp. [946](#)  
- POSCAR: pp. [947](#)

# Sodium Chlorate ( $\text{NaClO}_3$ , $G3$ ) Structure: ABC3\_cP20\_198\_a\_a\_b



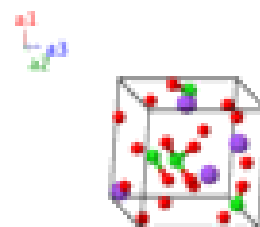
**Prototype** :  $\text{NaClO}_3$   
**AFLOW prototype label** : ABC3\_cP20\_198\_a\_a\_b  
**Strukturbericht designation** :  $G3$   
**Pearson symbol** : cP20  
**Space group number** : 198  
**Space group symbol** :  $P2_13$   
**AFLOW prototype command** : aflow --proto=ABC3\_cP20\_198\_a\_a\_b  
 --params= $a, x_1, x_2, x_3, y_3, z_3$

## Other compounds with this structure:

- $\text{NaBrO}_3$

## Simple Cubic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= a \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + x_1 a \hat{\mathbf{z}}$	(4a)	Cl
$\mathbf{B}_2$	$= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{1}{2} + x_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{z}}$	(4a)	Cl

$$\begin{aligned}
\mathbf{B}_3 &= -x_1 \mathbf{a}_1 + \left(\frac{1}{2} + x_1\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_1\right) \mathbf{a}_3 = -x_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{z}} & (4a) & \text{Cl} \\
\mathbf{B}_4 &= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_1\right) \mathbf{a}_2 - x_1 \mathbf{a}_3 = \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{y}} - x_1 a \hat{\mathbf{z}} & (4a) & \text{Cl} \\
\mathbf{B}_5 &= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3 = x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}} & (4a) & \text{Na} \\
\mathbf{B}_6 &= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{z}} & (4a) & \text{Na} \\
\mathbf{B}_7 &= -x_2 \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{z}} & (4a) & \text{Na} \\
\mathbf{B}_8 &= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 - x_2 \mathbf{a}_3 = \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}} & (4a) & \text{Na} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 a \hat{\mathbf{z}} & (12b) & \text{O} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_3\right) a \hat{\mathbf{z}} & (12b) & \text{O} \\
\mathbf{B}_{11} &= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_3 = -x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) a \hat{\mathbf{z}} & (12b) & \text{O} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 = \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} - z_3 a \hat{\mathbf{z}} & (12b) & \text{O} \\
\mathbf{B}_{13} &= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3 = z_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + y_3 a \hat{\mathbf{z}} & (12b) & \text{O} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} + z_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 - y_3 \mathbf{a}_3 = \left(\frac{1}{2} + z_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} - y_3 a \hat{\mathbf{z}} & (12b) & \text{O} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} - z_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} + y_3\right) \mathbf{a}_3 = \left(\frac{1}{2} - z_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{z}} & (12b) & \text{O} \\
\mathbf{B}_{16} &= -z_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_3\right) \mathbf{a}_3 = -z_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{z}} & (12b) & \text{O} \\
\mathbf{B}_{17} &= y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3 = y_3 a \hat{\mathbf{x}} + z_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}} & (12b) & \text{O} \\
\mathbf{B}_{18} &= -y_3 \mathbf{a}_1 + \left(\frac{1}{2} + z_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_3 = -y_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{z}} & (12b) & \text{O} \\
\mathbf{B}_{19} &= \left(\frac{1}{2} + y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - z_3\right) \mathbf{a}_2 - x_3 \mathbf{a}_3 = \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_3\right) a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}} & (12b) & \text{O} \\
\mathbf{B}_{20} &= \left(\frac{1}{2} - y_3\right) \mathbf{a}_1 - z_3 \mathbf{a}_2 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_3 = \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{x}} - z_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{z}} & (12b) & \text{O}
\end{aligned}$$

---

### References:

- G. N. Ramachandran and K. S. Chandrasekaran, *The absolute configuration of sodium chlorate*, *Acta Cryst.* **10**, 671–675 (1957), doi:[10.1107/S0365110X57002327](https://doi.org/10.1107/S0365110X57002327).

### Found in:

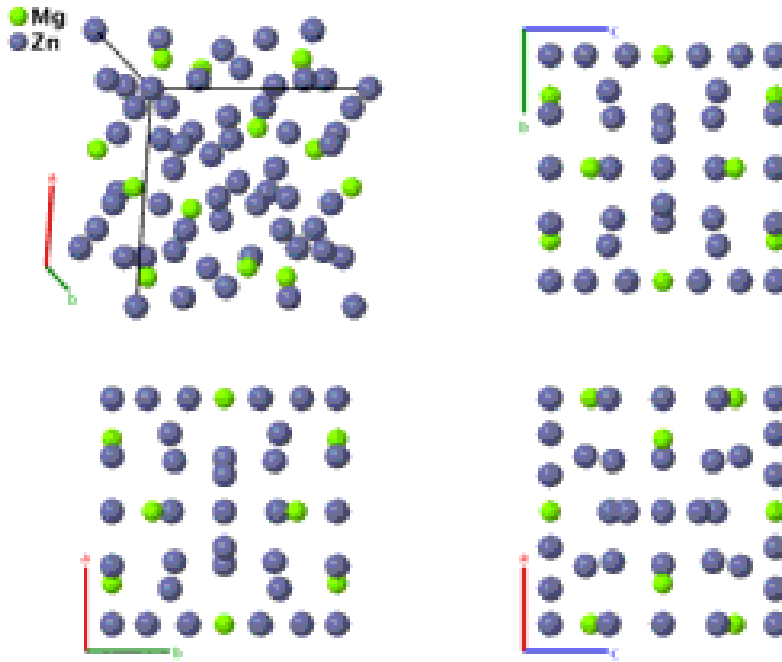
- A. A. Kaminskii, S. N. Bagayev, J. Hulliger, H. Eichler, J. Findeisen, and R. Macdonald, *Acentric cubic NaClO<sub>3</sub>—a new crystal for Raman lasers*, *Appl. Phys. B* **67**, 157–162 (1998), doi:[10.1007/s003400050487](https://doi.org/10.1007/s003400050487).

---

### Geometry files:

- CIF: pp. [947](#)
- POSCAR: pp. [948](#)

# Mg<sub>2</sub>Zn<sub>11</sub> Structure: A2B11\_cP39\_200\_f\_aghij



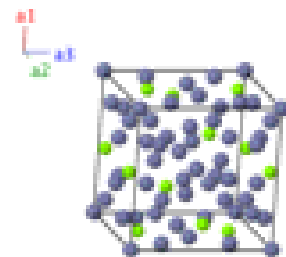
<b>Prototype</b>	:	Mg <sub>2</sub> Zn <sub>11</sub>
<b>AFLOW prototype label</b>	:	A2B11_cP39_200_f_aghij
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cP39
<b>Space group number</b>	:	200
<b>Space group symbol</b>	:	$Pm\bar{3}$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B11_cP39_200_f_aghij --params= $a, x_2, x_3, x_4, x_5, y_6, z_6$

**Simple Cubic primitive vectors:**

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Zn I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$= x_2 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Mg
$\mathbf{B}_3$	$= -x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$= -x_2 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Mg
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + x_2 \mathbf{a}_2$	$= \frac{1}{2} a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}}$	(6f)	Mg

$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}}$	(6f)	Mg
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}}$	(6f)	Mg
$\mathbf{B}_7$	$=$	$\frac{1}{2} \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}}$	(6f)	Mg
$\mathbf{B}_8$	$=$	$x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$x_3 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6g)	Zn II
$\mathbf{B}_9$	$=$	$-x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$-x_3 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6g)	Zn II
$\mathbf{B}_{10}$	$=$	$x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6g)	Zn II
$\mathbf{B}_{11}$	$=$	$-x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6g)	Zn II
$\mathbf{B}_{12}$	$=$	$\frac{1}{2} \mathbf{a}_1 + x_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{z}}$	(6g)	Zn II
$\mathbf{B}_{13}$	$=$	$\frac{1}{2} \mathbf{a}_1 + -x_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + -x_3 a \hat{\mathbf{z}}$	(6g)	Zn II
$\mathbf{B}_{14}$	$=$	$x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6h)	Zn III
$\mathbf{B}_{15}$	$=$	$-x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6h)	Zn III
$\mathbf{B}_{16}$	$=$	$\frac{1}{2} \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6h)	Zn III
$\mathbf{B}_{17}$	$=$	$\frac{1}{2} \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6h)	Zn III
$\mathbf{B}_{18}$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}}$	(6h)	Zn III
$\mathbf{B}_{19}$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}}$	(6h)	Zn III
$\mathbf{B}_{20}$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{21}$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{22}$	$=$	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{23}$	$=$	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{24}$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{25}$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{26}$	$=$	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{27}$	$=$	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{28}$	$=$	$y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{y}} + z_6 a \hat{\mathbf{z}}$	(12j)	Zn V
$\mathbf{B}_{29}$	$=$	$-y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{y}} + z_6 a \hat{\mathbf{z}}$	(12j)	Zn V
$\mathbf{B}_{30}$	$=$	$y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{y}} - z_6 a \hat{\mathbf{z}}$	(12j)	Zn V
$\mathbf{B}_{31}$	$=$	$-y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{y}} - z_6 a \hat{\mathbf{z}}$	(12j)	Zn V
$\mathbf{B}_{32}$	$=$	$z_6 \mathbf{a}_1 + y_6 \mathbf{a}_3$	$=$	$z_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{z}}$	(12j)	Zn V
$\mathbf{B}_{33}$	$=$	$z_6 \mathbf{a}_1 + -y_6 \mathbf{a}_3$	$=$	$z_6 a \hat{\mathbf{x}} + -y_6 a \hat{\mathbf{z}}$	(12j)	Zn V
$\mathbf{B}_{34}$	$=$	$-z_6 \mathbf{a}_1 + y_6 \mathbf{a}_3$	$=$	$-z_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{z}}$	(12j)	Zn V
$\mathbf{B}_{35}$	$=$	$-z_6 \mathbf{a}_1 + -y_6 \mathbf{a}_3$	$=$	$-z_6 a \hat{\mathbf{x}} + -y_6 a \hat{\mathbf{z}}$	(12j)	Zn V
$\mathbf{B}_{36}$	$=$	$y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2$	$=$	$y_6 a \hat{\mathbf{x}} + z_6 a \hat{\mathbf{y}}$	(12j)	Zn V
$\mathbf{B}_{37}$	$=$	$-y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2$	$=$	$-y_6 a \hat{\mathbf{x}} + z_6 a \hat{\mathbf{y}}$	(12j)	Zn V
$\mathbf{B}_{38}$	$=$	$y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2$	$=$	$y_6 a \hat{\mathbf{x}} - z_6 a \hat{\mathbf{y}}$	(12j)	Zn V
$\mathbf{B}_{39}$	$=$	$-y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2$	$=$	$-y_6 a \hat{\mathbf{x}} - z_6 a \hat{\mathbf{y}}$	(12j)	Zn V

---

## References:



- S. Samson, *Die Kristallstruktur von  $Mg_2Zn_{11}$  Isomorphie zwischen  $Mg_2Zn_{11}$  und  $Mg_2Cu_6Al_5$* , Acta Chem. Scand. **3**, 835–843 (1949), doi:[10.3891/acta.chem.scand.03-0835](https://doi.org/10.3891/acta.chem.scand.03-0835).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

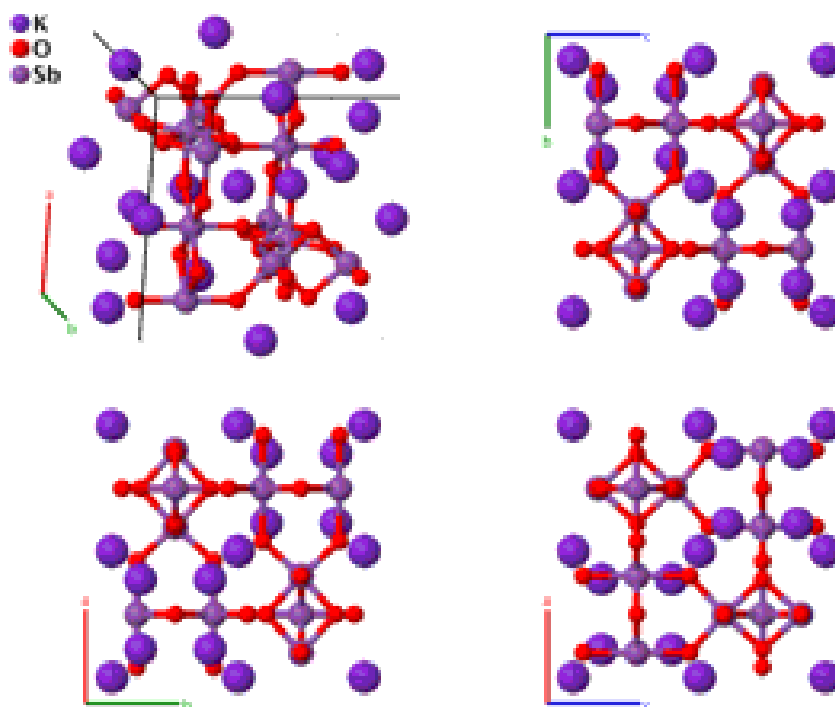
**Geometry files:**

- CIF: pp. [948](#)

- POSCAR: pp. [948](#)

# KSbO<sub>3</sub> (High-temperature) Structure:

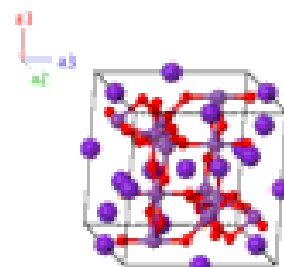
AB3C\_cP60\_201\_ce\_fh\_g



**Prototype** : KSbO<sub>3</sub>  
**AFLOW prototype label** : AB3C\_cP60\_201\_ce\_fh\_g  
**Strukturbericht designation** : None  
**Pearson symbol** : cP60  
**Space group number** : 201  
**Space group symbol** :  $Pn\bar{3}$   
**AFLOW prototype command** : aflow --proto=AB3C\_cP60\_201\_ce\_fh\_g  
 --params= $a, x_2, x_3, x_4, x_5, y_5, z_5$

## Simple Cubic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= a \hat{\mathbf{z}}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4c)	K I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{z}}$	(4c)	K I



$$\begin{aligned}
\mathbf{B}_{39} &= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{40} &= x_5 \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3 = x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{41} &= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3 = z_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + y_5 a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{42} &= z_5 \mathbf{a}_1 + \left(\frac{1}{2} - x_5\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_3 = z_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_5\right) a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{43} &= \left(\frac{1}{2} - z_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_5\right) \mathbf{a}_2 + y_5 \mathbf{a}_3 = \left(\frac{1}{2} - z_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{y}} + y_5 a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{44} &= \left(\frac{1}{2} - z_5\right) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_3 = \left(\frac{1}{2} - z_5\right) a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_5\right) a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{45} &= y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3 = y_5 a \hat{\mathbf{x}} + z_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{46} &= \left(\frac{1}{2} - y_5\right) \mathbf{a}_1 + z_5 \mathbf{a}_2 + \left(\frac{1}{2} - x_5\right) \mathbf{a}_3 = \left(\frac{1}{2} - y_5\right) a \hat{\mathbf{x}} + z_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{47} &= y_5 \mathbf{a}_1 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_5\right) \mathbf{a}_3 = y_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{48} &= \left(\frac{1}{2} - y_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_2 + x_5 \mathbf{a}_3 = \left(\frac{1}{2} - y_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_5\right) a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{49} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = -x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{50} &= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 - z_5 \mathbf{a}_3 = \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{51} &= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{52} &= -x_5 \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3 = -x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{53} &= -z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3 = -z_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{54} &= -z_5 \mathbf{a}_1 + \left(\frac{1}{2} + x_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_3 = -z_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_5\right) a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{55} &= \left(\frac{1}{2} + z_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_5\right) \mathbf{a}_2 - y_5 \mathbf{a}_3 = \left(\frac{1}{2} + z_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{56} &= \left(\frac{1}{2} + z_5\right) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_3 = \left(\frac{1}{2} + z_5\right) a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_5\right) a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{57} &= -y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3 = -y_5 a \hat{\mathbf{x}} - z_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{58} &= \left(\frac{1}{2} + y_5\right) \mathbf{a}_1 - z_5 \mathbf{a}_2 + \left(\frac{1}{2} + x_5\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_5\right) a \hat{\mathbf{x}} - z_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{59} &= -y_5 \mathbf{a}_1 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_5\right) \mathbf{a}_3 = -y_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{z}} & (24h) & \text{O II} \\
\mathbf{B}_{60} &= \left(\frac{1}{2} + y_5\right) \mathbf{a}_1 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_2 - x_5 \mathbf{a}_3 = \left(\frac{1}{2} + y_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_5\right) a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}} & (24h) & \text{O II}
\end{aligned}$$

---

### References:

- P. Spiegelberg, *X-ray studies on potassium antimonates*, Ark. Kem. Mineral. Geol. **14A**, 1–12 (1940).

### Found in:

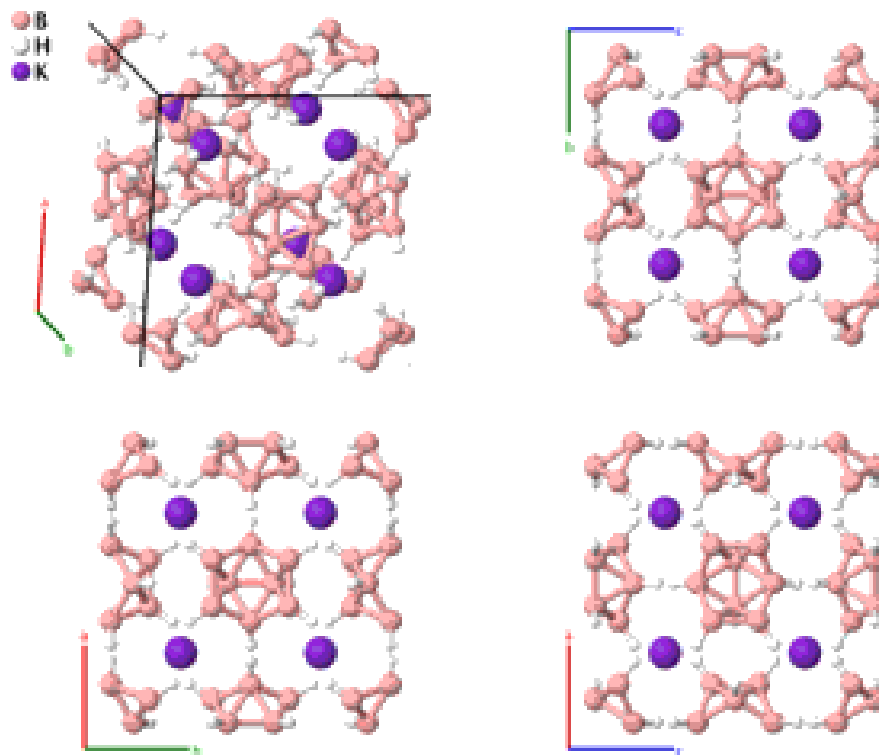
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

### Geometry files:

- CIF: pp. [949](#)
- POSCAR: pp. [949](#)

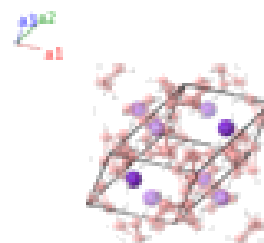
# KB<sub>6</sub>H<sub>6</sub> Structure: A6B6C\_cF104\_202\_h\_h\_c



**Prototype** : KB<sub>6</sub>H<sub>6</sub>  
**AFLOW prototype label** : A6B6C\_cF104\_202\_h\_h\_c  
**Strukturbericht designation** : None  
**Pearson symbol** : cF104  
**Space group number** : 202  
**Space group symbol** :  $Fm\bar{3}$   
**AFLOW prototype command** : `aflow --proto=A6B6C_cF104_202_h_h_c --params=a, y2, z2, y3, z3`

Face-centered Cubic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{y} + \frac{1}{2} a \hat{z} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{x} + \frac{1}{2} a \hat{z} \\
 \mathbf{a}_3 &= \frac{1}{2} a \hat{x} + \frac{1}{2} a \hat{y}
 \end{aligned}$$



Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$ =	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{4} a \hat{x} + \frac{1}{4} a \hat{y} + \frac{1}{4} a \hat{z}$	(8c)	K
$\mathbf{B}_2$ =	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{3}{4} a \hat{x} + \frac{3}{4} a \hat{y} + \frac{3}{4} a \hat{z}$	(8c)	K

$\mathbf{B}_3$	$=$	$(y_2 + z_2) \mathbf{a}_1 + (-y_2 + z_2) \mathbf{a}_2 + (y_2 - z_2) \mathbf{a}_3$	$=$	$y_2 a \hat{\mathbf{y}} + z_2 a \hat{\mathbf{z}}$	$(48h)$	B
$\mathbf{B}_4$	$=$	$(-y_2 + z_2) \mathbf{a}_1 + (y_2 + z_2) \mathbf{a}_2 + (-y_2 - z_2) \mathbf{a}_3$	$=$	$-y_2 a \hat{\mathbf{y}} + z_2 a \hat{\mathbf{z}}$	$(48h)$	B
$\mathbf{B}_5$	$=$	$(y_2 - z_2) \mathbf{a}_1 + (-y_2 - z_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3$	$=$	$y_2 a \hat{\mathbf{y}} - z_2 a \hat{\mathbf{z}}$	$(48h)$	B
$\mathbf{B}_6$	$=$	$(-y_2 - z_2) \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (-y_2 + z_2) \mathbf{a}_3$	$=$	$-y_2 a \hat{\mathbf{y}} - z_2 a \hat{\mathbf{z}}$	$(48h)$	B
$\mathbf{B}_7$	$=$	$(y_2 - z_2) \mathbf{a}_1 + (y_2 + z_2) \mathbf{a}_2 + (-y_2 + z_2) \mathbf{a}_3$	$=$	$z_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{z}}$	$(48h)$	B
$\mathbf{B}_8$	$=$	$(-y_2 - z_2) \mathbf{a}_1 + (-y_2 + z_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3$	$=$	$z_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{z}}$	$(48h)$	B
$\mathbf{B}_9$	$=$	$(y_2 + z_2) \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (-y_2 - z_2) \mathbf{a}_3$	$=$	$-z_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{z}}$	$(48h)$	B
$\mathbf{B}_{10}$	$=$	$(-y_2 + z_2) \mathbf{a}_1 + (-y_2 - z_2) \mathbf{a}_2 + (y_2 - z_2) \mathbf{a}_3$	$=$	$-z_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{z}}$	$(48h)$	B
$\mathbf{B}_{11}$	$=$	$(-y_2 + z_2) \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3$	$=$	$y_2 a \hat{\mathbf{x}} + z_2 a \hat{\mathbf{y}}$	$(48h)$	B
$\mathbf{B}_{12}$	$=$	$(y_2 + z_2) \mathbf{a}_1 + (-y_2 - z_2) \mathbf{a}_2 + (-y_2 + z_2) \mathbf{a}_3$	$=$	$-y_2 a \hat{\mathbf{x}} + z_2 a \hat{\mathbf{y}}$	$(48h)$	B
$\mathbf{B}_{13}$	$=$	$(-y_2 - z_2) \mathbf{a}_1 + (y_2 + z_2) \mathbf{a}_2 + (y_2 - z_2) \mathbf{a}_3$	$=$	$y_2 a \hat{\mathbf{x}} - z_2 a \hat{\mathbf{y}}$	$(48h)$	B
$\mathbf{B}_{14}$	$=$	$(y_2 - z_2) \mathbf{a}_1 + (-y_2 + z_2) \mathbf{a}_2 + (-y_2 - z_2) \mathbf{a}_3$	$=$	$-y_2 a \hat{\mathbf{x}} - z_2 a \hat{\mathbf{y}}$	$(48h)$	B
$\mathbf{B}_{15}$	$=$	$(y_3 + z_3) \mathbf{a}_1 + (-y_3 + z_3) \mathbf{a}_2 + (y_3 - z_3) \mathbf{a}_3$	$=$	$y_3 a \hat{\mathbf{y}} + z_3 a \hat{\mathbf{z}}$	$(48h)$	H
$\mathbf{B}_{16}$	$=$	$(-y_3 + z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 + (-y_3 - z_3) \mathbf{a}_3$	$=$	$-y_3 a \hat{\mathbf{y}} + z_3 a \hat{\mathbf{z}}$	$(48h)$	H
$\mathbf{B}_{17}$	$=$	$(y_3 - z_3) \mathbf{a}_1 + (-y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$=$	$y_3 a \hat{\mathbf{y}} - z_3 a \hat{\mathbf{z}}$	$(48h)$	H
$\mathbf{B}_{18}$	$=$	$(-y_3 - z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (-y_3 + z_3) \mathbf{a}_3$	$=$	$-y_3 a \hat{\mathbf{y}} - z_3 a \hat{\mathbf{z}}$	$(48h)$	H
$\mathbf{B}_{19}$	$=$	$(y_3 - z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 + (-y_3 + z_3) \mathbf{a}_3$	$=$	$z_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{z}}$	$(48h)$	H
$\mathbf{B}_{20}$	$=$	$(-y_3 - z_3) \mathbf{a}_1 + (-y_3 + z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$=$	$z_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{z}}$	$(48h)$	H
$\mathbf{B}_{21}$	$=$	$(y_3 + z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (-y_3 - z_3) \mathbf{a}_3$	$=$	$-z_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{z}}$	$(48h)$	H
$\mathbf{B}_{22}$	$=$	$(-y_3 + z_3) \mathbf{a}_1 + (-y_3 - z_3) \mathbf{a}_2 + (y_3 - z_3) \mathbf{a}_3$	$=$	$-z_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{z}}$	$(48h)$	H
$\mathbf{B}_{23}$	$=$	$(-y_3 + z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$=$	$y_3 a \hat{\mathbf{x}} + z_3 a \hat{\mathbf{y}}$	$(48h)$	H
$\mathbf{B}_{24}$	$=$	$(y_3 + z_3) \mathbf{a}_1 + (-y_3 - z_3) \mathbf{a}_2 + (-y_3 + z_3) \mathbf{a}_3$	$=$	$-y_3 a \hat{\mathbf{x}} + z_3 a \hat{\mathbf{y}}$	$(48h)$	H
$\mathbf{B}_{25}$	$=$	$(-y_3 - z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 + (y_3 - z_3) \mathbf{a}_3$	$=$	$y_3 a \hat{\mathbf{x}} - z_3 a \hat{\mathbf{y}}$	$(48h)$	H
$\mathbf{B}_{26}$	$=$	$(y_3 - z_3) \mathbf{a}_1 + (-y_3 + z_3) \mathbf{a}_2 + (-y_3 - z_3) \mathbf{a}_3$	$=$	$-y_3 a \hat{\mathbf{x}} - z_3 a \hat{\mathbf{y}}$	$(48h)$	H

---

#### References:

- J. A. Wunderlich and W. N. Lipscomb, *Structure of  $B_{12}H_{12}^{-2}$  Ion*, J. Am. Ceram. Soc. **82**, 4427–4428 (1960), [doi:10.1021/ja01501a076](https://doi.org/10.1021/ja01501a076).

#### Found in:

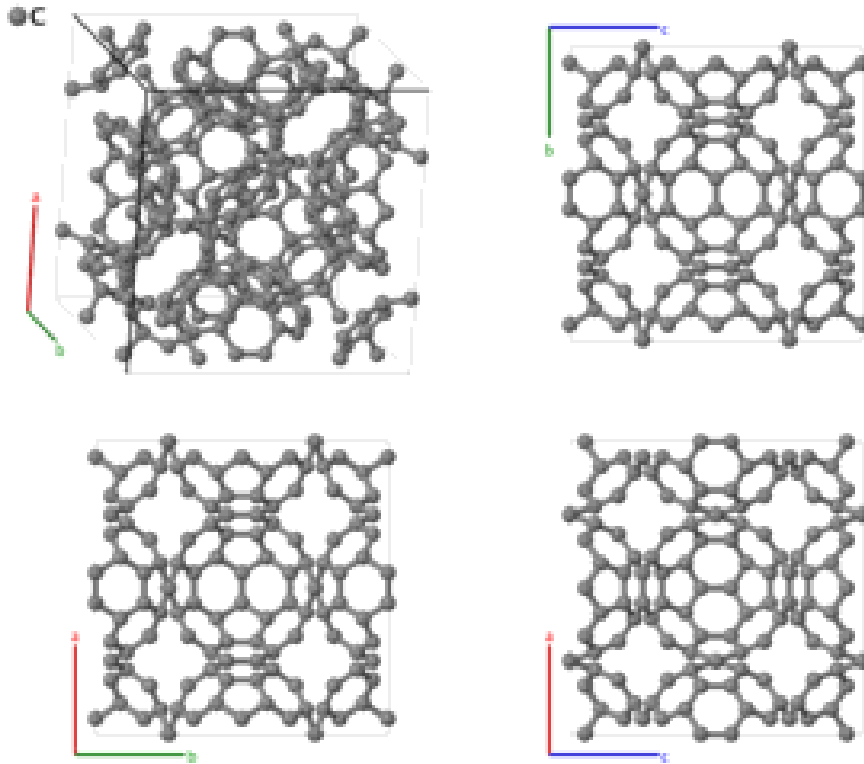
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [949](#)  
- POSCAR: pp. [950](#)

# FCC C<sub>60</sub> Buckminsterfullerene Structure: A\_cF240\_202\_h2i

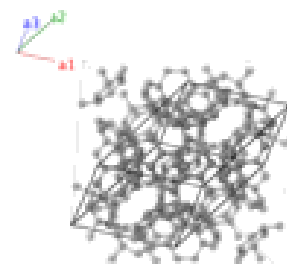


<b>Prototype</b>	:	C
<b>AFLOW prototype label</b>	:	A_cF240_202_h2i
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cF240
<b>Space group number</b>	:	202
<b>Space group symbol</b>	:	$Fm\bar{3}$
<b>AFLOW prototype command</b>	:	aflow --proto=A_cF240_202_h2i --params=a, y <sub>1</sub> , z <sub>1</sub> , x <sub>2</sub> , y <sub>2</sub> , z <sub>2</sub> , x <sub>3</sub> , y <sub>3</sub> , z <sub>3</sub>

- This is an *approximate* representation of the structure of C<sub>60</sub> buckminsterfullerene. As noted by the authors, “a careful analysis of the intensity data reveals that the molecules must pack in an uncorrelated array, in full agreement with the results from most previous diffraction and spectroscopic determinations.” The C<sub>60</sub> molecules are on the sites of an fcc lattice. Below 249 K there is a transition to a [simple cubic phase of C<sub>60</sub>](#).

**Face-centered Cubic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	= (y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>1</sub> + (-y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>2</sub> + (y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>3</sub>	=	y <sub>1</sub> a <b>ŷ</b> + z <sub>1</sub> a <b>ẑ</b>	(48h)	C I
<b>B<sub>2</sub></b>	= (-y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>1</sub> + (y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>2</sub> + (-y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>3</sub>	=	-y <sub>1</sub> a <b>ŷ</b> + z <sub>1</sub> a <b>ẑ</b>	(48h)	C I
<b>B<sub>3</sub></b>	= (y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>1</sub> + (-y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>2</sub> + (y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>3</sub>	=	y <sub>1</sub> a <b>ŷ</b> - z <sub>1</sub> a <b>ẑ</b>	(48h)	C I
<b>B<sub>4</sub></b>	= (-y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>1</sub> + (y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>2</sub> + (-y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>3</sub>	=	-y <sub>1</sub> a <b>ŷ</b> - z <sub>1</sub> a <b>ẑ</b>	(48h)	C I
<b>B<sub>5</sub></b>	= (y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>1</sub> + (y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>2</sub> + (-y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>3</sub>	=	z <sub>1</sub> a <b>ẋ</b> + y <sub>1</sub> a <b>ẑ</b>	(48h)	C I
<b>B<sub>6</sub></b>	= (-y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>1</sub> + (-y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>2</sub> + (y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>3</sub>	=	z <sub>1</sub> a <b>ẋ</b> + -y <sub>1</sub> a <b>ẑ</b>	(48h)	C I
<b>B<sub>7</sub></b>	= (y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>1</sub> + (y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>2</sub> + (-y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>3</sub>	=	-z <sub>1</sub> a <b>ẋ</b> + y <sub>1</sub> a <b>ẑ</b>	(48h)	C I
<b>B<sub>8</sub></b>	= (-y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>1</sub> + (-y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>2</sub> + (y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>3</sub>	=	-z <sub>1</sub> a <b>ẋ</b> + -y <sub>1</sub> a <b>ẑ</b>	(48h)	C I
<b>B<sub>9</sub></b>	= (-y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>1</sub> + (y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>2</sub> + (y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>3</sub>	=	y <sub>1</sub> a <b>ẋ</b> + z <sub>1</sub> a <b>ŷ</b>	(48h)	C I
<b>B<sub>10</sub></b>	= (y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>1</sub> + (-y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>2</sub> + (-y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>3</sub>	=	-y <sub>1</sub> a <b>ẋ</b> + z <sub>1</sub> a <b>ŷ</b>	(48h)	C I
<b>B<sub>11</sub></b>	= (-y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>1</sub> + (y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>2</sub> + (y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>3</sub>	=	y <sub>1</sub> a <b>ẋ</b> - z <sub>1</sub> a <b>ŷ</b>	(48h)	C I
<b>B<sub>12</sub></b>	= (y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>1</sub> + (-y <sub>1</sub> + z <sub>1</sub> ) <b>a</b> <sub>2</sub> + (-y <sub>1</sub> - z <sub>1</sub> ) <b>a</b> <sub>3</sub>	=	-y <sub>1</sub> a <b>ẋ</b> - z <sub>1</sub> a <b>ŷ</b>	(48h)	C I
<b>B<sub>13</sub></b>	= (-x <sub>2</sub> + y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (x <sub>2</sub> - y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (x <sub>2</sub> + y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	x <sub>2</sub> a <b>ẋ</b> + y <sub>2</sub> a <b>ŷ</b> + z <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>14</sub></b>	= (x <sub>2</sub> - y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (-x <sub>2</sub> + y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (-x <sub>2</sub> - y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	-x <sub>2</sub> a <b>ẋ</b> - y <sub>2</sub> a <b>ŷ</b> + z <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>15</sub></b>	= (x <sub>2</sub> + y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (-x <sub>2</sub> - y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (-x <sub>2</sub> + y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	-x <sub>2</sub> a <b>ẋ</b> + y <sub>2</sub> a <b>ŷ</b> - z <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>16</sub></b>	= (-x <sub>2</sub> - y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (x <sub>2</sub> + y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (x <sub>2</sub> - y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	x <sub>2</sub> a <b>ẋ</b> - y <sub>2</sub> a <b>ŷ</b> - z <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>17</sub></b>	= (x <sub>2</sub> + y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (-x <sub>2</sub> + y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (x <sub>2</sub> - y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	z <sub>2</sub> a <b>ẋ</b> + x <sub>2</sub> a <b>ŷ</b> + y <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>18</sub></b>	= (-x <sub>2</sub> - y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (x <sub>2</sub> - y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (-x <sub>2</sub> + y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	z <sub>2</sub> a <b>ẋ</b> - x <sub>2</sub> a <b>ŷ</b> - y <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>19</sub></b>	= (-x <sub>2</sub> + y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (x <sub>2</sub> + y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (-x <sub>2</sub> - y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	-z <sub>2</sub> a <b>ẋ</b> - x <sub>2</sub> a <b>ŷ</b> + y <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>20</sub></b>	= (x <sub>2</sub> - y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (-x <sub>2</sub> - y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (x <sub>2</sub> + y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	-z <sub>2</sub> a <b>ẋ</b> + x <sub>2</sub> a <b>ŷ</b> - y <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>21</sub></b>	= (x <sub>2</sub> - y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (x <sub>2</sub> + y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (-x <sub>2</sub> + y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	y <sub>2</sub> a <b>ẋ</b> + z <sub>2</sub> a <b>ŷ</b> + x <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>22</sub></b>	= (-x <sub>2</sub> + y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (-x <sub>2</sub> - y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (x <sub>2</sub> - y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	-y <sub>2</sub> a <b>ẋ</b> + z <sub>2</sub> a <b>ŷ</b> - x <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>23</sub></b>	= (-x <sub>2</sub> - y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (-x <sub>2</sub> + y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (x <sub>2</sub> + y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	y <sub>2</sub> a <b>ẋ</b> - z <sub>2</sub> a <b>ŷ</b> - x <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>24</sub></b>	= (x <sub>2</sub> + y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (x <sub>2</sub> - y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (-x <sub>2</sub> - y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	-y <sub>2</sub> a <b>ẋ</b> - z <sub>2</sub> a <b>ŷ</b> + x <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>25</sub></b>	= (x <sub>2</sub> - y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (-x <sub>2</sub> + y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (-x <sub>2</sub> - y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	-x <sub>2</sub> a <b>ẋ</b> - y <sub>2</sub> a <b>ŷ</b> - z <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>26</sub></b>	= (-x <sub>2</sub> + y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (x <sub>2</sub> - y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (x <sub>2</sub> + y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	x <sub>2</sub> a <b>ẋ</b> + y <sub>2</sub> a <b>ŷ</b> - z <sub>2</sub> a <b>ẑ</b>	(96i)	C II
<b>B<sub>27</sub></b>	= (-x <sub>2</sub> - y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>1</sub> + (x <sub>2</sub> + y <sub>2</sub> + z <sub>2</sub> ) <b>a</b> <sub>2</sub> + (x <sub>2</sub> - y <sub>2</sub> - z <sub>2</sub> ) <b>a</b> <sub>3</sub>	=	x <sub>2</sub> a <b>ẋ</b> - y <sub>2</sub> a <b>ŷ</b> + z <sub>2</sub> a <b>ẑ</b>	(96i)	C II





$$\begin{aligned}
\mathbf{B}_{52} &= (x_3 + y_3 + z_3) \mathbf{a}_1 + (-x_3 - y_3 + z_3) \mathbf{a}_2 + (-x_3 + y_3 - z_3) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 a \hat{\mathbf{z}} &(96i) & \text{C III} \\
\mathbf{B}_{53} &= (-x_3 - y_3 + z_3) \mathbf{a}_1 + (x_3 - y_3 - z_3) \mathbf{a}_2 + (-x_3 + y_3 - z_3) \mathbf{a}_3 &= -z_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - y_3 a \hat{\mathbf{z}} &(96i) & \text{C III} \\
\mathbf{B}_{54} &= (x_3 + y_3 + z_3) \mathbf{a}_1 + (-x_3 + y_3 - z_3) \mathbf{a}_2 + (x_3 - y_3 - z_3) \mathbf{a}_3 &= -z_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + y_3 a \hat{\mathbf{z}} &(96i) & \text{C III} \\
\mathbf{B}_{55} &= (x_3 - y_3 - z_3) \mathbf{a}_1 + (-x_3 - y_3 + z_3) \mathbf{a}_2 + (x_3 + y_3 + z_3) \mathbf{a}_3 &= z_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - y_3 a \hat{\mathbf{z}} &(96i) & \text{C III} \\
\mathbf{B}_{56} &= (-x_3 + y_3 - z_3) \mathbf{a}_1 + (x_3 + y_3 + z_3) \mathbf{a}_2 + (-x_3 - y_3 + z_3) \mathbf{a}_3 &= z_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + y_3 a \hat{\mathbf{z}} &(96i) & \text{C III} \\
\mathbf{B}_{57} &= (-x_3 + y_3 - z_3) \mathbf{a}_1 + (-x_3 - y_3 + z_3) \mathbf{a}_2 + (x_3 - y_3 - z_3) \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} - z_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}} &(96i) & \text{C III} \\
\mathbf{B}_{58} &= (x_3 - y_3 - z_3) \mathbf{a}_1 + (x_3 + y_3 + z_3) \mathbf{a}_2 + (-x_3 + y_3 - z_3) \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} - z_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}} &(96i) & \text{C III} \\
\mathbf{B}_{59} &= (x_3 + y_3 + z_3) \mathbf{a}_1 + (x_3 - y_3 - z_3) \mathbf{a}_2 + (-x_3 - y_3 + z_3) \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} + z_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}} &(96i) & \text{C III} \\
\mathbf{B}_{60} &= (-x_3 - y_3 + z_3) \mathbf{a}_1 + (-x_3 + y_3 - z_3) \mathbf{a}_2 + (x_3 + y_3 + z_3) \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} + z_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}} &(96i) & \text{C III}
\end{aligned}$$

---

#### References:

- D. L. Dorset and M. P. McCourt, *Disorder and the molecular packing of C<sub>60</sub> buckminsterfullerene: a direct electron-crystallographic analysis*, Acta Crystallogr. Sect. A **50**, 344–351 (1994), doi:10.1107/S0108767393012607.

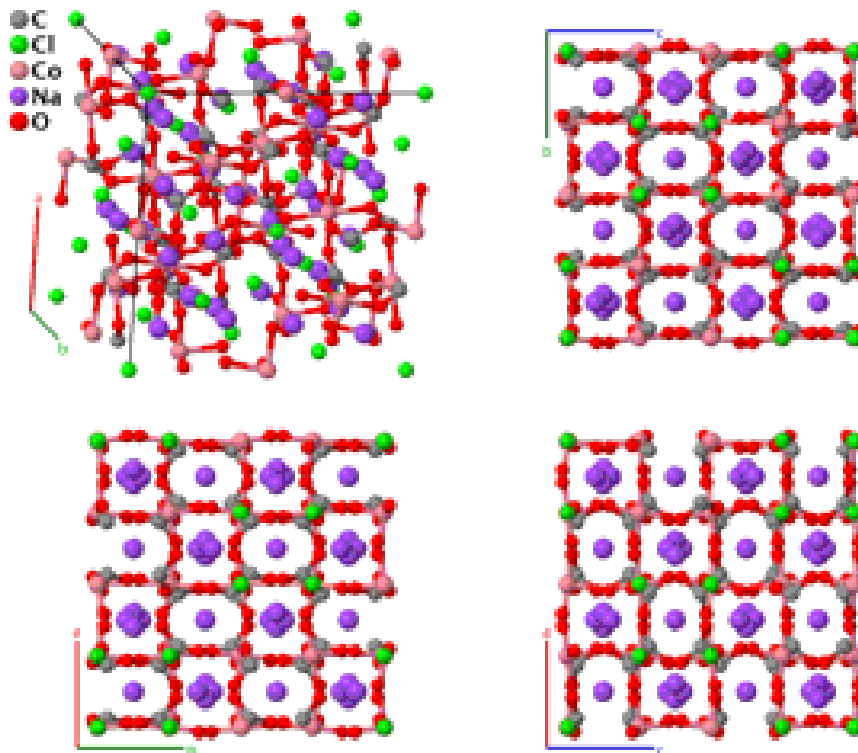
---

#### Geometry files:

- CIF: pp. 950  
- POSCAR: pp. 951

# Pyrochlore ( $\text{Na}_3\text{Co}(\text{CO}_3)_2\text{Cl}$ ) Structure: A2BCD3E6\_cF208\_203\_e\_c\_d\_f\_g

---



<b>Prototype</b>	:	$\text{Na}_3\text{Co}(\text{CO}_3)_2\text{Cl}$
<b>AFLOW prototype label</b>	:	A2BCD3E6_cF208_203_e_c_d_f_g
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cF208
<b>Space group number</b>	:	203
<b>Space group symbol</b>	:	$Fd\bar{3}$
<b>AFLOW prototype command</b>	:	aflow --proto=A2BCD3E6_cF208_203_e_c_d_f_g --params= $a, x_3, x_4, x_5, y_5, z_5$

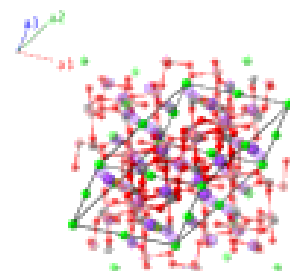
- This structure was suggested to us by Prof. Joel Helton, United States Naval Academy. This is a pyrochlore-like antiferromagnet, which we loosely define as a structure with magnetic ions on the corners of corner-sharing tetrahedra.

**Face-centered Cubic primitive vectors:**

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$	$=$	$0\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}}$	(16c)	Cl
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(16c)	Cl
$\mathbf{B}_3$	$= \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16c)	Cl
$\mathbf{B}_4$	$= \frac{1}{2}\mathbf{a}_1$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16c)	Cl
$\mathbf{B}_5$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(16d)	Co
$\mathbf{B}_6$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(16d)	Co
$\mathbf{B}_7$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16d)	Co
$\mathbf{B}_8$	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16d)	Co
$\mathbf{B}_9$	$= x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$x_3a\hat{\mathbf{x}} + x_3a\hat{\mathbf{y}} + x_3a\hat{\mathbf{z}}$	(32e)	C
$\mathbf{B}_{10}$	$= x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + \left(\frac{1}{2} - 3x_3\right)\mathbf{a}_3$	$=$	$\left(\frac{1}{4} - x_3\right)a\hat{\mathbf{x}} + \left(\frac{1}{4} - x_3\right)a\hat{\mathbf{y}} + x_3a\hat{\mathbf{z}}$	(32e)	C
$\mathbf{B}_{11}$	$= x_3\mathbf{a}_1 + \left(\frac{1}{2} - 3x_3\right)\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$\left(\frac{1}{4} - x_3\right)a\hat{\mathbf{x}} + x_3a\hat{\mathbf{y}} + \left(\frac{1}{4} - x_3\right)a\hat{\mathbf{z}}$	(32e)	C
$\mathbf{B}_{12}$	$= \left(\frac{1}{2} - 3x_3\right)\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$x_3a\hat{\mathbf{x}} + \left(\frac{1}{4} - x_3\right)a\hat{\mathbf{y}} + \left(\frac{1}{4} - x_3\right)a\hat{\mathbf{z}}$	(32e)	C
$\mathbf{B}_{13}$	$= -x_3\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-x_3a\hat{\mathbf{x}} - x_3a\hat{\mathbf{y}} - x_3a\hat{\mathbf{z}}$	(32e)	C
$\mathbf{B}_{14}$	$= -x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + \left(\frac{1}{2} + 3x_3\right)\mathbf{a}_3$	$=$	$\left(\frac{1}{4} + x_3\right)a\hat{\mathbf{x}} + \left(\frac{1}{4} + x_3\right)a\hat{\mathbf{y}} - x_3a\hat{\mathbf{z}}$	(32e)	C
$\mathbf{B}_{15}$	$= -x_3\mathbf{a}_1 + \left(\frac{1}{2} + 3x_3\right)\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$\left(\frac{1}{4} + x_3\right)a\hat{\mathbf{x}} - x_3a\hat{\mathbf{y}} + \left(\frac{1}{4} + x_3\right)a\hat{\mathbf{z}}$	(32e)	C
$\mathbf{B}_{16}$	$= \left(\frac{1}{2} + 3x_3\right)\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-x_3a\hat{\mathbf{x}} + \left(\frac{1}{4} + x_3\right)a\hat{\mathbf{y}} + \left(\frac{1}{4} + x_3\right)a\hat{\mathbf{z}}$	(32e)	C
$\mathbf{B}_{17}$	$= \left(\frac{1}{4} - x_4\right)\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$x_4a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48f)	Na
$\mathbf{B}_{18}$	$= x_4\mathbf{a}_1 + \left(\frac{1}{4} - x_4\right)\mathbf{a}_2 + \left(\frac{1}{4} - x_4\right)\mathbf{a}_3$	$=$	$\left(\frac{1}{4} - x_4\right)a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48f)	Na
$\mathbf{B}_{19}$	$= x_4\mathbf{a}_1 + \left(\frac{1}{4} - x_4\right)\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + x_4a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48f)	Na
$\mathbf{B}_{20}$	$= \left(\frac{1}{4} - x_4\right)\mathbf{a}_1 + x_4\mathbf{a}_2 + \left(\frac{1}{4} - x_4\right)\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \left(\frac{1}{4} - x_4\right)a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48f)	Na
$\mathbf{B}_{21}$	$= x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + \left(\frac{1}{4} - x_4\right)\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + x_4a\hat{\mathbf{z}}$	(48f)	Na
$\mathbf{B}_{22}$	$= \left(\frac{1}{4} - x_4\right)\mathbf{a}_1 + \left(\frac{1}{4} - x_4\right)\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \left(\frac{1}{4} - x_4\right)a\hat{\mathbf{z}}$	(48f)	Na
$\mathbf{B}_{23}$	$= \left(\frac{3}{4} + x_4\right)\mathbf{a}_1 - x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$-x_4a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(48f)	Na
$\mathbf{B}_{24}$	$= -x_4\mathbf{a}_1 + \left(\frac{3}{4} + x_4\right)\mathbf{a}_2 + \left(\frac{3}{4} + x_4\right)\mathbf{a}_3$	$=$	$\left(\frac{3}{4} + x_4\right)a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(48f)	Na
$\mathbf{B}_{25}$	$= -x_4\mathbf{a}_1 + \left(\frac{3}{4} + x_4\right)\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} - x_4a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(48f)	Na
$\mathbf{B}_{26}$	$= \left(\frac{3}{4} + x_4\right)\mathbf{a}_1 - x_4\mathbf{a}_2 + \left(\frac{3}{4} + x_4\right)\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \left(\frac{3}{4} + x_4\right)a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(48f)	Na
$\mathbf{B}_{27}$	$= -x_4\mathbf{a}_1 - x_4\mathbf{a}_2 + \left(\frac{3}{4} + x_4\right)\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} - x_4a\hat{\mathbf{z}}$	(48f)	Na
$\mathbf{B}_{28}$	$= \left(\frac{3}{4} + x_4\right)\mathbf{a}_1 + \left(\frac{3}{4} + x_4\right)\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \left(\frac{3}{4} + x_4\right)a\hat{\mathbf{z}}$	(48f)	Na
$\mathbf{B}_{29}$	$= (-x_5 + y_5 + z_5)\mathbf{a}_1 +$ $(x_5 - y_5 + z_5)\mathbf{a}_2 +$ $(x_5 + y_5 - z_5)\mathbf{a}_3$	$=$	$x_5a\hat{\mathbf{x}} + y_5a\hat{\mathbf{y}} + z_5a\hat{\mathbf{z}}$	(96g)	O
$\mathbf{B}_{30}$	$= (x_5 - y_5 + z_5)\mathbf{a}_1 +$ $(-x_5 + y_5 + z_5)\mathbf{a}_2 +$ $\left(\frac{1}{2} - x_5 - y_5 - z_5\right)\mathbf{a}_3$	$=$	$\left(\frac{1}{4} - x_5\right)a\hat{\mathbf{x}} + \left(\frac{1}{4} - y_5\right)a\hat{\mathbf{y}} + z_5a\hat{\mathbf{z}}$	(96g)	O
$\mathbf{B}_{31}$	$= (x_5 + y_5 - z_5)\mathbf{a}_1 +$ $\left(\frac{1}{2} - x_5 - y_5 - z_5\right)\mathbf{a}_2 +$ $(-x_5 + y_5 + z_5)\mathbf{a}_3$	$=$	$\left(\frac{1}{4} - x_5\right)a\hat{\mathbf{x}} + y_5a\hat{\mathbf{y}} + \left(\frac{1}{4} - z_5\right)a\hat{\mathbf{z}}$	(96g)	O

$$\begin{aligned}
\mathbf{B}_{32} &= \begin{pmatrix} \frac{1}{2} - x_5 - y_5 - z_5 \\ x_5 + y_5 - z_5 \\ x_5 - y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + &= x_5 a \hat{\mathbf{x}} + \left(\frac{1}{4} - y_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_5\right) a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{33} &= \begin{pmatrix} x_5 + y_5 - z_5 \\ -x_5 + y_5 + z_5 \\ x_5 - y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + &= z_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + y_5 a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{34} &= \begin{pmatrix} \frac{1}{2} - x_5 - y_5 - z_5 \\ x_5 - y_5 + z_5 \\ -x_5 + y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + &= z_5 a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - y_5\right) a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{35} &= \begin{pmatrix} -x_5 + y_5 + z_5 \\ x_5 + y_5 - z_5 \\ \frac{1}{2} - x_5 - y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + &= \left(\frac{1}{4} - z_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_5\right) a \hat{\mathbf{y}} + y_5 a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{36} &= \begin{pmatrix} x_5 - y_5 + z_5 \\ \frac{1}{2} - x_5 - y_5 - z_5 \\ x_5 + y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + &= \left(\frac{1}{4} - z_5\right) a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + \left(\frac{1}{4} - y_5\right) a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{37} &= \begin{pmatrix} x_5 - y_5 + z_5 \\ x_5 + y_5 - z_5 \\ -x_5 + y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + &= y_5 a \hat{\mathbf{x}} + z_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{38} &= \begin{pmatrix} -x_5 + y_5 + z_5 \\ \frac{1}{2} - x_5 - y_5 - z_5 \\ x_5 - y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + &= \left(\frac{1}{4} - y_5\right) a \hat{\mathbf{x}} + z_5 a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_5\right) a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{39} &= \begin{pmatrix} \frac{1}{2} - x_5 - y_5 - z_5 \\ -x_5 + y_5 + z_5 \\ x_5 + y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + &= y_5 a \hat{\mathbf{x}} + \left(\frac{1}{4} - z_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_5\right) a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{40} &= \begin{pmatrix} x_5 + y_5 - z_5 \\ x_5 - y_5 + z_5 \\ \frac{1}{2} - x_5 - y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + &= \left(\frac{1}{4} - y_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - z_5\right) a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{41} &= \begin{pmatrix} x_5 - y_5 - z_5 \\ -x_5 + y_5 - z_5 \\ -x_5 - y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + &= -x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{42} &= \begin{pmatrix} -x_5 + y_5 - z_5 \\ x_5 - y_5 - z_5 \\ \frac{1}{2} + x_5 + y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + &= \left(\frac{1}{4} + x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + y_5\right) a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{43} &= \begin{pmatrix} -x_5 - y_5 + z_5 \\ \frac{1}{2} + x_5 + y_5 + z_5 \\ x_5 - y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + &= \left(\frac{1}{4} + x_5\right) a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_5\right) a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{44} &= \begin{pmatrix} \frac{1}{2} + x_5 + y_5 + z_5 \\ -x_5 - y_5 + z_5 \\ -x_5 + y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + &= -x_5 a \hat{\mathbf{x}} + \left(\frac{1}{4} + y_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_5\right) a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{45} &= \begin{pmatrix} -x_5 - y_5 + z_5 \\ x_5 - y_5 - z_5 \\ -x_5 + y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + &= -z_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{46} &= \begin{pmatrix} \frac{1}{2} + x_5 + y_5 + z_5 \\ -x_5 + y_5 - z_5 \\ x_5 - y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + &= -z_5 a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + y_5\right) a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O} \\
\mathbf{B}_{47} &= \begin{pmatrix} x_5 - y_5 - z_5 \\ -x_5 - y_5 + z_5 \\ \frac{1}{2} + x_5 + y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + &= \left(\frac{1}{4} + z_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_5\right) a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}} & (96g) & \quad \mathbf{O}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{48} &= \begin{pmatrix} (-x_5 + y_5 - z_5) \mathbf{a}_1 + \\ (\frac{1}{2} + x_5 + y_5 + z_5) \mathbf{a}_2 + \\ (-x_5 - y_5 + z_5) \mathbf{a}_3 \end{pmatrix} &= \left(\frac{1}{4} + z_5\right) a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{1}{4} + y_5\right) a \hat{\mathbf{z}} && (96g) && \text{O} \\
\mathbf{B}_{49} &= \begin{pmatrix} (-x_5 + y_5 - z_5) \mathbf{a}_1 + \\ (-x_5 - y_5 + z_5) \mathbf{a}_2 + \\ (x_5 - y_5 - z_5) \mathbf{a}_3 \end{pmatrix} &= -y_5 a \hat{\mathbf{x}} - z_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}} && (96g) && \text{O} \\
\mathbf{B}_{50} &= \begin{pmatrix} (x_5 - y_5 - z_5) \mathbf{a}_1 + \\ (\frac{1}{2} + x_5 + y_5 + z_5) \mathbf{a}_2 + \\ (-x_5 + y_5 - z_5) \mathbf{a}_3 \end{pmatrix} &= \left(\frac{1}{4} + y_5\right) a \hat{\mathbf{x}} - z_5 a \hat{\mathbf{y}} + \left(\frac{1}{4} + x_5\right) a \hat{\mathbf{z}} && (96g) && \text{O} \\
\mathbf{B}_{51} &= \begin{pmatrix} (\frac{1}{2} + x_5 + y_5 + z_5) \mathbf{a}_1 + \\ (x_5 - y_5 - z_5) \mathbf{a}_2 + \\ (-x_5 - y_5 + z_5) \mathbf{a}_3 \end{pmatrix} &= -y_5 a \hat{\mathbf{x}} + \left(\frac{1}{4} + z_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + x_5\right) a \hat{\mathbf{z}} && (96g) && \text{O} \\
\mathbf{B}_{52} &= \begin{pmatrix} (-x_5 - y_5 + z_5) \mathbf{a}_1 + \\ (-x_5 + y_5 - z_5) \mathbf{a}_2 + \\ (\frac{1}{2} + x_5 + y_5 + z_5) \mathbf{a}_3 \end{pmatrix} &= \left(\frac{1}{4} + y_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + z_5\right) a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}} && (96g) && \text{O}
\end{aligned}$$

---

### References:

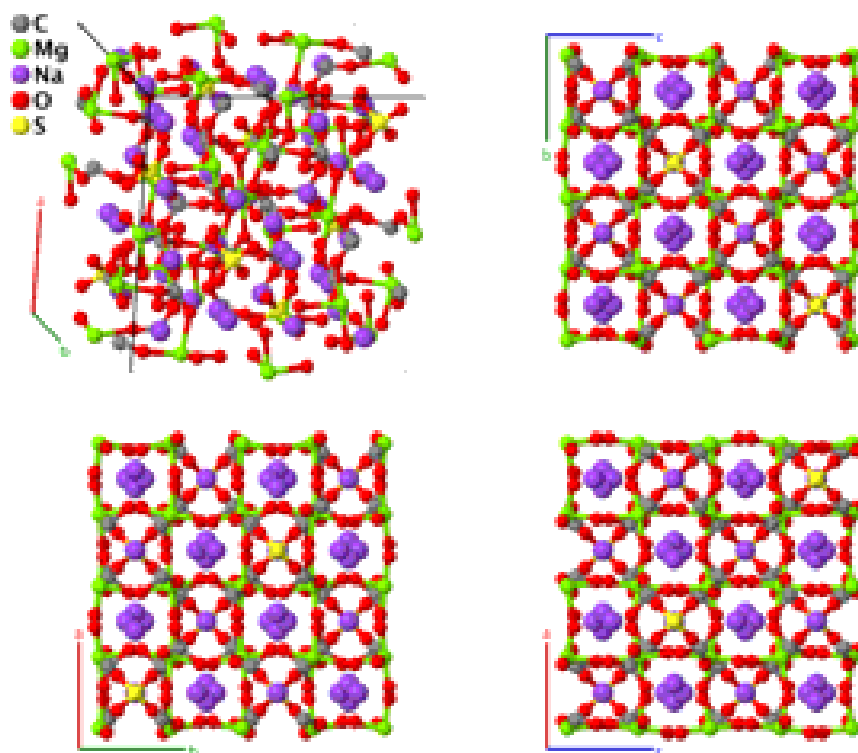
- Z. Fu, Y. Zheng, Y. Xiao, S. Bedanta, A. Senyshyn, G. G. Simeoni, Y. Su, U. Rucker, P. Kögerler, and T. Brückel, *Coexistence of magnetic order and spin-glass-like phase in the pyrochlore antiferromagnet  $\text{Na}_3\text{Co}(\text{CO}_3)_2\text{Cl}$* , Phys. Rev. B **87**, 214406 (2013), [doi:10.1103/PhysRevB.87.214406](https://doi.org/10.1103/PhysRevB.87.214406).

---

### Geometry files:

- CIF: pp. [951](#)  
- POSCAR: pp. [952](#)

# Tychite ( $\text{Na}_6\text{Mg}_2(\text{SO}_4)(\text{CO}_3)_4$ ) Structure: A4B2C6D16E\_cF232\_203\_e\_d\_f\_eg\_a

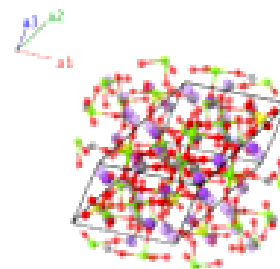


<b>Prototype</b>	:	$\text{Na}_6\text{Mg}_2(\text{SO}_4)(\text{CO}_3)_4$
<b>AFLOW prototype label</b>	:	A4B2C6D16E_cF232_203_e_d_f_eg_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cF232
<b>Space group number</b>	:	203
<b>Space group symbol</b>	:	$Fd\bar{3}$
<b>AFLOW prototype command</b>	:	aflow --proto=A4B2C6D16E_cF232_203_e_d_f_eg_a --params= $a, x_3, x_4, x_5, x_6, y_6, z_6$

- The data was obtained from an X-ray diffraction study of a single crystal at room temperature (298 K).

## Face-centered Cubic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{y} + \frac{1}{2} a \hat{z} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{x} + \frac{1}{2} a \hat{z} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{x} + \frac{1}{2} a \hat{y} \end{aligned}$$



## Basis vectors:





$$\begin{aligned}
\mathbf{B}_{35} &= (-x_6 + y_6 + z_6) \mathbf{a}_1 + (x_6 - y_6 + z_6) \mathbf{a}_2 + (x_6 + y_6 - z_6) \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + z_6 a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{36} &= (x_6 - y_6 + z_6) \mathbf{a}_1 + (-x_6 + y_6 + z_6) \mathbf{a}_2 + \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_3 &= \left(\frac{1}{4} - x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - y_6\right) a \hat{\mathbf{y}} + z_6 a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{37} &= (x_6 + y_6 - z_6) \mathbf{a}_1 + \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_2 + (-x_6 + y_6 + z_6) \mathbf{a}_3 &= \left(\frac{1}{4} - x_6\right) a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_6\right) a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{38} &= \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_1 + (x_6 + y_6 - z_6) \mathbf{a}_2 + (x_6 - y_6 + z_6) \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} + \left(\frac{1}{4} - y_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_6\right) a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{39} &= (x_6 + y_6 - z_6) \mathbf{a}_1 + (-x_6 + y_6 + z_6) \mathbf{a}_2 + (x_6 - y_6 + z_6) \mathbf{a}_3 &= z_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + y_6 a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{40} &= \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_1 + (x_6 - y_6 + z_6) \mathbf{a}_2 + (-x_6 + y_6 + z_6) \mathbf{a}_3 &= z_6 a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - y_6\right) a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{41} &= (-x_6 + y_6 + z_6) \mathbf{a}_1 + (x_6 + y_6 - z_6) \mathbf{a}_2 + \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_3 &= \left(\frac{1}{4} - z_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_6\right) a \hat{\mathbf{y}} + y_6 a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{42} &= (x_6 - y_6 + z_6) \mathbf{a}_1 + \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_2 + (x_6 + y_6 - z_6) \mathbf{a}_3 &= \left(\frac{1}{4} - z_6\right) a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + \left(\frac{1}{4} - y_6\right) a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{43} &= (x_6 - y_6 + z_6) \mathbf{a}_1 + (x_6 + y_6 - z_6) \mathbf{a}_2 + (-x_6 + y_6 + z_6) \mathbf{a}_3 &= y_6 a \hat{\mathbf{x}} + z_6 a \hat{\mathbf{y}} + x_6 a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{44} &= (-x_6 + y_6 + z_6) \mathbf{a}_1 + \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_2 + (x_6 - y_6 + z_6) \mathbf{a}_3 &= \left(\frac{1}{4} - y_6\right) a \hat{\mathbf{x}} + z_6 a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_6\right) a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{45} &= \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_1 + (-x_6 + y_6 + z_6) \mathbf{a}_2 + (x_6 + y_6 - z_6) \mathbf{a}_3 &= y_6 a \hat{\mathbf{x}} + \left(\frac{1}{4} - z_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_6\right) a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{46} &= (x_6 + y_6 - z_6) \mathbf{a}_1 + (x_6 - y_6 + z_6) \mathbf{a}_2 + \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_3 &= \left(\frac{1}{4} - y_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - z_6\right) a \hat{\mathbf{y}} + x_6 a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{47} &= (x_6 - y_6 - z_6) \mathbf{a}_1 + (-x_6 + y_6 - z_6) \mathbf{a}_2 + (-x_6 - y_6 + z_6) \mathbf{a}_3 &= -x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} - z_6 a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{48} &= (-x_6 + y_6 - z_6) \mathbf{a}_1 + (x_6 - y_6 - z_6) \mathbf{a}_2 + \left(\frac{1}{2} + x_6 + y_6 + z_6\right) \mathbf{a}_3 &= \left(\frac{1}{4} + x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + y_6\right) a \hat{\mathbf{y}} - z_6 a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{49} &= (-x_6 - y_6 + z_6) \mathbf{a}_1 + \left(\frac{1}{2} + x_6 + y_6 + z_6\right) \mathbf{a}_2 + (x_6 - y_6 - z_6) \mathbf{a}_3 &= \left(\frac{1}{4} + x_6\right) a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_6\right) a \hat{\mathbf{z}} & (96g) & \text{O II} \\
\mathbf{B}_{50} &= \left(\frac{1}{2} + x_6 + y_6 + z_6\right) \mathbf{a}_1 + (-x_6 - y_6 + z_6) \mathbf{a}_2 + (-x_6 + y_6 - z_6) \mathbf{a}_3 &= -x_6 a \hat{\mathbf{x}} + \left(\frac{1}{4} + y_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_6\right) a \hat{\mathbf{z}} & (96g) & \text{O II}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{51} &= \begin{aligned} &(-x_6 - y_6 + z_6) \mathbf{a}_1 + \\ &(x_6 - y_6 - z_6) \mathbf{a}_2 + \\ &(-x_6 + y_6 - z_6) \mathbf{a}_3 \end{aligned} &= -z_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} - y_6 a \hat{\mathbf{z}} &(96g) & \quad \text{O II} \\
\mathbf{B}_{52} &= \begin{aligned} &\left(\frac{1}{2} + x_6 + y_6 + z_6\right) \mathbf{a}_1 + \\ &(-x_6 + y_6 - z_6) \mathbf{a}_2 + \\ &(x_6 - y_6 - z_6) \mathbf{a}_3 \end{aligned} &= -z_6 a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + y_6\right) a \hat{\mathbf{z}} &(96g) & \quad \text{O II} \\
\mathbf{B}_{53} &= \begin{aligned} &(x_6 - y_6 - z_6) \mathbf{a}_1 + \\ &(-x_6 - y_6 + z_6) \mathbf{a}_2 + \\ &\left(\frac{1}{2} + x_6 + y_6 + z_6\right) \mathbf{a}_3 \end{aligned} &= \left(\frac{1}{4} + z_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_6\right) a \hat{\mathbf{y}} - y_6 a \hat{\mathbf{z}} &(96g) & \quad \text{O II} \\
\mathbf{B}_{54} &= \begin{aligned} &(-x_6 + y_6 - z_6) \mathbf{a}_1 + \\ &\left(\frac{1}{2} + x_6 + y_6 + z_6\right) \mathbf{a}_2 + \\ &(-x_6 - y_6 + z_6) \mathbf{a}_3 \end{aligned} &= \left(\frac{1}{4} + z_6\right) a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + \left(\frac{1}{4} + y_6\right) a \hat{\mathbf{z}} &(96g) & \quad \text{O II} \\
\mathbf{B}_{55} &= \begin{aligned} &(-x_6 + y_6 - z_6) \mathbf{a}_1 + \\ &(-x_6 - y_6 + z_6) \mathbf{a}_2 + \\ &(x_6 - y_6 - z_6) \mathbf{a}_3 \end{aligned} &= -y_6 a \hat{\mathbf{x}} - z_6 a \hat{\mathbf{y}} - x_6 a \hat{\mathbf{z}} &(96g) & \quad \text{O II} \\
\mathbf{B}_{56} &= \begin{aligned} &(x_6 - y_6 - z_6) \mathbf{a}_1 + \\ &\left(\frac{1}{2} + x_6 + y_6 + z_6\right) \mathbf{a}_2 + \\ &(-x_6 + y_6 - z_6) \mathbf{a}_3 \end{aligned} &= \left(\frac{1}{4} + y_6\right) a \hat{\mathbf{x}} - z_6 a \hat{\mathbf{y}} + \left(\frac{1}{4} + x_6\right) a \hat{\mathbf{z}} &(96g) & \quad \text{O II} \\
\mathbf{B}_{57} &= \begin{aligned} &\left(\frac{1}{2} + x_6 + y_6 + z_6\right) \mathbf{a}_1 + \\ &(x_6 - y_6 - z_6) \mathbf{a}_2 + \\ &(-x_6 - y_6 + z_6) \mathbf{a}_3 \end{aligned} &= -y_6 a \hat{\mathbf{x}} + \left(\frac{1}{4} + z_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + x_6\right) a \hat{\mathbf{z}} &(96g) & \quad \text{O II} \\
\mathbf{B}_{58} &= \begin{aligned} &(-x_6 - y_6 + z_6) \mathbf{a}_1 + \\ &(-x_6 + y_6 - z_6) \mathbf{a}_2 + \\ &\left(\frac{1}{2} + x_6 + y_6 + z_6\right) \mathbf{a}_3 \end{aligned} &= \left(\frac{1}{4} + y_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + z_6\right) a \hat{\mathbf{y}} - x_6 a \hat{\mathbf{z}} &(96g) & \quad \text{O II}
\end{aligned}$$

---

#### References:

- G. R. Schmidt, R. Jacqueline, H. Yang, and R. T. Downs, *Tychite, Na<sub>6</sub>Mg<sub>2</sub>(SO<sub>4</sub>)(CO<sub>3</sub>)<sub>4</sub>: Structure analysis and Raman spectroscopic data*, Acta Crystallogr. E **62**, i207–i209 (2006), doi:10.1107/S160053680603491X.

#### Found in:

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

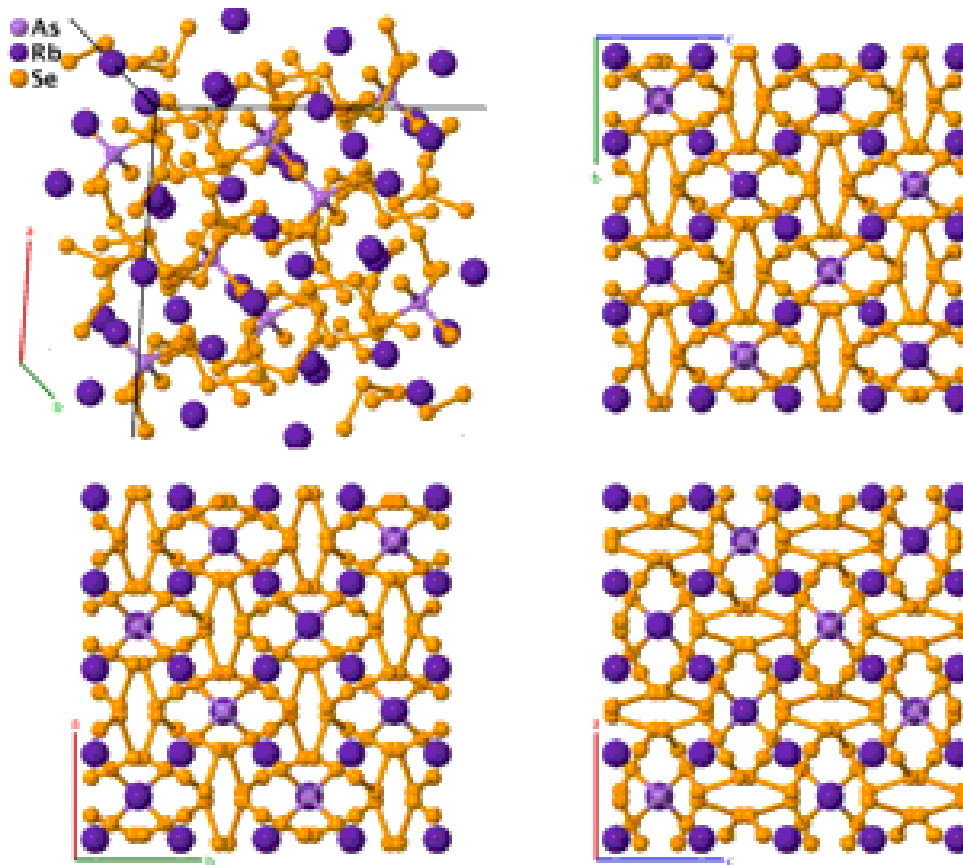
---

#### Geometry files:

- CIF: pp. 953

- POSCAR: pp. 953

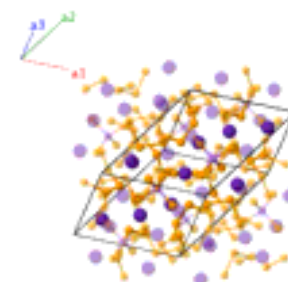
# Rb<sub>3</sub>AsSe<sub>16</sub> Structure: AB3C16\_cF160\_203\_b\_ad\_eg



**Prototype** : Rb<sub>3</sub>AsSe<sub>16</sub>  
**AFLOW prototype label** : AB3C16\_cF160\_203\_b\_ad\_eg  
**Strukturbericht designation** : None  
**Pearson symbol** : cF160  
**Space group number** : 203  
**Space group symbol** :  $Fd\bar{3}$   
**AFLOW prototype command** : aflow --proto=AB3C16\_cF160\_203\_b\_ad\_eg  
 --params= $a, x_4, x_5, y_5, z_5$

**Face-centered Cubic primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{y} + \frac{1}{2} a \hat{z} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{x} + \frac{1}{2} a \hat{z} \\
 \mathbf{a}_3 &= \frac{1}{2} a \hat{x} + \frac{1}{2} a \hat{y}
 \end{aligned}$$



**Basis vectors:**

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type

$$\begin{aligned}
\mathbf{B}_1 &= \frac{1}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3 &= \frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}} & (8a) & \text{Rb I} \\
\mathbf{B}_2 &= \frac{7}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3 &= \frac{7}{8}a\hat{\mathbf{x}} + \frac{7}{8}a\hat{\mathbf{y}} + \frac{7}{8}a\hat{\mathbf{z}} & (8a) & \text{Rb I} \\
\mathbf{B}_3 &= \frac{5}{8}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3 &= \frac{5}{8}a\hat{\mathbf{x}} + \frac{5}{8}a\hat{\mathbf{y}} + \frac{5}{8}a\hat{\mathbf{z}} & (8b) & \text{As} \\
\mathbf{B}_4 &= \frac{3}{8}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3 &= \frac{3}{8}a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}} & (8b) & \text{As} \\
\mathbf{B}_5 &= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} & (16d) & \text{Rb II} \\
\mathbf{B}_6 &= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 &= \frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} & (16d) & \text{Rb II} \\
\mathbf{B}_7 &= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3 &= \frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}} & (16d) & \text{Rb II} \\
\mathbf{B}_8 &= \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}} & (16d) & \text{Rb II} \\
\mathbf{B}_9 &= x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3 &= x_4a\hat{\mathbf{x}} + x_4a\hat{\mathbf{y}} + x_4a\hat{\mathbf{z}} & (32e) & \text{Se I} \\
\mathbf{B}_{10} &= x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + \left(\frac{1}{2} - 3x_4\right)\mathbf{a}_3 &= \left(\frac{1}{4} - x_4\right)a\hat{\mathbf{x}} + \left(\frac{1}{4} - x_4\right)a\hat{\mathbf{y}} + x_4a\hat{\mathbf{z}} & (32e) & \text{Se I} \\
\mathbf{B}_{11} &= x_4\mathbf{a}_1 + \left(\frac{1}{2} - 3x_4\right)\mathbf{a}_2 + x_4\mathbf{a}_3 &= \left(\frac{1}{4} - x_4\right)a\hat{\mathbf{x}} + x_4a\hat{\mathbf{y}} + \left(\frac{1}{4} - x_4\right)a\hat{\mathbf{z}} & (32e) & \text{Se I} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} - 3x_4\right)\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3 &= x_4a\hat{\mathbf{x}} + \left(\frac{1}{4} - x_4\right)a\hat{\mathbf{y}} + \left(\frac{1}{4} - x_4\right)a\hat{\mathbf{z}} & (32e) & \text{Se I} \\
\mathbf{B}_{13} &= -x_4\mathbf{a}_1 - x_4\mathbf{a}_2 - x_4\mathbf{a}_3 &= -x_4a\hat{\mathbf{x}} - x_4a\hat{\mathbf{y}} - x_4a\hat{\mathbf{z}} & (32e) & \text{Se I} \\
\mathbf{B}_{14} &= -x_4\mathbf{a}_1 - x_4\mathbf{a}_2 + \left(\frac{1}{2} + 3x_4\right)\mathbf{a}_3 &= \left(\frac{1}{4} + x_4\right)a\hat{\mathbf{x}} + \left(\frac{1}{4} + x_4\right)a\hat{\mathbf{y}} - x_4a\hat{\mathbf{z}} & (32e) & \text{Se I} \\
\mathbf{B}_{15} &= -x_4\mathbf{a}_1 + \left(\frac{1}{2} + 3x_4\right)\mathbf{a}_2 - x_4\mathbf{a}_3 &= \left(\frac{1}{4} + x_4\right)a\hat{\mathbf{x}} - x_4a\hat{\mathbf{y}} + \left(\frac{1}{4} + x_4\right)a\hat{\mathbf{z}} & (32e) & \text{Se I} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} + 3x_4\right)\mathbf{a}_1 - x_4\mathbf{a}_2 - x_4\mathbf{a}_3 &= -x_4a\hat{\mathbf{x}} + \left(\frac{1}{4} + x_4\right)a\hat{\mathbf{y}} + \left(\frac{1}{4} + x_4\right)a\hat{\mathbf{z}} & (32e) & \text{Se I} \\
\mathbf{B}_{17} &= (-x_5 + y_5 + z_5)\mathbf{a}_1 + &= x_5a\hat{\mathbf{x}} + y_5a\hat{\mathbf{y}} + z_5a\hat{\mathbf{z}} & (96g) & \text{Se II} \\
& (x_5 - y_5 + z_5)\mathbf{a}_2 + \\
& (x_5 + y_5 - z_5)\mathbf{a}_3 \\
\mathbf{B}_{18} &= (x_5 - y_5 + z_5)\mathbf{a}_1 + &= \left(\frac{1}{4} - x_5\right)a\hat{\mathbf{x}} + \left(\frac{1}{4} - y_5\right)a\hat{\mathbf{y}} + z_5a\hat{\mathbf{z}} & (96g) & \text{Se II} \\
& (-x_5 + y_5 + z_5)\mathbf{a}_2 + \\
& \left(\frac{1}{2} - x_5 - y_5 - z_5\right)\mathbf{a}_3 \\
\mathbf{B}_{19} &= (x_5 + y_5 - z_5)\mathbf{a}_1 + &= \left(\frac{1}{4} - x_5\right)a\hat{\mathbf{x}} + y_5a\hat{\mathbf{y}} + \left(\frac{1}{4} - z_5\right)a\hat{\mathbf{z}} & (96g) & \text{Se II} \\
& \left(\frac{1}{2} - x_5 - y_5 - z_5\right)\mathbf{a}_2 + \\
& (-x_5 + y_5 + z_5)\mathbf{a}_3 \\
\mathbf{B}_{20} &= \left(\frac{1}{2} - x_5 - y_5 - z_5\right)\mathbf{a}_1 + &= x_5a\hat{\mathbf{x}} + \left(\frac{1}{4} - y_5\right)a\hat{\mathbf{y}} + \left(\frac{1}{4} - z_5\right)a\hat{\mathbf{z}} & (96g) & \text{Se II} \\
& (x_5 + y_5 - z_5)\mathbf{a}_2 + \\
& (x_5 - y_5 + z_5)\mathbf{a}_3 \\
\mathbf{B}_{21} &= (x_5 + y_5 - z_5)\mathbf{a}_1 + &= z_5a\hat{\mathbf{x}} + x_5a\hat{\mathbf{y}} + y_5a\hat{\mathbf{z}} & (96g) & \text{Se II} \\
& (-x_5 + y_5 + z_5)\mathbf{a}_2 + \\
& (x_5 - y_5 + z_5)\mathbf{a}_3 \\
\mathbf{B}_{22} &= \left(\frac{1}{2} - x_5 - y_5 - z_5\right)\mathbf{a}_1 + &= z_5a\hat{\mathbf{x}} + \left(\frac{1}{4} - x_5\right)a\hat{\mathbf{y}} + \left(\frac{1}{4} - y_5\right)a\hat{\mathbf{z}} & (96g) & \text{Se II} \\
& (x_5 - y_5 + z_5)\mathbf{a}_2 + \\
& (-x_5 + y_5 + z_5)\mathbf{a}_3 \\
\mathbf{B}_{23} &= (-x_5 + y_5 + z_5)\mathbf{a}_1 + &= \left(\frac{1}{4} - z_5\right)a\hat{\mathbf{x}} + \left(\frac{1}{4} - x_5\right)a\hat{\mathbf{y}} + y_5a\hat{\mathbf{z}} & (96g) & \text{Se II} \\
& (x_5 + y_5 - z_5)\mathbf{a}_2 + \\
& \left(\frac{1}{2} - x_5 - y_5 - z_5\right)\mathbf{a}_3 \\
\mathbf{B}_{24} &= (x_5 - y_5 + z_5)\mathbf{a}_1 + &= \left(\frac{1}{4} - z_5\right)a\hat{\mathbf{x}} + x_5a\hat{\mathbf{y}} + \left(\frac{1}{4} - y_5\right)a\hat{\mathbf{z}} & (96g) & \text{Se II} \\
& \left(\frac{1}{2} - x_5 - y_5 - z_5\right)\mathbf{a}_2 + \\
& (x_5 + y_5 - z_5)\mathbf{a}_3 \\
\mathbf{B}_{25} &= (x_5 - y_5 + z_5)\mathbf{a}_1 + &= y_5a\hat{\mathbf{x}} + z_5a\hat{\mathbf{y}} + x_5a\hat{\mathbf{z}} & (96g) & \text{Se II} \\
& (x_5 + y_5 - z_5)\mathbf{a}_2 + \\
& (-x_5 + y_5 + z_5)\mathbf{a}_3
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{26} &= \begin{pmatrix} -x_5 + y_5 + z_5 \\ \frac{1}{2} - x_5 - y_5 - z_5 \\ x_5 - y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{4} - y_5 \\ \frac{1}{4} - z_5 \\ \frac{1}{4} - x_5 \end{pmatrix} a \hat{\mathbf{x}} + z_5 a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{4} - x_5 \\ \frac{1}{4} - z_5 \\ \frac{1}{4} - x_5 \end{pmatrix} a \hat{\mathbf{z}} &= \begin{pmatrix} \frac{1}{4} - y_5 \\ \frac{1}{4} - z_5 \\ \frac{1}{4} - x_5 \end{pmatrix} a \hat{\mathbf{x}} + z_5 a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{4} - x_5 \\ \frac{1}{4} - z_5 \\ \frac{1}{4} - x_5 \end{pmatrix} a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{27} &= \begin{pmatrix} \frac{1}{2} - x_5 - y_5 - z_5 \\ -x_5 + y_5 + z_5 \\ x_5 + y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_5 a \hat{\mathbf{x}} + (\frac{1}{4} - z_5) a \hat{\mathbf{y}} + (\frac{1}{4} - x_5) a \hat{\mathbf{z}} \end{pmatrix} &= y_5 a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} - z_5 \\ \frac{1}{4} - x_5 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{4} - x_5 \\ \frac{1}{4} - z_5 \end{pmatrix} a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{28} &= \begin{pmatrix} x_5 + y_5 - z_5 \\ x_5 - y_5 + z_5 \\ \frac{1}{2} - x_5 - y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{4} - y_5 \\ \frac{1}{4} - z_5 \\ x_5 a \hat{\mathbf{z}} \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} - z_5 \\ \frac{1}{4} - z_5 \end{pmatrix} a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}} &= \begin{pmatrix} \frac{1}{4} - y_5 \\ \frac{1}{4} - z_5 \\ \frac{1}{4} - z_5 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} - z_5 \\ \frac{1}{4} - z_5 \end{pmatrix} a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{29} &= \begin{pmatrix} x_5 - y_5 - z_5 \\ -x_5 + y_5 - z_5 \\ -x_5 - y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} -x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}} \end{pmatrix} &= -x_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{30} &= \begin{pmatrix} -x_5 + y_5 - z_5 \\ x_5 - y_5 - z_5 \\ \frac{1}{2} + x_5 + y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{4} + x_5 \\ \frac{1}{4} + y_5 \\ -z_5 a \hat{\mathbf{z}} \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + y_5 \\ \frac{1}{4} + y_5 \end{pmatrix} a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}} &= \begin{pmatrix} \frac{1}{4} + x_5 \\ \frac{1}{4} + y_5 \\ \frac{1}{4} + y_5 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + y_5 \\ \frac{1}{4} + y_5 \end{pmatrix} a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{31} &= \begin{pmatrix} -x_5 - y_5 + z_5 \\ \frac{1}{2} + x_5 + y_5 + z_5 \\ x_5 - y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{4} + x_5 \\ \frac{1}{4} + z_5 \\ -y_5 a \hat{\mathbf{y}} + (\frac{1}{4} + z_5) a \hat{\mathbf{z}} \end{pmatrix} a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{4} + z_5 \\ \frac{1}{4} + z_5 \end{pmatrix} a \hat{\mathbf{z}} &= \begin{pmatrix} \frac{1}{4} + x_5 \\ \frac{1}{4} + z_5 \\ \frac{1}{4} + z_5 \end{pmatrix} a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{4} + z_5 \\ \frac{1}{4} + z_5 \end{pmatrix} a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{32} &= \begin{pmatrix} \frac{1}{2} + x_5 + y_5 + z_5 \\ -x_5 - y_5 + z_5 \\ -x_5 + y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} -x_5 a \hat{\mathbf{x}} + (\frac{1}{4} + y_5) a \hat{\mathbf{y}} + (\frac{1}{4} + z_5) a \hat{\mathbf{z}} \end{pmatrix} &= -x_5 a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + y_5 \\ \frac{1}{4} + z_5 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{4} + z_5 \\ \frac{1}{4} + z_5 \end{pmatrix} a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{33} &= \begin{pmatrix} -x_5 - y_5 + z_5 \\ x_5 - y_5 - z_5 \\ -x_5 + y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} -z_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}} \end{pmatrix} &= -z_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{34} &= \begin{pmatrix} \frac{1}{2} + x_5 + y_5 + z_5 \\ -x_5 + y_5 - z_5 \\ x_5 - y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} -z_5 a \hat{\mathbf{x}} + (\frac{1}{4} + x_5) a \hat{\mathbf{y}} + (\frac{1}{4} + y_5) a \hat{\mathbf{z}} \end{pmatrix} &= -z_5 a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + x_5 \\ \frac{1}{4} + y_5 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{4} + y_5 \\ \frac{1}{4} + y_5 \end{pmatrix} a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{35} &= \begin{pmatrix} x_5 - y_5 - z_5 \\ -x_5 - y_5 + z_5 \\ \frac{1}{2} + x_5 + y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{4} + z_5 \\ \frac{1}{4} + x_5 \\ -y_5 a \hat{\mathbf{z}} \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + x_5 \\ \frac{1}{4} + x_5 \end{pmatrix} a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}} &= \begin{pmatrix} \frac{1}{4} + z_5 \\ \frac{1}{4} + x_5 \\ \frac{1}{4} + x_5 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + x_5 \\ \frac{1}{4} + x_5 \end{pmatrix} a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{36} &= \begin{pmatrix} -x_5 + y_5 - z_5 \\ \frac{1}{2} + x_5 + y_5 + z_5 \\ -x_5 - y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{4} + z_5 \\ \frac{1}{4} + z_5 \\ -x_5 a \hat{\mathbf{y}} + (\frac{1}{4} + y_5) a \hat{\mathbf{z}} \end{pmatrix} a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{4} + y_5 \\ \frac{1}{4} + y_5 \end{pmatrix} a \hat{\mathbf{z}} &= \begin{pmatrix} \frac{1}{4} + z_5 \\ \frac{1}{4} + z_5 \\ \frac{1}{4} + y_5 \end{pmatrix} a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{4} + y_5 \\ \frac{1}{4} + y_5 \end{pmatrix} a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{37} &= \begin{pmatrix} -x_5 + y_5 - z_5 \\ -x_5 - y_5 + z_5 \\ x_5 - y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} -y_5 a \hat{\mathbf{x}} - z_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}} \end{pmatrix} &= -y_5 a \hat{\mathbf{x}} - z_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{38} &= \begin{pmatrix} x_5 - y_5 - z_5 \\ \frac{1}{2} + x_5 + y_5 + z_5 \\ -x_5 + y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{4} + y_5 \\ \frac{1}{4} + y_5 \\ -z_5 a \hat{\mathbf{y}} + (\frac{1}{4} + x_5) a \hat{\mathbf{z}} \end{pmatrix} a \hat{\mathbf{x}} - z_5 a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{4} + x_5 \\ \frac{1}{4} + x_5 \end{pmatrix} a \hat{\mathbf{z}} &= \begin{pmatrix} \frac{1}{4} + y_5 \\ \frac{1}{4} + y_5 \\ \frac{1}{4} + x_5 \end{pmatrix} a \hat{\mathbf{x}} - z_5 a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{4} + x_5 \\ \frac{1}{4} + x_5 \end{pmatrix} a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{39} &= \begin{pmatrix} \frac{1}{2} + x_5 + y_5 + z_5 \\ x_5 - y_5 - z_5 \\ -x_5 - y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} -y_5 a \hat{\mathbf{x}} + (\frac{1}{4} + z_5) a \hat{\mathbf{y}} + (\frac{1}{4} + x_5) a \hat{\mathbf{z}} \end{pmatrix} &= -y_5 a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + z_5 \\ \frac{1}{4} + x_5 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{4} + x_5 \\ \frac{1}{4} + x_5 \end{pmatrix} a \hat{\mathbf{z}} & (96g) & \text{Se II} \\
\mathbf{B}_{40} &= \begin{pmatrix} -x_5 - y_5 + z_5 \\ -x_5 + y_5 - z_5 \\ \frac{1}{2} + x_5 + y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{4} + y_5 \\ \frac{1}{4} + z_5 \\ -x_5 a \hat{\mathbf{z}} \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + z_5 \\ \frac{1}{4} + z_5 \end{pmatrix} a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}} &= \begin{pmatrix} \frac{1}{4} + y_5 \\ \frac{1}{4} + z_5 \\ \frac{1}{4} + z_5 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + z_5 \\ \frac{1}{4} + z_5 \end{pmatrix} a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}} & (96g) & \text{Se II}
\end{aligned}$$

## References:

- M. Wachhold and W. S. Sheldrick, *Methanolothermale Synthese von  $Rb_3AsSe_4 \cdot 2Se_6$  und  $Cs_3AsSe_4 \cdot 2Cs_2As_2Se_4 \cdot 6Te_4Se_2$ , zwei Selenidoarsenate mit sechsgliedrigen Chalkogenringen/Methanolothermal Synthesis of  $Rb_3AsSe_4 \cdot 2Se_6$  and*

$Cs_3AsSe_4 \cdot 2Cs_2As_2Se_4 \cdot 6Te_4Se_2$ . *Two Selenidoarsenates with Six-Membered Chalcogen Rings*, Z. Naturforsch. B **52**, 169–175 (1997), doi:[10.1515/znb-1997-0204](https://doi.org/10.1515/znb-1997-0204).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

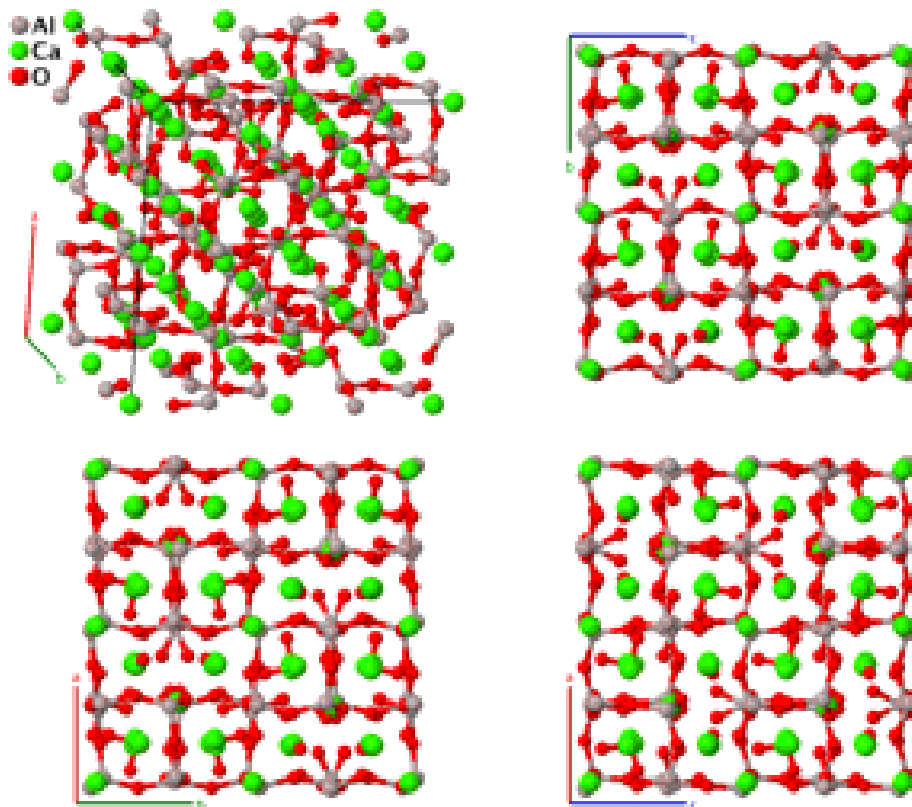
---

**Geometry files:**

- CIF: pp. [954](#)

- POSCAR: pp. [954](#)

# Ca<sub>3</sub>Al<sub>2</sub>O<sub>6</sub> Structure: A2B3C6\_cP264\_205\_2d\_ab2c2d\_6d

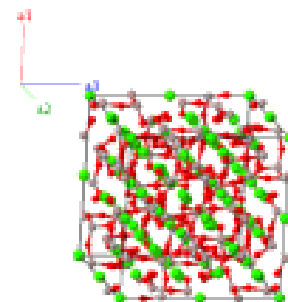


<b>Prototype</b>	:	Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub>
<b>AFLOW prototype label</b>	:	A2B3C6_cP264_205_2d_ab2c2d_6d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cP264
<b>Space group number</b>	:	205
<b>Space group symbol</b>	:	$Pa\bar{3}$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3C6_cP264_205_2d_ab2c2d_6d --params= $a, x_3, x_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}$

- This is a redetermination of the  $E9_1$  (Ca<sub>3</sub>Al<sub>2</sub>O<sub>6</sub>) structure. The lattice constant of the new unit cell is twice the original, giving a volume eight times larger.

**Simple Cubic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= a \hat{y} \\ \mathbf{a}_3 &= a \hat{z} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(4a)	Ca I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4b)	Ca II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(4b)	Ca II
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(4b)	Ca II
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{z}}$	(4b)	Ca II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}}$	(8c)	Ca III
$\mathbf{B}_{10}$	$= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{z}}$	(8c)	Ca III
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{z}}$	(8c)	Ca III
$\mathbf{B}_{12}$	$= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}}$	(8c)	Ca III
$\mathbf{B}_{13}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}}$	(8c)	Ca III
$\mathbf{B}_{14}$	$= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{z}}$	(8c)	Ca III
$\mathbf{B}_{15}$	$= x_3 \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{z}}$	(8c)	Ca III
$\mathbf{B}_{16}$	$= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}}$	(8c)	Ca III
$\mathbf{B}_{17}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}}$	(8c)	Ca IV
$\mathbf{B}_{18}$	$= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{z}}$	(8c)	Ca IV
$\mathbf{B}_{19}$	$= -x_4 \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{z}}$	(8c)	Ca IV
$\mathbf{B}_{20}$	$= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}}$	(8c)	Ca IV
$\mathbf{B}_{21}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}}$	(8c)	Ca IV
$\mathbf{B}_{22}$	$= \left(\frac{1}{2} + x_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{z}}$	(8c)	Ca IV
$\mathbf{B}_{23}$	$= x_4 \mathbf{a}_1 + \left(\frac{1}{2} - x_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{z}}$	(8c)	Ca IV
$\mathbf{B}_{24}$	$= \left(\frac{1}{2} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4\right) \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}}$	(8c)	Ca IV
$\mathbf{B}_{25}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$x_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}} + z_5 a \hat{\mathbf{z}}$	(24d)	Al I
$\mathbf{B}_{26}$	$= \left(\frac{1}{2} - x_5\right) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_5\right) a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_5\right) a \hat{\mathbf{z}}$	(24d)	Al I
$\mathbf{B}_{27}$	$= -x_5 \mathbf{a}_1 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_3$	$=$	$-x_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_5\right) a \hat{\mathbf{z}}$	(24d)	Al I
$\mathbf{B}_{28}$	$= \left(\frac{1}{2} + x_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_5\right) a \hat{\mathbf{y}} - z_5 a \hat{\mathbf{z}}$	(24d)	Al I
$\mathbf{B}_{29}$	$= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$z_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + y_5 a \hat{\mathbf{z}}$	(24d)	Al I
$\mathbf{B}_{30}$	$= \left(\frac{1}{2} + z_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_5\right) \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + z_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}}$	(24d)	Al I
$\mathbf{B}_{31}$	$= \left(\frac{1}{2} - z_5\right) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(\frac{1}{2} + y_5\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - z_5\right) a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_5\right) a \hat{\mathbf{z}}$	(24d)	Al I
$\mathbf{B}_{32}$	$= -z_5 \mathbf{a}_1 + \left(\frac{1}{2} + x_5\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_5\right) \mathbf{a}_3$	$=$	$-z_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_5\right) a \hat{\mathbf{z}}$	(24d)	Al I
$\mathbf{B}_{33}$	$= y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} + z_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(24d)	Al I
$\mathbf{B}_{34}$	$= -y_5 \mathbf{a}_1 + \left(\frac{1}{2} + z_5\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_5\right) \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_5\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_5\right) a \hat{\mathbf{z}}$	(24d)	Al I
$\mathbf{B}_{35}$	$= \left(\frac{1}{2} + y_5\right) \mathbf{a}_1 + \left(\frac{1}{2} - z_5\right) \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + y_5\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_5\right) a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(24d)	Al I















$$\begin{aligned}
\mathbf{B}_{242} &= \left(\frac{1}{2} - x_{14}\right) \mathbf{a}_1 - y_{14} \mathbf{a}_2 + \left(\frac{1}{2} + z_{14}\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_{14}\right) a \hat{\mathbf{x}} - y_{14} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{14}\right) a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{243} &= -x_{14} \mathbf{a}_1 + \left(\frac{1}{2} + y_{14}\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_{14}\right) \mathbf{a}_3 = -x_{14} a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_{14}\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{14}\right) a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{244} &= \left(\frac{1}{2} + x_{14}\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_{14}\right) \mathbf{a}_2 - z_{14} \mathbf{a}_3 = \left(\frac{1}{2} + x_{14}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_{14}\right) a \hat{\mathbf{y}} - z_{14} a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{245} &= z_{14} \mathbf{a}_1 + x_{14} \mathbf{a}_2 + y_{14} \mathbf{a}_3 = z_{14} a \hat{\mathbf{x}} + x_{14} a \hat{\mathbf{y}} + y_{14} a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{246} &= \left(\frac{1}{2} + z_{14}\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_{14}\right) \mathbf{a}_2 - y_{14} \mathbf{a}_3 = \left(\frac{1}{2} + z_{14}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_{14}\right) a \hat{\mathbf{y}} - y_{14} a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{247} &= \left(\frac{1}{2} - z_{14}\right) \mathbf{a}_1 - x_{14} \mathbf{a}_2 + \left(\frac{1}{2} + y_{14}\right) \mathbf{a}_3 = \left(\frac{1}{2} - z_{14}\right) a \hat{\mathbf{x}} - x_{14} a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_{14}\right) a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{248} &= -z_{14} \mathbf{a}_1 + \left(\frac{1}{2} + x_{14}\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_{14}\right) \mathbf{a}_3 = -z_{14} a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_{14}\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_{14}\right) a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{249} &= y_{14} \mathbf{a}_1 + z_{14} \mathbf{a}_2 + x_{14} \mathbf{a}_3 = y_{14} a \hat{\mathbf{x}} + z_{14} a \hat{\mathbf{y}} + x_{14} a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{250} &= -y_{14} \mathbf{a}_1 + \left(\frac{1}{2} + z_{14}\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_{14}\right) \mathbf{a}_3 = -y_{14} a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_{14}\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_{14}\right) a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{251} &= \left(\frac{1}{2} + y_{14}\right) \mathbf{a}_1 + \left(\frac{1}{2} - z_{14}\right) \mathbf{a}_2 - x_{14} \mathbf{a}_3 = \left(\frac{1}{2} + y_{14}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_{14}\right) a \hat{\mathbf{y}} - x_{14} a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{252} &= \left(\frac{1}{2} - y_{14}\right) \mathbf{a}_1 - z_{14} \mathbf{a}_2 + \left(\frac{1}{2} + x_{14}\right) \mathbf{a}_3 = \left(\frac{1}{2} - y_{14}\right) a \hat{\mathbf{x}} - z_{14} a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_{14}\right) a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{253} &= -x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3 = -x_{14} a \hat{\mathbf{x}} - y_{14} a \hat{\mathbf{y}} - z_{14} a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{254} &= \left(\frac{1}{2} + x_{14}\right) \mathbf{a}_1 + y_{14} \mathbf{a}_2 + \left(\frac{1}{2} - z_{14}\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_{14}\right) a \hat{\mathbf{x}} + y_{14} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{14}\right) a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{255} &= x_{14} \mathbf{a}_1 + \left(\frac{1}{2} - y_{14}\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_{14}\right) \mathbf{a}_3 = x_{14} a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_{14}\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{14}\right) a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{256} &= \left(\frac{1}{2} - x_{14}\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_{14}\right) \mathbf{a}_2 + z_{14} \mathbf{a}_3 = \left(\frac{1}{2} - x_{14}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_{14}\right) a \hat{\mathbf{y}} + z_{14} a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{257} &= -z_{14} \mathbf{a}_1 - x_{14} \mathbf{a}_2 - y_{14} \mathbf{a}_3 = -z_{14} a \hat{\mathbf{x}} - x_{14} a \hat{\mathbf{y}} - y_{14} a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{258} &= \left(\frac{1}{2} - z_{14}\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_{14}\right) \mathbf{a}_2 + y_{14} \mathbf{a}_3 = \left(\frac{1}{2} - z_{14}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_{14}\right) a \hat{\mathbf{y}} + y_{14} a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{259} &= \left(\frac{1}{2} + z_{14}\right) \mathbf{a}_1 + x_{14} \mathbf{a}_2 + \left(\frac{1}{2} - y_{14}\right) \mathbf{a}_3 = \left(\frac{1}{2} + z_{14}\right) a \hat{\mathbf{x}} + x_{14} a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_{14}\right) a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{260} &= z_{14} \mathbf{a}_1 + \left(\frac{1}{2} - x_{14}\right) \mathbf{a}_2 + \left(\frac{1}{2} + y_{14}\right) \mathbf{a}_3 = z_{14} a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_{14}\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_{14}\right) a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{261} &= -y_{14} \mathbf{a}_1 - z_{14} \mathbf{a}_2 - x_{14} \mathbf{a}_3 = -y_{14} a \hat{\mathbf{x}} - z_{14} a \hat{\mathbf{y}} - x_{14} a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{262} &= y_{14} \mathbf{a}_1 + \left(\frac{1}{2} - z_{14}\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_{14}\right) \mathbf{a}_3 = y_{14} a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_{14}\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_{14}\right) a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{263} &= \left(\frac{1}{2} - y_{14}\right) \mathbf{a}_1 + \left(\frac{1}{2} + z_{14}\right) \mathbf{a}_2 + x_{14} \mathbf{a}_3 = \left(\frac{1}{2} - y_{14}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_{14}\right) a \hat{\mathbf{y}} + x_{14} a \hat{\mathbf{z}} & (24d) & \text{O VI} \\
\mathbf{B}_{264} &= \left(\frac{1}{2} + y_{14}\right) \mathbf{a}_1 + z_{14} \mathbf{a}_2 + \left(\frac{1}{2} - x_{14}\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_{14}\right) a \hat{\mathbf{x}} + z_{14} a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_{14}\right) a \hat{\mathbf{z}} & (24d) & \text{O VI}
\end{aligned}$$

---

## References:

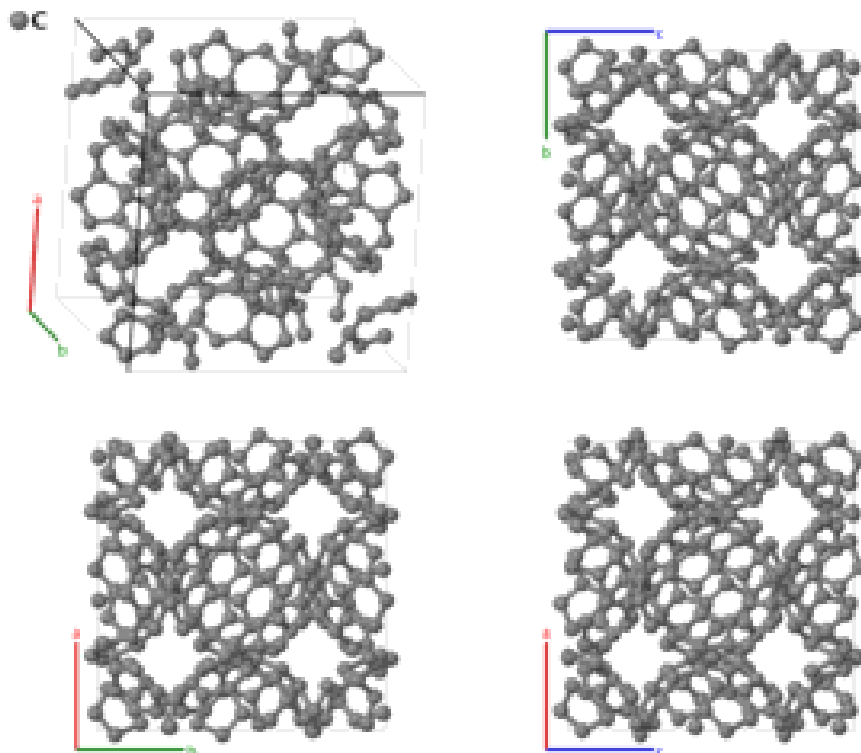
- P. Mondal and J. W. Jeffery, *The crystal structure of tricalcium aluminate, Ca<sub>3</sub>Al<sub>2</sub>O<sub>6</sub>*, Acta Crystallogr. Sect. B Struct. Sci. **31**, 689–697 (1975), doi:10.1107/S0567740875003639.

---

## Geometry files:

- CIF: pp. 955  
- POSCAR: pp. 955

# Simple Cubic C<sub>60</sub> Buckminsterfullerine Structure: A\_cP240\_205\_10d



<b>Prototype</b>	:	C
<b>AFLOW prototype label</b>	:	A_cP240_205_10d
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cP240
<b>Space group number</b>	:	205
<b>Space group symbol</b>	:	$Pa\bar{3}$
<b>AFLOW prototype command</b>	:	aflow --proto=A_cP240_205_10d --params= $a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

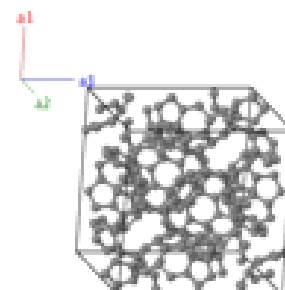
- This is the experimentally determined structure of C<sub>60</sub> buckminsterfullerene (*a.k.a.* “buckyballs”) below 249 K. Above that temperature the C<sub>60</sub> molecules are orientationally disordered and set on a face-centered cubic lattice. For computational purposes that structure is approximated by the [FCC C<sub>60</sub> buckminsterfullerine structure](#).

**Simple Cubic primitive vectors:**

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$





**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + z_1 a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_2$	$= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_4$	$= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) a \hat{\mathbf{y}} - z_1 a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_5$	$= z_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	$= z_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + y_1 a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_6$	$= \left(\frac{1}{2} + z_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_1\right) \mathbf{a}_2 - y_1 \mathbf{a}_3$	$= \left(\frac{1}{2} + z_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{y}} - y_1 a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_7$	$= \left(\frac{1}{2} - z_1\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - z_1\right) a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_1\right) a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_8$	$= -z_1 \mathbf{a}_1 + \left(\frac{1}{2} + x_1\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_3$	$= -z_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_1\right) a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_9$	$= y_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$= y_1 a \hat{\mathbf{x}} + z_1 a \hat{\mathbf{y}} + x_1 a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{10}$	$= -y_1 \mathbf{a}_1 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_1\right) \mathbf{a}_3$	$= -y_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{11}$	$= \left(\frac{1}{2} + y_1\right) \mathbf{a}_1 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_2 - x_1 \mathbf{a}_3$	$= \left(\frac{1}{2} + y_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_1\right) a \hat{\mathbf{y}} - x_1 a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{12}$	$= \left(\frac{1}{2} - y_1\right) \mathbf{a}_1 - z_1 \mathbf{a}_2 + \left(\frac{1}{2} + x_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - y_1\right) a \hat{\mathbf{x}} - z_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{13}$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}} - z_1 a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{14}$	$= \left(\frac{1}{2} + x_1\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_1\right) a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{15}$	$= x_1 \mathbf{a}_1 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_1\right) a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{16}$	$= \left(\frac{1}{2} - x_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_1\right) a \hat{\mathbf{y}} + z_1 a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{17}$	$= -z_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	$= -z_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} - y_1 a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{18}$	$= \left(\frac{1}{2} - z_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_1\right) \mathbf{a}_2 + y_1 \mathbf{a}_3$	$= \left(\frac{1}{2} - z_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{y}} + y_1 a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{19}$	$= \left(\frac{1}{2} + z_1\right) \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(\frac{1}{2} - y_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} + z_1\right) a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_1\right) a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{20}$	$= z_1 \mathbf{a}_1 + \left(\frac{1}{2} - x_1\right) \mathbf{a}_2 + \left(\frac{1}{2} + y_1\right) \mathbf{a}_3$	$= z_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_1\right) a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{21}$	$= -y_1 \mathbf{a}_1 - z_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$= -y_1 a \hat{\mathbf{x}} - z_1 a \hat{\mathbf{y}} - x_1 a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{22}$	$= y_1 \mathbf{a}_1 + \left(\frac{1}{2} - z_1\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_1\right) \mathbf{a}_3$	$= y_1 a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_1\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_1\right) a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{23}$	$= \left(\frac{1}{2} - y_1\right) \mathbf{a}_1 + \left(\frac{1}{2} + z_1\right) \mathbf{a}_2 + x_1 \mathbf{a}_3$	$= \left(\frac{1}{2} - y_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_1\right) a \hat{\mathbf{y}} + x_1 a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{24}$	$= \left(\frac{1}{2} + y_1\right) \mathbf{a}_1 + z_1 \mathbf{a}_2 + \left(\frac{1}{2} - x_1\right) \mathbf{a}_3$	$= \left(\frac{1}{2} + y_1\right) a \hat{\mathbf{x}} + z_1 a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_1\right) a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{25}$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 a \hat{\mathbf{z}}$	(24d)	C II
$\mathbf{B}_{26}$	$= \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_2\right) a \hat{\mathbf{z}}$	(24d)	C II
$\mathbf{B}_{27}$	$= -x_2 \mathbf{a}_1 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_2\right) \mathbf{a}_3$	$= -x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_2\right) a \hat{\mathbf{z}}$	(24d)	C II
$\mathbf{B}_{28}$	$= \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$= \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{y}} - z_2 a \hat{\mathbf{z}}$	(24d)	C II
$\mathbf{B}_{29}$	$= z_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + y_2 \mathbf{a}_3$	$= z_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + y_2 a \hat{\mathbf{z}}$	(24d)	C II
$\mathbf{B}_{30}$	$= \left(\frac{1}{2} + z_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 - y_2 \mathbf{a}_3$	$= \left(\frac{1}{2} + z_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} - y_2 a \hat{\mathbf{z}}$	(24d)	C II
$\mathbf{B}_{31}$	$= \left(\frac{1}{2} - z_2\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{2} + y_2\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - z_2\right) a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{z}}$	(24d)	C II
$\mathbf{B}_{32}$	$= -z_2 \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_2\right) \mathbf{a}_3$	$= -z_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{z}}$	(24d)	C II
$\mathbf{B}_{33}$	$= y_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$= y_2 a \hat{\mathbf{x}} + z_2 a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}}$	(24d)	C II
$\mathbf{B}_{34}$	$= -y_2 \mathbf{a}_1 + \left(\frac{1}{2} + z_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_3$	$= -y_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{z}}$	(24d)	C II











$$\begin{aligned}
\mathbf{B}_{215} &= \left(\frac{1}{2} - y_9\right) \mathbf{a}_1 + \left(\frac{1}{2} + z_9\right) \mathbf{a}_2 + x_9 \mathbf{a}_3 = \left(\frac{1}{2} - y_9\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_9\right) a \hat{\mathbf{y}} + x_9 a \hat{\mathbf{z}} & (24d) & \text{C IX} \\
\mathbf{B}_{216} &= \left(\frac{1}{2} + y_9\right) \mathbf{a}_1 + z_9 \mathbf{a}_2 + \left(\frac{1}{2} - x_9\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_9\right) a \hat{\mathbf{x}} + z_9 a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_9\right) a \hat{\mathbf{z}} & (24d) & \text{C IX} \\
\mathbf{B}_{217} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = x_{10} a \hat{\mathbf{x}} + y_{10} a \hat{\mathbf{y}} + z_{10} a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{218} &= \left(\frac{1}{2} - x_{10}\right) \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_{10}\right) a \hat{\mathbf{x}} - y_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{219} &= -x_{10} \mathbf{a}_1 + \left(\frac{1}{2} + y_{10}\right) \mathbf{a}_2 + \left(\frac{1}{2} - z_{10}\right) \mathbf{a}_3 = -x_{10} a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_{10}\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{10}\right) a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{220} &= \left(\frac{1}{2} + x_{10}\right) \mathbf{a}_1 + \left(\frac{1}{2} - y_{10}\right) \mathbf{a}_2 - z_{10} \mathbf{a}_3 = \left(\frac{1}{2} + x_{10}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_{10}\right) a \hat{\mathbf{y}} - z_{10} a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{221} &= z_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + y_{10} \mathbf{a}_3 = z_{10} a \hat{\mathbf{x}} + x_{10} a \hat{\mathbf{y}} + y_{10} a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{222} &= \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_{10}\right) \mathbf{a}_2 - y_{10} \mathbf{a}_3 = \left(\frac{1}{2} + z_{10}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_{10}\right) a \hat{\mathbf{y}} - y_{10} a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{223} &= \left(\frac{1}{2} - z_{10}\right) \mathbf{a}_1 - x_{10} \mathbf{a}_2 + \left(\frac{1}{2} + y_{10}\right) \mathbf{a}_3 = \left(\frac{1}{2} - z_{10}\right) a \hat{\mathbf{x}} - x_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_{10}\right) a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{224} &= -z_{10} \mathbf{a}_1 + \left(\frac{1}{2} + x_{10}\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_{10}\right) \mathbf{a}_3 = -z_{10} a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_{10}\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_{10}\right) a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{225} &= y_{10} \mathbf{a}_1 + z_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3 = y_{10} a \hat{\mathbf{x}} + z_{10} a \hat{\mathbf{y}} + x_{10} a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{226} &= -y_{10} \mathbf{a}_1 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_{10}\right) \mathbf{a}_3 = -y_{10} a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_{10}\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_{10}\right) a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{227} &= \left(\frac{1}{2} + y_{10}\right) \mathbf{a}_1 + \left(\frac{1}{2} - z_{10}\right) \mathbf{a}_2 - x_{10} \mathbf{a}_3 = \left(\frac{1}{2} + y_{10}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_{10}\right) a \hat{\mathbf{y}} - x_{10} a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{228} &= \left(\frac{1}{2} - y_{10}\right) \mathbf{a}_1 - z_{10} \mathbf{a}_2 + \left(\frac{1}{2} + x_{10}\right) \mathbf{a}_3 = \left(\frac{1}{2} - y_{10}\right) a \hat{\mathbf{x}} - z_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_{10}\right) a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{229} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 = -x_{10} a \hat{\mathbf{x}} - y_{10} a \hat{\mathbf{y}} - z_{10} a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{230} &= \left(\frac{1}{2} + x_{10}\right) \mathbf{a}_1 + y_{10} \mathbf{a}_2 + \left(\frac{1}{2} - z_{10}\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_{10}\right) a \hat{\mathbf{x}} + y_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_{10}\right) a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{231} &= x_{10} \mathbf{a}_1 + \left(\frac{1}{2} - y_{10}\right) \mathbf{a}_2 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_3 = x_{10} a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_{10}\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_{10}\right) a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{232} &= \left(\frac{1}{2} - x_{10}\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_{10}\right) \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \left(\frac{1}{2} - x_{10}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_{10}\right) a \hat{\mathbf{y}} + z_{10} a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{233} &= -z_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - y_{10} \mathbf{a}_3 = -z_{10} a \hat{\mathbf{x}} - x_{10} a \hat{\mathbf{y}} - y_{10} a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{234} &= \left(\frac{1}{2} - z_{10}\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_{10}\right) \mathbf{a}_2 + y_{10} \mathbf{a}_3 = \left(\frac{1}{2} - z_{10}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_{10}\right) a \hat{\mathbf{y}} + y_{10} a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{235} &= \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_1 + x_{10} \mathbf{a}_2 + \left(\frac{1}{2} - y_{10}\right) \mathbf{a}_3 = \left(\frac{1}{2} + z_{10}\right) a \hat{\mathbf{x}} + x_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_{10}\right) a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{236} &= z_{10} \mathbf{a}_1 + \left(\frac{1}{2} - x_{10}\right) \mathbf{a}_2 + \left(\frac{1}{2} + y_{10}\right) \mathbf{a}_3 = z_{10} a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_{10}\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_{10}\right) a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{237} &= -y_{10} \mathbf{a}_1 - z_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3 = -y_{10} a \hat{\mathbf{x}} - z_{10} a \hat{\mathbf{y}} - x_{10} a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{238} &= y_{10} \mathbf{a}_1 + \left(\frac{1}{2} - z_{10}\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_{10}\right) \mathbf{a}_3 = y_{10} a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_{10}\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_{10}\right) a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{239} &= \left(\frac{1}{2} - y_{10}\right) \mathbf{a}_1 + \left(\frac{1}{2} + z_{10}\right) \mathbf{a}_2 + x_{10} \mathbf{a}_3 = \left(\frac{1}{2} - y_{10}\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_{10}\right) a \hat{\mathbf{y}} + x_{10} a \hat{\mathbf{z}} & (24d) & \text{C X} \\
\mathbf{B}_{240} &= \left(\frac{1}{2} + y_{10}\right) \mathbf{a}_1 + z_{10} \mathbf{a}_2 + \left(\frac{1}{2} - x_{10}\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_{10}\right) a \hat{\mathbf{x}} + z_{10} a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_{10}\right) a \hat{\mathbf{z}} & (24d) & \text{C X}
\end{aligned}$$

---

### References:

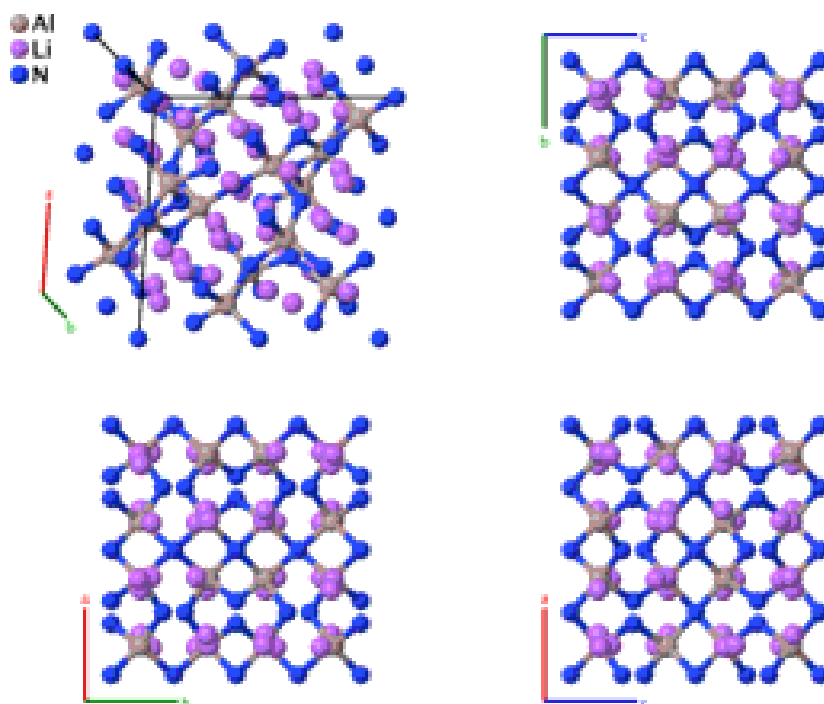
- W. I. F. David, R. M. Ibberson, J. C. Matthewman, K. Prassides, T. J. S. Dennis, J. P. Hare, H. W. Kroto, R. Taylor, and D. R. M. Walton, *Crystal structure and bonding of ordered C<sub>60</sub>*, *Nature* **353**, 147–149 (1991), [doi:10.1038/353147a0](https://doi.org/10.1038/353147a0).

---

### Geometry files:

- CIF: pp. [957](#)  
- POSCAR: pp. [957](#)

# AlLi<sub>3</sub>N<sub>2</sub> (*E9<sub>d</sub>*) Structure: AB3C2\_cI96\_206\_c\_e\_ad



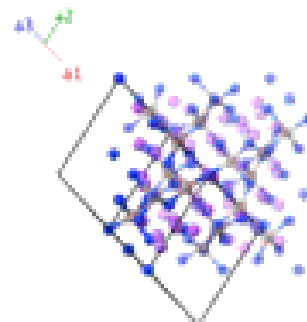
<b>Prototype</b>	:	AlLi <sub>3</sub> N <sub>2</sub>
<b>AFLOW prototype label</b>	:	AB3C2_cI96_206_c_e_ad
<b>Strukturbericht designation</b>	:	<i>E9<sub>d</sub></i>
<b>Pearson symbol</b>	:	cI96
<b>Space group number</b>	:	206
<b>Space group symbol</b>	:	<i>Ia</i> $\bar{3}$
<b>AFLOW prototype command</b>	:	aflow --proto=AB3C2_cI96_206_c_e_ad --params= <i>a</i> , <i>x</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub>

## Other compounds with this structure:

- GaLi<sub>3</sub>N<sub>2</sub>, ScLi<sub>3</sub>N<sub>2</sub>, TiLi<sub>3</sub>N<sub>2</sub>, ZnLi<sub>3</sub>N<sub>2</sub>, SiLi<sub>3</sub>N<sub>2</sub>, GeLi<sub>3</sub>N<sub>2</sub>

## Body-centered Cubic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} a \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type



$$\begin{aligned}
\mathbf{B}_1 &= 0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3 &= 0\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}} & (8a) & \text{NI} \\
\mathbf{B}_2 &= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{y}} & (8a) & \text{NI} \\
\mathbf{B}_3 &= \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} & (8a) & \text{NI} \\
\mathbf{B}_4 &= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{z}} & (8a) & \text{NI} \\
\mathbf{B}_5 &= 2x_2\mathbf{a}_1 + 2x_2\mathbf{a}_2 + 2x_2\mathbf{a}_3 &= x_2a\hat{\mathbf{x}} + x_2a\hat{\mathbf{y}} + x_2a\hat{\mathbf{z}} & (16c) & \text{Al} \\
\mathbf{B}_6 &= \frac{1}{2}\mathbf{a}_1 + \left(\frac{1}{2} - 2x_2\right)\mathbf{a}_3 &= -x_2a\hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right)a\hat{\mathbf{y}} + x_2a\hat{\mathbf{z}} & (16c) & \text{Al} \\
\mathbf{B}_7 &= \left(\frac{1}{2} - 2x_2\right)\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right)a\hat{\mathbf{x}} + x_2a\hat{\mathbf{y}} - x_2a\hat{\mathbf{z}} & (16c) & \text{Al} \\
\mathbf{B}_8 &= \left(\frac{1}{2} - 2x_2\right)\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 &= x_2a\hat{\mathbf{x}} - x_2a\hat{\mathbf{y}} + \left(\frac{1}{2} - x_2\right)a\hat{\mathbf{z}} & (16c) & \text{Al} \\
\mathbf{B}_9 &= -2x_2\mathbf{a}_1 - 2x_2\mathbf{a}_2 - 2x_2\mathbf{a}_3 &= -x_2a\hat{\mathbf{x}} - x_2a\hat{\mathbf{y}} - x_2a\hat{\mathbf{z}} & (16c) & \text{Al} \\
\mathbf{B}_{10} &= \frac{1}{2}\mathbf{a}_1 + \left(\frac{1}{2} + 2x_2\right)\mathbf{a}_3 &= x_2a\hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right)a\hat{\mathbf{y}} - x_2a\hat{\mathbf{z}} & (16c) & \text{Al} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} + 2x_2\right)\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3 &= \left(\frac{1}{2} + x_2\right)a\hat{\mathbf{x}} - x_2a\hat{\mathbf{y}} + x_2a\hat{\mathbf{z}} & (16c) & \text{Al} \\
\mathbf{B}_{12} &= \left(\frac{1}{2} + 2x_2\right)\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 &= -x_2a\hat{\mathbf{x}} + x_2a\hat{\mathbf{y}} + \left(\frac{1}{2} + x_2\right)a\hat{\mathbf{z}} & (16c) & \text{Al} \\
\mathbf{B}_{13} &= \frac{1}{4}\mathbf{a}_1 + \left(\frac{1}{4} + x_3\right)\mathbf{a}_2 + x_3\mathbf{a}_3 &= x_3a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}} & (24d) & \text{N II} \\
\mathbf{B}_{14} &= \frac{3}{4}\mathbf{a}_1 + \left(\frac{1}{4} - x_3\right)\mathbf{a}_2 + \left(\frac{1}{2} - x_3\right)\mathbf{a}_3 &= -x_3a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}} & (24d) & \text{N II} \\
\mathbf{B}_{15} &= x_3\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \left(\frac{1}{4} + x_3\right)\mathbf{a}_3 &= \frac{1}{4}a\hat{\mathbf{x}} + x_3a\hat{\mathbf{y}} & (24d) & \text{N II} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} - x_3\right)\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \left(\frac{1}{4} - x_3\right)\mathbf{a}_3 &= \frac{1}{4}a\hat{\mathbf{x}} - x_3a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} & (24d) & \text{N II} \\
\mathbf{B}_{17} &= \left(\frac{1}{4} + x_3\right)\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3 &= \frac{1}{4}a\hat{\mathbf{y}} + x_3a\hat{\mathbf{z}} & (24d) & \text{N II} \\
\mathbf{B}_{18} &= \left(\frac{1}{4} - x_3\right)\mathbf{a}_1 + \left(\frac{1}{2} - x_3\right)\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - x_3a\hat{\mathbf{z}} & (24d) & \text{N II} \\
\mathbf{B}_{19} &= \frac{3}{4}\mathbf{a}_1 + \left(\frac{3}{4} - x_3\right)\mathbf{a}_2 - x_3\mathbf{a}_3 &= -x_3a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{z}} & (24d) & \text{N II} \\
\mathbf{B}_{20} &= \frac{1}{4}\mathbf{a}_1 + \left(\frac{3}{4} + x_3\right)\mathbf{a}_2 + \left(\frac{1}{2} + x_3\right)\mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right)a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}} & (24d) & \text{N II} \\
\mathbf{B}_{21} &= -x_3\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \left(\frac{3}{4} - x_3\right)\mathbf{a}_3 &= \frac{3}{4}a\hat{\mathbf{x}} - x_3a\hat{\mathbf{y}} & (24d) & \text{N II} \\
\mathbf{B}_{22} &= \left(\frac{1}{2} + x_3\right)\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \left(\frac{3}{4} + x_3\right)\mathbf{a}_3 &= \frac{1}{4}a\hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right)a\hat{\mathbf{y}} & (24d) & \text{N II} \\
\mathbf{B}_{23} &= \left(\frac{3}{4} - x_3\right)\mathbf{a}_1 - x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3 &= \frac{3}{4}a\hat{\mathbf{y}} - x_3a\hat{\mathbf{z}} & (24d) & \text{N II} \\
\mathbf{B}_{24} &= \left(\frac{3}{4} + x_3\right)\mathbf{a}_1 + \left(\frac{1}{2} + x_3\right)\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3 &= \frac{1}{4}a\hat{\mathbf{y}} + \left(\frac{1}{2} + x_3\right)a\hat{\mathbf{z}} & (24d) & \text{N II} \\
\mathbf{B}_{25} &= (y_4 + z_4)\mathbf{a}_1 + (x_4 + z_4)\mathbf{a}_2 + (x_4 + y_4)\mathbf{a}_3 &= x_4a\hat{\mathbf{x}} + y_4a\hat{\mathbf{y}} + z_4a\hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{26} &= \left(\frac{1}{2} - y_4 + z_4\right)\mathbf{a}_1 + (-x_4 + z_4)\mathbf{a}_2 + \left(\frac{1}{2} - x_4 - y_4\right)\mathbf{a}_3 &= -x_4a\hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right)a\hat{\mathbf{y}} + z_4a\hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{27} &= (y_4 - z_4)\mathbf{a}_1 + \left(\frac{1}{2} - x_4 - z_4\right)\mathbf{a}_2 + \left(\frac{1}{2} - x_4 + y_4\right)\mathbf{a}_3 &= \left(\frac{1}{2} - x_4\right)a\hat{\mathbf{x}} + y_4a\hat{\mathbf{y}} - z_4a\hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{28} &= \left(\frac{1}{2} - y_4 - z_4\right)\mathbf{a}_1 + \left(\frac{1}{2} + x_4 - z_4\right)\mathbf{a}_2 + (x_4 - y_4)\mathbf{a}_3 &= x_4a\hat{\mathbf{x}} - y_4a\hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right)a\hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{29} &= (x_4 + y_4)\mathbf{a}_1 + (y_4 + z_4)\mathbf{a}_2 + (x_4 + z_4)\mathbf{a}_3 &= z_4a\hat{\mathbf{x}} + x_4a\hat{\mathbf{y}} + y_4a\hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{30} &= \left(\frac{1}{2} - x_4 - y_4\right)\mathbf{a}_1 + \left(\frac{1}{2} - y_4 + z_4\right)\mathbf{a}_2 + (-x_4 + z_4)\mathbf{a}_3 &= z_4a\hat{\mathbf{x}} - x_4a\hat{\mathbf{y}} + \left(\frac{1}{2} - y_4\right)a\hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{31} &= \left(\frac{1}{2} - x_4 + y_4\right)\mathbf{a}_1 + (y_4 - z_4)\mathbf{a}_2 + \left(\frac{1}{2} - x_4 - z_4\right)\mathbf{a}_3 &= -z_4a\hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right)a\hat{\mathbf{y}} + y_4a\hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{32} &= (x_4 - y_4)\mathbf{a}_1 + \left(\frac{1}{2} - y_4 - z_4\right)\mathbf{a}_2 + \left(\frac{1}{2} + x_4 - z_4\right)\mathbf{a}_3 &= \left(\frac{1}{2} - z_4\right)a\hat{\mathbf{x}} + x_4a\hat{\mathbf{y}} - y_4a\hat{\mathbf{z}} & (48e) & \text{Li}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{33} &= (x_4 + z_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3 = y_4 a \hat{\mathbf{x}} + z_4 a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{34} &= (-x_4 + z_4) \mathbf{a}_1 + \left(\frac{1}{2} - x_4 - y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - y_4 + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{x}} + z_4 a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{35} &= \left(\frac{1}{2} - x_4 - z_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4 + y_4\right) \mathbf{a}_2 + (y_4 - z_4) \mathbf{a}_3 = y_4 a \hat{\mathbf{x}} - z_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{36} &= \left(\frac{1}{2} + x_4 - z_4\right) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \left(\frac{1}{2} - y_4 - z_4\right) \mathbf{a}_3 = -y_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_4\right) a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{37} &= (-y_4 - z_4) \mathbf{a}_1 + (-x_4 - z_4) \mathbf{a}_2 + (-x_4 - y_4) \mathbf{a}_3 = -x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} - z_4 a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{38} &= \left(\frac{1}{2} + y_4 - z_4\right) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + \left(\frac{1}{2} + x_4 + y_4\right) \mathbf{a}_3 = x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{y}} - z_4 a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{39} &= (-y_4 + z_4) \mathbf{a}_1 + \left(\frac{1}{2} + x_4 + z_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_4 - y_4\right) \mathbf{a}_3 = \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + z_4 a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{40} &= \left(\frac{1}{2} + y_4 + z_4\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_4 + z_4\right) \mathbf{a}_2 + (-x_4 + y_4) \mathbf{a}_3 = -x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_4\right) a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{41} &= (-x_4 - y_4) \mathbf{a}_1 + (-y_4 - z_4) \mathbf{a}_2 + (-x_4 - z_4) \mathbf{a}_3 = -z_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - y_4 a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{42} &= \left(\frac{1}{2} + x_4 + y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + y_4 - z_4\right) \mathbf{a}_2 + (x_4 - z_4) \mathbf{a}_3 = -z_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{43} &= \left(\frac{1}{2} + x_4 - y_4\right) \mathbf{a}_1 + (-y_4 + z_4) \mathbf{a}_2 + \left(\frac{1}{2} + x_4 + z_4\right) \mathbf{a}_3 = z_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{y}} - y_4 a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{44} &= (-x_4 + y_4) \mathbf{a}_1 + \left(\frac{1}{2} + y_4 + z_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_4 + z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} + z_4\right) a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + y_4 a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{45} &= (-x_4 - z_4) \mathbf{a}_1 + (-x_4 - y_4) \mathbf{a}_2 + (-y_4 - z_4) \mathbf{a}_3 = -y_4 a \hat{\mathbf{x}} - z_4 a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{46} &= (x_4 - z_4) \mathbf{a}_1 + \left(\frac{1}{2} + x_4 + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + y_4 - z_4\right) \mathbf{a}_3 = \left(\frac{1}{2} + y_4\right) a \hat{\mathbf{x}} - z_4 a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{47} &= \left(\frac{1}{2} + x_4 + z_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4 - y_4\right) \mathbf{a}_2 + (-y_4 + z_4) \mathbf{a}_3 = -y_4 a \hat{\mathbf{x}} + z_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_4\right) a \hat{\mathbf{z}} & (48e) & \text{Li} \\
\mathbf{B}_{48} &= \left(\frac{1}{2} - x_4 + z_4\right) \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + \left(\frac{1}{2} + y_4 + z_4\right) \mathbf{a}_3 = y_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_4\right) a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}} & (48e) & \text{Li}
\end{aligned}$$

---

### References:

- R. Juza and F. Hund, *Die ternären Nitride Li<sub>3</sub>AlN<sub>2</sub> und Li<sub>3</sub>GaN<sub>2</sub>. 17. Mitteilung über Metallamide und Metallnitride*, Z. Anorg. Allg. Chem. **257**, 13–25 (1948), [doi:10.1002/zaac.19482570102](https://doi.org/10.1002/zaac.19482570102).

### Found in:

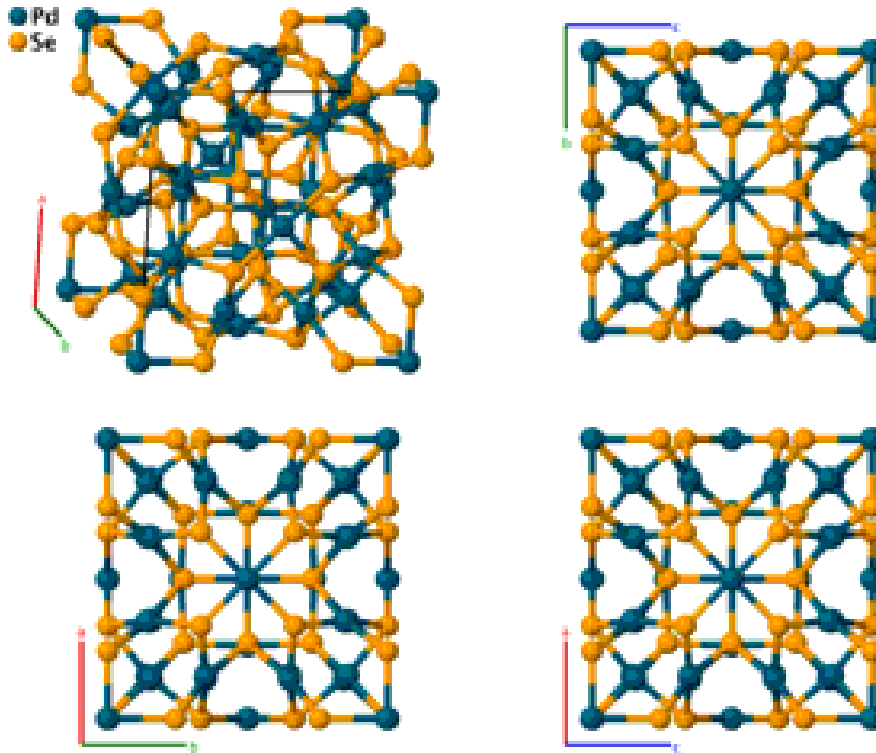
- J. F. Herbst and L. G. Hector, Jr., *Exploration of the formation of XLi<sub>3</sub>N<sub>2</sub> compounds (X=Sc-Zn) by means of density functional theory*, Phys. Rev. B **85**, 195137 (2012), [doi:10.1103/PhysRevB.85.195137](https://doi.org/10.1103/PhysRevB.85.195137).

---

### Geometry files:

- CIF: pp. [958](#)  
- POSCAR: pp. [959](#)

# Pd<sub>17</sub>Se<sub>15</sub> Structure: A17B15\_cP64\_207\_acfk\_eij



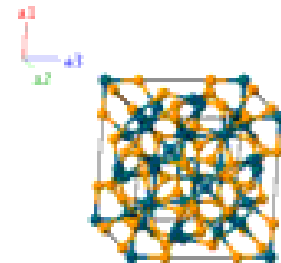
**Prototype** : Pd<sub>17</sub>Se<sub>15</sub>  
**AFLOW prototype label** : A17B15\_cP64\_207\_acfk\_eij  
**Strukturbericht designation** : None  
**Pearson symbol** : cP64  
**Space group number** : 207  
**Space group symbol** : *P*432  
**AFLOW prototype command** : aflow --proto=A17B15\_cP64\_207\_acfk\_eij  
 --params=*a*, *x*<sub>3</sub>, *x*<sub>4</sub>, *y*<sub>5</sub>, *y*<sub>6</sub>, *x*<sub>7</sub>, *y*<sub>7</sub>, *z*<sub>7</sub>

Simple Cubic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a)	Pd I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c)	Pd II

$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c)	Pd II
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(3c)	Pd II
$\mathbf{B}_5$	$=$	$x_3 \mathbf{a}_1$	$=$	$x_3 a \hat{\mathbf{x}}$	(6e)	Se I
$\mathbf{B}_6$	$=$	$-x_3 \mathbf{a}_1$	$=$	$-x_3 a \hat{\mathbf{x}}$	(6e)	Se I
$\mathbf{B}_7$	$=$	$x_3 \mathbf{a}_2$	$=$	$x_3 a \hat{\mathbf{y}}$	(6e)	Se I
$\mathbf{B}_8$	$=$	$-x_3 \mathbf{a}_2$	$=$	$-x_3 a \hat{\mathbf{y}}$	(6e)	Se I
$\mathbf{B}_9$	$=$	$x_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{z}}$	(6e)	Se I
$\mathbf{B}_{10}$	$=$	$-x_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{z}}$	(6e)	Se I
$\mathbf{B}_{11}$	$=$	$x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$x_4 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B}_{12}$	$=$	$-x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-x_4 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B}_{13}$	$=$	$\frac{1}{2} \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B}_{14}$	$=$	$\frac{1}{2} \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B}_{15}$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B}_{16}$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B}_{17}$	$=$	$y_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{y}} + y_5 a \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{18}$	$=$	$-y_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{y}} + y_5 a \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{19}$	$=$	$y_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{20}$	$=$	$-y_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{y}} - y_5 a \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{21}$	$=$	$y_5 \mathbf{a}_1 + y_5 \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{22}$	$=$	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_3$	$=$	$y_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{23}$	$=$	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{24}$	$=$	$-y_5 \mathbf{a}_1 - y_5 \mathbf{a}_3$	$=$	$-y_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{25}$	$=$	$y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$y_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}}$	(12i)	Se II
$\mathbf{B}_{26}$	$=$	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$-y_5 a \hat{\mathbf{x}} + y_5 a \hat{\mathbf{y}}$	(12i)	Se II
$\mathbf{B}_{27}$	$=$	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$y_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}}$	(12i)	Se II
$\mathbf{B}_{28}$	$=$	$-y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$-y_5 a \hat{\mathbf{x}} - y_5 a \hat{\mathbf{y}}$	(12i)	Se II
$\mathbf{B}_{29}$	$=$	$\frac{1}{2} \mathbf{a}_1 + y_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + y_6 a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{30}$	$=$	$\frac{1}{2} \mathbf{a}_1 - y_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + y_6 a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{31}$	$=$	$\frac{1}{2} \mathbf{a}_1 + y_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} - y_6 a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{32}$	$=$	$\frac{1}{2} \mathbf{a}_1 - y_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} - y_6 a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{33}$	$=$	$y_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + y_6 a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{34}$	$=$	$y_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - y_6 a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{35}$	$=$	$-y_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + y_6 a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{36}$	$=$	$-y_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - y_6 a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{37}$	$=$	$y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$y_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{38}$	$=$	$-y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-y_6 a \hat{\mathbf{x}} + y_6 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12j)	Se III

<b>B</b> <sub>39</sub>	=	$y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$y_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12j)	Se III
<b>B</b> <sub>40</sub>	=	$-y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-y_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12j)	Se III
<b>B</b> <sub>41</sub>	=	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + z_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>42</sub>	=	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + z_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>43</sub>	=	$-x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} - z_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>44</sub>	=	$x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} - z_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>45</sub>	=	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	=	$z_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + y_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>46</sub>	=	$z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - y_7 \mathbf{a}_3$	=	$z_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} - y_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>47</sub>	=	$-z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	=	$-z_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + y_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>48</sub>	=	$-z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - y_7 \mathbf{a}_3$	=	$-z_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} - y_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>49</sub>	=	$y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$y_7 a \hat{\mathbf{x}} + z_7 a \hat{\mathbf{y}} + x_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>50</sub>	=	$-y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$-y_7 a \hat{\mathbf{x}} + z_7 a \hat{\mathbf{y}} - x_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>51</sub>	=	$y_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$y_7 a \hat{\mathbf{x}} - z_7 a \hat{\mathbf{y}} - x_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>52</sub>	=	$-y_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$-y_7 a \hat{\mathbf{x}} - z_7 a \hat{\mathbf{y}} + x_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>53</sub>	=	$y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} - z_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>54</sub>	=	$-y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} - z_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>55</sub>	=	$y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$y_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + z_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>56</sub>	=	$-y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$-y_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + z_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>57</sub>	=	$x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 - y_7 \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} + z_7 a \hat{\mathbf{y}} - y_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>58</sub>	=	$-x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} + z_7 a \hat{\mathbf{y}} + y_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>59</sub>	=	$-x_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - y_7 \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} - z_7 a \hat{\mathbf{y}} - y_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>60</sub>	=	$x_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} - z_7 a \hat{\mathbf{y}} + y_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>61</sub>	=	$z_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$z_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} - x_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>62</sub>	=	$z_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$z_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} + x_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>63</sub>	=	$-z_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$-z_7 a \hat{\mathbf{x}} + y_7 a \hat{\mathbf{y}} + x_7 a \hat{\mathbf{z}}$	(24k)	Pd IV
<b>B</b> <sub>64</sub>	=	$-z_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$-z_7 a \hat{\mathbf{x}} - y_7 a \hat{\mathbf{y}} - x_7 a \hat{\mathbf{z}}$	(24k)	Pd IV

---

#### References:

- S. Geller, *The crystal structure of Pd<sub>17</sub>Se<sub>15</sub>*, Acta Cryst. **15**, 713–721 (1962), doi:10.1107/S0365110X62001929.

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

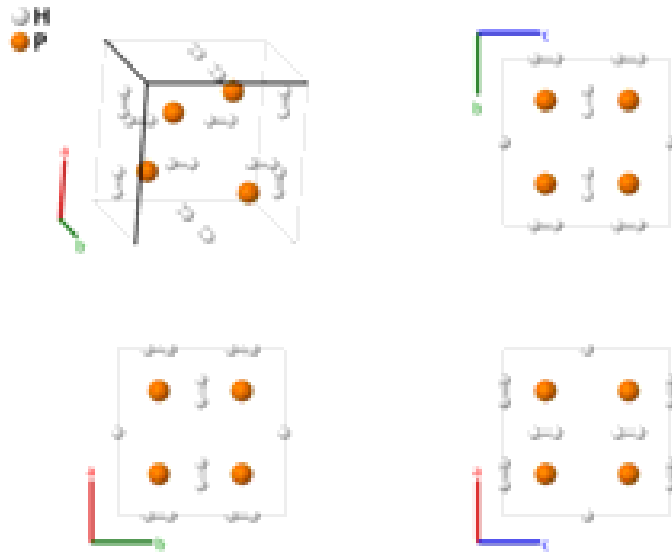
---

#### Geometry files:

- CIF: pp. 959

- POSCAR: pp. 960

# PH<sub>3</sub> Structure: A3B\_cP16\_208\_j\_b



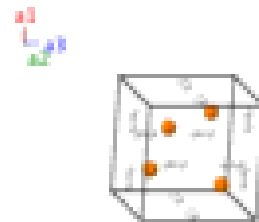
<b>Prototype</b>	:	PH <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B_cP16_208_j_b
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cP16
<b>Space group number</b>	:	208
<b>Space group symbol</b>	:	<i>P</i> 4 <sub>2</sub> 32
<b>AFLOW prototype command</b>	:	aflow --proto=A3B_cP16_208_j_b --params= <i>a</i> , <i>x</i> <sub>2</sub>

## Simple Cubic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	= $\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4 <i>b</i> )	P
<b>B</b> <sub>2</sub>	= $\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	= $\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4 <i>b</i> )	P
<b>B</b> <sub>3</sub>	= $\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	= $\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4 <i>b</i> )	P
<b>B</b> <sub>4</sub>	= $\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	= $\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4 <i>b</i> )	P
<b>B</b> <sub>5</sub>	= $x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	= $x_2 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(12 <i>j</i> )	H
<b>B</b> <sub>6</sub>	= $-x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	= $-x_2 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(12 <i>j</i> )	H

$$\begin{array}{llllll}
\mathbf{B}_7 & = & x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & x_2 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (12j) & \text{H} \\
\mathbf{B}_8 & = & -x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & -x_2 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (12j) & \text{H} \\
\mathbf{B}_9 & = & \frac{1}{2} \mathbf{a}_1 + x_2 \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{z}} & (12j) & \text{H} \\
\mathbf{B}_{10} & = & \frac{1}{2} \mathbf{a}_1 + -x_2 \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + -x_2 a \hat{\mathbf{z}} & (12j) & \text{H} \\
\mathbf{B}_{11} & = & \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (12j) & \text{H} \\
\mathbf{B}_{12} & = & \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (12j) & \text{H} \\
\mathbf{B}_{13} & = & \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 & = & \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} & (12j) & \text{H} \\
\mathbf{B}_{14} & = & \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 & = & \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} & (12j) & \text{H} \\
\mathbf{B}_{15} & = & \frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{z}} & (12j) & \text{H} \\
\mathbf{B}_{16} & = & \frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_3 & = & \frac{1}{2} a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{z}} & (12j) & \text{H}
\end{array}$$

---

**References:**

- G. Natta and E. Casazza, *La struttura dell'idrogeno fosforato (PH<sub>3</sub>) e dell'idrogeno arsenicale (AsH<sub>3</sub>)*, Gazz. Chim. Ital. **60**, 851–859 (1930).

**Found in:**

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

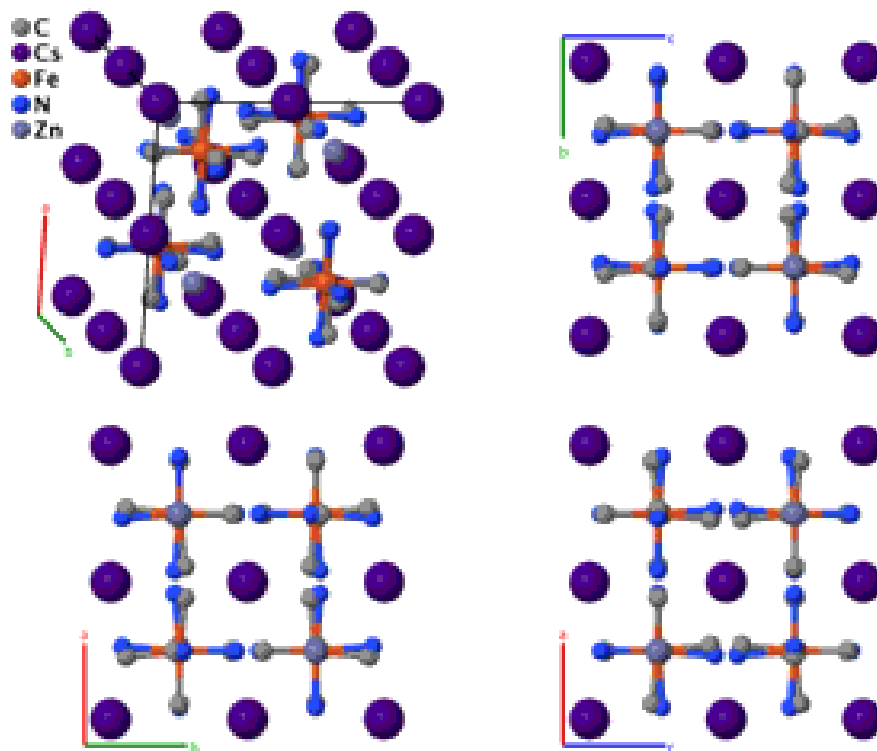
---

**Geometry files:**

- CIF: pp. [960](#)

- POSCAR: pp. [960](#)

# Cs<sub>2</sub>ZnFe[CN]<sub>6</sub> Structure: A6B2CD6E\_cP64\_208\_m\_ad\_b\_m\_c



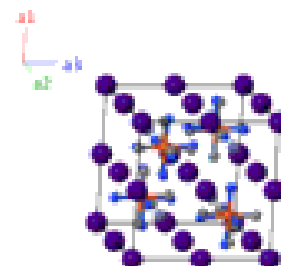
**Prototype** : Cs<sub>2</sub>ZnFe[CN]<sub>6</sub>  
**AFLOW prototype label** : A6B2CD6E\_cP64\_208\_m\_ad\_b\_m\_c  
**Strukturbericht designation** : None  
**Pearson symbol** : cP64  
**Space group number** : 208  
**Space group symbol** : *P*4<sub>2</sub>32  
**AFLOW prototype command** : aflow --proto=A6B2CD6E\_cP64\_208\_m\_ad\_b\_m\_c  
 --params=*a*, *x*<sub>5</sub>, *y*<sub>5</sub>, *z*<sub>5</sub>, *x*<sub>6</sub>, *y*<sub>6</sub>, *z*<sub>6</sub>

Simple Cubic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2 <i>a</i> )	Cs I







$$\begin{aligned}
\mathbf{B}_{59} &= \begin{pmatrix} \frac{1}{2} - x_6 \\ \frac{1}{2} - y_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} - y_6 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} - x_6 \\ \frac{1}{2} - y_6 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} - y_6 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} - x_6 \\ \frac{1}{2} - y_6 \end{pmatrix} a \hat{\mathbf{z}} &= & (24m) & \text{N} \\
\mathbf{B}_{60} &= \begin{pmatrix} \frac{1}{2} + x_6 \\ \frac{1}{2} + y_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} + y_6 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} + x_6 \\ \frac{1}{2} + y_6 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} + y_6 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} + x_6 \\ \frac{1}{2} + y_6 \end{pmatrix} a \hat{\mathbf{z}} &= & (24m) & \text{N} \\
\mathbf{B}_{61} &= \begin{pmatrix} \frac{1}{2} + z_6 \\ \frac{1}{2} - x_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_6 \\ \frac{1}{2} - x_6 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} + z_6 \\ \frac{1}{2} - x_6 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_6 \\ \frac{1}{2} - x_6 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} + z_6 \\ \frac{1}{2} - x_6 \end{pmatrix} a \hat{\mathbf{z}} &= & (24m) & \text{N} \\
\mathbf{B}_{62} &= \begin{pmatrix} \frac{1}{2} + z_6 \\ \frac{1}{2} + x_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - y_6 \\ \frac{1}{2} + x_6 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} + z_6 \\ \frac{1}{2} + x_6 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - y_6 \\ \frac{1}{2} + x_6 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} + z_6 \\ \frac{1}{2} + x_6 \end{pmatrix} a \hat{\mathbf{z}} &= & (24m) & \text{N} \\
\mathbf{B}_{63} &= \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} + x_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_6 \\ \frac{1}{2} + x_6 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} + x_6 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_6 \\ \frac{1}{2} + x_6 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} + x_6 \end{pmatrix} a \hat{\mathbf{z}} &= & (24m) & \text{N} \\
\mathbf{B}_{64} &= \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} - x_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - y_6 \\ \frac{1}{2} - x_6 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} - x_6 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - y_6 \\ \frac{1}{2} - x_6 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} - x_6 \end{pmatrix} a \hat{\mathbf{z}} &= & (24m) & \text{N}
\end{aligned}$$

---

#### References:

- V. G. Kuznetsov, Z. V. Popova, and G. B. Seifer, *X-ray diffraction study of ferrocyanides of copper, cobalt, nickel, trivalent iron and mixed copper ferrocyanide with potassium*, Russ. J. Inorg. Chem. **15**, 1084–1088 (1970).

#### Found in:

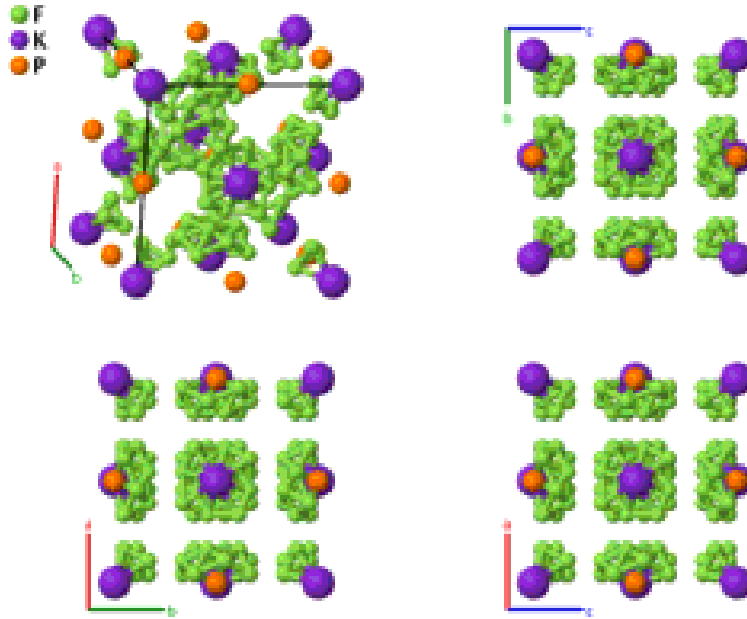
- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

---

#### Geometry files:

- CIF: pp. [960](#)  
- POSCAR: pp. [961](#)

# F<sub>6</sub>KP Structure: A24BC\_cF104\_209\_j\_a\_b

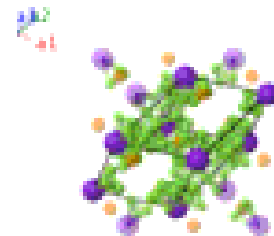


**Prototype** : F<sub>6</sub>KP  
**AFLOW prototype label** : A24BC\_cF104\_209\_j\_a\_b  
**Strukturbericht designation** : None  
**Pearson symbol** : cF104  
**Space group number** : 209  
**Space group symbol** : *F*432  
**AFLOW prototype command** : `aflow --proto=A24BC_cF104_209_j_a_b`  
                                   `--params=a, x3, y3, z3`

- The (96j) Wyckoff positions are decorated by F atoms with a site occupation of 0.25. Hence, the prototype material is F<sub>6</sub>KP as opposed to F<sub>24</sub>KP.

## Face-centered Cubic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{y} + \frac{1}{2} a \hat{z} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{x} + \frac{1}{2} a \hat{z} \\
 \mathbf{a}_3 &= \frac{1}{2} a \hat{x} + \frac{1}{2} a \hat{y}
 \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub> =	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{x} + 0 \hat{y} + 0 \hat{z}$	(4a)	K
<b>B</b> <sub>2</sub> =	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} a \hat{x} + \frac{1}{2} a \hat{y} + \frac{1}{2} a \hat{z}$	(4b)	P



**References:**

- Y. P. Mascarenhas and S. H. Pulcinelli, *A redetermination of the structure of  $\alpha$ -potassium fluorophosphate*, Acta Crystallogr. Sect. A **37**, C175 (1981), doi:[10.1107/S0108767381094294](https://doi.org/10.1107/S0108767381094294).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

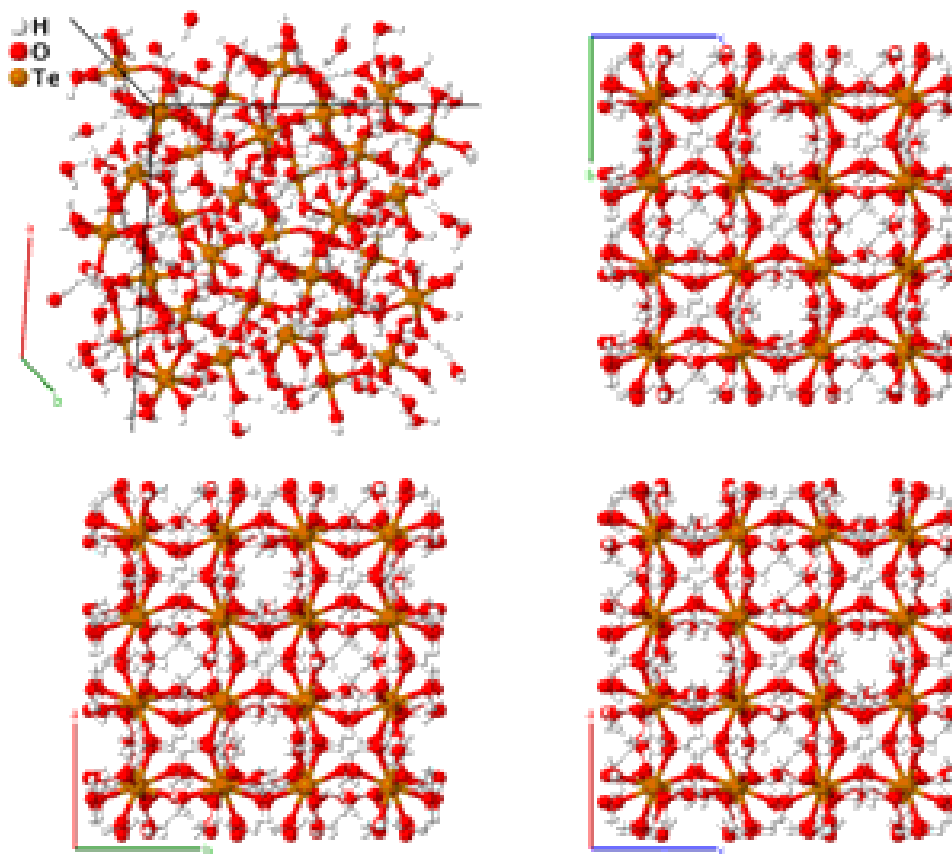
---

**Geometry files:**

- CIF: pp. [961](#)

- POSCAR: pp. [962](#)

# Te[OH]<sub>6</sub> Structure: A12B6C\_cF608\_210\_4h\_2h\_e

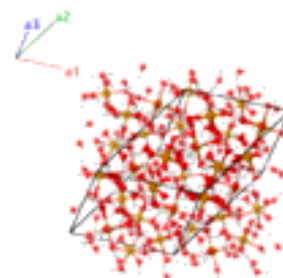


<b>Prototype</b>	:	Te[OH] <sub>6</sub>
<b>AFLOW prototype label</b>	:	A12B6C_cF608_210_4h_2h_e
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cF608
<b>Space group number</b>	:	210
<b>Space group symbol</b>	:	$F4_132$
<b>AFLOW prototype command</b>	:	aflow --proto=A12B6C_cF608_210_4h_2h_e --params= $a, x_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- All H sites are half occupation. Polytypes appear in space groups #14, #228, and #225.

**Face-centered Cubic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$x_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + x_1 a \hat{\mathbf{z}}$	(32e)	Te
$\mathbf{B}_2$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - 3x_1 \mathbf{a}_3$	$=$	$-x_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + x_1 a \hat{\mathbf{z}}$	(32e)	Te
$\mathbf{B}_3$	$= x_1 \mathbf{a}_1 - 3x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$-x_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} - x_1 a \hat{\mathbf{z}}$	(32e)	Te
$\mathbf{B}_4$	$= -3x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$x_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} - x_1 a \hat{\mathbf{z}}$	(32e)	Te
$\mathbf{B}_5$	$= \left(\frac{1}{4} - x_1\right) \mathbf{a}_1 + \left(\frac{1}{4} - x_1\right) \mathbf{a}_2 +$ $\left(\frac{1}{4} + 3x_1\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_1\right) a \hat{\mathbf{y}} +$ $\left(\frac{1}{4} - x_1\right) a \hat{\mathbf{z}}$	(32e)	Te
$\mathbf{B}_6$	$= \left(\frac{1}{4} - x_1\right) \mathbf{a}_1 + \left(\frac{1}{4} - x_1\right) \mathbf{a}_2 +$ $\left(\frac{1}{4} - x_1\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_1\right) a \hat{\mathbf{y}} +$ $\left(\frac{1}{4} - x_1\right) a \hat{\mathbf{z}}$	(32e)	Te
$\mathbf{B}_7$	$= \left(\frac{1}{4} - x_1\right) \mathbf{a}_1 + \left(\frac{1}{4} + 3x_1\right) \mathbf{a}_2 +$ $\left(\frac{1}{4} - x_1\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} + x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_1\right) a \hat{\mathbf{y}} +$ $\left(\frac{1}{4} + x_1\right) a \hat{\mathbf{z}}$	(32e)	Te
$\mathbf{B}_8$	$= \left(\frac{1}{4} + 3x_1\right) \mathbf{a}_1 + \left(\frac{1}{4} - x_1\right) \mathbf{a}_2 +$ $\left(\frac{1}{4} - x_1\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} - x_1\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_1\right) a \hat{\mathbf{y}} +$ $\left(\frac{1}{4} + x_1\right) a \hat{\mathbf{z}}$	(32e)	Te
$\mathbf{B}_9$	$= (-x_2 + y_2 + z_2) \mathbf{a}_1 +$ $(x_2 - y_2 + z_2) \mathbf{a}_2 +$ $(x_2 + y_2 - z_2) \mathbf{a}_3$	$=$	$x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + z_2 a \hat{\mathbf{z}}$	(96h)	H I
$\mathbf{B}_{10}$	$= (x_2 - y_2 + z_2) \mathbf{a}_1 +$ $(-x_2 + y_2 + z_2) \mathbf{a}_2 +$ $(-x_2 - y_2 - z_2) \mathbf{a}_3$	$=$	$-x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + z_2 a \hat{\mathbf{z}}$	(96h)	H I
$\mathbf{B}_{11}$	$= (x_2 + y_2 - z_2) \mathbf{a}_1 +$ $(-x_2 - y_2 - z_2) \mathbf{a}_2 +$ $(-x_2 + y_2 + z_2) \mathbf{a}_3$	$=$	$-x_2 a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} - z_2 a \hat{\mathbf{z}}$	(96h)	H I
$\mathbf{B}_{12}$	$= (-x_2 - y_2 - z_2) \mathbf{a}_1 +$ $(x_2 + y_2 - z_2) \mathbf{a}_2 +$ $(x_2 - y_2 + z_2) \mathbf{a}_3$	$=$	$x_2 a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} - z_2 a \hat{\mathbf{z}}$	(96h)	H I
$\mathbf{B}_{13}$	$= (x_2 + y_2 - z_2) \mathbf{a}_1 +$ $(-x_2 + y_2 + z_2) \mathbf{a}_2 +$ $(x_2 - y_2 + z_2) \mathbf{a}_3$	$=$	$z_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + y_2 a \hat{\mathbf{z}}$	(96h)	H I
$\mathbf{B}_{14}$	$= (-x_2 - y_2 - z_2) \mathbf{a}_1 +$ $(x_2 - y_2 + z_2) \mathbf{a}_2 +$ $(-x_2 + y_2 + z_2) \mathbf{a}_3$	$=$	$z_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} - y_2 a \hat{\mathbf{z}}$	(96h)	H I
$\mathbf{B}_{15}$	$= (-x_2 + y_2 + z_2) \mathbf{a}_1 +$ $(x_2 + y_2 - z_2) \mathbf{a}_2 +$ $(-x_2 - y_2 - z_2) \mathbf{a}_3$	$=$	$-z_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + y_2 a \hat{\mathbf{z}}$	(96h)	H I
$\mathbf{B}_{16}$	$= (x_2 - y_2 + z_2) \mathbf{a}_1 +$ $(-x_2 - y_2 - z_2) \mathbf{a}_2 +$ $(x_2 + y_2 - z_2) \mathbf{a}_3$	$=$	$-z_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} - y_2 a \hat{\mathbf{z}}$	(96h)	H I
$\mathbf{B}_{17}$	$= (x_2 - y_2 + z_2) \mathbf{a}_1 +$ $(x_2 + y_2 - z_2) \mathbf{a}_2 +$ $(-x_2 + y_2 + z_2) \mathbf{a}_3$	$=$	$y_2 a \hat{\mathbf{x}} + z_2 a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}}$	(96h)	H I
$\mathbf{B}_{18}$	$= (-x_2 + y_2 + z_2) \mathbf{a}_1 +$ $(-x_2 - y_2 - z_2) \mathbf{a}_2 +$ $(x_2 - y_2 + z_2) \mathbf{a}_3$	$=$	$-y_2 a \hat{\mathbf{x}} + z_2 a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}}$	(96h)	H I
$\mathbf{B}_{19}$	$= (-x_2 - y_2 - z_2) \mathbf{a}_1 +$ $(-x_2 + y_2 + z_2) \mathbf{a}_2 +$ $(x_2 + y_2 - z_2) \mathbf{a}_3$	$=$	$y_2 a \hat{\mathbf{x}} - z_2 a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}}$	(96h)	H I





$$\begin{aligned}
\mathbf{B}_{34} &= (x_3 - y_3 + z_3) \mathbf{a}_1 + (-x_3 + y_3 + z_3) \mathbf{a}_2 + (-x_3 - y_3 - z_3) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + z_3 a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{35} &= (x_3 + y_3 - z_3) \mathbf{a}_1 + (-x_3 - y_3 - z_3) \mathbf{a}_2 + (-x_3 + y_3 + z_3) \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} - z_3 a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{36} &= (-x_3 - y_3 - z_3) \mathbf{a}_1 + (x_3 + y_3 - z_3) \mathbf{a}_2 + (x_3 - y_3 + z_3) \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} - z_3 a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{37} &= (x_3 + y_3 - z_3) \mathbf{a}_1 + (-x_3 + y_3 + z_3) \mathbf{a}_2 + (x_3 - y_3 + z_3) \mathbf{a}_3 &= z_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + y_3 a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{38} &= (-x_3 - y_3 - z_3) \mathbf{a}_1 + (x_3 - y_3 + z_3) \mathbf{a}_2 + (-x_3 + y_3 + z_3) \mathbf{a}_3 &= z_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - y_3 a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{39} &= (-x_3 + y_3 + z_3) \mathbf{a}_1 + (x_3 + y_3 - z_3) \mathbf{a}_2 + (-x_3 - y_3 - z_3) \mathbf{a}_3 &= -z_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + y_3 a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{40} &= (x_3 - y_3 + z_3) \mathbf{a}_1 + (-x_3 - y_3 - z_3) \mathbf{a}_2 + (x_3 + y_3 - z_3) \mathbf{a}_3 &= -z_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - y_3 a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{41} &= (x_3 - y_3 + z_3) \mathbf{a}_1 + (x_3 + y_3 - z_3) \mathbf{a}_2 + (-x_3 + y_3 + z_3) \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} + z_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{42} &= (-x_3 + y_3 + z_3) \mathbf{a}_1 + (-x_3 - y_3 - z_3) \mathbf{a}_2 + (x_3 - y_3 + z_3) \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} + z_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{43} &= (-x_3 - y_3 - z_3) \mathbf{a}_1 + (-x_3 + y_3 + z_3) \mathbf{a}_2 + (x_3 + y_3 - z_3) \mathbf{a}_3 &= y_3 a \hat{\mathbf{x}} - z_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{44} &= (x_3 + y_3 - z_3) \mathbf{a}_1 + (x_3 - y_3 + z_3) \mathbf{a}_2 + (-x_3 - y_3 - z_3) \mathbf{a}_3 &= -y_3 a \hat{\mathbf{x}} - z_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{45} &= \left(\frac{1}{4} + x_3 - y_3 - z_3\right) \mathbf{a}_1 + \left(\frac{1}{4} - x_3 + y_3 - z_3\right) \mathbf{a}_2 + \left(\frac{1}{4} + x_3 + y_3 + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{4} + y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_3\right) a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{46} &= \left(\frac{1}{4} - x_3 + y_3 - z_3\right) \mathbf{a}_1 + \left(\frac{1}{4} + x_3 - y_3 - z_3\right) \mathbf{a}_2 + \left(\frac{1}{4} - x_3 - y_3 + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{4} - y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - z_3\right) a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{47} &= \left(\frac{1}{4} - x_3 - y_3 + z_3\right) \mathbf{a}_1 + \left(\frac{1}{4} + x_3 + y_3 + z_3\right) \mathbf{a}_2 + \left(\frac{1}{4} - x_3 + y_3 - z_3\right) \mathbf{a}_3 &= \left(\frac{1}{4} + y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_3\right) a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{48} &= \left(\frac{1}{4} + x_3 + y_3 + z_3\right) \mathbf{a}_1 + \left(\frac{1}{4} - x_3 - y_3 + z_3\right) \mathbf{a}_2 + \left(\frac{1}{4} + x_3 - y_3 - z_3\right) \mathbf{a}_3 &= \left(\frac{1}{4} - y_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_3\right) a \hat{\mathbf{z}} &(96h) & \text{H II} \\
\mathbf{B}_{49} &= \left(\frac{1}{4} - x_3 - y_3 + z_3\right) \mathbf{a}_1 + \left(\frac{1}{4} + x_3 - y_3 - z_3\right) \mathbf{a}_2 + \left(\frac{1}{4} + x_3 + y_3 + z_3\right) \mathbf{a}_3 &= \left(\frac{1}{4} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + z_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - y_3\right) a \hat{\mathbf{z}} &(96h) & \text{H II}
\end{aligned}$$















$$\begin{aligned}
\mathbf{B}_{140} &= (x_7 + y_7 - z_7) \mathbf{a}_1 + &= -y_7 a \hat{\mathbf{x}} - z_7 a \hat{\mathbf{y}} + x_7 a \hat{\mathbf{z}} & (96h) & \text{O II} \\
&(x_7 - y_7 + z_7) \mathbf{a}_2 + \\
&(-x_7 - y_7 - z_7) \mathbf{a}_3 \\
\mathbf{B}_{141} &= \left(\frac{1}{4} + x_7 - y_7 - z_7\right) \mathbf{a}_1 + &= \left(\frac{1}{4} + y_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_7\right) a \hat{\mathbf{y}} + & (96h) & \text{O II} \\
&\left(\frac{1}{4} - x_7 + y_7 - z_7\right) \mathbf{a}_2 + \\
&\left(\frac{1}{4} + x_7 + y_7 + z_7\right) \mathbf{a}_3 \\
\mathbf{B}_{142} &= \left(\frac{1}{4} - x_7 + y_7 - z_7\right) \mathbf{a}_1 + &= \left(\frac{1}{4} - y_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_7\right) a \hat{\mathbf{y}} + & (96h) & \text{O II} \\
&\left(\frac{1}{4} + x_7 - y_7 - z_7\right) \mathbf{a}_2 + \\
&\left(\frac{1}{4} - x_7 - y_7 + z_7\right) \mathbf{a}_3 \\
\mathbf{B}_{143} &= \left(\frac{1}{4} - x_7 - y_7 + z_7\right) \mathbf{a}_1 + &= \left(\frac{1}{4} + y_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_7\right) a \hat{\mathbf{y}} + & (96h) & \text{O II} \\
&\left(\frac{1}{4} + x_7 + y_7 + z_7\right) \mathbf{a}_2 + \\
&\left(\frac{1}{4} - x_7 + y_7 - z_7\right) \mathbf{a}_3 \\
\mathbf{B}_{144} &= \left(\frac{1}{4} + x_7 + y_7 + z_7\right) \mathbf{a}_1 + &= \left(\frac{1}{4} - y_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_7\right) a \hat{\mathbf{y}} + & (96h) & \text{O II} \\
&\left(\frac{1}{4} - x_7 - y_7 + z_7\right) \mathbf{a}_2 + \\
&\left(\frac{1}{4} + x_7 - y_7 - z_7\right) \mathbf{a}_3 \\
\mathbf{B}_{145} &= \left(\frac{1}{4} - x_7 - y_7 + z_7\right) \mathbf{a}_1 + &= \left(\frac{1}{4} + x_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + z_7\right) a \hat{\mathbf{y}} + & (96h) & \text{O II} \\
&\left(\frac{1}{4} + x_7 - y_7 - z_7\right) \mathbf{a}_2 + \\
&\left(\frac{1}{4} + x_7 + y_7 + z_7\right) \mathbf{a}_3 \\
\mathbf{B}_{146} &= \left(\frac{1}{4} + x_7 + y_7 + z_7\right) \mathbf{a}_1 + &= \left(\frac{1}{4} - x_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + z_7\right) a \hat{\mathbf{y}} + & (96h) & \text{O II} \\
&\left(\frac{1}{4} - x_7 + y_7 - z_7\right) \mathbf{a}_2 + \\
&\left(\frac{1}{4} - x_7 - y_7 + z_7\right) \mathbf{a}_3 \\
\mathbf{B}_{147} &= \left(\frac{1}{4} + x_7 - y_7 - z_7\right) \mathbf{a}_1 + &= \left(\frac{1}{4} - x_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - z_7\right) a \hat{\mathbf{y}} + & (96h) & \text{O II} \\
&\left(\frac{1}{4} - x_7 - y_7 + z_7\right) \mathbf{a}_2 + \\
&\left(\frac{1}{4} - x_7 + y_7 - z_7\right) \mathbf{a}_3 \\
\mathbf{B}_{148} &= \left(\frac{1}{4} - x_7 + y_7 - z_7\right) \mathbf{a}_1 + &= \left(\frac{1}{4} + x_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - z_7\right) a \hat{\mathbf{y}} + & (96h) & \text{O II} \\
&\left(\frac{1}{4} + x_7 + y_7 + z_7\right) \mathbf{a}_2 + \\
&\left(\frac{1}{4} + x_7 - y_7 - z_7\right) \mathbf{a}_3 \\
\mathbf{B}_{149} &= \left(\frac{1}{4} - x_7 + y_7 - z_7\right) \mathbf{a}_1 + &= \left(\frac{1}{4} + z_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + y_7\right) a \hat{\mathbf{y}} + & (96h) & \text{O II} \\
&\left(\frac{1}{4} - x_7 - y_7 + z_7\right) \mathbf{a}_2 + \\
&\left(\frac{1}{4} + x_7 + y_7 + z_7\right) \mathbf{a}_3 \\
\mathbf{B}_{150} &= \left(\frac{1}{4} + x_7 - y_7 - z_7\right) \mathbf{a}_1 + &= \left(\frac{1}{4} + z_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - y_7\right) a \hat{\mathbf{y}} + & (96h) & \text{O II} \\
&\left(\frac{1}{4} + x_7 + y_7 + z_7\right) \mathbf{a}_2 + \\
&\left(\frac{1}{4} - x_7 - y_7 + z_7\right) \mathbf{a}_3 \\
\mathbf{B}_{151} &= \left(\frac{1}{4} + x_7 + y_7 + z_7\right) \mathbf{a}_1 + &= \left(\frac{1}{4} - z_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + y_7\right) a \hat{\mathbf{y}} + & (96h) & \text{O II} \\
&\left(\frac{1}{4} + x_7 - y_7 - z_7\right) \mathbf{a}_2 + \\
&\left(\frac{1}{4} - x_7 + y_7 - z_7\right) \mathbf{a}_3 \\
\mathbf{B}_{152} &= \left(\frac{1}{4} - x_7 - y_7 + z_7\right) \mathbf{a}_1 + &= \left(\frac{1}{4} - z_7\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - y_7\right) a \hat{\mathbf{y}} + & (96h) & \text{O II} \\
&\left(\frac{1}{4} - x_7 + y_7 - z_7\right) \mathbf{a}_2 + \\
&\left(\frac{1}{4} + x_7 - y_7 - z_7\right) \mathbf{a}_3
\end{aligned}$$

## References:

- D. F. Mullica, J. D. Korp, W. O. Milligan, G. W. Beall, and I. Bernal, *Neutron structural refinement of cubic orthotelluric acid*, Acta Crystallogr. Sect. B Struct. Sci. **36**, 2565–2570 (1980), doi:10.1107/S0567740880009454.

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

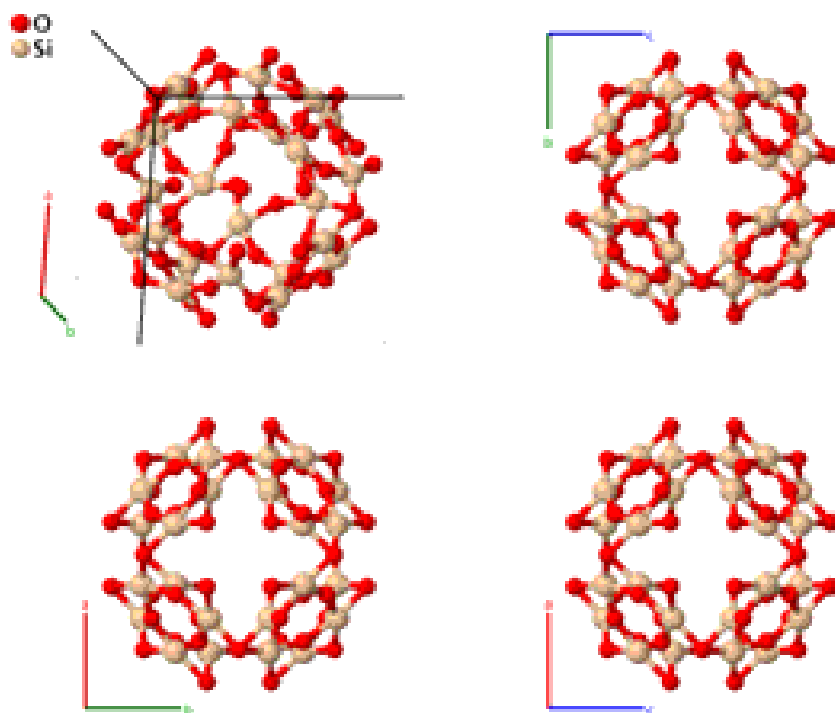
---

**Geometry files:**

- CIF: pp. [962](#)

- POSCAR: pp. [963](#)

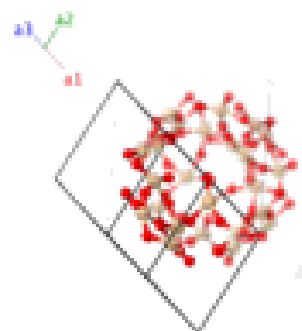
# SiO<sub>2</sub> Structure: A2B\_cI72\_211\_hi\_i



**Prototype** : SiO<sub>2</sub>  
**AFLOW prototype label** : A2B\_cI72\_211\_hi\_i  
**Strukturbericht designation** : None  
**Pearson symbol** : cI72  
**Space group number** : 211  
**Space group symbol** : *I*432  
**AFLOW prototype command** : `aflow --proto=A2B_cI72_211_hi_i`  
                                   `--params=a, y1, y2, y3`

**Body-centered Cubic primitive vectors:**

$$\begin{aligned}
 \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\
 \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}a\hat{\mathbf{z}}
 \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub> =	$2y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	=	$y_1 a \hat{\mathbf{y}} + y_1 a \hat{\mathbf{z}}$	(24h)	O I
<b>B</b> <sub>2</sub> =	$y_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	=	$-y_1 a \hat{\mathbf{y}} + y_1 a \hat{\mathbf{z}}$	(24h)	O I
<b>B</b> <sub>3</sub> =	$-y_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	=	$y_1 a \hat{\mathbf{y}} - y_1 a \hat{\mathbf{z}}$	(24h)	O I

$\mathbf{B}_4$	$=$	$-2y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	$=$	$-y_1 a \hat{\mathbf{y}} - y_1 a \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_5$	$=$	$y_1 \mathbf{a}_1 + 2y_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	$=$	$y_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_6$	$=$	$-y_1 \mathbf{a}_1 + y_1 \mathbf{a}_3$	$=$	$y_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_7$	$=$	$y_1 \mathbf{a}_1 + -y_1 \mathbf{a}_3$	$=$	$-y_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_8$	$=$	$-y_1 \mathbf{a}_1 - 2y_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	$=$	$-y_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_9$	$=$	$y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + 2y_1 \mathbf{a}_3$	$=$	$y_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}}$	(24h)	O I
$\mathbf{B}_{10}$	$=$	$y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	$=$	$-y_1 a \hat{\mathbf{x}} + y_1 a \hat{\mathbf{y}}$	(24h)	O I
$\mathbf{B}_{11}$	$=$	$-y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$=$	$y_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}}$	(24h)	O I
$\mathbf{B}_{12}$	$=$	$-y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - 2y_1 \mathbf{a}_3$	$=$	$-y_1 a \hat{\mathbf{x}} - y_1 a \hat{\mathbf{y}}$	(24h)	O I
$\mathbf{B}_{13}$	$=$	$\frac{1}{2} \mathbf{a}_1 + \left(\frac{3}{4} - y_2\right) \mathbf{a}_2 + \left(\frac{1}{4} + y_2\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{14}$	$=$	$\left(\frac{1}{2} - 2y_2\right) \mathbf{a}_1 + \left(\frac{1}{4} - y_2\right) \mathbf{a}_2 + \left(\frac{3}{4} - y_2\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{y}} - y_2 a \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{15}$	$=$	$\left(\frac{1}{2} + 2y_2\right) \mathbf{a}_1 + \left(\frac{1}{4} + y_2\right) \mathbf{a}_2 + \left(\frac{3}{4} + y_2\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{y}} + y_2 a \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{16}$	$=$	$\frac{1}{2} \mathbf{a}_1 + \left(\frac{3}{4} + y_2\right) \mathbf{a}_2 + \left(\frac{1}{4} - y_2\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{17}$	$=$	$\left(\frac{1}{4} + y_2\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{3}{4} - y_2\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - y_2\right) a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + y_2 a \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{18}$	$=$	$\left(\frac{3}{4} - y_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - 2y_2\right) \mathbf{a}_2 + \left(\frac{1}{4} - y_2\right) \mathbf{a}_3$	$=$	$-y_2 a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{19}$	$=$	$\left(\frac{3}{4} + y_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + 2y_2\right) \mathbf{a}_2 + \left(\frac{1}{4} + y_2\right) \mathbf{a}_3$	$=$	$y_2 a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{20}$	$=$	$\left(\frac{1}{4} - y_2\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{3}{4} + y_2\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + y_2\right) a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - y_2 a \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{21}$	$=$	$\left(\frac{3}{4} - y_2\right) \mathbf{a}_1 + \left(\frac{1}{4} + y_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$y_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_2\right) a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{22}$	$=$	$\left(\frac{1}{4} - y_2\right) \mathbf{a}_1 + \left(\frac{3}{4} - y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - 2y_2\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - y_2\right) a \hat{\mathbf{x}} - y_2 a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{23}$	$=$	$\left(\frac{1}{4} + y_2\right) \mathbf{a}_1 + \left(\frac{3}{4} + y_2\right) \mathbf{a}_2 + \left(\frac{1}{2} + 2y_2\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + y_2\right) a \hat{\mathbf{x}} + y_2 a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{24}$	$=$	$\left(\frac{3}{4} + y_2\right) \mathbf{a}_1 + \left(\frac{1}{4} - y_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-y_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_2\right) a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{25}$	$=$	$\frac{1}{2} \mathbf{a}_1 + \left(\frac{3}{4} - y_3\right) \mathbf{a}_2 + \left(\frac{1}{4} + y_3\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{z}}$	(24i)	Si
$\mathbf{B}_{26}$	$=$	$\left(\frac{1}{2} - 2y_3\right) \mathbf{a}_1 + \left(\frac{1}{4} - y_3\right) \mathbf{a}_2 + \left(\frac{3}{4} - y_3\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} - y_3 a \hat{\mathbf{z}}$	(24i)	Si
$\mathbf{B}_{27}$	$=$	$\left(\frac{1}{2} + 2y_3\right) \mathbf{a}_1 + \left(\frac{1}{4} + y_3\right) \mathbf{a}_2 + \left(\frac{3}{4} + y_3\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} + y_3 a \hat{\mathbf{z}}$	(24i)	Si
$\mathbf{B}_{28}$	$=$	$\frac{1}{2} \mathbf{a}_1 + \left(\frac{3}{4} + y_3\right) \mathbf{a}_2 + \left(\frac{1}{4} - y_3\right) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{z}}$	(24i)	Si
$\mathbf{B}_{29}$	$=$	$\left(\frac{1}{4} + y_3\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{3}{4} - y_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - y_3\right) a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + y_3 a \hat{\mathbf{z}}$	(24i)	Si
$\mathbf{B}_{30}$	$=$	$\left(\frac{3}{4} - y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - 2y_3\right) \mathbf{a}_2 + \left(\frac{1}{4} - y_3\right) \mathbf{a}_3$	$=$	$-y_3 a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{z}}$	(24i)	Si
$\mathbf{B}_{31}$	$=$	$\left(\frac{3}{4} + y_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + 2y_3\right) \mathbf{a}_2 + \left(\frac{1}{4} + y_3\right) \mathbf{a}_3$	$=$	$y_3 a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{z}}$	(24i)	Si
$\mathbf{B}_{32}$	$=$	$\left(\frac{1}{4} - y_3\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(\frac{3}{4} + y_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + y_3\right) a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - y_3 a \hat{\mathbf{z}}$	(24i)	Si
$\mathbf{B}_{33}$	$=$	$\left(\frac{3}{4} - y_3\right) \mathbf{a}_1 + \left(\frac{1}{4} + y_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$y_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24i)	Si
$\mathbf{B}_{34}$	$=$	$\left(\frac{1}{4} - y_3\right) \mathbf{a}_1 + \left(\frac{3}{4} - y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - 2y_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - y_3\right) a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24i)	Si
$\mathbf{B}_{35}$	$=$	$\left(\frac{1}{4} + y_3\right) \mathbf{a}_1 + \left(\frac{3}{4} + y_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + 2y_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{2} + y_3\right) a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24i)	Si
$\mathbf{B}_{36}$	$=$	$\left(\frac{3}{4} + y_3\right) \mathbf{a}_1 + \left(\frac{1}{4} - y_3\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-y_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24i)	Si

## References:

- M. D. Foster, O. Delgado Friedrichs, R. G. Bell, and F. A. Almeida Pazand J. Klinowski, *Chemical Evaluation of Hypothetical Uninodal Zeolites*, J. Am. Chem. Soc. **126**, 9769–9775 (2004), doi:10.1021/ja037334j.

**Found in:**

- ICSD, *Inorganic Crystal Structure Database*. ID 170506.

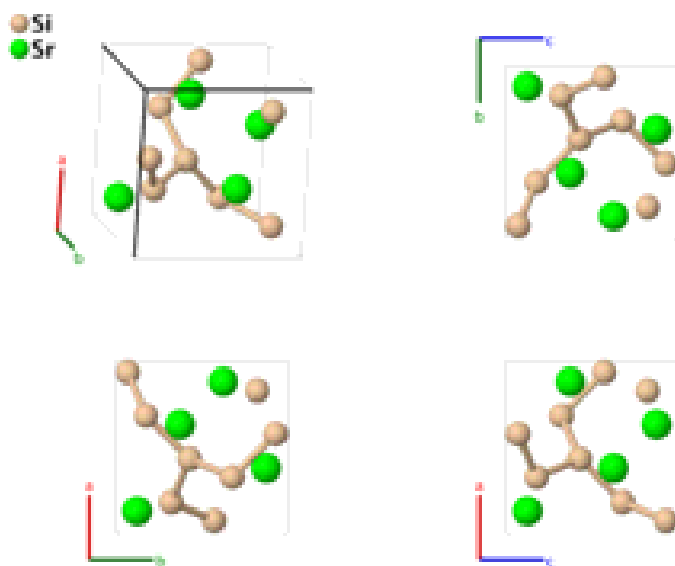
---

**Geometry files:**

- CIF: pp. [964](#)

- POSCAR: pp. [964](#)

# SrSi<sub>2</sub> Structure: A2B\_cP12\_212\_c\_a



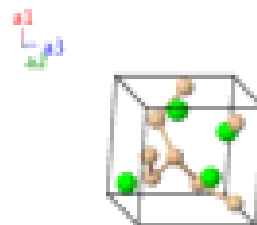
<b>Prototype</b>	:	SrSi <sub>2</sub>
<b>AFLOW prototype label</b>	:	A2B_cP12_212_c_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cP12
<b>Space group number</b>	:	212
<b>Space group symbol</b>	:	<i>P</i> 4 <sub>3</sub> 32
<b>AFLOW prototype command</b>	:	aflow --proto=A2B_cP12_212_c_a --params= <i>a</i> , <i>x</i> <sub>2</sub>

## Other compounds with this structure:

- BaSi<sub>2</sub>, BaSi<sub>4</sub>Sr

## Simple Cubic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub> =	$\frac{1}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$	=	$\frac{1}{8} a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}}$	(4 <i>a</i> )	Sr
<b>B</b> <sub>2</sub> =	$\frac{3}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3$	=	$\frac{3}{8} a \hat{\mathbf{x}} + \frac{7}{8} a \hat{\mathbf{y}} + \frac{5}{8} a \hat{\mathbf{z}}$	(4 <i>a</i> )	Sr
<b>B</b> <sub>3</sub> =	$\frac{7}{8} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3$	=	$\frac{7}{8} a \hat{\mathbf{x}} + \frac{5}{8} a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}}$	(4 <i>a</i> )	Sr

$$\mathbf{B}_4 = \frac{5}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3 = \frac{5}{8} a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} + \frac{7}{8} a \hat{\mathbf{z}} \quad (4a) \quad \text{Sr}$$

$$\mathbf{B}_5 = x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3 = x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}} \quad (8c) \quad \text{Si}$$

$$\mathbf{B}_6 = \left(\frac{1}{2} - x_2\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_3 = \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{z}} \quad (8c) \quad \text{Si}$$

$$\mathbf{B}_7 = -x_2 \mathbf{a}_1 + \left(\frac{1}{2} + x_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_3 = -x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{z}} \quad (8c) \quad \text{Si}$$

$$\mathbf{B}_8 = \left(\frac{1}{2} + x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_2\right) \mathbf{a}_2 - x_2 \mathbf{a}_3 = \left(\frac{1}{2} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}} \quad (8c) \quad \text{Si}$$

$$\mathbf{B}_9 = \left(\frac{1}{4} + x_2\right) \mathbf{a}_1 + \left(\frac{3}{4} + x_2\right) \mathbf{a}_2 + \left(\frac{3}{4} - x_2\right) \mathbf{a}_3 = \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{3}{4} + x_2\right) a \hat{\mathbf{y}} + \left(\frac{3}{4} - x_2\right) a \hat{\mathbf{z}} \quad (8c) \quad \text{Si}$$

$$\mathbf{B}_{10} = \left(\frac{1}{4} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{4} - x_2\right) \mathbf{a}_2 + \left(\frac{1}{4} - x_2\right) \mathbf{a}_3 = \left(\frac{1}{4} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_2\right) a \hat{\mathbf{z}} \quad (8c) \quad \text{Si}$$

$$\mathbf{B}_{11} = \left(\frac{3}{4} + x_2\right) \mathbf{a}_1 + \left(\frac{3}{4} - x_2\right) \mathbf{a}_2 + \left(\frac{1}{4} + x_2\right) \mathbf{a}_3 = \left(\frac{3}{4} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{3}{4} - x_2\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{z}} \quad (8c) \quad \text{Si}$$

$$\mathbf{B}_{12} = \left(\frac{3}{4} - x_2\right) \mathbf{a}_1 + \left(\frac{1}{4} + x_2\right) \mathbf{a}_2 + \left(\frac{3}{4} + x_2\right) \mathbf{a}_3 = \left(\frac{3}{4} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{y}} + \left(\frac{3}{4} + x_2\right) a \hat{\mathbf{z}} \quad (8c) \quad \text{Si}$$

### References:

- K. Janzon, H. Schäfer, and A. Weiss, *Kristallstruktur von Strontiumdisilicid SrSi<sub>2</sub>*, *Angew. Chem. Int. Ed.* **77**, 258–259 (1965), doi:10.1002/ange.19650770605.

### Found in:

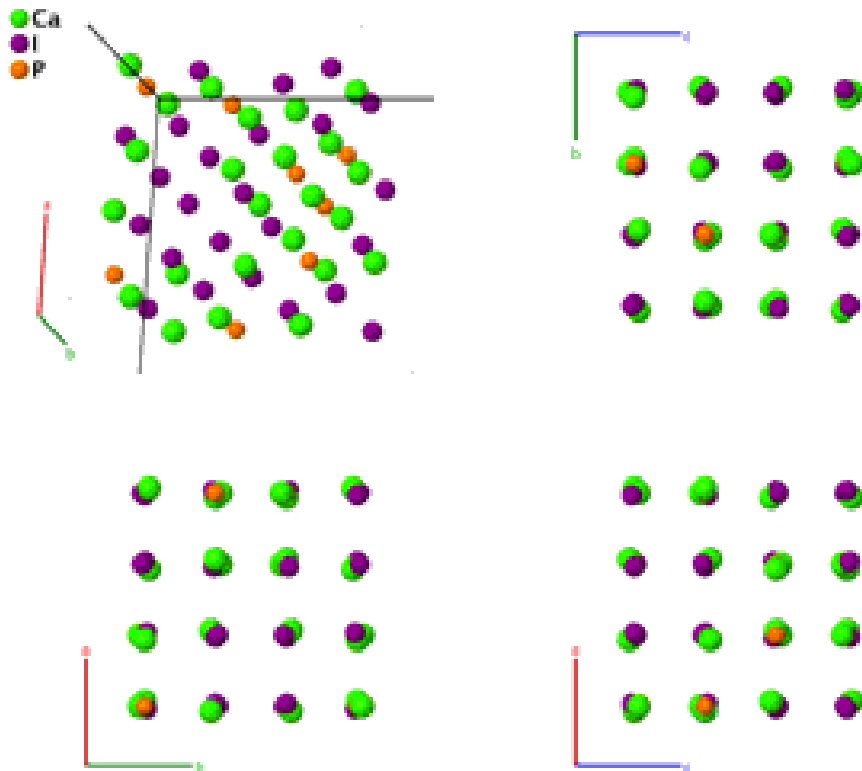
- P. Villars and L. D. Calvert, eds., *Pearson's Handbook of Crystallographic Data for Intermetallic Phases*, vol. 1 (American Society of Metals, Materials Park, Ohio, 1985).

### Geometry files:

- CIF: pp. 965

- POSCAR: pp. 965

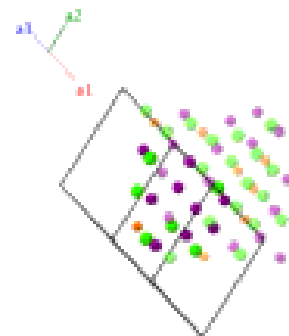
# Ca<sub>3</sub>PI<sub>3</sub> Structure: A3B3C\_cI56\_214\_g\_h\_a



<b>Prototype</b>	:	Ca <sub>3</sub> PI <sub>3</sub>
<b>AFLOW prototype label</b>	:	A3B3C_cI56_214_g_h_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cI56
<b>Space group number</b>	:	214
<b>Space group symbol</b>	:	<i>I</i> 4 <sub>1</sub> 32
<b>AFLOW prototype command</b>	:	aflow --proto=A3B3C_cI56_214_g_h_a --params= <i>a</i> , <i>y</i> <sub>2</sub> , <i>y</i> <sub>3</sub>

**Body-centered Cubic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} a \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b> =	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{8} a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}}$	(8 <i>a</i> )	P





---

**References:**

- C. Hamon, R. Marchand, Y. Laurent, and J. Lang, *Etude d'halogenopictures. m. Structures de  $Ca_2PI$  et  $Ca_3Pl_3$ . Sur structures de type  $NaCl$* , Bull. Soc. fr. Mineral. Crystallogr. **97**, 6–12 (1974).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

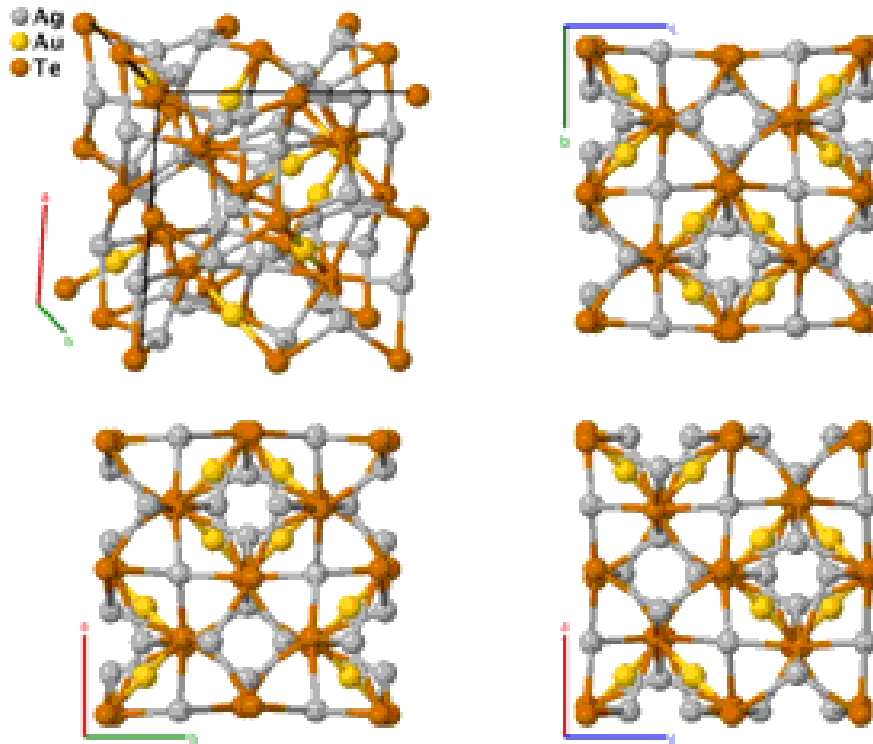
---

**Geometry files:**

- CIF: pp. [965](#)

- POSCAR: pp. [966](#)

# Petzite ( $\text{Ag}_3\text{AuTe}_2$ ) Structure: A3BC2\_cI48\_214\_f\_a\_e

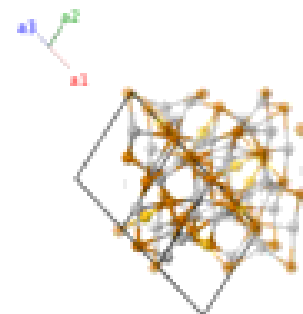


<b>Prototype</b>	:	$\text{Ag}_3\text{AuTe}_2$
<b>AFLOW prototype label</b>	:	A3BC2_cI48_214_f_a_e
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cI48
<b>Space group number</b>	:	214
<b>Space group symbol</b>	:	$I4_132$
<b>AFLOW prototype command</b>	:	aflow --proto=A3BC2_cI48_214_f_a_e --params= $a, x_2, x_3$

- The Wyckoff positions given in the *International Tables* have been shifted by one or more body-centered cubic primitive lattice vectors to provide a more compact set of coordinates in both Cartesian and lattice space.

## Body-centered Cubic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} a \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{8}a \hat{\mathbf{x}} + \frac{1}{8}a \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$	(8a)	Au
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{8}a \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$	(8a)	Au
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{8}a \hat{\mathbf{x}} + \frac{1}{8}a \hat{\mathbf{y}} - \frac{1}{8}a \hat{\mathbf{z}}$	(8a)	Au
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{8}a \hat{\mathbf{x}} - \frac{1}{8}a \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}}$	(8a)	Au
$\mathbf{B}_5$	$= 2x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + 2x_2 \mathbf{a}_3$	$=$	$x_2a \hat{\mathbf{x}} + x_2a \hat{\mathbf{y}} + x_2a \hat{\mathbf{z}}$	(16e)	Te
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} - 2x_2\right) \mathbf{a}_3$	$=$	$-x_2a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right)a \hat{\mathbf{y}} + x_2a \hat{\mathbf{z}}$	(16e)	Te
$\mathbf{B}_7$	$= \left(\frac{1}{2} - 2x_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_2\right)a \hat{\mathbf{x}} + x_2a \hat{\mathbf{y}} - x_2a \hat{\mathbf{z}}$	(16e)	Te
$\mathbf{B}_8$	$= \left(\frac{1}{2} - 2x_2\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$x_2a \hat{\mathbf{x}} - x_2a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_2\right)a \hat{\mathbf{z}}$	(16e)	Te
$\mathbf{B}_9$	$= \frac{1}{2} \mathbf{a}_1 + 2x_2 \mathbf{a}_3$	$=$	$\left(\frac{3}{4} + x_2\right)a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_2\right)a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_2\right)a \hat{\mathbf{z}}$	(16e)	Te
$\mathbf{B}_{10}$	$= \left(\frac{1}{2} - 2x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} - 2x_2\right) \mathbf{a}_2 + \left(\frac{1}{2} - 2x_2\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} - x_2\right)a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_2\right)a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_2\right)a \hat{\mathbf{z}}$	(16e)	Te
$\mathbf{B}_{11}$	$= 2x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{1}{4} + x_2\right)a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_2\right)a \hat{\mathbf{y}} + \left(\frac{3}{4} + x_2\right)a \hat{\mathbf{z}}$	(16e)	Te
$\mathbf{B}_{12}$	$= 2x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\left(\frac{1}{4} - x_2\right)a \hat{\mathbf{x}} + \left(\frac{3}{4} + x_2\right)a \hat{\mathbf{y}} + \left(\frac{1}{4} + x_2\right)a \hat{\mathbf{z}}$	(16e)	Te
$\mathbf{B}_{13}$	$= \frac{1}{4} \mathbf{a}_1 + \left(\frac{1}{4} + x_3\right) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$x_3a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24f)	Ag
$\mathbf{B}_{14}$	$= \frac{3}{4} \mathbf{a}_1 + \left(\frac{1}{4} - x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_3$	$=$	$-x_3a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24f)	Ag
$\mathbf{B}_{15}$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{4} + x_3\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + x_3a \hat{\mathbf{y}}$	(24f)	Ag
$\mathbf{B}_{16}$	$= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(\frac{1}{4} - x_3\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - x_3a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(24f)	Ag
$\mathbf{B}_{17}$	$= \left(\frac{1}{4} + x_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{y}} + x_3a \hat{\mathbf{z}}$	(24f)	Ag
$\mathbf{B}_{18}$	$= \left(\frac{1}{4} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - x_3a \hat{\mathbf{z}}$	(24f)	Ag
$\mathbf{B}_{19}$	$= \left(\frac{1}{4} + x_3\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \left(-\frac{1}{4} + x_3\right)a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(24f)	Ag
$\mathbf{B}_{20}$	$= \left(\frac{1}{4} - x_3\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_3\right)a \hat{\mathbf{y}}$	(24f)	Ag
$\mathbf{B}_{21}$	$= \frac{3}{4} \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{4} + x_3\right) \mathbf{a}_3$	$=$	$\left(\frac{3}{4} + x_3\right)a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24f)	Ag
$\mathbf{B}_{22}$	$= \frac{1}{4} \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \left(\frac{1}{4} - x_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} - x_3\right)a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24f)	Ag
$\mathbf{B}_{23}$	$= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{4} - x_3\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_3\right)a \hat{\mathbf{z}}$	(24f)	Ag
$\mathbf{B}_{24}$	$= x_3 \mathbf{a}_1 + \left(\frac{1}{4} + x_3\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \left(\frac{3}{4} + x_3\right)a \hat{\mathbf{z}}$	(24f)	Ag

---

#### References:

- A. J. Frueh, Jr., *Crystallography of petzite, Ag<sub>3</sub>AuTe<sub>2</sub>*, Am. Mineral. **44**, 693–701 (1959).

#### Found in:

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

---

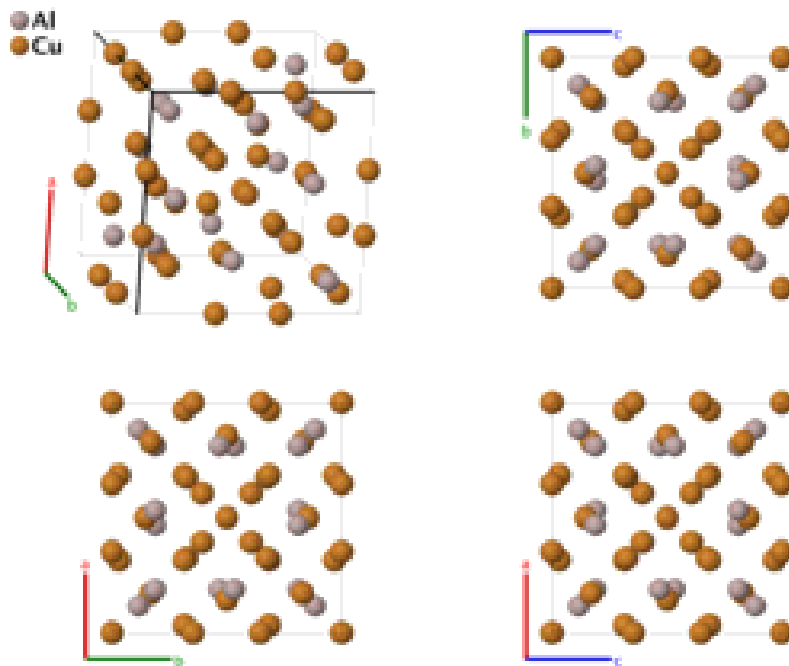
#### Geometry files:

- CIF: pp. 966

- POSCAR: pp. 966

# $\gamma$ -brass ( $\text{Cu}_9\text{Al}_4$ , $D8_3$ ) Structure: A4B9\_cP52\_215\_ei\_3efgi

---



<b>Prototype</b>	:	$\gamma$ - $\text{Cu}_9\text{Al}_4$
<b>AFLOW prototype label</b>	:	A4B9_cP52_215_ei_3efgi
<b>Strukturbericht designation</b>	:	$D8_3$
<b>Pearson symbol</b>	:	cP52
<b>Space group number</b>	:	215
<b>Space group symbol</b>	:	$P\bar{4}3m$
<b>AFLOW prototype command</b>	:	aflow --proto=A4B9_cP52_215_ei_3efgi --params= $a, x_1, x_2, x_3, x_4, x_5, x_6, x_7, z_7, x_8, z_8$

---

## Other compounds with this structure:

- $\text{Cu}_9\text{Ga}_4$ . (Pearson, 1958), pp. 252, gives a list of compounds which can take on the  $D8_1$ ,  $D8_2$ , or  $D8_3$  structure, depending on the exact composition.
- (Arnberg, 1978) give the Wyckoff positions of the Cu IV and Cu V atoms as (6g) ( $x, 1/2, 1/2$ ), but give the coordinates in the form ( $x, 0, 0$ ) corresponding to the (6f) site. (Stokhuyzen, 1974) used (6f) for both types of atoms in the isostructural system  $\text{Ga}_9\text{Al}_4$ . (Pearson, 1958) places the Cu IV atoms on a (6f) site and Cu V on (6g), but does not give explicit coordinates.
- Placing the Cu V atoms on (6f) sites yields an interatomic distance of  $1.8\text{\AA}$ . This contradicts (Arnberg, 1978), who say that the minimum interatomic distance is  $2.48\text{\AA}$  between the Cu IV and Cu V atoms. Placing the Cu V atoms on (6g) sites gives this distance, in agreement with (Pearson, 1958), so we make this choice for the crystal structure. This is a variety of  $\gamma$ -brass comparable to the [D8<sub>2</sub> structure](#). In fact, if we
  - Replace the Al and Cu III atoms by Zn, while setting  $x_4 = x_1 + 1/2$ ,
  - Replace the Al II and Cu VI atoms by Zn, with  $x_8 = x_7 + 1/2$  and  $z_8 = z_7 + 1/2$ ,

– Set  $x_3 = x_2 + 1/2$  and

– Set  $x_6 = x_5 + 1/2$ ,

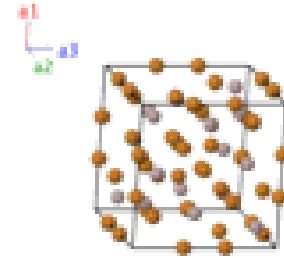
then this structure is identical to  $D8_2$   $\gamma$ -brass.

### Simple Cubic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



### Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} + x_1 a \hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} + x_1 a \hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}} + x_1 a \hat{\mathbf{y}} - x_1 a \hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B}_4$	$= x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}} - x_1 a \hat{\mathbf{y}} - x_1 a \hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$= x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}}$	(4e)	Cu I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$= -x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}}$	(4e)	Cu I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$= -x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}}$	(4e)	Cu I
$\mathbf{B}_8$	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$= x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}}$	(4e)	Cu I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$= -x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$= -x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B}_{12}$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$= x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}}$	(4e)	Cu III
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$= -x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}}$	(4e)	Cu III
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$= -x_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}}$	(4e)	Cu III
$\mathbf{B}_{16}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$= x_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}}$	(4e)	Cu III
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1$	$= x_5 a \hat{\mathbf{x}}$	(6f)	Cu IV
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1$	$= -x_5 a \hat{\mathbf{x}}$	(6f)	Cu IV
$\mathbf{B}_{19}$	$= x_5 \mathbf{a}_2$	$= x_5 a \hat{\mathbf{y}}$	(6f)	Cu IV
$\mathbf{B}_{20}$	$= -x_5 \mathbf{a}_2$	$= -x_5 a \hat{\mathbf{y}}$	(6f)	Cu IV
$\mathbf{B}_{21}$	$= x_5 \mathbf{a}_3$	$= x_5 a \hat{\mathbf{z}}$	(6f)	Cu IV
$\mathbf{B}_{22}$	$= -x_5 \mathbf{a}_3$	$= -x_5 a \hat{\mathbf{z}}$	(6f)	Cu IV
$\mathbf{B}_{23}$	$= x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= x_6 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6g)	Cu V
$\mathbf{B}_{24}$	$= -x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= -x_6 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6g)	Cu V

<b>B</b> <sub>25</sub>	=	$\frac{1}{2} \mathbf{a}_1 + x_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6g)	Cu V
<b>B</b> <sub>26</sub>	=	$\frac{1}{2} \mathbf{a}_1 - x_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6g)	Cu V
<b>B</b> <sub>27</sub>	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + x_6 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + x_6 a \hat{\mathbf{z}}$	(6g)	Cu V
<b>B</b> <sub>28</sub>	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - x_6 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - x_6 a \hat{\mathbf{z}}$	(6g)	Cu V
<b>B</b> <sub>29</sub>	=	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + z_7 a \hat{\mathbf{z}}$	(12i)	Al II
<b>B</b> <sub>30</sub>	=	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + z_7 a \hat{\mathbf{z}}$	(12i)	Al II
<b>B</b> <sub>31</sub>	=	$-x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} - z_7 a \hat{\mathbf{z}}$	(12i)	Al II
<b>B</b> <sub>32</sub>	=	$x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} - z_7 a \hat{\mathbf{z}}$	(12i)	Al II
<b>B</b> <sub>33</sub>	=	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$z_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} + x_7 a \hat{\mathbf{z}}$	(12i)	Al II
<b>B</b> <sub>34</sub>	=	$z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$z_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} - x_7 a \hat{\mathbf{z}}$	(12i)	Al II
<b>B</b> <sub>35</sub>	=	$-z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$-z_7 a \hat{\mathbf{x}} - x_7 a \hat{\mathbf{y}} + x_7 a \hat{\mathbf{z}}$	(12i)	Al II
<b>B</b> <sub>36</sub>	=	$-z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$-z_7 a \hat{\mathbf{x}} + x_7 a \hat{\mathbf{y}} - x_7 a \hat{\mathbf{z}}$	(12i)	Al II
<b>B</b> <sub>37</sub>	=	$x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} + z_7 a \hat{\mathbf{y}} + x_7 a \hat{\mathbf{z}}$	(12i)	Al II
<b>B</b> <sub>38</sub>	=	$-x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} + z_7 a \hat{\mathbf{y}} - x_7 a \hat{\mathbf{z}}$	(12i)	Al II
<b>B</b> <sub>39</sub>	=	$x_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$x_7 a \hat{\mathbf{x}} - z_7 a \hat{\mathbf{y}} - x_7 a \hat{\mathbf{z}}$	(12i)	Al II
<b>B</b> <sub>40</sub>	=	$-x_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$-x_7 a \hat{\mathbf{x}} - z_7 a \hat{\mathbf{y}} + x_7 a \hat{\mathbf{z}}$	(12i)	Al II
<b>B</b> <sub>41</sub>	=	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$x_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} + z_8 a \hat{\mathbf{z}}$	(12i)	Cu VI
<b>B</b> <sub>42</sub>	=	$-x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$-x_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} + z_8 a \hat{\mathbf{z}}$	(12i)	Cu VI
<b>B</b> <sub>43</sub>	=	$-x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	=	$-x_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} - z_8 a \hat{\mathbf{z}}$	(12i)	Cu VI
<b>B</b> <sub>44</sub>	=	$x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	=	$x_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} - z_8 a \hat{\mathbf{z}}$	(12i)	Cu VI
<b>B</b> <sub>45</sub>	=	$z_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	=	$z_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} + x_8 a \hat{\mathbf{z}}$	(12i)	Cu VI
<b>B</b> <sub>46</sub>	=	$z_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - x_8 \mathbf{a}_3$	=	$z_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} - x_8 a \hat{\mathbf{z}}$	(12i)	Cu VI
<b>B</b> <sub>47</sub>	=	$-z_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	=	$-z_8 a \hat{\mathbf{x}} - x_8 a \hat{\mathbf{y}} + x_8 a \hat{\mathbf{z}}$	(12i)	Cu VI
<b>B</b> <sub>48</sub>	=	$-z_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - x_8 \mathbf{a}_3$	=	$-z_8 a \hat{\mathbf{x}} + x_8 a \hat{\mathbf{y}} - x_8 a \hat{\mathbf{z}}$	(12i)	Cu VI
<b>B</b> <sub>49</sub>	=	$x_8 \mathbf{a}_1 + z_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	=	$x_8 a \hat{\mathbf{x}} + z_8 a \hat{\mathbf{y}} + x_8 a \hat{\mathbf{z}}$	(12i)	Cu VI
<b>B</b> <sub>50</sub>	=	$-x_8 \mathbf{a}_1 + z_8 \mathbf{a}_2 - x_8 \mathbf{a}_3$	=	$-x_8 a \hat{\mathbf{x}} + z_8 a \hat{\mathbf{y}} - x_8 a \hat{\mathbf{z}}$	(12i)	Cu VI
<b>B</b> <sub>51</sub>	=	$x_8 \mathbf{a}_1 - z_8 \mathbf{a}_2 - x_8 \mathbf{a}_3$	=	$x_8 a \hat{\mathbf{x}} - z_8 a \hat{\mathbf{y}} - x_8 a \hat{\mathbf{z}}$	(12i)	Cu VI
<b>B</b> <sub>52</sub>	=	$-x_8 \mathbf{a}_1 - z_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	=	$-x_8 a \hat{\mathbf{x}} - z_8 a \hat{\mathbf{y}} + x_8 a \hat{\mathbf{z}}$	(12i)	Cu VI

## References:

- L. Arnberg and S. Westman, *Crystal perfection in a noncentrosymmetric alloy. Refinement and test of twinning of the  $\gamma\text{Cu}_9\text{Al}_4$  structure*, Acta Crystallogr. Sect. A **34**, 399–404 (1978), doi:10.1107/S0567739478000807.
- R. Stokhuyzen, J. K. Brandon, P. C. Chieh, and W. B. Pearson, *Copper-Gallium,  $\gamma_1\text{Cu}_9\text{Ga}_4$* , Acta Crystallogr. Sect. B Struct. Sci. **30**, 2910–2911 (1974), doi:10.1107/S0567740874008478.
- W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

## Found in:

- P. Villars and K. Cenzual, eds., *Structure Types* (Springer, Berlin, Heidelberg, 2005), *Landolt-Börnstein - Group III*

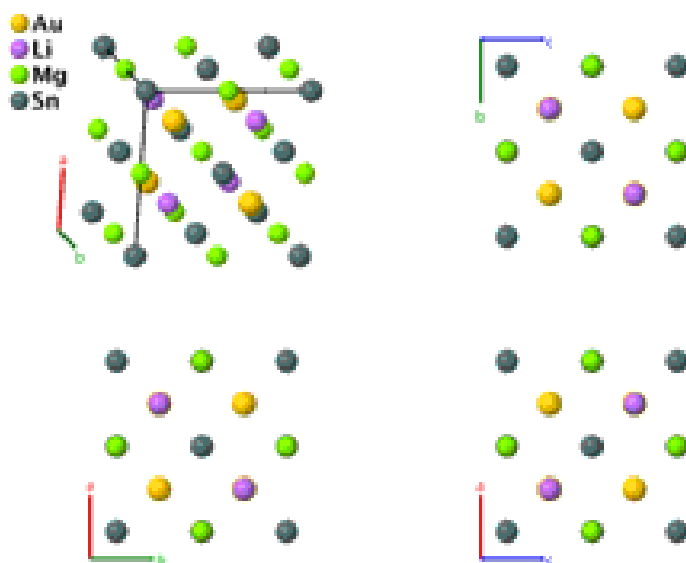
**Geometry files:**

- CIF: pp. [966](#)

- POSCAR: pp. [967](#)



# Quaternary Heusler (LiMgAuSn) Structure: ABCD\_cF16\_216\_c\_d\_b\_a



<b>Prototype</b>	:	LiMgAuSn
<b>AFLOW prototype label</b>	:	ABCD_cF16_216_c_d_b_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cF16
<b>Space group number</b>	:	216
<b>Space group symbol</b>	:	$F\bar{4}3m$
<b>AFLOW prototype command</b>	:	aflow --proto=ABCD_cF16_216_c_d_b_a --params=a

## Other compounds with this structure:

- AuLiMgSn, CuMg<sub>2</sub>Ti, AuBiLi<sub>2</sub>, AgLi<sub>2</sub>Sn, AuLi<sub>2</sub>Sn, CuHfHg<sub>2</sub>, MnPd<sub>2</sub>Sn, and many more. See (Eberz, 1980).
- This “quaternary-Heusler” structure can be considered as the parent of a wide variety of structures, depending on the occupancy of the (4a), (4b), (4c), and (4d) Wyckoff positions. Consider atoms of type A, B, C, D, distributed in this structure. By placing these atoms on the appropriate Wyckoff positions we find the following structures:

Structure	Strukturbericht	AFLOW label	(4a)	(4b)	(4c)	(4d)
simple cubic	$A_h$	A_cP1_221_a	A	A	-	-
fcc	$A1$	A_cF4_225_a	A	-	-	-
bcc	$A2$	A_cI2_229_a	A	A	-	-
diamond	$A4$	A_cF8_227_a	A	-	A	-
NaCl	$B1$	AB_cF8_225_a_b	A	B	-	-
CsCl	$B2$	AB_cP2_221_a_b	A	B	-	-
ZnS (zincblende)	$B3$	AB_cF8_216_c_a	B	-	A	-
half-Heusler	$C1_b$	ABC_cF12_216_b_c_a	C	A	B	-
Heusler	$L2_1$	AB2C_cF16_225_a_c_b	A	C	B	B

The ordering of this structure is somewhat arbitrary. So long as Sn and Mg are on either the (4a)/(4b) or (4c)/(4d) sites, with Au and Li on the opposite sites, we will get the same structure.

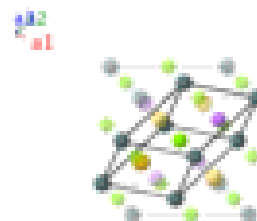
---

### Face-centered Cubic primitive vectors:

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$$




---

### Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(4a)	Sn
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4b)	Mg
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4c)	Au
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4d)	Li

---

### References:

- U. Eberz, W. Seelentag, and H.-U. Schuster, *Zur Kenntnis farbiger ternärer und quaternärer Zintl-Phasen / Coloured Ternary and Quaternary Zintl-Phases*, Z. Naturforsch. B **35**, 1341–1343 (1980), doi:10.1515/znb-1980-1103.

### Found in:

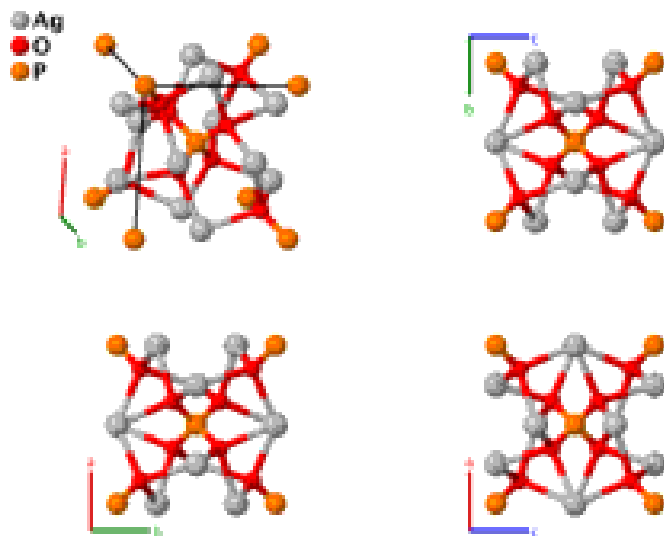
- P. V. C. Editor), ed., *PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database)* (Springer Materials, Heidelberg, 2016), chap. LiMgPdSn Crystal Structure, doi:[https://materials.springer.com/isp/crystallographic/docs/sd\\_1703124](https://materials.springer.com/isp/crystallographic/docs/sd_1703124).

---

### Geometry files:

- CIF: pp. 967  
 - POSCAR: pp. 968

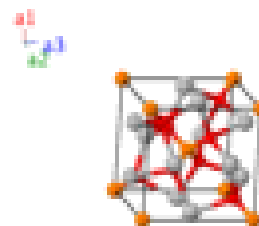
# Ag<sub>3</sub>[PO<sub>4</sub>] Structure: A3B4C\_cP16\_218\_c\_e\_a



**Prototype** : Ag<sub>3</sub>[PO<sub>4</sub>]  
**AFLOW prototype label** : A3B4C\_cP16\_218\_c\_e\_a  
**Strukturbericht designation** : None  
**Pearson symbol** : cP16  
**Space group number** : 218  
**Space group symbol** :  $P\bar{4}3n$   
**AFLOW prototype command** : aflow --proto=A3B4C\_cP16\_218\_c\_e\_a  
 --params= $a, x_3$

Simple Cubic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= a \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(2a)	P
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(2a)	P
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6c)	Ag
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6c)	Ag
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6c)	Ag
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6c)	Ag

$$\begin{aligned}
\mathbf{B}_7 &= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{z}} & (6c) & \text{Ag} \\
\mathbf{B}_8 &= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{z}} & (6c) & \text{Ag} \\
\mathbf{B}_9 &= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}} & (8e) & \text{O} \\
\mathbf{B}_{10} &= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}} & (8e) & \text{O} \\
\mathbf{B}_{11} &= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3 &= -x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}} & (8e) & \text{O} \\
\mathbf{B}_{12} &= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3 &= x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}} & (8e) & \text{O} \\
\mathbf{B}_{13} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{z}} & (8e) & \text{O} \\
\mathbf{B}_{14} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{z}} & (8e) & \text{O} \\
\mathbf{B}_{15} &= \left(\frac{1}{2} + x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{z}} & (8e) & \text{O} \\
\mathbf{B}_{16} &= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{z}} & (8e) & \text{O}
\end{aligned}$$

---

#### References:

- R. Masse, I. Tordjman, and A. Durif, *Affinement de la structure cristalline du monophosphate d'argent Ag<sub>3</sub>PO<sub>4</sub>. Existence d'une forme haute temperature*, Zeitschrift für Kristallographie - Crystalline Materials **144**, 76–81 (1976), [doi:10.1524/zkri.1976.144.1-6.76](https://doi.org/10.1524/zkri.1976.144.1-6.76).

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

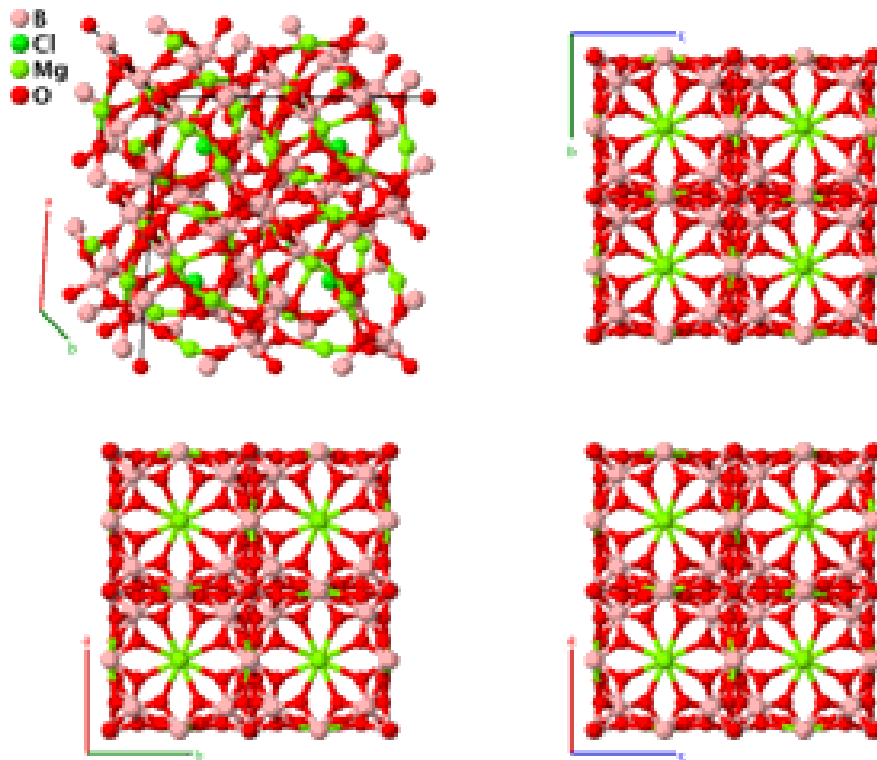
---

#### Geometry files:

- CIF: pp. [968](#)  
- POSCAR: pp. [968](#)

# Boracite ( $\text{Mg}_3\text{B}_7\text{ClO}_{13}$ ) Structure: A7BC3D13\_cF192\_219\_de\_b\_c\_ah

---



<b>Prototype</b>	:	$\text{Mg}_3\text{B}_7\text{ClO}_{13}$
<b>AFLOW prototype label</b>	:	A7BC3D13_cF192_219_de_b_c_ah
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cF192
<b>Space group number</b>	:	219
<b>Space group symbol</b>	:	$F\bar{4}3c$
<b>AFLOW prototype command</b>	:	aflow --proto=A7BC3D13_cF192_219_de_b_c_ah --params= $a, x_5, x_6, y_6, z_6$

---

## Other compounds with this structure:

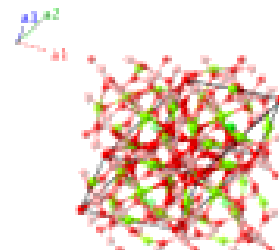
- $M_3\text{B}_7\text{O}_{13}X$ ;  $M = \text{Mg, Cr, Mn, Fe, Co}$ ;  $X = \text{Cl, Br, I}$

- Experimental data was obtained at 400° C.

---

## Face-centered Cubic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{y} + \frac{1}{2} a \hat{z} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{x} + \frac{1}{2} a \hat{z} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{x} + \frac{1}{2} a \hat{y} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$	$=$	$0\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}}$	(8a)	O I
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(8a)	O I
$\mathbf{B}_3$	$= \frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(8b)	Cl
$\mathbf{B}_4$	$= \frac{3}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}} + \frac{3}{4}a\hat{\mathbf{z}}$	(8b)	Cl
$\mathbf{B}_5$	$= \frac{1}{2}\mathbf{a}_1$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	Mg
$\mathbf{B}_6$	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	Mg
$\mathbf{B}_7$	$= \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	Mg
$\mathbf{B}_8$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	Mg
$\mathbf{B}_9$	$= \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(24c)	Mg
$\mathbf{B}_{10}$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24c)	Mg
$\mathbf{B}_{11}$	$= \frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{12}$	$= \frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{13}$	$= \frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{14}$	$= \frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{15}$	$= \frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{16}$	$= \frac{3}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{3}{4}a\hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{17}$	$= x_5\mathbf{a}_1 + x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$x_5a\hat{\mathbf{x}} + x_5a\hat{\mathbf{y}} + x_5a\hat{\mathbf{z}}$	(32e)	B II
$\mathbf{B}_{18}$	$= x_5\mathbf{a}_1 + x_5\mathbf{a}_2 - 3x_5\mathbf{a}_3$	$=$	$-x_5a\hat{\mathbf{x}} - x_5a\hat{\mathbf{y}} + x_5a\hat{\mathbf{z}}$	(32e)	B II
$\mathbf{B}_{19}$	$= x_5\mathbf{a}_1 - 3x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$-x_5a\hat{\mathbf{x}} + x_5a\hat{\mathbf{y}} - x_5a\hat{\mathbf{z}}$	(32e)	B II
$\mathbf{B}_{20}$	$= -3x_5\mathbf{a}_1 + x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$x_5a\hat{\mathbf{x}} - x_5a\hat{\mathbf{y}} - x_5a\hat{\mathbf{z}}$	(32e)	B II
$\mathbf{B}_{21}$	$= \left(\frac{1}{2} + x_5\right)\mathbf{a}_1 + \left(\frac{1}{2} + x_5\right)\mathbf{a}_2 + \left(\frac{1}{2} + x_5\right)\mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_5\right)a\hat{\mathbf{x}} + \left(\frac{1}{2} + x_5\right)a\hat{\mathbf{y}} + \left(\frac{1}{2} + x_5\right)a\hat{\mathbf{z}}$	(32e)	B II
$\mathbf{B}_{22}$	$= \left(\frac{1}{2} + x_5\right)\mathbf{a}_1 + \left(\frac{1}{2} + x_5\right)\mathbf{a}_2 + \left(\frac{1}{2} - 3x_5\right)\mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_5\right)a\hat{\mathbf{x}} + \left(\frac{1}{2} - x_5\right)a\hat{\mathbf{y}} + \left(\frac{1}{2} + x_5\right)a\hat{\mathbf{z}}$	(32e)	B II
$\mathbf{B}_{23}$	$= \left(\frac{1}{2} - 3x_5\right)\mathbf{a}_1 + \left(\frac{1}{2} + x_5\right)\mathbf{a}_2 + \left(\frac{1}{2} + x_5\right)\mathbf{a}_3$	$=$	$\left(\frac{1}{2} + x_5\right)a\hat{\mathbf{x}} + \left(\frac{1}{2} - x_5\right)a\hat{\mathbf{y}} + \left(\frac{1}{2} - x_5\right)a\hat{\mathbf{z}}$	(32e)	B II
$\mathbf{B}_{24}$	$= \left(\frac{1}{2} + x_5\right)\mathbf{a}_1 + \left(\frac{1}{2} - 3x_5\right)\mathbf{a}_2 + \left(\frac{1}{2} + x_5\right)\mathbf{a}_3$	$=$	$\left(\frac{1}{2} - x_5\right)a\hat{\mathbf{x}} + \left(\frac{1}{2} + x_5\right)a\hat{\mathbf{y}} + \left(\frac{1}{2} - x_5\right)a\hat{\mathbf{z}}$	(32e)	B II
$\mathbf{B}_{25}$	$= (-x_6 + y_6 + z_6)\mathbf{a}_1 + (x_6 - y_6 + z_6)\mathbf{a}_2 + (x_6 + y_6 - z_6)\mathbf{a}_3$	$=$	$x_6a\hat{\mathbf{x}} + y_6a\hat{\mathbf{y}} + z_6a\hat{\mathbf{z}}$	(96h)	O II
$\mathbf{B}_{26}$	$= (x_6 - y_6 + z_6)\mathbf{a}_1 + (-x_6 + y_6 + z_6)\mathbf{a}_2 + (-x_6 - y_6 - z_6)\mathbf{a}_3$	$=$	$-x_6a\hat{\mathbf{x}} - y_6a\hat{\mathbf{y}} + z_6a\hat{\mathbf{z}}$	(96h)	O II
$\mathbf{B}_{27}$	$= (x_6 + y_6 - z_6)\mathbf{a}_1 + (-x_6 - y_6 - z_6)\mathbf{a}_2 + (-x_6 + y_6 + z_6)\mathbf{a}_3$	$=$	$-x_6a\hat{\mathbf{x}} + y_6a\hat{\mathbf{y}} - z_6a\hat{\mathbf{z}}$	(96h)	O II

$$\begin{aligned}
\mathbf{B}_{28} &= (-x_6 - y_6 - z_6) \mathbf{a}_1 + (x_6 + y_6 - z_6) \mathbf{a}_2 + (x_6 - y_6 + z_6) \mathbf{a}_3 &= x_6 a \hat{\mathbf{x}} - y_6 a \hat{\mathbf{y}} - z_6 a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{29} &= (x_6 + y_6 - z_6) \mathbf{a}_1 + (-x_6 + y_6 + z_6) \mathbf{a}_2 + (x_6 - y_6 + z_6) \mathbf{a}_3 &= z_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} + y_6 a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{30} &= (-x_6 - y_6 - z_6) \mathbf{a}_1 + (x_6 - y_6 + z_6) \mathbf{a}_2 + (-x_6 + y_6 + z_6) \mathbf{a}_3 &= z_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} - y_6 a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{31} &= (-x_6 + y_6 + z_6) \mathbf{a}_1 + (x_6 + y_6 - z_6) \mathbf{a}_2 + (-x_6 - y_6 - z_6) \mathbf{a}_3 &= -z_6 a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}} + y_6 a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{32} &= (x_6 - y_6 + z_6) \mathbf{a}_1 + (-x_6 - y_6 - z_6) \mathbf{a}_2 + (x_6 + y_6 - z_6) \mathbf{a}_3 &= -z_6 a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}} - y_6 a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{33} &= (x_6 - y_6 + z_6) \mathbf{a}_1 + (x_6 + y_6 - z_6) \mathbf{a}_2 + (-x_6 + y_6 + z_6) \mathbf{a}_3 &= y_6 a \hat{\mathbf{x}} + z_6 a \hat{\mathbf{y}} + x_6 a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{34} &= (-x_6 + y_6 + z_6) \mathbf{a}_1 + (-x_6 - y_6 - z_6) \mathbf{a}_2 + (x_6 - y_6 + z_6) \mathbf{a}_3 &= -y_6 a \hat{\mathbf{x}} + z_6 a \hat{\mathbf{y}} - x_6 a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{35} &= (-x_6 - y_6 - z_6) \mathbf{a}_1 + (-x_6 + y_6 + z_6) \mathbf{a}_2 + (x_6 + y_6 - z_6) \mathbf{a}_3 &= y_6 a \hat{\mathbf{x}} - z_6 a \hat{\mathbf{y}} - x_6 a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{36} &= (x_6 + y_6 - z_6) \mathbf{a}_1 + (x_6 - y_6 + z_6) \mathbf{a}_2 + (-x_6 - y_6 - z_6) \mathbf{a}_3 &= -y_6 a \hat{\mathbf{x}} - z_6 a \hat{\mathbf{y}} + x_6 a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{37} &= \left(\frac{1}{2} + x_6 - y_6 + z_6\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_6 + y_6 + z_6\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_6 + y_6 - z_6\right) \mathbf{a}_3 &= \left(\frac{1}{2} + y_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{38} &= \left(\frac{1}{2} - x_6 + y_6 + z_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_6 - y_6 + z_6\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_3 &= \left(\frac{1}{2} - y_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + z_6\right) a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{39} &= \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_6 + y_6 - z_6\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_6 + y_6 + z_6\right) \mathbf{a}_3 &= \left(\frac{1}{2} + y_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{40} &= \left(\frac{1}{2} + x_6 + y_6 - z_6\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_6 - y_6 + z_6\right) \mathbf{a}_3 &= \left(\frac{1}{2} - y_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_6\right) a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{41} &= \left(\frac{1}{2} - x_6 + y_6 + z_6\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_6 + y_6 - z_6\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_6 - y_6 + z_6\right) \mathbf{a}_3 &= \left(\frac{1}{2} + x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_6\right) a \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{42} &= \left(\frac{1}{2} + x_6 - y_6 + z_6\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_6 - y_6 - z_6\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_6 + y_6 + z_6\right) \mathbf{a}_3 &= \left(\frac{1}{2} - x_6\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + z_6\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_6\right) a \hat{\mathbf{z}} & (96h) & \text{O II}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{43} &= \begin{pmatrix} \frac{1}{2} + x_6 + y_6 - z_6 \\ \frac{1}{2} - x_6 + y_6 + z_6 \\ \frac{1}{2} - x_6 - y_6 - z_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - x_6 \\ \frac{1}{2} + y_6 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} + y_6 \end{pmatrix} a \hat{\mathbf{y}} + a \hat{\mathbf{z}} &= (96h) & \text{O II} \\
\mathbf{B}_{44} &= \begin{pmatrix} \frac{1}{2} - x_6 - y_6 - z_6 \\ \frac{1}{2} + x_6 - y_6 + z_6 \\ \frac{1}{2} + x_6 + y_6 - z_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + x_6 \\ \frac{1}{2} - y_6 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} - y_6 \end{pmatrix} a \hat{\mathbf{y}} + a \hat{\mathbf{z}} &= (96h) & \text{O II} \\
\mathbf{B}_{45} &= \begin{pmatrix} \frac{1}{2} + x_6 + y_6 - z_6 \\ \frac{1}{2} + x_6 - y_6 + z_6 \\ \frac{1}{2} - x_6 + y_6 + z_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + z_6 \\ \frac{1}{2} + x_6 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_6 \\ \frac{1}{2} + x_6 \end{pmatrix} a \hat{\mathbf{y}} + a \hat{\mathbf{z}} &= (96h) & \text{O II} \\
\mathbf{B}_{46} &= \begin{pmatrix} \frac{1}{2} - x_6 - y_6 - z_6 \\ \frac{1}{2} - x_6 + y_6 + z_6 \\ \frac{1}{2} + x_6 - y_6 + z_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + z_6 \\ \frac{1}{2} - x_6 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - y_6 \\ \frac{1}{2} - x_6 \end{pmatrix} a \hat{\mathbf{y}} + a \hat{\mathbf{z}} &= (96h) & \text{O II} \\
\mathbf{B}_{47} &= \begin{pmatrix} \frac{1}{2} - x_6 + y_6 + z_6 \\ \frac{1}{2} - x_6 - y_6 - z_6 \\ \frac{1}{2} + x_6 + y_6 - z_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} - x_6 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_6 \\ \frac{1}{2} - x_6 \end{pmatrix} a \hat{\mathbf{y}} + a \hat{\mathbf{z}} &= (96h) & \text{O II} \\
\mathbf{B}_{48} &= \begin{pmatrix} \frac{1}{2} + x_6 - y_6 + z_6 \\ \frac{1}{2} + x_6 + y_6 - z_6 \\ \frac{1}{2} - x_6 - y_6 - z_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - z_6 \\ \frac{1}{2} + x_6 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} - y_6 \\ \frac{1}{2} + x_6 \end{pmatrix} a \hat{\mathbf{y}} + a \hat{\mathbf{z}} &= (96h) & \text{O II}
\end{aligned}$$

---

#### References:

- S. Sueng, J. R. Clark, J. J. Papike, and J. A. Konnert, *Crystal-Structure Refinement of Cubic Boracite*, Am. Mineral. **58**, 691–697 (1973).

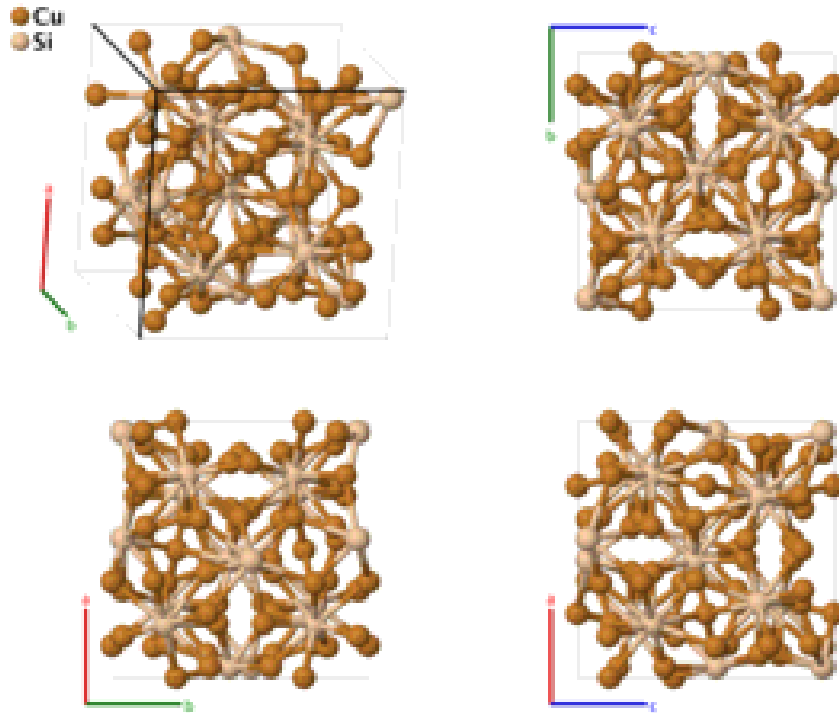
---

#### Geometry files:

- CIF: pp. [969](#)  
- POSCAR: pp. [969](#)



# Cu<sub>15</sub>Si<sub>4</sub> (*D*8<sub>6</sub>) Structure: A15B4\_cI76\_220\_ae\_c



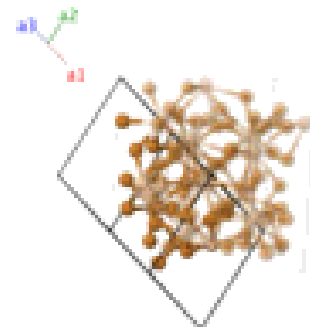
<b>Prototype</b>	:	Cu <sub>15</sub> Si <sub>4</sub>
<b>AFLOW prototype label</b>	:	A15B4_cI76_220_ae_c
<b>Strukturbericht designation</b>	:	<i>D</i> 8 <sub>6</sub>
<b>Pearson symbol</b>	:	cI76
<b>Space group number</b>	:	220
<b>Space group symbol</b>	:	<i>I</i> $\bar{4}$ 3 <i>d</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A15B4_cI76_220_ae_c --params= <i>a</i> , <i>x</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub>

## Other compounds with this structure:

- Cu<sub>15</sub>As<sub>4</sub>, Li<sub>15</sub>Si<sub>4</sub>, Na<sub>15</sub>Pb<sub>4</sub>

## Body-centered Cubic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{2} a \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

Lattice Coordinates

Cartesian Coordinates

Wyckoff Position

Atom Type

$$\begin{aligned}
\mathbf{B}_1 &= \frac{1}{4} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3 &= \frac{3}{8} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{z}} & (12a) & \text{Cu I} \\
\mathbf{B}_2 &= \frac{3}{4} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3 &= \frac{1}{8} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{z}} & (12a) & \text{Cu I} \\
\mathbf{B}_3 &= \frac{3}{8} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} & (12a) & \text{Cu I} \\
\mathbf{B}_4 &= \frac{1}{8} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} & (12a) & \text{Cu I} \\
\mathbf{B}_5 &= \frac{5}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (12a) & \text{Cu I} \\
\mathbf{B}_6 &= \frac{7}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}} & (12a) & \text{Cu I} \\
\mathbf{B}_7 &= 2x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + 2x_2 \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}} & (16c) & \text{Si} \\
\mathbf{B}_8 &= \frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} - 2x_2\right) \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}} & (16c) & \text{Si} \\
\mathbf{B}_9 &= \left(\frac{1}{2} - 2x_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}} & (16c) & \text{Si} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - 2x_2\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 &= x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{z}} & (16c) & \text{Si} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} + 2x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + 2x_2\right) \mathbf{a}_2 + &= \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{y}} + & (16c) & \text{Si} \\
&\quad \left(\frac{1}{2} + 2x_2\right) \mathbf{a}_3 &\quad \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{z}} & & \\
\mathbf{B}_{12} &= \frac{1}{2} \mathbf{a}_1 + -2x_2 \mathbf{a}_3 &= -a \left(x_2 + \frac{1}{4}\right) \hat{\mathbf{x}} + \left(\frac{1}{4} - x_2\right) a \hat{\mathbf{y}} + & (16c) & \text{Si} \\
&&\quad \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{z}} & & \\
\mathbf{B}_{13} &= -2x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 &= \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{x}} - a \left(x_2 + \frac{1}{4}\right) \hat{\mathbf{y}} + & (16c) & \text{Si} \\
&&\quad \left(\frac{1}{4} - x_2\right) a \hat{\mathbf{z}} & & \\
\mathbf{B}_{14} &= -2x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{4} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{y}} - & (16c) & \text{Si} \\
&&\quad a \left(x_2 + \frac{1}{4}\right) \hat{\mathbf{z}} & & \\
\mathbf{B}_{15} &= (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + &= x_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} + z_3 a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
&\quad (x_3 + y_3) \mathbf{a}_3 & & & \\
\mathbf{B}_{16} &= \left(\frac{1}{2} - y_3 + z_3\right) \mathbf{a}_1 + (-x_3 + z_3) \mathbf{a}_2 + &= -x_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} + z_3 a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
&\quad \left(\frac{1}{2} - x_3 - y_3\right) \mathbf{a}_3 & & & \\
\mathbf{B}_{17} &= (y_3 - z_3) \mathbf{a}_1 + \left(\frac{1}{2} - x_3 - z_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}} - z_3 a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
&\quad \left(\frac{1}{2} - x_3 + y_3\right) \mathbf{a}_3 & & & \\
\mathbf{B}_{18} &= \left(\frac{1}{2} - y_3 - z_3\right) \mathbf{a}_1 + &= x_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_3\right) a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
&\quad \left(\frac{1}{2} + x_3 - z_3\right) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3 & & & \\
\mathbf{B}_{19} &= (x_3 + y_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 + &= z_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + y_3 a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
&\quad (x_3 + z_3) \mathbf{a}_3 & & & \\
\mathbf{B}_{20} &= \left(\frac{1}{2} - x_3 - y_3\right) \mathbf{a}_1 + &= z_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
&\quad \left(\frac{1}{2} - y_3 + z_3\right) \mathbf{a}_2 + (-x_3 + z_3) \mathbf{a}_3 & & & \\
\mathbf{B}_{21} &= \left(\frac{1}{2} - x_3 + y_3\right) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + &= -z_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + y_3 a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
&\quad \left(\frac{1}{2} - x_3 - z_3\right) \mathbf{a}_3 & & & \\
\mathbf{B}_{22} &= (x_3 - y_3) \mathbf{a}_1 + \left(\frac{1}{2} - y_3 - z_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - z_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - y_3 a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
&\quad \left(\frac{1}{2} + x_3 - z_3\right) \mathbf{a}_3 & & & \\
\mathbf{B}_{23} &= (x_3 + z_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + &= y_3 a \hat{\mathbf{x}} + z_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
&\quad (y_3 + z_3) \mathbf{a}_3 & & & \\
\mathbf{B}_{24} &= (-x_3 + z_3) \mathbf{a}_1 + \left(\frac{1}{2} - x_3 - y_3\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{x}} + z_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
&\quad \left(\frac{1}{2} - y_3 + z_3\right) \mathbf{a}_3 & & & \\
\mathbf{B}_{25} &= \left(\frac{1}{2} - x_3 - z_3\right) \mathbf{a}_1 + &= y_3 a \hat{\mathbf{x}} - z_3 a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
&\quad \left(\frac{1}{2} - x_3 + y_3\right) \mathbf{a}_2 + (y_3 - z_3) \mathbf{a}_3 & & &
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{26} &= \begin{pmatrix} \frac{1}{2} + x_3 - z_3 \\ \frac{1}{2} - y_3 - z_3 \end{pmatrix} \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \mathbf{a}_3 = -y_3 a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_3\right) a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{27} &= \begin{pmatrix} \frac{1}{2} + x_3 + z_3 \\ \frac{1}{2} + y_3 + z_3 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + x_3 + y_3 \\ \frac{1}{2} + x_3 + z_3 \end{pmatrix} \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} + y_3 \\ \frac{1}{4} + z_3 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + x_3 \\ \frac{1}{4} + z_3 \end{pmatrix} a \hat{\mathbf{y}} + a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{28} &= \begin{pmatrix} \frac{1}{2} - x_3 + z_3 \\ -x_3 - y_3 \end{pmatrix} \mathbf{a}_1 + (-y_3 + z_3) \mathbf{a}_2 + \mathbf{a}_3 = -a \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{x}} + \left(\frac{1}{4} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + z_3\right) a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{29} &= (-x_3 - z_3) \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_3 - z_3 \\ -x_3 + y_3 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} + y_3 \\ \frac{1}{4} - z_3 \end{pmatrix} a \hat{\mathbf{x}} - a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{y}} + \left(\frac{1}{4} - z_3\right) a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{30} &= (x_3 - z_3) \mathbf{a}_1 + (-y_3 - z_3) \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} + x_3 - y_3 \\ \frac{1}{2} + x_3 - y_3 \end{pmatrix} \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} - y_3 \\ a \left(z_3 + \frac{1}{4}\right) \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + x_3 \\ a \left(z_3 + \frac{1}{4}\right) \end{pmatrix} a \hat{\mathbf{y}} - a \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{31} &= \begin{pmatrix} \frac{1}{2} + y_3 + z_3 \\ \frac{1}{2} + x_3 + y_3 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + x_3 + z_3 \\ \frac{1}{2} + x_3 + z_3 \end{pmatrix} \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} + x_3 \\ \frac{1}{4} + y_3 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + z_3 \\ \frac{1}{4} + y_3 \end{pmatrix} a \hat{\mathbf{y}} + a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{32} &= (-y_3 + z_3) \mathbf{a}_1 + (-x_3 - y_3) \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} - x_3 + z_3 \\ \frac{1}{2} - x_3 + z_3 \end{pmatrix} \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} - x_3 \\ a \left(y_3 + \frac{1}{4}\right) \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + z_3 \\ a \left(y_3 + \frac{1}{4}\right) \end{pmatrix} a \hat{\mathbf{y}} - a \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{33} &= \begin{pmatrix} \frac{1}{2} + y_3 - z_3 \\ -x_3 - z_3 \end{pmatrix} \mathbf{a}_1 + (-x_3 + y_3) \mathbf{a}_2 + \mathbf{a}_3 = -a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} - z_3 \\ \frac{1}{4} + y_3 \end{pmatrix} a \hat{\mathbf{y}} + \left(\frac{1}{4} + y_3\right) a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{34} &= (-y_3 - z_3) \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + x_3 - y_3 \\ x_3 - z_3 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} + x_3 \\ \frac{1}{4} - y_3 \end{pmatrix} a \hat{\mathbf{x}} - a \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{y}} + \left(\frac{1}{4} - y_3\right) a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{35} &= \begin{pmatrix} \frac{1}{2} + x_3 + y_3 \\ \frac{1}{2} + x_3 + z_3 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_3 + z_3 \\ \frac{1}{2} + y_3 + z_3 \end{pmatrix} \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} + z_3 \\ \frac{1}{4} + x_3 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + y_3 \\ \frac{1}{4} + x_3 \end{pmatrix} a \hat{\mathbf{y}} + a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{36} &= (-x_3 - y_3) \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - x_3 + z_3 \\ -y_3 + z_3 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} + z_3 \\ \frac{1}{4} - x_3 \end{pmatrix} a \hat{\mathbf{x}} - a \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{y}} + \left(\frac{1}{4} - x_3\right) a \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{37} &= (-x_3 + y_3) \mathbf{a}_1 + (-x_3 - z_3) \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} + y_3 - z_3 \\ \frac{1}{2} + y_3 - z_3 \end{pmatrix} \mathbf{a}_3 = \begin{pmatrix} \frac{1}{4} - z_3 \\ a \left(x_3 + \frac{1}{4}\right) \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} + y_3 \\ a \left(x_3 + \frac{1}{4}\right) \end{pmatrix} a \hat{\mathbf{y}} - a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{38} &= \begin{pmatrix} \frac{1}{2} + x_3 - y_3 \\ -y_3 - z_3 \end{pmatrix} \mathbf{a}_1 + (x_3 - z_3) \mathbf{a}_2 + \mathbf{a}_3 = -a \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} - y_3 \\ \frac{1}{4} + x_3 \end{pmatrix} a \hat{\mathbf{y}} + \left(\frac{1}{4} + x_3\right) a \hat{\mathbf{z}} & (48e) & \text{Cu II}
\end{aligned}$$

---

### References:

- M. Mattern, R. Seyrich, L. Wilde, C. Baetz, M. Knapp, and J. Acker, *Phase formation of rapidly quenched Cu-Si alloys*, *J. Alloys Compd.* **429**, 211–215 (2007), [doi:10.1016/j.jallcom.2006.04.046](https://doi.org/10.1016/j.jallcom.2006.04.046).

### Found in:

- K. Sufryd, N. Ponweiser, P. Riani, K. W. Richter, and G. Cacciamani, *Experimental investigation of the Cu-Si phase diagram at  $x(\text{Cu}) > 0.72$* , *Intermetallics* **19**, 1479–1488 (2011), [doi:10.1016/j.intermet.2011.05.017](https://doi.org/10.1016/j.intermet.2011.05.017).

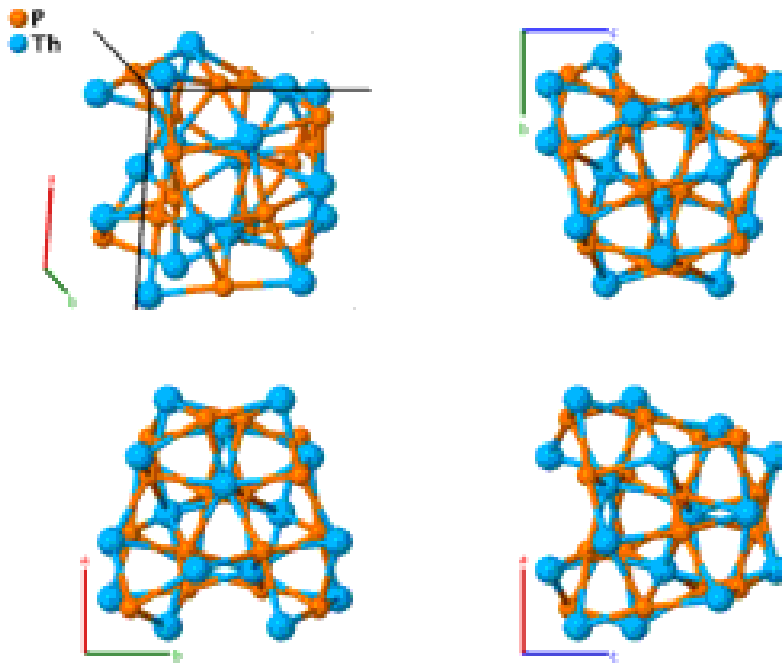
---

### Geometry files:

- CIF: pp. [970](#)

- POSCAR: pp. [970](#)

# Th<sub>3</sub>P<sub>4</sub> (*D*7<sub>3</sub>) Structure: A4B3\_cI28\_220\_c\_a



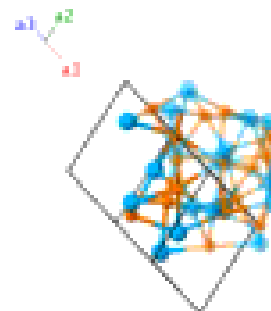
<b>Prototype</b>	:	Th <sub>3</sub> P <sub>4</sub>
<b>AFLOW prototype label</b>	:	A4B3_cI28_220_c_a
<b>Strukturbericht designation</b>	:	<i>D</i> 7 <sub>3</sub>
<b>Pearson symbol</b>	:	cI28
<b>Space group number</b>	:	220
<b>Space group symbol</b>	:	<i>I</i> $\bar{4}$ 3 <i>d</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A4B3_cI28_220_c_a --params= <i>a</i> , <i>x</i> <sub>2</sub>

## Other compounds with this structure:

- Th<sub>3</sub>As<sub>4</sub>, U<sub>3</sub>As<sub>4</sub>, U<sub>3</sub>Bi<sub>4</sub>, N<sub>3</sub>P<sub>4</sub>, Th<sub>3</sub>P<sub>4</sub>, U<sub>3</sub>P<sub>4</sub>, Th<sub>3</sub>Sb<sub>4</sub>, U<sub>3</sub>Sb<sub>4</sub>, U<sub>3</sub>Te<sub>4</sub>

## Body-centered Cubic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}a\hat{\mathbf{z}} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub> =	$\frac{1}{4}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	=	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(12 <i>a</i> )	Th

$$\begin{aligned}
\mathbf{B}_2 &= \frac{3}{4} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3 &= \frac{1}{8} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{z}} & (12a) & \text{Th} \\
\mathbf{B}_3 &= \frac{3}{8} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} & (12a) & \text{Th} \\
\mathbf{B}_4 &= \frac{1}{8} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} & (12a) & \text{Th} \\
\mathbf{B}_5 &= \frac{5}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (12a) & \text{Th} \\
\mathbf{B}_6 &= \frac{7}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}} & (12a) & \text{Th} \\
\mathbf{B}_7 &= 2x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + 2x_2 \mathbf{a}_3 &= x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}} & (16c) & \text{P} \\
\mathbf{B}_8 &= \frac{1}{2} \mathbf{a}_1 + \left(\frac{1}{2} - 2x_2\right) \mathbf{a}_3 &= -x_2 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}} & (16c) & \text{P} \\
\mathbf{B}_9 &= \left(\frac{1}{2} - 2x_2\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}} & (16c) & \text{P} \\
\mathbf{B}_{10} &= \left(\frac{1}{2} - 2x_2\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 &= x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_2\right) a \hat{\mathbf{z}} & (16c) & \text{P} \\
\mathbf{B}_{11} &= \left(\frac{1}{2} + 2x_2\right) \mathbf{a}_1 + \left(\frac{1}{2} + 2x_2\right) \mathbf{a}_2 + &= \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{y}} + & (16c) & \text{P} \\
&\quad \left(\frac{1}{2} + 2x_2\right) \mathbf{a}_3 &\quad \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{z}} & & \\
\mathbf{B}_{12} &= \frac{1}{2} \mathbf{a}_1 + -2x_2 \mathbf{a}_3 &= -a \left(x_2 + \frac{1}{4}\right) \hat{\mathbf{x}} + \left(\frac{1}{4} - x_2\right) a \hat{\mathbf{y}} + & (16c) & \text{P} \\
&&\quad \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{z}} & & \\
\mathbf{B}_{13} &= -2x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 &= \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{x}} - a \left(x_2 + \frac{1}{4}\right) \hat{\mathbf{y}} + & (16c) & \text{P} \\
&&\quad \left(\frac{1}{4} - x_2\right) a \hat{\mathbf{z}} & & \\
\mathbf{B}_{14} &= -2x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \left(\frac{1}{4} - x_2\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_2\right) a \hat{\mathbf{y}} - & (16c) & \text{P} \\
&&\quad a \left(x_2 + \frac{1}{4}\right) \hat{\mathbf{z}} & &
\end{aligned}$$

---

#### References:

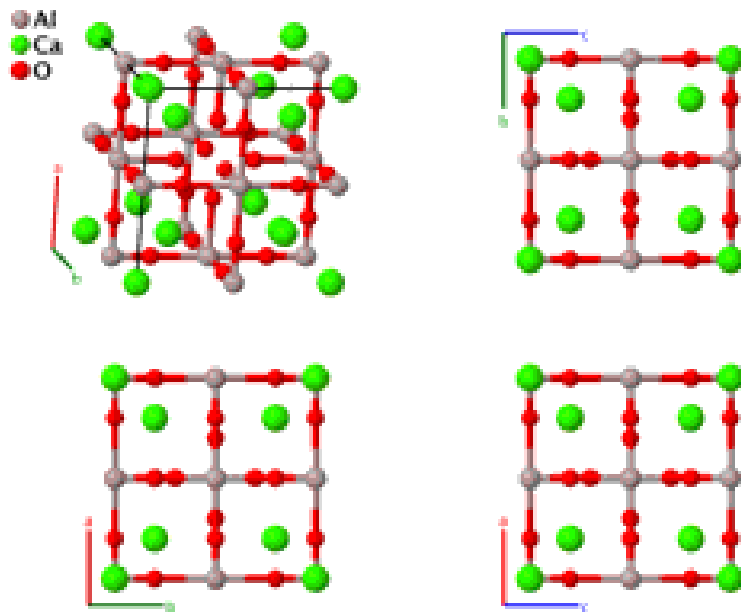
- K. Meisel, *Kristallstrukturen von Thoriumphosphiden*, Z. Anorg. Allg. Chem. **240**, 300–312 (1939), doi:10.1002/zaac.19392400403.

---

#### Geometry files:

- CIF: pp. 970  
- POSCAR: pp. 971

# Ca<sub>3</sub>Al<sub>2</sub>O<sub>6</sub> (*E9*<sub>1</sub>) Structure: A2B3C6\_cP33\_221\_cd\_ag\_fh



<b>Prototype</b>	:	Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub>
<b>AFLOW prototype label</b>	:	A2B3C6_cP33_221_cd_ag_fh
<b>Strukturbericht designation</b>	:	<i>E9</i> <sub>1</sub>
<b>Pearson symbol</b>	:	cP33
<b>Space group number</b>	:	221
<b>Space group symbol</b>	:	<i>Pm</i> $\bar{3}$ <i>m</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3C6_cP33_221_cd_ag_fh --params= <i>a</i> , <i>x</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>x</i> <sub>6</sub>

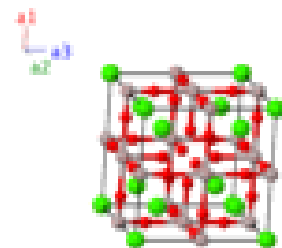
- (Steele, 1929) do not use the standard Wyckoff position notation to describe the atomic positions, so we use the parameters found in (Herman, 1937). An alternative description of the structure places the O I atoms on the (6e) ( $\pm x, 0, 0$ )... site rather than the (6f) site.
- (Mondal, 1975) reanalyzed this structure and concluded that the true structure was one where the lattice constant was doubled and contained 264 atoms. See [the Ca<sub>3</sub>Al<sub>2</sub>O<sub>6</sub> structure page](#).

## Simple Cubic primitive vectors:

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	=	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(1a) Ca I
<b>B</b> <sub>2</sub>	=	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c) Al I
<b>B</b> <sub>3</sub>	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c) Al I
<b>B</b> <sub>4</sub>	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(3c) Al I
<b>B</b> <sub>5</sub>	=	$\frac{1}{2} \mathbf{a}_1$	=	$\frac{1}{2} a \hat{\mathbf{x}}$	(3d) Al II
<b>B</b> <sub>6</sub>	=	$\frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{y}}$	(3d) Al II
<b>B</b> <sub>7</sub>	=	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{z}}$	(3d) Al II
<b>B</b> <sub>8</sub>	=	$x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$x_4 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f) O I
<b>B</b> <sub>9</sub>	=	$-x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-x_4 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f) O I
<b>B</b> <sub>10</sub>	=	$\frac{1}{2} \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f) O I
<b>B</b> <sub>11</sub>	=	$\frac{1}{2} \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f) O I
<b>B</b> <sub>12</sub>	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}}$	(6f) O I
<b>B</b> <sub>13</sub>	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - x_4 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}}$	(6f) O I
<b>B</b> <sub>14</sub>	=	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(8g) Ca II
<b>B</b> <sub>15</sub>	=	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$-x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(8g) Ca II
<b>B</b> <sub>16</sub>	=	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	=	$-x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(8g) Ca II
<b>B</b> <sub>17</sub>	=	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	=	$x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(8g) Ca II
<b>B</b> <sub>18</sub>	=	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	=	$x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(8g) Ca II
<b>B</b> <sub>19</sub>	=	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	=	$-x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} - x_5 a \hat{\mathbf{z}}$	(8g) Ca II
<b>B</b> <sub>20</sub>	=	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$x_5 a \hat{\mathbf{x}} - x_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(8g) Ca II
<b>B</b> <sub>21</sub>	=	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$-x_5 a \hat{\mathbf{x}} + x_5 a \hat{\mathbf{y}} + x_5 a \hat{\mathbf{z}}$	(8g) Ca II
<b>B</b> <sub>22</sub>	=	$x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$x_6 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(12h) O II
<b>B</b> <sub>23</sub>	=	$-x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$-x_6 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(12h) O II
<b>B</b> <sub>24</sub>	=	$x_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$x_6 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12h) O II
<b>B</b> <sub>25</sub>	=	$-x_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-x_6 a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12h) O II
<b>B</b> <sub>26</sub>	=	$\frac{1}{2} \mathbf{a}_1 + x_6 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{z}}$	(12h) O II
<b>B</b> <sub>27</sub>	=	$\frac{1}{2} \mathbf{a}_1 - x_6 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{z}}$	(12h) O II
<b>B</b> <sub>28</sub>	=	$\frac{1}{2} \mathbf{a}_1 + x_6 \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} + x_6 a \hat{\mathbf{y}}$	(12h) O II
<b>B</b> <sub>29</sub>	=	$\frac{1}{2} \mathbf{a}_1 - x_6 \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} - x_6 a \hat{\mathbf{y}}$	(12h) O II
<b>B</b> <sub>30</sub>	=	$x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$x_6 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12h) O II
<b>B</b> <sub>31</sub>	=	$-x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$-x_6 a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12h) O II
<b>B</b> <sub>32</sub>	=	$\frac{1}{2} \mathbf{a}_2 - x_6 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} - x_6 a \hat{\mathbf{z}}$	(12h) O II
<b>B</b> <sub>33</sub>	=	$\frac{1}{2} \mathbf{a}_2 + x_6 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + x_6 a \hat{\mathbf{z}}$	(12h) O II

## References:

- F. A. Steele and W. P. Davey, *The Crystal Structure of Tricalcium Aluminate*, J. Am. Chem. Soc. **51**, 689–697 (1929),

[doi:10.1021/ja01383a001](https://doi.org/10.1021/ja01383a001).

- C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II, 1928-1932* (Akademische Verlagsgesellschaft M. B. H, Leipzig, 1937).

**Found in:**

- P. Mondal and J. W. Jeffery, *The crystal structure of tricalcium aluminate,  $Ca_3Al_2O_6$* , Acta Crystallogr. Sect. B Struct. Sci. **31**, 689–697 (1975), [doi:10.1107/S0567740875003639](https://doi.org/10.1107/S0567740875003639).

---

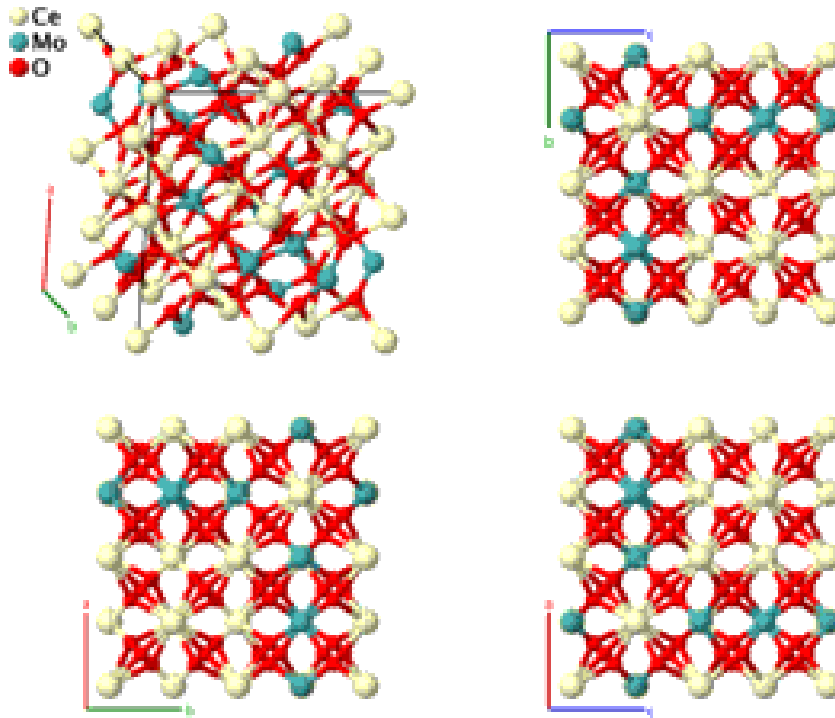
**Geometry files:**

- CIF: pp. [971](#)

- POSCAR: pp. [972](#)



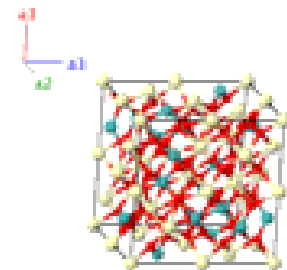
# Ce<sub>5</sub>Mo<sub>3</sub>O<sub>16</sub> Structure: A5B3C16\_cP96\_222\_ce\_d\_fi



<b>Prototype</b>	:	Ce <sub>5</sub> Mo <sub>3</sub> O <sub>16</sub>
<b>AFLOW prototype label</b>	:	A5B3C16_cP96_222_ce_d_fi
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cP96
<b>Space group number</b>	:	222
<b>Space group symbol</b>	:	$Pn\bar{3}n$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A5B3C16_cP96_222_ce_d_fi --params=a, x3, x4, x5, y5, z5</code>

**Simple Cubic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$=$	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(8c)	Ce I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(8c)	Ce I

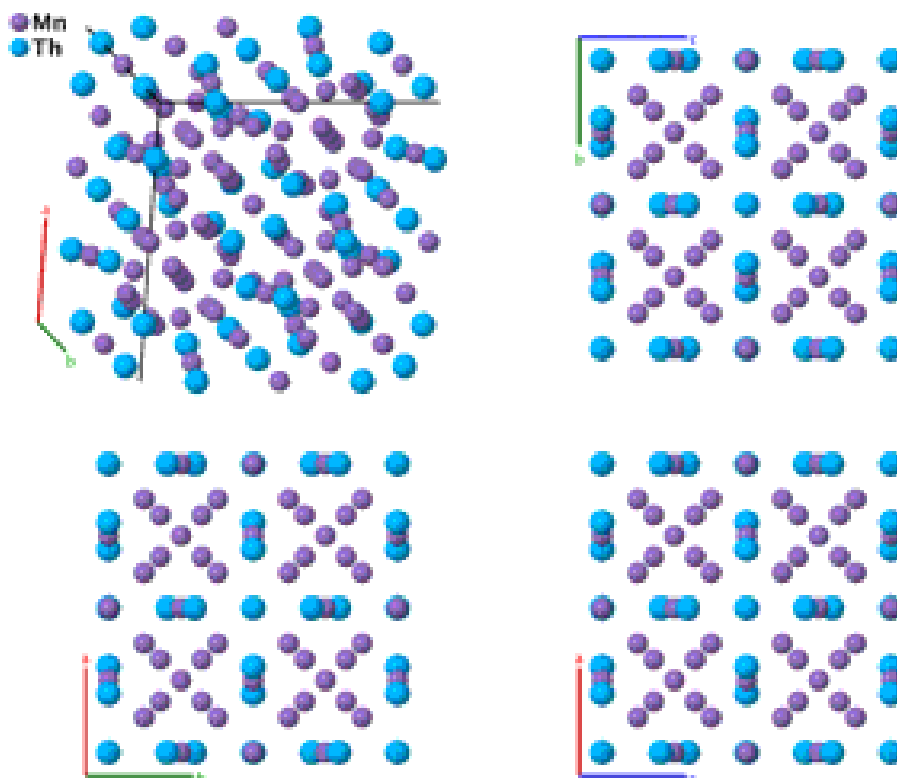






- POSCAR: pp. [972](#)

# Th<sub>6</sub>Mn<sub>23</sub> (*D*8<sub>a</sub>) Structure: A23B6\_cF116\_225\_bd2f\_e



<b>Prototype</b>	:	Th <sub>6</sub> Mn <sub>23</sub>
<b>AFLOW prototype label</b>	:	A23B6_cF116_225_bd2f_e
<b>Strukturbericht designation</b>	:	<i>D</i> 8 <sub>a</sub>
<b>Pearson symbol</b>	:	cF116
<b>Space group number</b>	:	225
<b>Space group symbol</b>	:	<i>Fm</i> $\bar{3}$ <i>m</i>
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A23B6_cF116_225_bd2f_e</code> <code>--params=a, x3, x4, x5</code>

## Other compounds with this structure:

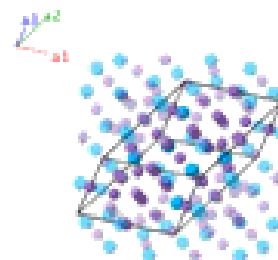
- Ba<sub>6</sub>Mg<sub>23</sub>, Cu<sub>16</sub>Mg<sub>4</sub>Si<sub>7</sub>, Er<sub>6</sub>Fe<sub>23</sub>, Fe<sub>10</sub>Ge<sub>13</sub>Ti<sub>6</sub>, Fe<sub>3</sub>Zn, Ho<sub>6</sub>Fe<sub>23</sub>, Mn<sub>6</sub>Ni<sub>16</sub>Si<sub>7</sub>, Sm<sub>6</sub>Fe<sub>23</sub>, Sr<sub>6</sub>Li<sub>23</sub>, Tb<sub>6</sub>Fe<sub>23</sub>, Th<sub>6-x</sub>Y<sub>x</sub>Mn<sub>23</sub>, Th<sub>6</sub>Mn<sub>23</sub>, Y<sub>6</sub>Mn<sub>23</sub>

## Face-centered Cubic primitive vectors:

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	= $\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(4b)	Mn I
<b>B</b> <sub>2</sub>	= $\frac{1}{2} \mathbf{a}_1$	= $\frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24d)	Mn II
<b>B</b> <sub>3</sub>	= $\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	= $\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24d)	Mn II
<b>B</b> <sub>4</sub>	= $\frac{1}{2} \mathbf{a}_2$	= $\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24d)	Mn II
<b>B</b> <sub>5</sub>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	= $\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24d)	Mn II
<b>B</b> <sub>6</sub>	= $\frac{1}{2} \mathbf{a}_3$	= $\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}}$	(24d)	Mn II
<b>B</b> <sub>7</sub>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	= $\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(24d)	Mn II
<b>B</b> <sub>8</sub>	= $-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	= $x_3a \hat{\mathbf{x}}$	(24e)	Th
<b>B</b> <sub>9</sub>	= $x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	= $-x_3a \hat{\mathbf{x}}$	(24e)	Th
<b>B</b> <sub>10</sub>	= $x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	= $x_3a \hat{\mathbf{y}}$	(24e)	Th
<b>B</b> <sub>11</sub>	= $-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	= $-x_3a \hat{\mathbf{y}}$	(24e)	Th
<b>B</b> <sub>12</sub>	= $x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	= $x_3a \hat{\mathbf{z}}$	(24e)	Th
<b>B</b> <sub>13</sub>	= $-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	= $-x_3a \hat{\mathbf{z}}$	(24e)	Th
<b>B</b> <sub>14</sub>	= $x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	= $x_4a \hat{\mathbf{x}} + x_4a \hat{\mathbf{y}} + x_4a \hat{\mathbf{z}}$	(32f)	Mn III
<b>B</b> <sub>15</sub>	= $x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - 3x_4 \mathbf{a}_3$	= $-x_4a \hat{\mathbf{x}} - x_4a \hat{\mathbf{y}} + x_4a \hat{\mathbf{z}}$	(32f)	Mn III
<b>B</b> <sub>16</sub>	= $x_4 \mathbf{a}_1 - 3x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	= $-x_4a \hat{\mathbf{x}} + x_4a \hat{\mathbf{y}} - x_4a \hat{\mathbf{z}}$	(32f)	Mn III
<b>B</b> <sub>17</sub>	= $-3x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	= $x_4a \hat{\mathbf{x}} - x_4a \hat{\mathbf{y}} - x_4a \hat{\mathbf{z}}$	(32f)	Mn III
<b>B</b> <sub>18</sub>	= $-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + 3x_4 \mathbf{a}_3$	= $x_4a \hat{\mathbf{x}} + x_4a \hat{\mathbf{y}} - x_4a \hat{\mathbf{z}}$	(32f)	Mn III
<b>B</b> <sub>19</sub>	= $-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	= $-x_4a \hat{\mathbf{x}} - x_4a \hat{\mathbf{y}} - x_4a \hat{\mathbf{z}}$	(32f)	Mn III
<b>B</b> <sub>20</sub>	= $-x_4 \mathbf{a}_1 + 3x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	= $x_4a \hat{\mathbf{x}} - x_4a \hat{\mathbf{y}} + x_4a \hat{\mathbf{z}}$	(32f)	Mn III
<b>B</b> <sub>21</sub>	= $3x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	= $-x_4a \hat{\mathbf{x}} + x_4a \hat{\mathbf{y}} + x_4a \hat{\mathbf{z}}$	(32f)	Mn III
<b>B</b> <sub>22</sub>	= $x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	= $x_5a \hat{\mathbf{x}} + x_5a \hat{\mathbf{y}} + x_5a \hat{\mathbf{z}}$	(32f)	Mn IV
<b>B</b> <sub>23</sub>	= $x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - 3x_5 \mathbf{a}_3$	= $-x_5a \hat{\mathbf{x}} - x_5a \hat{\mathbf{y}} + x_5a \hat{\mathbf{z}}$	(32f)	Mn IV
<b>B</b> <sub>24</sub>	= $x_5 \mathbf{a}_1 - 3x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	= $-x_5a \hat{\mathbf{x}} + x_5a \hat{\mathbf{y}} - x_5a \hat{\mathbf{z}}$	(32f)	Mn IV
<b>B</b> <sub>25</sub>	= $-3x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	= $x_5a \hat{\mathbf{x}} - x_5a \hat{\mathbf{y}} - x_5a \hat{\mathbf{z}}$	(32f)	Mn IV
<b>B</b> <sub>26</sub>	= $-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + 3x_5 \mathbf{a}_3$	= $x_5a \hat{\mathbf{x}} + x_5a \hat{\mathbf{y}} - x_5a \hat{\mathbf{z}}$	(32f)	Mn IV
<b>B</b> <sub>27</sub>	= $-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	= $-x_5a \hat{\mathbf{x}} - x_5a \hat{\mathbf{y}} - x_5a \hat{\mathbf{z}}$	(32f)	Mn IV
<b>B</b> <sub>28</sub>	= $-x_5 \mathbf{a}_1 + 3x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	= $x_5a \hat{\mathbf{x}} - x_5a \hat{\mathbf{y}} + x_5a \hat{\mathbf{z}}$	(32f)	Mn IV
<b>B</b> <sub>29</sub>	= $3x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	= $-x_5a \hat{\mathbf{x}} + x_5a \hat{\mathbf{y}} + x_5a \hat{\mathbf{z}}$	(32f)	Mn IV

#### References:

- J. V. Florio, R. E. Rundle, and A. I. Snow, *Compounds of thorium with transition metals. I. The thorium-manganese system*, Acta Cryst. **5**, 445–457 (1952), doi:10.1107/S0365110X52001337.

#### Found in:

- W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

---

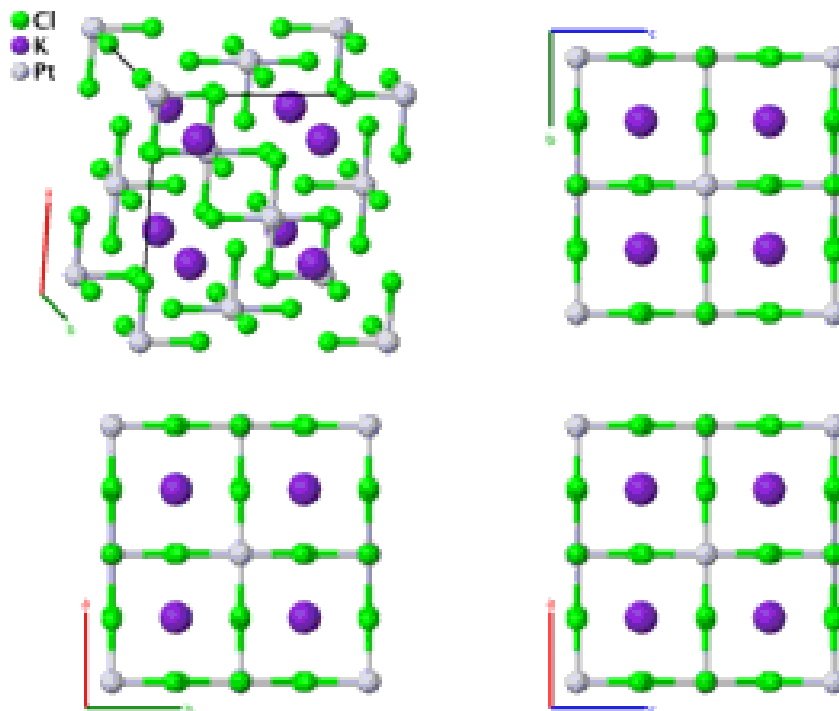
**Geometry files:**

- CIF: pp. [973](#)

- POSCAR: pp. [974](#)



# K<sub>2</sub>PtCl<sub>6</sub> (*J1*<sub>1</sub>) Structure: A6B2C\_cF36\_225\_e\_c\_a



<b>Prototype</b>	:	K <sub>2</sub> PtCl <sub>6</sub>
<b>AFLOW prototype label</b>	:	A6B2C_cF36_225_e_c_a
<b>Strukturbericht designation</b>	:	<i>J1</i> <sub>1</sub>
<b>Pearson symbol</b>	:	cF36
<b>Space group number</b>	:	225
<b>Space group symbol</b>	:	<i>Fm</i> $\bar{3}$ <i>m</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A6B2C_cF36_225_e_c_a --params= <i>a</i> , <i>x</i> <sub>3</sub>

## Other compounds with this structure:

- Gd<sub>2</sub>MnGa<sub>6</sub>, K<sub>2</sub>TeBr<sub>6</sub>, Sr<sub>2</sub>RuH<sub>6</sub>

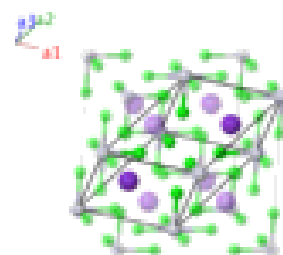
- In (Douglas, 2006), Table 6.6 provides an extensive list of compounds with this structure. Most have the formula *A*<sub>2</sub>*MX*<sub>6</sub>, where *A* is an alkali metal, *M* is a metal, and *X* is a halide. An ammonium ion (NH<sub>4</sub><sup>+</sup>) can also substitute for the alkali.

## Face-centered Cubic primitive vectors:

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$$



## Basis vectors:

	Lattice Coordinates	=	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B<sub>1</sub></b>	=	$0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(4a) Pt
<b>B<sub>2</sub></b>	=	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(8c) K
<b>B<sub>3</sub></b>	=	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{3}{4}a \hat{\mathbf{z}}$	(8c) K
<b>B<sub>4</sub></b>	=	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$x_3a \hat{\mathbf{x}}$	(24e) Cl
<b>B<sub>5</sub></b>	=	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-x_3a \hat{\mathbf{x}}$	(24e) Cl
<b>B<sub>6</sub></b>	=	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$x_3a \hat{\mathbf{y}}$	(24e) Cl
<b>B<sub>7</sub></b>	=	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-x_3a \hat{\mathbf{y}}$	(24e) Cl
<b>B<sub>8</sub></b>	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$x_3a \hat{\mathbf{z}}$	(24e) Cl
<b>B<sub>9</sub></b>	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$-x_3a \hat{\mathbf{z}}$	(24e) Cl

---

#### References:

- G. Engel, *Die Kristallstrukturen einiger Hexachlorokomplexsalze*, Z. Kristallogr. **90**, 341–373 (1935), [doi:10.1524/zkri.1935.90.1.341](https://doi.org/10.1524/zkri.1935.90.1.341).
- B. Douglas and S.-M. Ho, *Structure and Chemistry of Crystalline Solids* (Springer, 2006).

#### Found in:

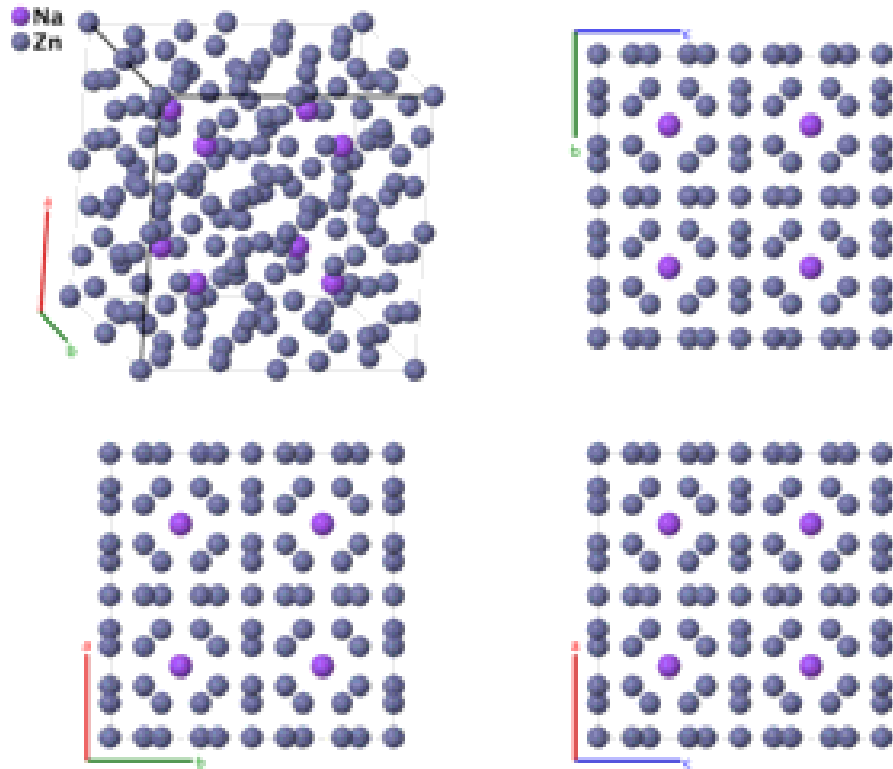
- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

---

#### Geometry files:

- CIF: pp. [974](#)
- POSCAR: pp. [976](#)

# NaZn<sub>13</sub> (*D*<sub>23</sub>) Structure: AB13\_cF112\_226\_a\_bi



<b>Prototype</b>	:	NaZn <sub>13</sub>
<b>AFLOW prototype label</b>	:	AB13_cF112_226_a_bi
<b>Strukturbericht designation</b>	:	<i>D</i> <sub>23</sub>
<b>Pearson symbol</b>	:	cF112
<b>Space group number</b>	:	226
<b>Space group symbol</b>	:	<i>Fm</i> $\bar{3}$ <i>c</i>
<b>AFLOW prototype command</b>	:	aflow --proto=AB13_cF112_226_a_bi --params= <i>a</i> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub>

## Other compounds with this structure:

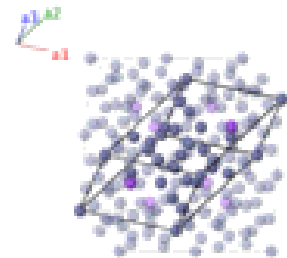
- AmBe<sub>13</sub>, BaZn<sub>13</sub>, CaBe<sub>13</sub>, CaZn<sub>13</sub>, CdZn<sub>13</sub>, CeBe<sub>13</sub>, CsCd<sub>13</sub>, KCd<sub>13</sub>, KZn<sub>13</sub>, MgBe<sub>13</sub>, NbBe<sub>13</sub>, RbCd<sub>13</sub>, SrZn<sub>13</sub>, ThBe<sub>13</sub>, UBe<sub>13</sub>, VBe<sub>13</sub>, ZrBe<sub>13</sub>, CeNi<sub>8.5</sub>Si<sub>4.5</sub>, LaFe<sub>13-x-y</sub>Co<sub>y</sub>Al<sub>x</sub>, LaFe<sub>13-x-y</sub>Co<sub>y</sub>Si<sub>x</sub>, NdFe<sub>13-x-y</sub>Co<sub>y</sub>Si<sub>x</sub>

## Face-centered Cubic primitive vectors:

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub>	= $\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(8a)	Na
<b>B</b> <sub>2</sub>	= $\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{3}{4}a \hat{\mathbf{z}}$	(8a)	Na
<b>B</b> <sub>3</sub>	= $0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	=	$0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(8b)	Zn I
<b>B</b> <sub>4</sub>	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(8b)	Zn I
<b>B</b> <sub>5</sub>	= $(y_3 + z_3) \mathbf{a}_1 + (-y_3 + z_3) \mathbf{a}_2 +$ $(y_3 - z_3) \mathbf{a}_3$	=	$y_3a \hat{\mathbf{y}} + z_3a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>6</sub>	= $(-y_3 + z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 +$ $(-y_3 - z_3) \mathbf{a}_3$	=	$-y_3a \hat{\mathbf{y}} + z_3a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>7</sub>	= $(y_3 - z_3) \mathbf{a}_1 + (-y_3 - z_3) \mathbf{a}_2 +$ $(y_3 + z_3) \mathbf{a}_3$	=	$y_3a \hat{\mathbf{y}} - z_3a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>8</sub>	= $(-y_3 - z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 +$ $(-y_3 + z_3) \mathbf{a}_3$	=	$-y_3a \hat{\mathbf{y}} - z_3a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>9</sub>	= $(y_3 - z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 +$ $(-y_3 + z_3) \mathbf{a}_3$	=	$z_3a \hat{\mathbf{x}} + y_3a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>10</sub>	= $(-y_3 - z_3) \mathbf{a}_1 + (-y_3 + z_3) \mathbf{a}_2 +$ $(y_3 + z_3) \mathbf{a}_3$	=	$z_3a \hat{\mathbf{x}} - y_3a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>11</sub>	= $(y_3 + z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 +$ $(-y_3 - z_3) \mathbf{a}_3$	=	$-z_3a \hat{\mathbf{x}} + y_3a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>12</sub>	= $(-y_3 + z_3) \mathbf{a}_1 + (-y_3 - z_3) \mathbf{a}_2 +$ $(y_3 - z_3) \mathbf{a}_3$	=	$-z_3a \hat{\mathbf{x}} - y_3a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>13</sub>	= $(-y_3 + z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 +$ $(y_3 + z_3) \mathbf{a}_3$	=	$y_3a \hat{\mathbf{x}} + z_3a \hat{\mathbf{y}}$	(96i)	Zn II
<b>B</b> <sub>14</sub>	= $(y_3 + z_3) \mathbf{a}_1 + (-y_3 - z_3) \mathbf{a}_2 +$ $(-y_3 + z_3) \mathbf{a}_3$	=	$-y_3a \hat{\mathbf{x}} + z_3a \hat{\mathbf{y}}$	(96i)	Zn II
<b>B</b> <sub>15</sub>	= $(-y_3 - z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 +$ $(y_3 - z_3) \mathbf{a}_3$	=	$y_3a \hat{\mathbf{x}} - z_3a \hat{\mathbf{y}}$	(96i)	Zn II
<b>B</b> <sub>16</sub>	= $(y_3 - z_3) \mathbf{a}_1 + (-y_3 + z_3) \mathbf{a}_2 +$ $(-y_3 - z_3) \mathbf{a}_3$	=	$-y_3a \hat{\mathbf{x}} - z_3a \hat{\mathbf{y}}$	(96i)	Zn II
<b>B</b> <sub>17</sub>	= $(\frac{1}{2} - y_3 - z_3) \mathbf{a}_1 + (\frac{1}{2} + y_3 - z_3) \mathbf{a}_2 +$ $(\frac{1}{2} + y_3 + z_3) \mathbf{a}_3$	=	$(\frac{1}{2} + y_3)a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + (\frac{1}{2} - z_3)a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>18</sub>	= $(\frac{1}{2} + y_3 - z_3) \mathbf{a}_1 + (\frac{1}{2} - y_3 - z_3) \mathbf{a}_2 +$ $(\frac{1}{2} - y_3 + z_3) \mathbf{a}_3$	=	$(\frac{1}{2} - y_3)a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + (\frac{1}{2} - z_3)a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>19</sub>	= $(\frac{1}{2} - y_3 + z_3) \mathbf{a}_1 + (\frac{1}{2} + y_3 + z_3) \mathbf{a}_2 +$ $(\frac{1}{2} + y_3 - z_3) \mathbf{a}_3$	=	$(\frac{1}{2} + y_3)a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + (\frac{1}{2} + z_3)a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>20</sub>	= $(\frac{1}{2} + y_3 + z_3) \mathbf{a}_1 + (\frac{1}{2} - y_3 + z_3) \mathbf{a}_2 +$ $(\frac{1}{2} - y_3 - z_3) \mathbf{a}_3$	=	$(\frac{1}{2} - y_3)a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + (\frac{1}{2} + z_3)a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>21</sub>	= $(\frac{1}{2} - y_3 + z_3) \mathbf{a}_1 + (\frac{1}{2} - y_3 - z_3) \mathbf{a}_2 +$ $(\frac{1}{2} + y_3 + z_3) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + (\frac{1}{2} + z_3)a \hat{\mathbf{y}} + (\frac{1}{2} - y_3)a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>22</sub>	= $(\frac{1}{2} + y_3 + z_3) \mathbf{a}_1 + (\frac{1}{2} + y_3 - z_3) \mathbf{a}_2 +$ $(\frac{1}{2} - y_3 + z_3) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + (\frac{1}{2} + z_3)a \hat{\mathbf{y}} + (\frac{1}{2} + y_3)a \hat{\mathbf{z}}$	(96i)	Zn II
<b>B</b> <sub>23</sub>	= $(\frac{1}{2} - y_3 - z_3) \mathbf{a}_1 + (\frac{1}{2} - y_3 + z_3) \mathbf{a}_2 +$ $(\frac{1}{2} + y_3 - z_3) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + (\frac{1}{2} - z_3)a \hat{\mathbf{y}} + (\frac{1}{2} - y_3)a \hat{\mathbf{z}}$	(96i)	Zn II

$$\mathbf{B}_{24} = \begin{pmatrix} \frac{1}{2} + y_3 - z_3 \\ \frac{1}{2} - y_3 - z_3 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_3 + z_3 \\ \frac{1}{2} - y_3 + z_3 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \frac{1}{2} a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{z}} \\ \left(\frac{1}{2} - y_3 - z_3\right) \mathbf{a}_3 \end{pmatrix} \quad (96i) \quad \text{Zn II}$$

$$\mathbf{B}_{25} = \begin{pmatrix} \frac{1}{2} + y_3 - z_3 \\ \frac{1}{2} + y_3 + z_3 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - y_3 + z_3 \\ \frac{1}{2} + y_3 - z_3 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \left(\frac{1}{2} + z_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \left(\frac{1}{2} + y_3 + z_3\right) \mathbf{a}_3 \end{pmatrix} \quad (96i) \quad \text{Zn II}$$

$$\mathbf{B}_{26} = \begin{pmatrix} \frac{1}{2} - y_3 - z_3 \\ \frac{1}{2} - y_3 + z_3 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_3 + z_3 \\ \frac{1}{2} - y_3 - z_3 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \left(\frac{1}{2} + z_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \left(\frac{1}{2} - y_3 + z_3\right) \mathbf{a}_3 \end{pmatrix} \quad (96i) \quad \text{Zn II}$$

$$\mathbf{B}_{27} = \begin{pmatrix} \frac{1}{2} + y_3 + z_3 \\ \frac{1}{2} + y_3 - z_3 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} - y_3 - z_3 \\ \frac{1}{2} + y_3 + z_3 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \left(\frac{1}{2} - z_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} + y_3\right) a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \left(\frac{1}{2} + y_3 - z_3\right) \mathbf{a}_3 \end{pmatrix} \quad (96i) \quad \text{Zn II}$$

$$\mathbf{B}_{28} = \begin{pmatrix} \frac{1}{2} - y_3 + z_3 \\ \frac{1}{2} - y_3 - z_3 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + y_3 - z_3 \\ \frac{1}{2} - y_3 + z_3 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \left(\frac{1}{2} - z_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_3\right) a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \left(\frac{1}{2} - y_3 - z_3\right) \mathbf{a}_3 \end{pmatrix} \quad (96i) \quad \text{Zn II}$$

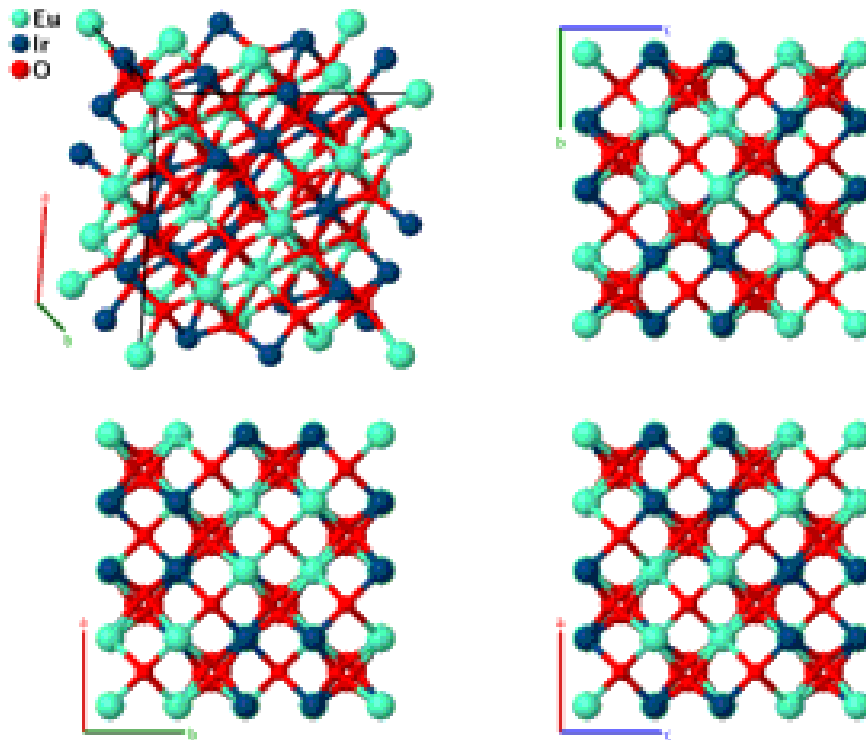
### References:

- D. P. Shoemaker, R. E. Marsh, F. J. Ewing, and L. Pauling, *Interatomic distances and atomic valences in NaZn<sub>13</sub>*, *Acta Cryst.* **5**, 637–644 (1952), [doi:10.1107/S0365110X52001763](https://doi.org/10.1107/S0365110X52001763).

### Geometry files:

- CIF: pp. [976](#)
- POSCAR: pp. [977](#)

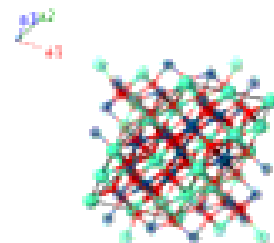
# Pyrochlore Iridate ( $\text{Eu}_2\text{Ir}_2\text{O}_7$ ) Structure: A2B2C7\_cF88\_227\_c\_d\_af



**Prototype** :  $\text{Eu}_2\text{Ir}_2\text{O}_7$   
**AFLOW prototype label** : A2B2C7\_cF88\_227\_c\_d\_af  
**Strukturbericht designation** : None  
**Pearson symbol** : cF88  
**Space group number** : 227  
**Space group symbol** :  $Fd\bar{3}m$   
**AFLOW prototype command** : aflow --proto=A2B2C7\_cF88\_227\_c\_d\_af  
 --params=a, x4

Face-centered Cubic primitive vectors:

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}} \\
 \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}
 \end{aligned}$$



Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$	=	$\frac{1}{8} a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}}$	(8a)	O I

$$\begin{aligned}
\mathbf{B}_2 &= \frac{7}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3 &= \frac{7}{8} a \hat{\mathbf{x}} + \frac{7}{8} a \hat{\mathbf{y}} + \frac{7}{8} a \hat{\mathbf{z}} & (8a) & \text{O I} \\
\mathbf{B}_3 &= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3 &= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}} & (16c) & \text{Eu} \\
\mathbf{B}_4 &= \frac{1}{2} \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} & (16c) & \text{Eu} \\
\mathbf{B}_5 &= \frac{1}{2} \mathbf{a}_2 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{z}} & (16c) & \text{Eu} \\
\mathbf{B}_6 &= \frac{1}{2} \mathbf{a}_1 &= \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}} & (16c) & \text{Eu} \\
\mathbf{B}_7 &= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (16d) & \text{Ir} \\
\mathbf{B}_8 &= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (16d) & \text{Ir} \\
\mathbf{B}_9 &= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}} & (16d) & \text{Ir} \\
\mathbf{B}_{10} &= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}} & (16d) & \text{Ir} \\
\mathbf{B}_{11} &= \left(\frac{1}{4} - x_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 &= x_4 a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}} & (48f) & \text{O II} \\
\mathbf{B}_{12} &= x_4 \mathbf{a}_1 + \left(\frac{1}{4} - x_4\right) \mathbf{a}_2 + \left(\frac{1}{4} - x_4\right) \mathbf{a}_3 &= \left(\frac{1}{4} - x_4\right) a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}} & (48f) & \text{O II} \\
\mathbf{B}_{13} &= x_4 \mathbf{a}_1 + \left(\frac{1}{4} - x_4\right) \mathbf{a}_2 + x_4 \mathbf{a}_3 &= \frac{1}{8} a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}} & (48f) & \text{O II} \\
\mathbf{B}_{14} &= \left(\frac{1}{4} - x_4\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{4} - x_4\right) \mathbf{a}_3 &= \frac{1}{8} a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_4\right) a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}} & (48f) & \text{O II} \\
\mathbf{B}_{15} &= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(\frac{1}{4} - x_4\right) \mathbf{a}_3 &= \frac{1}{8} a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}} & (48f) & \text{O II} \\
\mathbf{B}_{16} &= \left(\frac{1}{4} - x_4\right) \mathbf{a}_1 + \left(\frac{1}{4} - x_4\right) \mathbf{a}_2 + x_4 \mathbf{a}_3 &= \frac{1}{8} a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_4\right) a \hat{\mathbf{z}} & (48f) & \text{O II} \\
\mathbf{B}_{17} &= \left(\frac{3}{4} + x_4\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{3}{4} + x_4\right) \mathbf{a}_3 &= \frac{3}{8} a \hat{\mathbf{x}} + \left(\frac{3}{4} + x_4\right) a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (48f) & \text{O II} \\
\mathbf{B}_{18} &= -x_4 \mathbf{a}_1 + \left(\frac{3}{4} + x_4\right) \mathbf{a}_2 - x_4 \mathbf{a}_3 &= \frac{3}{8} a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (48f) & \text{O II} \\
\mathbf{B}_{19} &= -x_4 \mathbf{a}_1 + \left(\frac{3}{4} + x_4\right) \mathbf{a}_2 + \left(\frac{3}{4} + x_4\right) \mathbf{a}_3 &= \left(\frac{3}{4} + x_4\right) a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (48f) & \text{O II} \\
\mathbf{B}_{20} &= \left(\frac{3}{4} + x_4\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3 &= -x_4 a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (48f) & \text{O II} \\
\mathbf{B}_{21} &= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(\frac{3}{4} + x_4\right) \mathbf{a}_3 &= \frac{3}{8} a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}} & (48f) & \text{O II} \\
\mathbf{B}_{22} &= \left(\frac{3}{4} + x_4\right) \mathbf{a}_1 + \left(\frac{3}{4} + x_4\right) \mathbf{a}_2 - x_4 \mathbf{a}_3 &= \frac{3}{8} a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} + \left(\frac{3}{4} + x_4\right) a \hat{\mathbf{z}} & (48f) & \text{O II}
\end{aligned}$$

---

### References:

- H. Sagayama, D. Uematsu, T. Arima, K. Sugimoto, J. J. Ishikawa, E. O'Farrell, and S. Nakatsuji, *Determination of long-range all-in-all-out ordering of Ir<sup>4+</sup> moments in a pyrochlore iridate Eu<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> by resonant x-ray diffraction*, Phys. Rev. B **87**, 100403 (2013), [doi:10.1103/PhysRevB.87.100403](https://doi.org/10.1103/PhysRevB.87.100403).

### Found in:

- S. H. Chun, B. Yuan, D. Casa, J. Kim, C.-Y. Kim, Z. Tian, Y. Qiu, S. Nakatsuji, and Y.-J. Kim, *Magnetic Excitations across the Metal-Insulator Transition in the Pyrochlore Iridate Eu<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>*, Phys. Rev. Lett. **120**, 177203 (2018), [doi:10.1103/PhysRevLett.120.177203](https://doi.org/10.1103/PhysRevLett.120.177203).

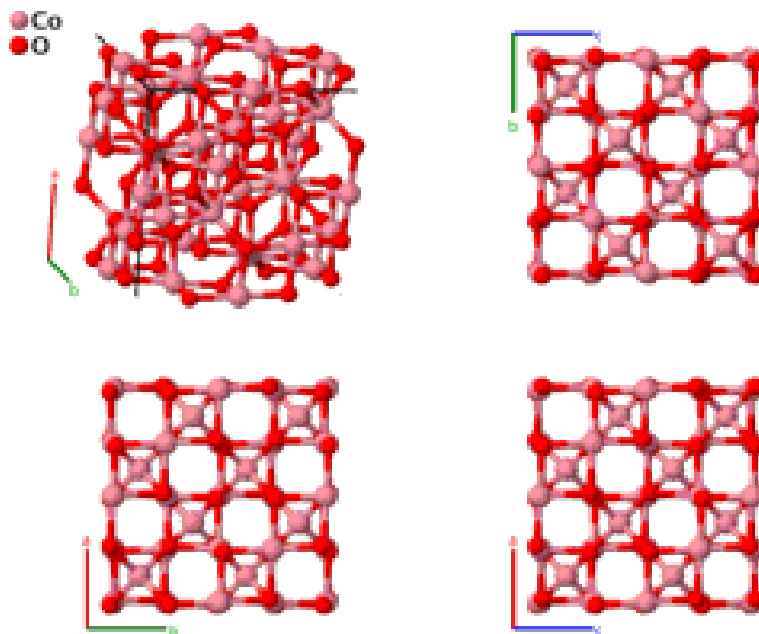
---

### Geometry files:

- CIF: pp. [977](#)  
- POSCAR: pp. [978](#)

# Spinel ( $\text{Co}_3\text{O}_4$ , $D7_2$ ) Structure: A3B4\_cF56\_227\_ad\_e

---



<b>Prototype</b>	:	$\text{Co}_3\text{O}_4$
<b>AFLOW prototype label</b>	:	A3B4_cF56_227_ad_e
<b>Strukturbericht designation</b>	:	$D7_2$
<b>Pearson symbol</b>	:	cF56
<b>Space group number</b>	:	227
<b>Space group symbol</b>	:	$Fd\bar{3}m$
<b>AFLOW prototype command</b>	:	aflow --proto=A3B4_cF56_227_ad_e --params=a, x3

---

## Other compounds with this structure:

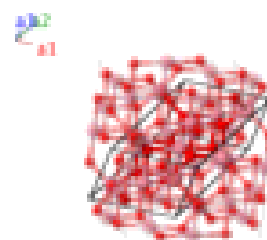
- $\text{NiCo}_2\text{O}_4$ ,  $\text{Co}_3\text{S}_4$ ,  $\text{NiCo}_2\text{S}_4$ ,  $\text{FeNi}_2\text{S}_4$

- The  $D7_2$  and  $H1_1$  Spinel structures are for all intents and purposes identical. We could use  $D7_3$  for the binary spinels and  $H1_1$  for the ternaries, but historically this has not been the case. We dual-list this structure only to keep the historical record intact. (Hahn, 1955) has an extensive list of ternary spinels and inverse spinels.

---

## Face-centered Cubic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} \end{aligned}$$




---

## Basis vectors:



	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$	$=$	$\frac{1}{8}a \hat{\mathbf{x}} + \frac{1}{8}a \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$	(8a)	Co I
$\mathbf{B}_2$	$= \frac{7}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3$	$=$	$\frac{7}{8}a \hat{\mathbf{x}} + \frac{7}{8}a \hat{\mathbf{y}} + \frac{7}{8}a \hat{\mathbf{z}}$	(8a)	Co I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(16d)	Co II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(16d)	Co II
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(16d)	Co II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(16d)	Co II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$x_3a \hat{\mathbf{x}} + x_3a \hat{\mathbf{y}} + x_3a \hat{\mathbf{z}}$	(32e)	O
$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} - 3x_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} - x_3\right)a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_3\right)a \hat{\mathbf{y}} + x_3a \hat{\mathbf{z}}$	(32e)	O
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + \left(\frac{1}{2} - 3x_3\right) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$\left(\frac{1}{4} - x_3\right)a \hat{\mathbf{x}} + x_3a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_3\right)a \hat{\mathbf{z}}$	(32e)	O
$\mathbf{B}_{10}$	$= \left(\frac{1}{2} - 3x_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$x_3a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_3\right)a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_3\right)a \hat{\mathbf{z}}$	(32e)	O
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(\frac{1}{2} + 3x_3\right) \mathbf{a}_3$	$=$	$\left(\frac{1}{4} + x_3\right)a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_3\right)a \hat{\mathbf{y}} - x_3a \hat{\mathbf{z}}$	(32e)	O
$\mathbf{B}_{12}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-x_3a \hat{\mathbf{x}} - x_3a \hat{\mathbf{y}} - x_3a \hat{\mathbf{z}}$	(32e)	O
$\mathbf{B}_{13}$	$= -x_3 \mathbf{a}_1 + \left(\frac{1}{2} + 3x_3\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\left(\frac{1}{4} + x_3\right)a \hat{\mathbf{x}} - x_3a \hat{\mathbf{y}} + \left(\frac{1}{4} + x_3\right)a \hat{\mathbf{z}}$	(32e)	O
$\mathbf{B}_{14}$	$= \left(\frac{1}{2} + 3x_3\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-x_3a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_3\right)a \hat{\mathbf{y}} + \left(\frac{1}{4} + x_3\right)a \hat{\mathbf{z}}$	(32e)	O

---

#### References:

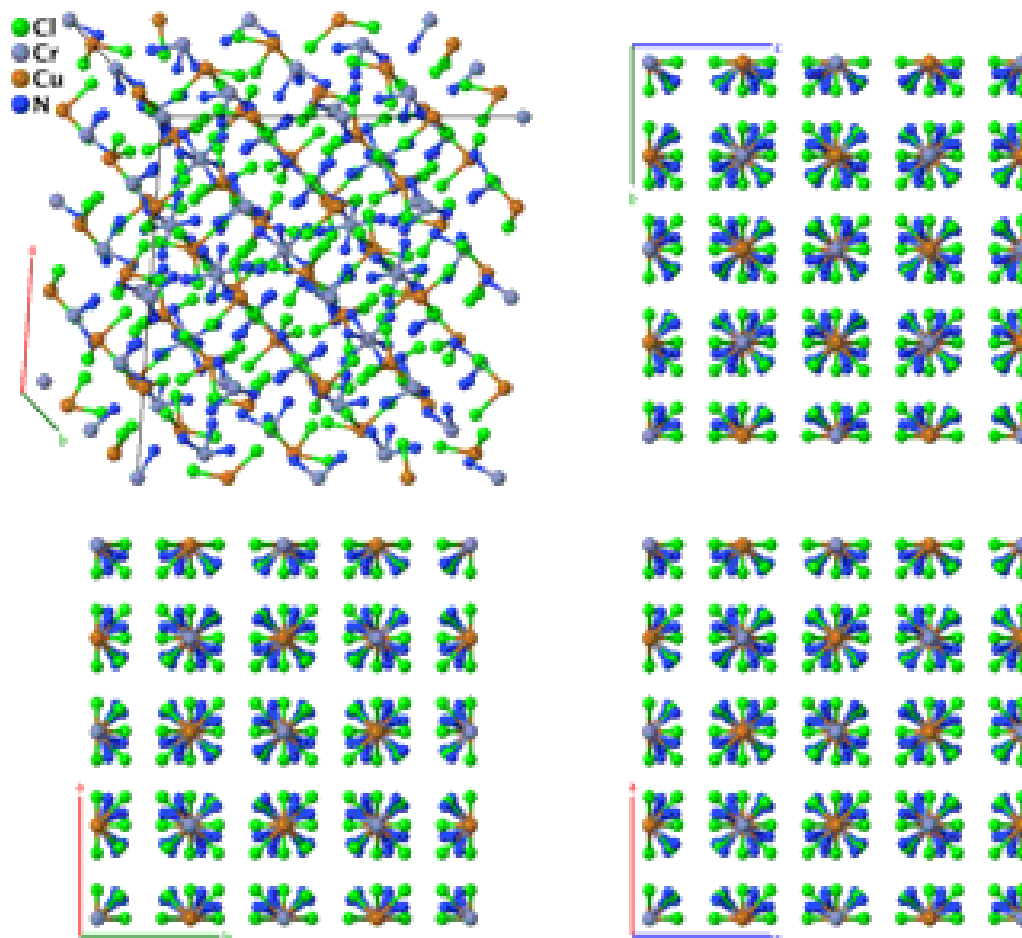
- O. Knop, K. I. G. Reid, Sutarno, and Y. Nakagawa, *Chalkogenides of the transition elements. VI. X-Ray, neutron, and magnetic investigation of the spinels  $\text{Co}_3\text{O}_4$ ,  $\text{NiCo}_2\text{O}_4$ ,  $\text{Co}_3\text{S}_4$ , and  $\text{NiCo}_2\text{S}_4$* , *Can. J. Chem.* **46**, 3463–3476 (1968), [doi:10.1139/v68-576](https://doi.org/10.1139/v68-576).
- H. Hahn, G. Frank, W. Klingler, A. D. Störger, and G. Störger, *Chalkogenide. VI. Über Ternäre Chalkogenide des Aluminiums, Galliums und Indiums mit Zink, Cadmium und Quecksilber*, *Z. Anorg. Allg. Chem.* **279**, 241–270 (1955), [doi:10.1002/zaac.19552790502](https://doi.org/10.1002/zaac.19552790502).

---

#### Geometry files:

- CIF: pp. 978
- POSCAR: pp. 980

# CuCrCl<sub>5</sub>[NH<sub>3</sub>]<sub>6</sub> Structure: A5BCD6\_cF416\_228\_eg\_c\_b\_h



<b>Prototype</b>	:	CuCrCl <sub>5</sub> [NH <sub>3</sub> ] <sub>6</sub>
<b>AFLOW prototype label</b>	:	A5BCD6_cF416_228_eg_c_b_h
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cF416
<b>Space group number</b>	:	228
<b>Space group symbol</b>	:	$Fd\bar{3}c$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A5BCD6_cF416_228_eg_c_b_h --params=a, x3, y4, x5, y5, z5</code>

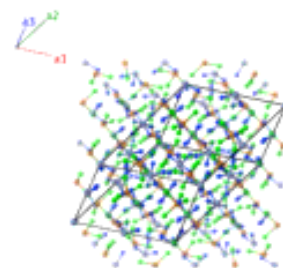
- The N atoms correspond to NH<sub>3</sub> units centered on the (192h) Wyckoff positions.

**Face-centered Cubic primitive vectors:**

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(32b)	Cu
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(32b)	Cu
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(32b)	Cu
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(32b)	Cu
$\mathbf{B}_5$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(32b)	Cu
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(32b)	Cu
$\mathbf{B}_7$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(32b)	Cu
$\mathbf{B}_8$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(32b)	Cu
$\mathbf{B}_9$	$= 0 \mathbf{a}_1 + 0 \mathbf{a}_2 + 0 \mathbf{a}_3$	$= 0 \hat{\mathbf{x}} + 0 \hat{\mathbf{y}} + 0 \hat{\mathbf{z}}$	(32c)	Cr
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(32c)	Cr
$\mathbf{B}_{11}$	$= \frac{1}{2} \mathbf{a}_2$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{z}}$	(32c)	Cr
$\mathbf{B}_{12}$	$= \frac{1}{2} \mathbf{a}_1$	$= \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(32c)	Cr
$\mathbf{B}_{13}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(32c)	Cr
$\mathbf{B}_{14}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(32c)	Cr
$\mathbf{B}_{15}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(32c)	Cr
$\mathbf{B}_{16}$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(32c)	Cr
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}}$	(64e)	Cl I
$\mathbf{B}_{18}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(\frac{1}{2} - 3x_3\right) \mathbf{a}_3$	$= \left(\frac{1}{4} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_3\right) a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}}$	(64e)	Cl I
$\mathbf{B}_{19}$	$= x_3 \mathbf{a}_1 + \left(\frac{1}{2} - 3x_3\right) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$= \left(\frac{1}{4} - x_3\right) a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_3\right) a \hat{\mathbf{z}}$	(64e)	Cl I
$\mathbf{B}_{20}$	$= \left(\frac{1}{2} - 3x_3\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$= x_3 a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} - x_3\right) a \hat{\mathbf{z}}$	(64e)	Cl I
$\mathbf{B}_{21}$	$= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + 3x_3 \mathbf{a}_3$	$= \left(\frac{1}{4} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{z}}$	(64e)	Cl I
$\mathbf{B}_{22}$	$= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_3$	$= \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{z}}$	(64e)	Cl I
$\mathbf{B}_{23}$	$= \left(\frac{1}{2} - x_3\right) \mathbf{a}_1 + 3x_3 \mathbf{a}_2 + \left(\frac{1}{2} - x_3\right) \mathbf{a}_3$	$= \left(\frac{1}{4} + x_3\right) a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_3\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + x_3\right) a \hat{\mathbf{z}}$	(64e)	Cl I









$$\mathbf{B}_{104} = \begin{pmatrix} \frac{1}{2} + x_5 + y_5 - z_5 \\ \frac{1}{2} + x_5 - y_5 + z_5 \\ \frac{1}{2} - x_5 + y_5 + z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} \frac{1}{2} + z_5 \\ \frac{1}{2} + x_5 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_5 \\ \frac{1}{2} + x_5 \end{pmatrix} a \hat{\mathbf{y}} + \begin{pmatrix} \frac{1}{2} + z_5 \\ \frac{1}{2} + x_5 \end{pmatrix} a \hat{\mathbf{z}} \quad (192h) \quad \text{N}$$

---

**References:**

- M. Masayasu, S. Yoshihiko, and W. Tokunosuké, *The Crystal Structure of [Cr(NH<sub>3</sub>)<sub>6</sub>] [CuCl<sub>5</sub>]*, Bull. Chem. Soc. Jpn. **34**, 295–296 (1961), [doi:10.1246/bcsj.34.295](https://doi.org/10.1246/bcsj.34.295).

**Found in:**

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

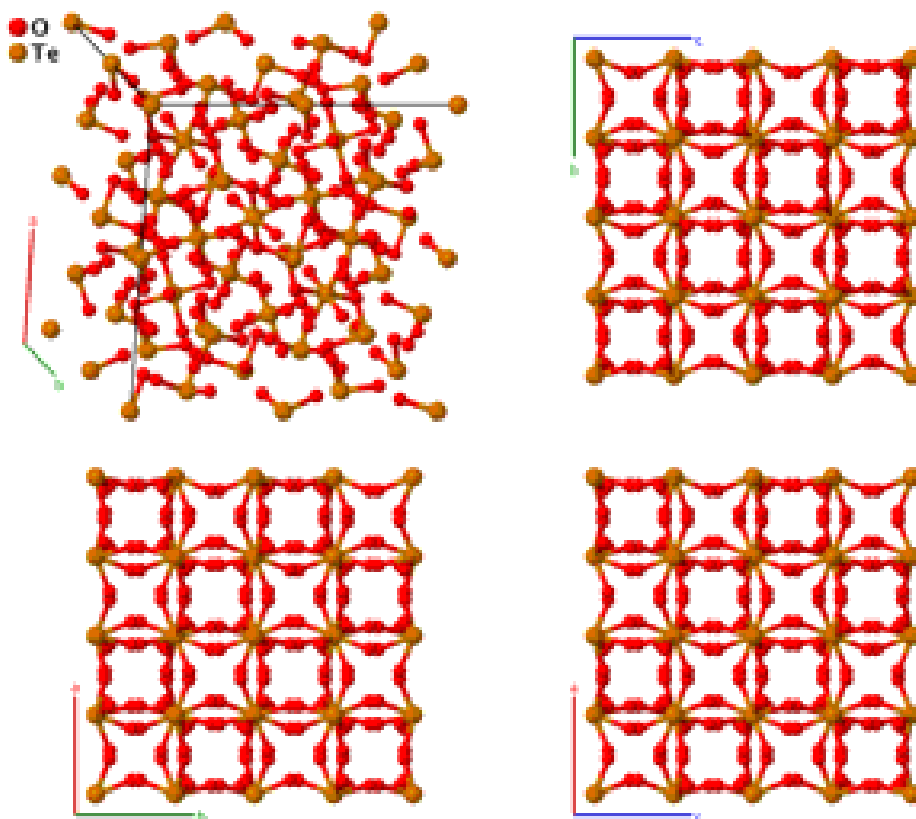
---

**Geometry files:**

- CIF: pp. [980](#)
- POSCAR: pp. [981](#)



# TeO<sub>6</sub>H<sub>6</sub> Structure: A6B\_cF224\_228\_h\_c



<b>Prototype</b>	:	TeO <sub>6</sub> H <sub>6</sub>
<b>AFLOW prototype label</b>	:	A6B_cF224_228_h_c
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cF224
<b>Space group number</b>	:	228
<b>Space group symbol</b>	:	$Fd\bar{3}c$
<b>AFLOW prototype command</b>	:	<code>aflow --proto=A6B_cF224_228_h_c --params=a, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub></code>

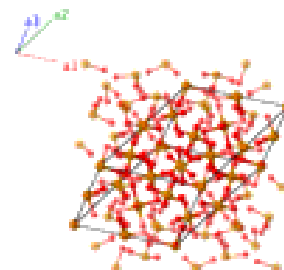
- Polytypes appear in space groups #14, #210 and #225. Only the non-hydrogen atoms are listed.

## Face-centered Cubic primitive vectors:

$$\mathbf{a}_1 = \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$$



## Basis vectors:

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$	$=$	$0\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}}$	(32c)	Te
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(32c)	Te
$\mathbf{B}_3$	$= \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(32c)	Te
$\mathbf{B}_4$	$= \frac{1}{2}\mathbf{a}_1$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(32c)	Te
$\mathbf{B}_5$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(32c)	Te
$\mathbf{B}_6$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(32c)	Te
$\mathbf{B}_7$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(32c)	Te
$\mathbf{B}_8$	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(32c)	Te
$\mathbf{B}_9$	$= (-x_2 + y_2 + z_2)\mathbf{a}_1 +$ $(x_2 - y_2 + z_2)\mathbf{a}_2 +$ $(x_2 + y_2 - z_2)\mathbf{a}_3$	$=$	$x_2a\hat{\mathbf{x}} + y_2a\hat{\mathbf{y}} + z_2a\hat{\mathbf{z}}$	(192h)	O
$\mathbf{B}_{10}$	$= (x_2 - y_2 + z_2)\mathbf{a}_1 +$ $(-x_2 + y_2 + z_2)\mathbf{a}_2 +$ $(\frac{1}{2} - x_2 - y_2 - z_2)\mathbf{a}_3$	$=$	$(\frac{1}{4} - x_2)a\hat{\mathbf{x}} + (\frac{1}{4} - y_2)a\hat{\mathbf{y}} + z_2a\hat{\mathbf{z}}$	(192h)	O
$\mathbf{B}_{11}$	$= (x_2 + y_2 - z_2)\mathbf{a}_1 +$ $(\frac{1}{2} - x_2 - y_2 - z_2)\mathbf{a}_2 +$ $(-x_2 + y_2 + z_2)\mathbf{a}_3$	$=$	$(\frac{1}{4} - x_2)a\hat{\mathbf{x}} + y_2a\hat{\mathbf{y}} + (\frac{1}{4} - z_2)a\hat{\mathbf{z}}$	(192h)	O
$\mathbf{B}_{12}$	$= (\frac{1}{2} - x_2 - y_2 - z_2)\mathbf{a}_1 +$ $(x_2 + y_2 - z_2)\mathbf{a}_2 +$ $(x_2 - y_2 + z_2)\mathbf{a}_3$	$=$	$x_2a\hat{\mathbf{x}} + (\frac{1}{4} - y_2)a\hat{\mathbf{y}} + (\frac{1}{4} - z_2)a\hat{\mathbf{z}}$	(192h)	O
$\mathbf{B}_{13}$	$= (x_2 + y_2 - z_2)\mathbf{a}_1 +$ $(-x_2 + y_2 + z_2)\mathbf{a}_2 +$ $(x_2 - y_2 + z_2)\mathbf{a}_3$	$=$	$z_2a\hat{\mathbf{x}} + x_2a\hat{\mathbf{y}} + y_2a\hat{\mathbf{z}}$	(192h)	O
$\mathbf{B}_{14}$	$= (\frac{1}{2} - x_2 - y_2 - z_2)\mathbf{a}_1 +$ $(x_2 - y_2 + z_2)\mathbf{a}_2 +$ $(-x_2 + y_2 + z_2)\mathbf{a}_3$	$=$	$z_2a\hat{\mathbf{x}} + (\frac{1}{4} - x_2)a\hat{\mathbf{y}} + (\frac{1}{4} - y_2)a\hat{\mathbf{z}}$	(192h)	O
$\mathbf{B}_{15}$	$= (-x_2 + y_2 + z_2)\mathbf{a}_1 +$ $(x_2 + y_2 - z_2)\mathbf{a}_2 +$ $(\frac{1}{2} - x_2 - y_2 - z_2)\mathbf{a}_3$	$=$	$(\frac{1}{4} - z_2)a\hat{\mathbf{x}} + (\frac{1}{4} - x_2)a\hat{\mathbf{y}} + y_2a\hat{\mathbf{z}}$	(192h)	O
$\mathbf{B}_{16}$	$= (x_2 - y_2 + z_2)\mathbf{a}_1 +$ $(\frac{1}{2} - x_2 - y_2 - z_2)\mathbf{a}_2 +$ $(x_2 + y_2 - z_2)\mathbf{a}_3$	$=$	$(\frac{1}{4} - z_2)a\hat{\mathbf{x}} + x_2a\hat{\mathbf{y}} + (\frac{1}{4} - y_2)a\hat{\mathbf{z}}$	(192h)	O
$\mathbf{B}_{17}$	$= (x_2 - y_2 + z_2)\mathbf{a}_1 +$ $(x_2 + y_2 - z_2)\mathbf{a}_2 +$ $(-x_2 + y_2 + z_2)\mathbf{a}_3$	$=$	$y_2a\hat{\mathbf{x}} + z_2a\hat{\mathbf{y}} + x_2a\hat{\mathbf{z}}$	(192h)	O
$\mathbf{B}_{18}$	$= (-x_2 + y_2 + z_2)\mathbf{a}_1 +$ $(\frac{1}{2} - x_2 - y_2 - z_2)\mathbf{a}_2 +$ $(x_2 - y_2 + z_2)\mathbf{a}_3$	$=$	$(\frac{1}{4} - y_2)a\hat{\mathbf{x}} + z_2a\hat{\mathbf{y}} + (\frac{1}{4} - x_2)a\hat{\mathbf{z}}$	(192h)	O
$\mathbf{B}_{19}$	$= (\frac{1}{2} - x_2 - y_2 - z_2)\mathbf{a}_1 +$ $(-x_2 + y_2 + z_2)\mathbf{a}_2 +$ $(x_2 + y_2 - z_2)\mathbf{a}_3$	$=$	$y_2a\hat{\mathbf{x}} + (\frac{1}{4} - z_2)a\hat{\mathbf{y}} + (\frac{1}{4} - x_2)a\hat{\mathbf{z}}$	(192h)	O
$\mathbf{B}_{20}$	$= (x_2 + y_2 - z_2)\mathbf{a}_1 +$ $(x_2 - y_2 + z_2)\mathbf{a}_2 +$ $(\frac{1}{2} - x_2 - y_2 - z_2)\mathbf{a}_3$	$=$	$(\frac{1}{4} - y_2)a\hat{\mathbf{x}} + (\frac{1}{4} - z_2)a\hat{\mathbf{y}} + x_2a\hat{\mathbf{z}}$	(192h)	O





$$\begin{aligned}
\mathbf{B}_{52} &= \begin{pmatrix} \frac{1}{2} + x_2 - y_2 + z_2 \\ -x_2 - y_2 - z_2 \\ \frac{1}{2} - x_2 + y_2 + z_2 \end{pmatrix} \mathbf{a}_1 + &= \begin{pmatrix} \frac{1}{4} - x_2 \\ \frac{1}{4} - y_2 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + z_2 \\ \frac{1}{4} - y_2 \end{pmatrix} a \hat{\mathbf{y}} + & (192h) & \text{O} \\
& \begin{pmatrix} -x_2 - y_2 - z_2 \\ \frac{1}{2} - x_2 + y_2 + z_2 \end{pmatrix} \mathbf{a}_2 + \\
& \begin{pmatrix} \frac{1}{2} + x_2 - y_2 + z_2 \\ \frac{1}{2} + x_2 + y_2 - z_2 \\ -x_2 - y_2 - z_2 \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{53} &= \begin{pmatrix} \frac{1}{2} + x_2 - y_2 + z_2 \\ \frac{1}{2} + x_2 + y_2 - z_2 \\ -x_2 - y_2 - z_2 \end{pmatrix} \mathbf{a}_1 + &= \begin{pmatrix} \frac{1}{4} - z_2 \\ \frac{1}{2} + x_2 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} - y_2 \\ \frac{1}{2} + x_2 \end{pmatrix} a \hat{\mathbf{y}} + & (192h) & \text{O} \\
& \begin{pmatrix} \frac{1}{2} + x_2 - y_2 + z_2 \\ -x_2 - y_2 - z_2 \\ \frac{1}{2} + x_2 + y_2 - z_2 \end{pmatrix} \mathbf{a}_2 + \\
& \begin{pmatrix} \frac{1}{2} - x_2 + y_2 + z_2 \\ -x_2 - y_2 - z_2 \\ \frac{1}{2} + x_2 + y_2 - z_2 \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{54} &= \begin{pmatrix} \frac{1}{2} - x_2 + y_2 + z_2 \\ -x_2 - y_2 - z_2 \\ \frac{1}{2} + x_2 + y_2 - z_2 \end{pmatrix} \mathbf{a}_1 + &= \begin{pmatrix} \frac{1}{4} - z_2 \\ \frac{1}{4} - x_2 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_2 \\ \frac{1}{4} - x_2 \end{pmatrix} a \hat{\mathbf{y}} + & (192h) & \text{O} \\
& \begin{pmatrix} -x_2 - y_2 - z_2 \\ \frac{1}{2} - x_2 + y_2 + z_2 \\ \frac{1}{2} + x_2 - y_2 + z_2 \end{pmatrix} \mathbf{a}_2 + \\
& \begin{pmatrix} -x_2 - y_2 - z_2 \\ \frac{1}{2} - x_2 + y_2 + z_2 \\ \frac{1}{2} + x_2 - y_2 + z_2 \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{55} &= \begin{pmatrix} -x_2 - y_2 - z_2 \\ \frac{1}{2} - x_2 + y_2 + z_2 \\ \frac{1}{2} + x_2 - y_2 + z_2 \end{pmatrix} \mathbf{a}_1 + &= \begin{pmatrix} \frac{1}{2} + z_2 \\ \frac{1}{4} - x_2 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{4} - y_2 \\ \frac{1}{4} - x_2 \end{pmatrix} a \hat{\mathbf{y}} + & (192h) & \text{O} \\
& \begin{pmatrix} \frac{1}{2} - x_2 + y_2 + z_2 \\ \frac{1}{2} + x_2 - y_2 + z_2 \\ \frac{1}{2} + x_2 - y_2 + z_2 \end{pmatrix} \mathbf{a}_2 + \\
& \begin{pmatrix} \frac{1}{2} + x_2 - y_2 + z_2 \\ \frac{1}{2} + x_2 - y_2 + z_2 \\ \frac{1}{2} - x_2 + y_2 + z_2 \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{56} &= \begin{pmatrix} \frac{1}{2} + x_2 + y_2 - z_2 \\ \frac{1}{2} + x_2 - y_2 + z_2 \\ \frac{1}{2} - x_2 + y_2 + z_2 \end{pmatrix} \mathbf{a}_1 + &= \begin{pmatrix} \frac{1}{2} + z_2 \\ \frac{1}{2} + x_2 \end{pmatrix} a \hat{\mathbf{x}} + \begin{pmatrix} \frac{1}{2} + y_2 \\ \frac{1}{2} + x_2 \end{pmatrix} a \hat{\mathbf{y}} + & (192h) & \text{O} \\
& \begin{pmatrix} \frac{1}{2} + x_2 + y_2 - z_2 \\ \frac{1}{2} + x_2 - y_2 + z_2 \\ \frac{1}{2} - x_2 + y_2 + z_2 \end{pmatrix} \mathbf{a}_2 + \\
& \begin{pmatrix} \frac{1}{2} + x_2 + y_2 - z_2 \\ \frac{1}{2} + x_2 - y_2 + z_2 \\ \frac{1}{2} - x_2 + y_2 + z_2 \end{pmatrix} \mathbf{a}_3
\end{aligned}$$

---

#### References:

- L. M. Kirkpatrick and L. Pauling, *XXVIII. Über die Kristallstruktur der kubischen Tellursäure*, *Zeitschrift für Kristallographie - Crystalline Materials* **63**, 502–506 (1926), doi:10.1524/zkri.1926.63.1.502.

#### Found in:

- P. Villars and K. Cenzual, *Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds*, ASM International (2013).

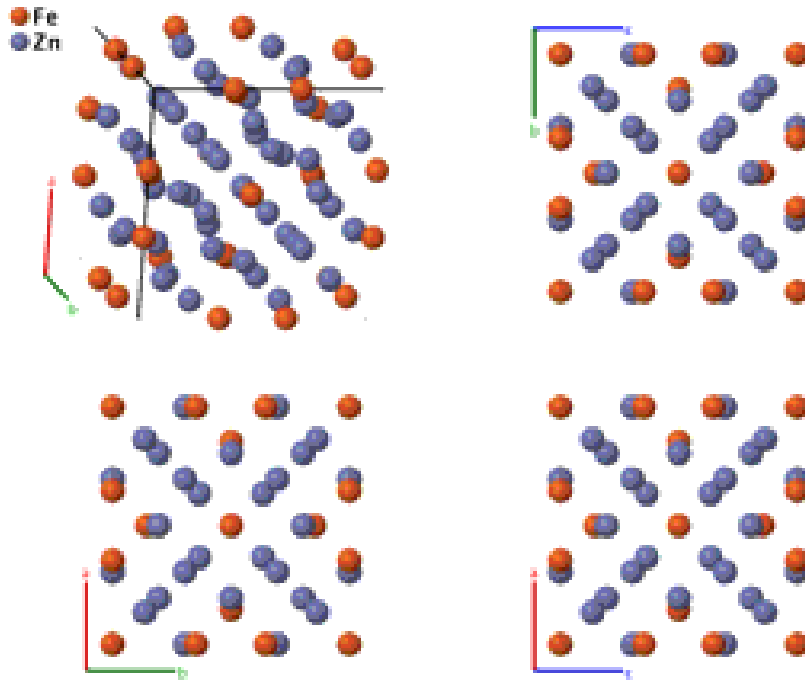
---

#### Geometry files:

- CIF: pp. 982  
- POSCAR: pp. 983

# $\gamma$ -brass ( $\text{Fe}_3\text{Zn}_{10}$ , $D8_1$ ) Structure: A3B10\_cI52\_229\_e\_fh

---



<b>Prototype</b>	:	$\gamma\text{-Fe}_3\text{Zn}_{10}$
<b>AFLOW prototype label</b>	:	A3B10_cI52_229_e_fh
<b>Strukturbericht designation</b>	:	$D8_1$
<b>Pearson symbol</b>	:	cI52
<b>Space group number</b>	:	229
<b>Space group symbol</b>	:	$Im\bar{3}m$
<b>AFLOW prototype command</b>	:	aflow --proto=A3B10_cI52_229_e_fh --params= $a, x_1, x_2, y_3$

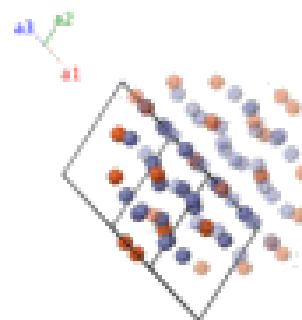
---

## Other compounds with this structure:

- (Pearson, 1958), p. 252, gives a list of compounds which can take on the  $D8_1$ ,  $D8_2$ , or  $D8_3$  structure, depending on the exact composition.
- Adding another atom at the origin changes this to the [L2<sub>2</sub> structure](#). This structure is defined in (Pearson, 1958) quoting (Schramm, 1938). More recent investigations such as (Johannsson, 1968), (Brandon, 1974) and (Yu, 2005) find that  $\gamma\text{-Fe}_3\text{Zn}_{10}$  forms in the [D8<sub>2</sub> structure](#), with Fe atoms on one (8c) site, Zn atoms on the other (8e) site and the (24g) sites, and a 50-50 alloy of Fe and Zn on the other (8e) site. We use Brandon's data, mapping (12g)  $\rightarrow$  (12e), (24g)  $\rightarrow$  (24h), and averaging the two (8e) sites to produce the (12e) coordinate here.

**Body-centered Cubic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}a\hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$= x_1 a \hat{\mathbf{x}}$	(12e)	Fe
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{x}}$	(12e)	Fe
$\mathbf{B}_3$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_3$	$= x_1 a \hat{\mathbf{y}}$	(12e)	Fe
$\mathbf{B}_4$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_3$	$= -x_1 a \hat{\mathbf{y}}$	(12e)	Fe
$\mathbf{B}_5$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$= x_1 a \hat{\mathbf{z}}$	(12e)	Fe
$\mathbf{B}_6$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$= -x_1 a \hat{\mathbf{z}}$	(12e)	Fe
$\mathbf{B}_7$	$= 2x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + 2x_2 \mathbf{a}_3$	$= x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}}$	(16f)	Zn I
$\mathbf{B}_8$	$= -2x_2 \mathbf{a}_3$	$= -x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}}$	(16f)	Zn I
$\mathbf{B}_9$	$= -2x_2 \mathbf{a}_2$	$= -x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}}$	(16f)	Zn I
$\mathbf{B}_{10}$	$= -2x_2 \mathbf{a}_1$	$= x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}}$	(16f)	Zn I
$\mathbf{B}_{11}$	$= 2x_2 \mathbf{a}_3$	$= x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}}$	(16f)	Zn I
$\mathbf{B}_{12}$	$= -2x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 - 2x_2 \mathbf{a}_3$	$= -x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} - x_2 a \hat{\mathbf{z}}$	(16f)	Zn I
$\mathbf{B}_{13}$	$= 2x_2 \mathbf{a}_2$	$= x_2 a \hat{\mathbf{x}} - x_2 a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}}$	(16f)	Zn I
$\mathbf{B}_{14}$	$= 2x_2 \mathbf{a}_1$	$= -x_2 a \hat{\mathbf{x}} + x_2 a \hat{\mathbf{y}} + x_2 a \hat{\mathbf{z}}$	(16f)	Zn I
$\mathbf{B}_{15}$	$= 2y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$= y_3 a \hat{\mathbf{y}} + y_3 a \hat{\mathbf{z}}$	(24h)	Zn II
$\mathbf{B}_{16}$	$= y_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$= -y_3 a \hat{\mathbf{y}} + y_3 a \hat{\mathbf{z}}$	(24h)	Zn II
$\mathbf{B}_{17}$	$= -y_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$= y_3 a \hat{\mathbf{y}} - y_3 a \hat{\mathbf{z}}$	(24h)	Zn II
$\mathbf{B}_{18}$	$= -2y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$= -y_3 a \hat{\mathbf{y}} - y_3 a \hat{\mathbf{z}}$	(24h)	Zn II
$\mathbf{B}_{19}$	$= y_3 \mathbf{a}_1 + 2y_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$= y_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{z}}$	(24h)	Zn II
$\mathbf{B}_{20}$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_3$	$= y_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{z}}$	(24h)	Zn II
$\mathbf{B}_{21}$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_3$	$= -y_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{z}}$	(24h)	Zn II
$\mathbf{B}_{22}$	$= -y_3 \mathbf{a}_1 - 2y_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$= -y_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{z}}$	(24h)	Zn II
$\mathbf{B}_{23}$	$= y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + 2y_3 \mathbf{a}_3$	$= y_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}}$	(24h)	Zn II
$\mathbf{B}_{24}$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$= -y_3 a \hat{\mathbf{x}} + y_3 a \hat{\mathbf{y}}$	(24h)	Zn II
$\mathbf{B}_{25}$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$= y_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}}$	(24h)	Zn II
$\mathbf{B}_{26}$	$= -y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - 2y_3 \mathbf{a}_3$	$= -y_3 a \hat{\mathbf{x}} - y_3 a \hat{\mathbf{y}}$	(24h)	Zn II

---

**References:**

- J. Schramm, *X-Ray Investigation of Phases and Phase Limits of the Zn Alloy Systems with Fe, Co and Ni*, Z. Metallkd. **30**, 122–130 (1938).
- A. Johansson, H. Ljung, and S. Westman, *X-Ray and Neutron Diffraction Studies on Gamma-Ni,Zn and Gamma-Fe,Zn*, Acta Chem. Scand. **22**, 2743–2753 (1968), [doi:10.3891/acta.chem.scand.22-2743](https://doi.org/10.3891/acta.chem.scand.22-2743).
- J. K. Brandon, R. Y. Brizard, P. C. Chieh, R. K. McMillan, and W. B. Pearson, *New refinements of the  $\gamma$ -brass type structures  $Cu_5Zn_8$ ,  $Cu_5Cd_8$  and  $Fe_3Zn_{10}$* , Acta Crystallogr. Sect. B Struct. Sci. **30**, 1412–1417 (1974), [doi:10.1107/S0567740874004997](https://doi.org/10.1107/S0567740874004997).
- J. Yu, J. Liu, J. Zhang, and J. Wu, *Electron Diffraction Study on Fe–Zn  $\Gamma$  intermetallic Phase of a Galvannealed IF Steel Sheet*, Mater. Trans. **46**, 1079–1082 (2005).

**Found in:**

- W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

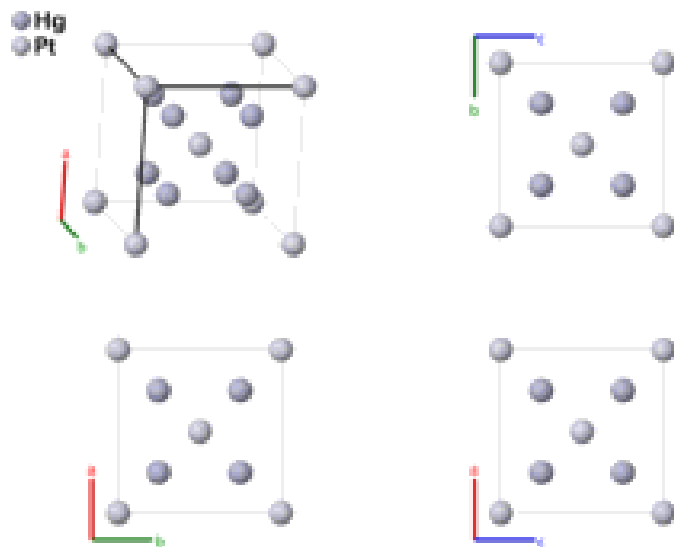
---

**Geometry files:**

- CIF: pp. [983](#)
- POSCAR: pp. [984](#)



# $\beta$ -Hg<sub>4</sub>Pt Structure: A4B\_cI10\_229\_c\_a



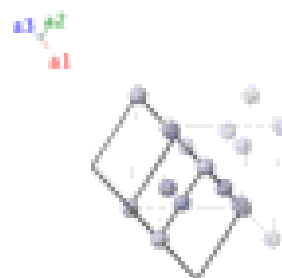
<b>Prototype</b>	:	$\beta$ -Hg <sub>4</sub> Pt
<b>AFLOW prototype label</b>	:	A4B_cI10_229_c_a
<b>Strukturbericht designation</b>	:	None
<b>Pearson symbol</b>	:	cI10
<b>Space group number</b>	:	229
<b>Space group symbol</b>	:	$Im\bar{3}m$
<b>AFLOW prototype command</b>	:	aflow --proto=A4B_cI10_229_c_a --params=a

## Other compounds with this structure:

- Hg<sub>4</sub>Pd, Hg<sub>4</sub>U

## Body-centered Cubic primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{x} - \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} - \frac{1}{2}a\hat{z} \end{aligned}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$	$= 0\hat{x} + 0\hat{y} + 0\hat{z}$	(2a)	Pt
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$= \frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y} + \frac{1}{4}a\hat{z}$	(8c)	Hg
$\mathbf{B}_3$	$= \frac{1}{2}\mathbf{a}_3$	$= \frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y} - \frac{1}{4}a\hat{z}$	(8c)	Hg

$$\mathbf{B}_4 = \frac{1}{2} \mathbf{a}_2 = \frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}} \quad (8c) \quad \text{Hg}$$

$$\mathbf{B}_5 = \frac{1}{2} \mathbf{a}_1 = -\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}} \quad (8c) \quad \text{Hg}$$

---

**References:**

- E. Bauer, H. Nowotny, and A. Stempf, *Röntgenographische Untersuchungen im System: Platin-Quecksilber*, *Monatsh. Chem.* **84**, 211–212 (1953), [doi:10.1007/BF00899140](https://doi.org/10.1007/BF00899140).

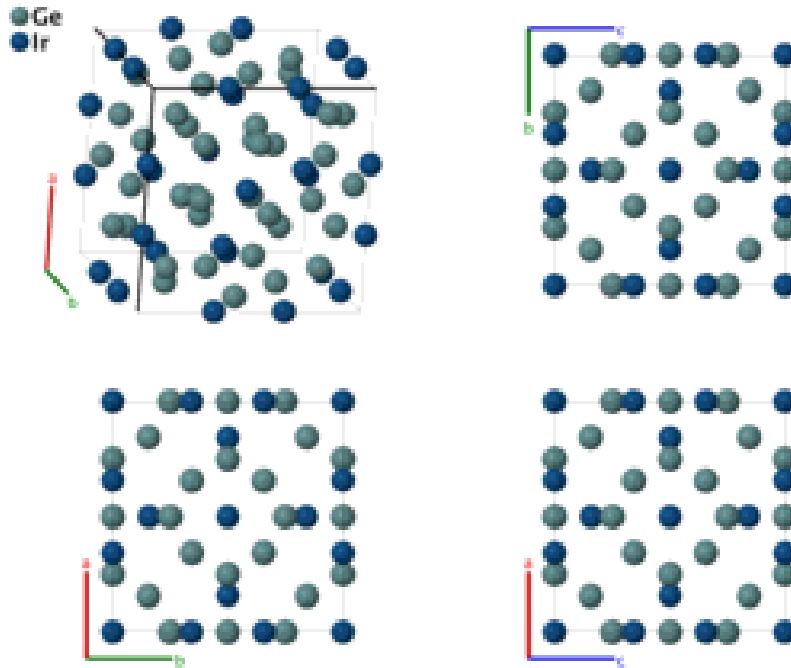
---

**Geometry files:**

- CIF: pp. [984](#)

- POSCAR: pp. [985](#)

# Ir<sub>3</sub>Ge<sub>7</sub> (*D*8<sub>*f*</sub>) Structure: A7B3\_cI40\_229\_df\_e



<b>Prototype</b>	:	Ir <sub>3</sub> Ge <sub>7</sub>
<b>AFLOW prototype label</b>	:	A7B3_cI40_229_df_e
<b>Strukturbericht designation</b>	:	<i>D</i> 8 <sub><i>f</i></sub>
<b>Pearson symbol</b>	:	cI40
<b>Space group number</b>	:	229
<b>Space group symbol</b>	:	<i>Im</i> $\bar{3}$ <i>m</i>
<b>AFLOW prototype command</b>	:	aflow --proto=A7B3_cI40_229_df_e --params= <i>a</i> , <i>x</i> <sub>2</sub> , <i>x</i> <sub>3</sub>

## Other compounds with this structure

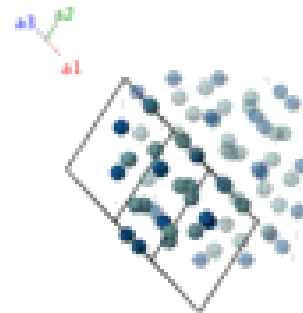
- Ga<sub>7</sub>Ni<sub>3</sub>, In<sub>7</sub>Pd<sub>3</sub>, Sb<sub>7</sub>Mo<sub>3</sub>, As<sub>7</sub>Re<sub>3</sub>, Sn<sub>7</sub>Ru<sub>3</sub>

## Body-centered Cubic primitive vectors:

$$\mathbf{a}_1 = -\frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z}$$

$$\mathbf{a}_2 = \frac{1}{2}a\hat{x} - \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z}$$

$$\mathbf{a}_3 = \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} - \frac{1}{2}a\hat{z}$$



## Basis vectors:

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom Type
<b>B</b> <sub>1</sub> =	$\frac{1}{2}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$\frac{1}{4}a\hat{x} + \frac{1}{2}a\hat{z}$	(12 <i>d</i> )	Ge I

$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(12d)	Ge I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(12d)	Ge I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B}_5$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B}_6$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B}_7$	$= x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$x_2 a \hat{\mathbf{x}}$	(12e)	Ir
$\mathbf{B}_8$	$= -x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-x_2 a \hat{\mathbf{x}}$	(12e)	Ir
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_3$	$=$	$x_2 a \hat{\mathbf{y}}$	(12e)	Ir
$\mathbf{B}_{10}$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_3$	$=$	$-x_2 a \hat{\mathbf{y}}$	(12e)	Ir
$\mathbf{B}_{11}$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$x_2 a \hat{\mathbf{z}}$	(12e)	Ir
$\mathbf{B}_{12}$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-x_2 a \hat{\mathbf{z}}$	(12e)	Ir
$\mathbf{B}_{13}$	$= 2x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + 2x_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{14}$	$= -2x_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{15}$	$= -2x_3 \mathbf{a}_2$	$=$	$-x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{16}$	$= -2x_3 \mathbf{a}_1$	$=$	$x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{17}$	$= 2x_3 \mathbf{a}_3$	$=$	$x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{18}$	$= -2x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 - 2x_3 \mathbf{a}_3$	$=$	$-x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} - x_3 a \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{19}$	$= 2x_3 \mathbf{a}_2$	$=$	$x_3 a \hat{\mathbf{x}} - x_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{20}$	$= 2x_3 \mathbf{a}_1$	$=$	$-x_3 a \hat{\mathbf{x}} + x_3 a \hat{\mathbf{y}} + x_3 a \hat{\mathbf{z}}$	(16f)	Ge II

---

#### References:

- U. Häussermann, M. Elding-Pontén, C. Svensson, and S. Lidin, *Compounds with the Ir<sub>3</sub>Ge<sub>7</sub> Structure Type: Interpenetrating Frameworks with Flexible Bonding Properties*, Chem. Euro. J. **4**, 1007–1015 (1998), doi:10.1002/(SICI)1521-3765(19980615)4:6<1007::AID-CHEM1007>3.0.CO;2-7.

#### Found in:

- F. Selim, J. P. Bevington, and G. S. Collins, *Diffusion of <sup>111</sup>Cd probes in Ga<sub>7</sub>Pt<sub>3</sub> studied via nuclear quadrupole relaxation*, Hyperfine Interact. **178**, 87–90 (2007), doi:10.1007/s10751-008-9663-3.

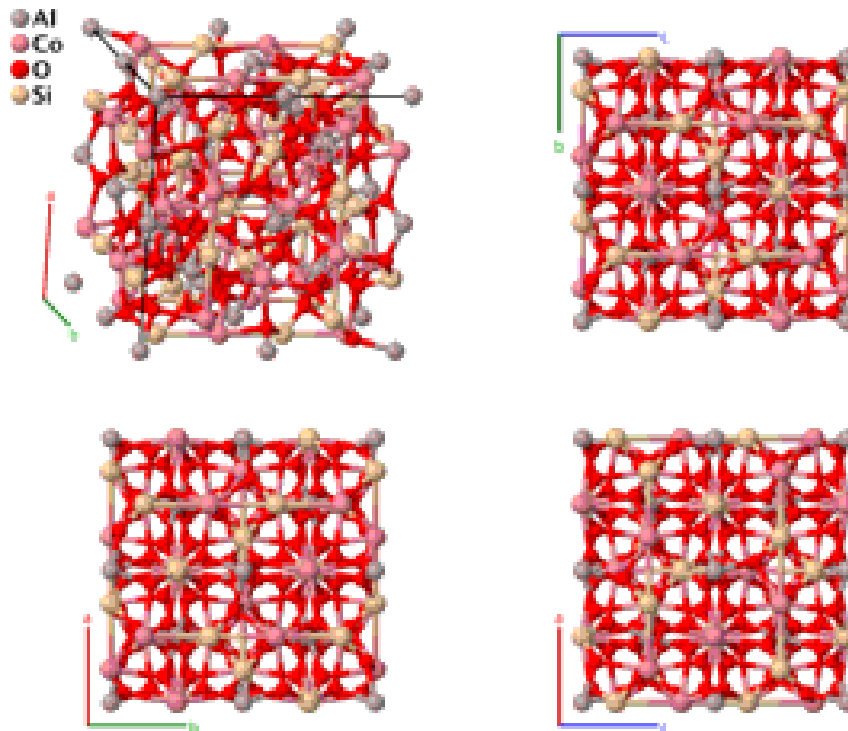
---

#### Geometry files:

- CIF: pp. 985  
 - POSCAR: pp. 986

# Garnet ( $\text{Co}_3\text{Al}_2\text{Si}_3\text{O}_{12}$ , $S 1_4$ ) Structure: A2B3C12D3\_cI160\_230\_a\_c\_h\_d

---



<b>Prototype</b>	:	$\text{Co}_3\text{Al}_2\text{Si}_3\text{O}_{12}$
<b>AFLOW prototype label</b>	:	A2B3C12D3_cI160_230_a_c_h_d
<b>Strukturbericht designation</b>	:	$S 1_4$
<b>Pearson symbol</b>	:	cI160
<b>Space group number</b>	:	230
<b>Space group symbol</b>	:	$Ia\bar{3}d$
<b>AFLOW prototype command</b>	:	aflow --proto=A2B3C12D3_cI160_230_a_c_h_d --params= $a, x_4, y_4, z_4$

---

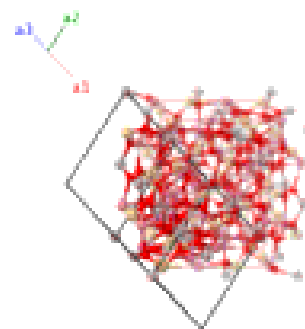
## Other compounds with this structure:

- $\text{Al}_2(\text{Mg},\text{Ni})_3\text{Si}_3\text{O}_{12}$ ,  $\text{Al}_2\text{Ca}_3\text{Si}_3\text{O}_{12}$ ,  $\text{Al}_2\text{Co}_3\text{Si}_3\text{O}_{12}$ ,  $\text{Al}_2\text{Mg}_3\text{Si}_3\text{O}_{12}$ ,  $\text{Al}_2\text{Mn}_3\text{Si}_3\text{O}_{12}$ ,  $\text{Cr}_2\text{Ca}_3\text{Si}_3\text{O}_{12}$ ,  $\text{Fe}_2\text{Ca}_3\text{Si}_3\text{O}_{12}$ ,  $\text{Fe}_2\text{Mn}_3\text{Ge}_3\text{O}_{12}$ ,  $\text{Mn}_5\text{Si}_3\text{O}_{12}$ ,  $\text{Sc}_2\text{Ca}_3\text{Si}_3\text{O}_{12}$

- (Ross, 1996) does not explicitly give the positions of the Al and Si atoms, which we take from (Downs, 2003).

**Body-centered Cubic primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}a\hat{\mathbf{z}} \end{aligned}$$



**Basis vectors:**

	Lattice Coordinates		Cartesian Coordinates	Wyckoff Position	Atom Type
$\mathbf{B}_1$	$= 0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$	$=$	$0\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}}$	(16a)	Al
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}}$	(16a)	Al
$\mathbf{B}_3$	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}}$	(16a)	Al
$\mathbf{B}_4$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{2}a\hat{\mathbf{z}}$	(16a)	Al
$\mathbf{B}_5$	$= \frac{1}{2}\mathbf{a}_1$	$=$	$\frac{3}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16a)	Al
$\mathbf{B}_6$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16a)	Al
$\mathbf{B}_7$	$= \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{4}a\hat{\mathbf{z}}$	(16a)	Al
$\mathbf{B}_8$	$= \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16a)	Al
$\mathbf{B}_9$	$= \frac{1}{4}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	Co
$\mathbf{B}_{10}$	$= \frac{3}{4}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$-\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	Co
$\mathbf{B}_{11}$	$= \frac{1}{8}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}}$	(24c)	Co
$\mathbf{B}_{12}$	$= \frac{3}{8}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24c)	Co
$\mathbf{B}_{13}$	$= \frac{3}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(24c)	Co
$\mathbf{B}_{14}$	$= \frac{1}{8}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - \frac{1}{8}a\hat{\mathbf{z}}$	(24c)	Co
$\mathbf{B}_{15}$	$= \frac{3}{4}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	Co
$\mathbf{B}_{16}$	$= \frac{1}{4}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	$=$	$\frac{5}{8}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	Co
$\mathbf{B}_{17}$	$= \frac{7}{8}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24c)	Co
$\mathbf{B}_{18}$	$= \frac{5}{8}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{5}{8}a\hat{\mathbf{y}}$	(24c)	Co
$\mathbf{B}_{19}$	$= \frac{5}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(24c)	Co
$\mathbf{B}_{20}$	$= \frac{7}{8}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{5}{8}a\hat{\mathbf{z}}$	(24c)	Co
$\mathbf{B}_{21}$	$= \frac{1}{4}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d)	Si
$\mathbf{B}_{22}$	$= \frac{3}{4}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{z}}$	(24d)	Si
$\mathbf{B}_{23}$	$= \frac{3}{8}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}}$	(24d)	Si
$\mathbf{B}_{24}$	$= \frac{1}{8}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}}$	(24d)	Si
$\mathbf{B}_{25}$	$= \frac{5}{8}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(24d)	Si
$\mathbf{B}_{26}$	$= \frac{7}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(24d)	Si
$\mathbf{B}_{27}$	$= \frac{5}{8}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d)	Si

$$\begin{aligned}
\mathbf{B}_{28} &= \frac{7}{8} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (24d) & \text{Si} \\
\mathbf{B}_{29} &= \frac{3}{4} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3 &= \frac{1}{8} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}} & (24d) & \text{Si} \\
\mathbf{B}_{30} &= \frac{1}{4} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3 &= \frac{3}{8} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{4} a \hat{\mathbf{z}} & (24d) & \text{Si} \\
\mathbf{B}_{31} &= \frac{1}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (24d) & \text{Si} \\
\mathbf{B}_{32} &= \frac{3}{8} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}} & (24d) & \text{Si} \\
\mathbf{B}_{33} &= (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + &= x_4 a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} + z_4 a \hat{\mathbf{z}} & (96h) & \text{O} \\
&\quad (x_4 + y_4) \mathbf{a}_3 \\
\mathbf{B}_{34} &= \left(\frac{1}{2} - y_4 + z_4\right) \mathbf{a}_1 + (-x_4 + z_4) \mathbf{a}_2 + &= -x_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{y}} + z_4 a \hat{\mathbf{z}} & (96h) & \text{O} \\
&\quad \left(\frac{1}{2} - x_4 - y_4\right) \mathbf{a}_3 \\
\mathbf{B}_{35} &= (y_4 - z_4) \mathbf{a}_1 + \left(\frac{1}{2} - x_4 - z_4\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{x}} + y_4 a \hat{\mathbf{y}} - z_4 a \hat{\mathbf{z}} & (96h) & \text{O} \\
&\quad \left(\frac{1}{2} - x_4 + y_4\right) \mathbf{a}_3 \\
\mathbf{B}_{36} &= \left(\frac{1}{2} - y_4 - z_4\right) \mathbf{a}_1 + &= x_4 a \hat{\mathbf{x}} - y_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - z_4\right) a \hat{\mathbf{z}} & (96h) & \text{O} \\
&\quad \left(\frac{1}{2} + x_4 - z_4\right) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3 \\
\mathbf{B}_{37} &= (x_4 + y_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + &= z_4 a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} + y_4 a \hat{\mathbf{z}} & (96h) & \text{O} \\
&\quad (x_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{38} &= \left(\frac{1}{2} - x_4 - y_4\right) \mathbf{a}_1 + &= z_4 a \hat{\mathbf{x}} - x_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{z}} & (96h) & \text{O} \\
&\quad \left(\frac{1}{2} - y_4 + z_4\right) \mathbf{a}_2 + (-x_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{39} &= \left(\frac{1}{2} - x_4 + y_4\right) \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + &= -z_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{y}} + y_4 a \hat{\mathbf{z}} & (96h) & \text{O} \\
&\quad \left(\frac{1}{2} - x_4 - z_4\right) \mathbf{a}_3 \\
\mathbf{B}_{40} &= (x_4 - y_4) \mathbf{a}_1 + \left(\frac{1}{2} - y_4 - z_4\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - z_4\right) a \hat{\mathbf{x}} + x_4 a \hat{\mathbf{y}} - y_4 a \hat{\mathbf{z}} & (96h) & \text{O} \\
&\quad \left(\frac{1}{2} + x_4 - z_4\right) \mathbf{a}_3 \\
\mathbf{B}_{41} &= (x_4 + z_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + &= y_4 a \hat{\mathbf{x}} + z_4 a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}} & (96h) & \text{O} \\
&\quad (y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{42} &= (-x_4 + z_4) \mathbf{a}_1 + \left(\frac{1}{2} - x_4 - y_4\right) \mathbf{a}_2 + &= \left(\frac{1}{2} - y_4\right) a \hat{\mathbf{x}} + z_4 a \hat{\mathbf{y}} - x_4 a \hat{\mathbf{z}} & (96h) & \text{O} \\
&\quad \left(\frac{1}{2} - y_4 + z_4\right) \mathbf{a}_3 \\
\mathbf{B}_{43} &= \left(\frac{1}{2} - x_4 - z_4\right) \mathbf{a}_1 + &= y_4 a \hat{\mathbf{x}} - z_4 a \hat{\mathbf{y}} + \left(\frac{1}{2} - x_4\right) a \hat{\mathbf{z}} & (96h) & \text{O} \\
&\quad \left(\frac{1}{2} - x_4 + y_4\right) \mathbf{a}_2 + (y_4 - z_4) \mathbf{a}_3 \\
\mathbf{B}_{44} &= \left(\frac{1}{2} + x_4 - z_4\right) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + &= -y_4 a \hat{\mathbf{x}} + \left(\frac{1}{2} - z_4\right) a \hat{\mathbf{y}} + x_4 a \hat{\mathbf{z}} & (96h) & \text{O} \\
&\quad \left(\frac{1}{2} - y_4 - z_4\right) \mathbf{a}_3 \\
\mathbf{B}_{45} &= \left(\frac{1}{2} + x_4 - z_4\right) \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + &= \left(\frac{3}{4} + y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + x_4\right) a \hat{\mathbf{y}} + & (96h) & \text{O} \\
&\quad (x_4 + y_4) \mathbf{a}_3 &\quad \left(\frac{1}{4} - z_4\right) a \hat{\mathbf{z}} \\
\mathbf{B}_{46} &= \left(\frac{1}{2} - x_4 - z_4\right) \mathbf{a}_1 + &= \left(\frac{1}{4} - y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_4\right) a \hat{\mathbf{y}} + & (96h) & \text{O} \\
&\quad \left(\frac{1}{2} - y_4 - z_4\right) \mathbf{a}_2 + \left(\frac{1}{2} - x_4 - y_4\right) \mathbf{a}_3 &\quad \left(\frac{1}{4} - z_4\right) a \hat{\mathbf{z}} \\
\mathbf{B}_{47} &= (-x_4 + z_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + &= \left(\frac{1}{4} + y_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} - x_4\right) a \hat{\mathbf{y}} + & (96h) & \text{O} \\
&\quad \left(\frac{1}{2} - x_4 + y_4\right) \mathbf{a}_3 &\quad \left(\frac{3}{4} + z_4\right) a \hat{\mathbf{z}} \\
\mathbf{B}_{48} &= (x_4 + z_4) \mathbf{a}_1 + \left(\frac{1}{2} - y_4 + z_4\right) \mathbf{a}_2 + &= \left(\frac{1}{4} - y_4\right) a \hat{\mathbf{x}} + \left(\frac{3}{4} + x_4\right) a \hat{\mathbf{y}} + & (96h) & \text{O} \\
&\quad (x_4 - y_4) \mathbf{a}_3 &\quad \left(\frac{1}{4} + z_4\right) a \hat{\mathbf{z}} \\
\mathbf{B}_{49} &= \left(\frac{1}{2} - y_4 + z_4\right) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + &= \left(\frac{3}{4} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + z_4\right) a \hat{\mathbf{y}} + & (96h) & \text{O} \\
&\quad (x_4 + z_4) \mathbf{a}_3 &\quad \left(\frac{1}{4} - y_4\right) a \hat{\mathbf{z}} \\
\mathbf{B}_{50} &= (y_4 + z_4) \mathbf{a}_1 + \left(\frac{1}{2} - x_4 + y_4\right) \mathbf{a}_2 + &= \left(\frac{1}{4} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{3}{4} + z_4\right) a \hat{\mathbf{y}} + & (96h) & \text{O} \\
&\quad (-x_4 + z_4) \mathbf{a}_3 &\quad \left(\frac{1}{4} + y_4\right) a \hat{\mathbf{z}}
\end{aligned}$$





$$\begin{aligned}
\mathbf{B}_{72} &= (-x_4 - z_4) \mathbf{a}_1 + \left(\frac{1}{2} + y_4 - z_4\right) \mathbf{a}_2 + (-x_4 + y_4) \mathbf{a}_3 = \left(\frac{1}{4} + y_4\right) a \hat{\mathbf{x}} - a\left(x_4 + \frac{1}{4}\right) \hat{\mathbf{y}} + \left(\frac{1}{4} - z_4\right) a \hat{\mathbf{z}} & (96h) & \quad \mathbf{O} \\
\mathbf{B}_{73} &= \left(\frac{1}{2} + y_4 - z_4\right) \mathbf{a}_1 + (-x_4 + y_4) \mathbf{a}_2 + (-x_4 - z_4) \mathbf{a}_3 = -a\left(x_4 + \frac{1}{4}\right) \hat{\mathbf{x}} + \left(\frac{1}{4} - z_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + y_4\right) a \hat{\mathbf{z}} & (96h) & \quad \mathbf{O} \\
\mathbf{B}_{74} &= (-y_4 - z_4) \mathbf{a}_1 + \left(\frac{1}{2} + x_4 - y_4\right) \mathbf{a}_2 + (x_4 - z_4) \mathbf{a}_3 = \left(\frac{1}{4} + x_4\right) a \hat{\mathbf{x}} - a\left(z_4 + \frac{1}{4}\right) \hat{\mathbf{y}} + \left(\frac{1}{4} - y_4\right) a \hat{\mathbf{z}} & (96h) & \quad \mathbf{O} \\
\mathbf{B}_{75} &= \left(\frac{1}{2} + y_4 + z_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4 + y_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + x_4 + z_4\right) \mathbf{a}_3 = \left(\frac{1}{4} + x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + z_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + y_4\right) a \hat{\mathbf{z}} & (96h) & \quad \mathbf{O} \\
\mathbf{B}_{76} &= (-y_4 + z_4) \mathbf{a}_1 + (-x_4 - y_4) \mathbf{a}_2 + \left(\frac{1}{2} - x_4 + z_4\right) \mathbf{a}_3 = \left(\frac{1}{4} - x_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + z_4\right) a \hat{\mathbf{y}} - a\left(y_4 + \frac{1}{4}\right) \hat{\mathbf{z}} & (96h) & \quad \mathbf{O} \\
\mathbf{B}_{77} &= \left(\frac{1}{2} + x_4 - y_4\right) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + (-y_4 - z_4) \mathbf{a}_3 = -a\left(z_4 + \frac{1}{4}\right) \hat{\mathbf{x}} + \left(\frac{1}{4} - y_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + x_4\right) a \hat{\mathbf{z}} & (96h) & \quad \mathbf{O} \\
\mathbf{B}_{78} &= (-x_4 + y_4) \mathbf{a}_1 + (-x_4 - z_4) \mathbf{a}_2 + \left(\frac{1}{2} + y_4 - z_4\right) \mathbf{a}_3 = \left(\frac{1}{4} - z_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + y_4\right) a \hat{\mathbf{y}} - a\left(x_4 + \frac{1}{4}\right) \hat{\mathbf{z}} & (96h) & \quad \mathbf{O} \\
\mathbf{B}_{79} &= (-x_4 - y_4) \mathbf{a}_1 + \left(\frac{1}{2} - x_4 + z_4\right) \mathbf{a}_2 + (-y_4 + z_4) \mathbf{a}_3 = \left(\frac{1}{4} + z_4\right) a \hat{\mathbf{x}} - a\left(y_4 + \frac{1}{4}\right) \hat{\mathbf{y}} + \left(\frac{1}{4} - x_4\right) a \hat{\mathbf{z}} & (96h) & \quad \mathbf{O} \\
\mathbf{B}_{80} &= \left(\frac{1}{2} + x_4 + y_4\right) \mathbf{a}_1 + \left(\frac{1}{2} + x_4 + z_4\right) \mathbf{a}_2 + \left(\frac{1}{2} + y_4 + z_4\right) \mathbf{a}_3 = \left(\frac{1}{4} + z_4\right) a \hat{\mathbf{x}} + \left(\frac{1}{4} + y_4\right) a \hat{\mathbf{y}} + \left(\frac{1}{4} + x_4\right) a \hat{\mathbf{z}} & (96h) & \quad \mathbf{O}
\end{aligned}$$

---

#### References:

- C. R. Ross II, H. Keppler, D. Canil, and H. S. C. O'Neill, *Structure and crystal-field spectra of  $\text{Co}_3\text{Al}_2(\text{SiO}_4)_3$  and  $(\text{Mg},\text{Ni})_3\text{Al}_2(\text{SiO}_4)_3$  garnet*, *Am. Mineral.* **81**, 61–66 (1996).

#### Found in:

- R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, *Am. Mineral.* **88**, 247–250 (2003).

---

#### Geometry files:

- CIF: pp. [986](#)  
- POSCAR: pp. [987](#)

## CIF and POSCAR Files

H<sub>2</sub>S (90 GPa): A2B\_ap6\_2\_acei\_i - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'H2S'
_chemical_formula_sum 'H2 S'

loop_
_publ_author_name
'Y. Li'
'J. Hao'
'H. Liu'
'Y. Li'
'Y. Ma'
_journal_name_full_name
:
Journal of Chemical Physics
:
_journal_volume 140
_journal_year 2014
_journal_page_first 174712
_journal_page_last 174712
_publ_section_title
:
The metallization and superconductivity of dense hydrogen sulfide
:
_aflow_title 'HS_{2}$S (90-GPa) Structure'
_aflow_proto 'A2B_ap6_2_acei_i'
_aflow_params 'a,b/a,c/a,\alpha,\beta,\gamma,x_{3},y_{3},z_{3},x_{4},y_{4},z_{4}'
_aflow_params_values '2.7804,1.00438785786,1.53100273342,78.28,76.53,70.42,0.259,0.415,0.663,0.192,0.183,0.255'
_aflow_Structurbericht 'None'
_aflow_Pearson 'aP6'

_symmetry_space_group_name_H-M "P -1"
_symmetry_Int_Tables_number 2

_cell_length_a 2.78040
_cell_length_b 2.79260
_cell_length_c 4.25680
_cell_angle_alpha 78.28000
_cell_angle_beta 76.53000
_cell_angle_gamma 70.42000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 1 a 0.00000 0.00000 0.00000 1.00000
H2 H 1 e 0.50000 0.50000 0.00000 1.00000
H3 H 2 i 0.25900 0.41500 0.66300 1.00000
S1 S 2 i 0.19200 0.18300 0.25500 1.00000
```

H<sub>2</sub>S (90 GPa): A2B\_ap6\_2\_acei\_i - POSCAR

```
A2B_ap6_2_acei_i & a,b/a,c/a,\alpha,\beta,\gamma,x_{3},y_{3},z_{3},x_{4},y_{4},z_{4} --params=
↳ 2.7804,1.00438785786,1.53100273342,78.28,76.53,70.42,0.259,
↳ 0.415,0.663,0.192,0.183,0.255 & P-1 C_{i}^{1} #2 (acei^2) & aP6
↳ & None & H2S & H2S & Y. Li et al., J. Chem. Phys. 140, 174712(
↳ 2014)
1.0000000000000000
2.7804000000000000 0.0000000000000000 0.0000000000000000
0.93586367780735 2.63111648099450 0.0000000000000000
0.99156281692297 0.56505957748759 4.10095807025448
H S
4 2
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 H (1a)
0.5000000000000000 0.5000000000000000 0.0000000000000000 H (1e)
0.2590000000000000 0.4150000000000000 0.6630000000000000 H (2i)
-0.2590000000000000 -0.4150000000000000 -0.6630000000000000 H (2i)
0.1920000000000000 0.1830000000000000 0.2550000000000000 S (2i)
-0.1920000000000000 -0.1830000000000000 -0.2550000000000000 S (2i)
```

MoP<sub>5</sub> (High-temperature): A8B5\_mP13\_6\_a7b\_3a2b - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Mo8P5'
_chemical_formula_sum 'Mo8 P5'

loop_
_publ_author_name
'T. Johansson'
_journal_name_full_name
```

```
;
Acta Chemica Scandinavica
;
_journal_volume 26
_journal_year 1972
_journal_page_first 365
_journal_page_last 382
_publ_section_title
;
The crystal structure of MoS_{8}$P_{5}$ from twin-crystal data
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'MoS_{8}$P_{5}$ (High-temperature) Structure'
_aflow_proto 'A8B5_mP13_6_a7b_3a2b'
_aflow_params 'a,b/a,c/a,\beta,x_{1},z_{1},x_{2},z_{2},x_{3},z_{3},x_{4},z_{4},x_{5},z_{5},x_{6},z_{6},x_{7},z_{7},x_{8},z_{8},x_{9},z_{9},x_{10},z_{10},x_{11},z_{11},x_{12},z_{12},x_{13},z_{13}'
_aflow_params_values '6.5369054321,0.490874879533,1.43786810261,109.592,
↳ 0.5119,0.7172,0.4546,0.4285,0.044,0.5911,0.37,0.0053,0.3887,
↳ 0.2195,0.6277,0.0001,0.1818,0.4663,0.7456,0.5256,0.1826,0.7901,
↳ 0.7824,0.2724,0.0,0.0,0.8188,0.8026,0.0123,0.2051'
_aflow_Structurbericht 'None'
_aflow_Pearson 'mP13'

_cell_length_a 6.5369054321
_cell_length_b 3.2088026665
_cell_length_c 9.3992078106
_cell_angle_alpha 90.0000000000
_cell_angle_beta 109.5920000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 1 m 1"
_symmetry_Int_Tables_number 6

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mo1 Mo 1 a 0.51190 0.00000 0.71720 1.00000
P1 P 1 a 0.45460 0.00000 0.42850 1.00000
P2 P 1 a 0.04400 0.00000 0.59110 1.00000
P3 P 1 a 0.37000 0.00000 0.00530 1.00000
Mo2 Mo 1 b 0.38870 0.50000 0.21950 1.00000
Mo3 Mo 1 b 0.62770 0.50000 0.00010 1.00000
Mo4 Mo 1 b 0.18180 0.50000 0.46630 1.00000
Mo5 Mo 1 b 0.74560 0.50000 0.52560 1.00000
Mo6 Mo 1 b 0.18260 0.50000 0.79010 1.00000
Mo7 Mo 1 b 0.78240 0.50000 0.27240 1.00000
Mo8 Mo 1 b 0.00000 0.50000 0.00000 1.00000
P4 P 1 b 0.81880 0.50000 0.80260 1.00000
P5 P 1 b 0.01230 0.50000 0.20510 1.00000
```

MoP<sub>5</sub> (High-temperature): A8B5\_mP13\_6\_a7b\_3a2b - POSCAR

```
A8B5_mP13_6_a7b_3a2b & a,b/a,c/a,\beta,x_{1},z_{1},x_{2},z_{2},x_{3},z_{3},x_{4},z_{4},x_{5},z_{5},x_{6},z_{6},x_{7},z_{7},x_{8},z_{8},x_{9},z_{9},x_{10},z_{10},x_{11},z_{11},x_{12},z_{12},x_{13},z_{13} --params=
↳ 6.5369054321,0.490874879533,1.43786810261,109.592,0.5119,0.7172,
↳ 0.4546,0.4285,0.044,0.5911,0.37,0.0053,0.3887,0.2195,0.6277,
↳ 0.0001,0.1818,0.4663,0.7456,0.5256,0.1826,0.7901,0.2195,0.6277,
↳ 0.0,0.0,0.8188,0.8026,0.0123,0.2051 & Pm C_{s}^{1} #6 (a^4b^9)
↳ & mP13 & None & Mo8P5 & T. Johansson, Acta Chem. Scand. 26,
↳ 365-382 (1972)
1.0000000000000000
6.53690543210000 0.00000000000000 0.0000000000000000
0.0000000000000000 3.20880266650000 0.0000000000000000
-3.15174264922271 0.0000000000000000 8.85503392087883
Mo P
8 5
Direct
0.5119000000000000 0.0000000000000000 0.7172000000000000 Mo (1a)
0.3887000000000000 0.5000000000000000 0.2195000000000000 Mo (1b)
0.6277000000000000 0.5000000000000000 0.0010000000000000 Mo (1b)
0.1818000000000000 0.5000000000000000 0.4663000000000000 Mo (1b)
0.7456000000000000 0.5000000000000000 0.5256000000000000 Mo (1b)
0.1826000000000000 0.5000000000000000 0.7901000000000000 Mo (1b)
0.7824000000000000 0.5000000000000000 0.2724000000000000 Mo (1b)
0.0000000000000000 0.5000000000000000 0.0000000000000000 Mo (1b)
0.4546000000000000 0.0000000000000000 0.4285000000000000 P (1a)
0.0440000000000000 0.0000000000000000 0.5911000000000000 P (1a)
0.3700000000000000 0.0000000000000000 0.0053000000000000 P (1a)
0.8188000000000000 0.5000000000000000 0.8026000000000000 P (1b)
0.0123000000000000 0.5000000000000000 0.2051000000000000 P (1b)
```

FeNi: AB\_mP4\_6\_2b\_2a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'FeNi'
_chemical_formula_sum 'Fe Ni'
```

```

loop_
_publ_author_name
'T. Tagai'
'H. Takeda'
'T. Fukuda'
_journal_name_full_name
:
Zeitschrift f{"u}r Kristallographie - Crystalline Materials
:
_journal_volume 210
_journal_year 1995
_journal_page_first 14
_journal_page_last 18
_publ_section_title
:
Superstructure of tetrataenite from the Saint Severin meteorite
:
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'FeNi Structure'
_aflow_proto 'AB_mP4_6_2b_2a'
_aflow_params 'a,b/a,c/a,\beta,x_{1},z_{1},x_{2},z_{2},x_{3},z_{3},x_{4},z_{4}'
↪ '3.580975428,1.00027925162,1.00167550965,90.04,0.0,0.0,0.518,0.507,0.026,0.026,0.501,0.529,0.027'
_aflow_strukturbericht 'None'
_aflow_pearson 'mP4'

_cell_length_a 3.5809754280
_cell_length_b 3.5819754212
_cell_length_c 3.5869753869
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0400000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 1 m 1"
_symmetry_Int_Tables_number 6

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ni1 Ni 1 a 0.00000 0.00000 1.00000
Ni2 Ni 1 a 0.51800 0.00000 0.50700 1.00000
Fe1 Fe 1 b 0.02600 0.50000 0.50100 1.00000
Fe2 Fe 1 b 0.52900 0.50000 0.02700 1.00000

```

FeNi: AB\_mP4\_6\_2b\_2a - POSCAR

```

AB_mP4_6_2b_2a & a,b/a,c/a,\beta,x1,x2,z2,x3,z3,x4,z4 --params=
↪ 3.580975428,1.00027925162,1.00167550965,90.04,0.0,0.0,0.518,
↪ 0.507,0.026,0.501,0.529,0.027 & Pm C_{s}^{1} #6 (a^2b^2) & mP4
↪ & None & FeNi & T. Tagai and H. Takeda and T. Fukuda,
↪ Zeitschrift f{"u}r Kristallographie - Crystalline Materials 210
↪ 14-18 (1995)
1.0000000000000000
3.580975428000000 0.000000000000000 0.000000000000000
0.000000000000000 3.58197542120000 0.000000000000000
-0.00250418102416 0.000000000000000 3.58697451277589
Fe Ni
2 2
Direct
0.026000000000000 0.500000000000000 0.501000000000000 Fe (1b)
0.529000000000000 0.500000000000000 0.027000000000000 Fe (1b)
0.000000000000000 0.000000000000000 0.000000000000000 Ni (1a)
0.518000000000000 0.000000000000000 0.507000000000000 Ni (1a)

```

H<sub>2</sub>S IV: A2B\_mP12\_7\_4a\_2a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'H2S IV'
_chemical_formula_sum 'H2 S'

loop_
_publ_author_name
'Y. Li'
'J. Hao'
'H. Liu'
'Y. Li'
'Y. Ma'
_journal_name_full_name
:
Journal of Chemical Physics
:
_journal_volume 140
_journal_year 2014
_journal_page_first 174712
_journal_page_last 174712

```

```

_publ_section_title
:
The metallization and superconductivity of dense hydrogen sulfide
:
_aflow_title 'HS_{2}SS IV Structure'
_aflow_proto 'A2B_mP12_7_4a_2a'
_aflow_params 'a,b/a,c/a,\beta,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6}'
↪ '0.062,0.472,-0.023,0.574,0.143,0.777,-0.052,0.799,0.271,0.151,0.261,-0.001,0.808,0.36,0.494,0.649,0.658'
_aflow_params_values '5.0942,0.627360527659,1.04603274312,90.38,0.498,-0.062,0.472,-0.023,0.574,0.143,0.777,-0.052,0.799,0.271,0.151,0.261,-0.001,0.808,0.36,0.494,0.649,0.658'
_aflow_strukturbericht 'None'
_aflow_pearson 'mP12'

_symmetry_space_group_name_H-M "P 1 c 1"
_symmetry_Int_Tables_number 7

_cell_length_a 5.09420
_cell_length_b 3.19590
_cell_length_c 5.32870
_cell_angle_alpha 90.00000
_cell_angle_beta 90.38000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 2 a 0.49800 -0.06200 0.47200 1.00000
H2 H 2 a -0.02300 0.57400 0.14300 1.00000
H3 H 2 a 0.77700 -0.05200 0.79900 1.00000
H4 H 2 a 0.27100 0.15100 0.26100 1.00000
S1 S 2 a -0.00100 0.80800 0.36000 1.00000
S2 S 2 a 0.49400 0.64900 0.65800 1.00000

```

H<sub>2</sub>S IV: A2B\_mP12\_7\_4a\_2a - POSCAR

```

A2B_mP12_7_4a_2a & a,b/a,c/a,\beta,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6 --params=5.0942,0.627360527659,1.04603274312,
↪ 90.38,0.498,-0.062,0.472,-0.023,0.574,0.143,0.777,-0.052,0.799,
↪ 0.271,0.151,0.261,-0.001,0.808,0.36,0.494,0.649,0.658 & Pc C_{s}^{1}
↪ #7 (a^6) & mP12 & None & H2S & H2S IV & Y. Li et al., J.
↪ Chem. Phys. 140, 174712 (2014)
1.0000000000000000
5.094200000000000 0.000000000000000 0.000000000000000
0.000000000000000 3.195900000000000 0.000000000000000
-0.03534101765261 0.000000000000000 5.32858280431779
H S
8 4
Direct
0.498000000000000 -0.062000000000000 0.472000000000000 H (2a)
0.498000000000000 0.062000000000000 0.972000000000000 H (2a)
-0.023000000000000 0.574000000000000 0.143000000000000 H (2a)
-0.023000000000000 -0.574000000000000 0.643000000000000 H (2a)
0.777000000000000 -0.052000000000000 0.799000000000000 H (2a)
0.777000000000000 0.052000000000000 1.299000000000000 H (2a)
0.271000000000000 0.151000000000000 0.261000000000000 H (2a)
0.271000000000000 -0.151000000000000 0.761000000000000 H (2a)
-0.001000000000000 0.808000000000000 0.360000000000000 S (2a)
-0.001000000000000 -0.808000000000000 0.860000000000000 S (2a)
0.494000000000000 0.649000000000000 0.658000000000000 S (2a)
0.494000000000000 -0.649000000000000 1.158000000000000 S (2a)

```

As<sub>2</sub>Ba: A2B\_mP18\_7\_6a\_3a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'As2Ba'
_chemical_formula_sum 'As2 Ba'

loop_
_publ_author_name
'F. Emmerling'
'D. Petri'
'C. R{"o}hr'
_journal_name_full_name
:
Zeitschrift fur Anorganische und Allgemeine Chemie
:
_journal_volume 630
_journal_year 2004
_journal_page_first 2490
_journal_page_last 2501
_publ_section_title
:
Neue Arsenide mit As^{n-}-Ketten und -Ringen: BaAs_{2}S und SA^{I}
↪ SBa_{2}SAs_{5}S (SA^{I}S = K, Rb)
:

```

```
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'As_{2}SbA Structure'
_aflow_proto 'A2B_mP18_7_6a_3a'
_aflow_params 'a,b/a,c/a,\beta,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},y_{7},z_{7},x_{8},y_{8},z_{8},x_{9},y_{9},z_{9}'
_aflow_params_values '6.5499839723,1.91328244277,1.22717557252,127.75,0.6753,0.4828,0.3393,0.4711,0.6498,0.3067,0.4174,0.3433,0.0893,0.2883,0.1551,0.3432,0.1472,0.1112,0.5582,0.0,0.0746,0.0,0.5693,0.07852,0.0933,0.1184,0.41567,0.2938,0.8473,0.27155,0.6656'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mP18'

_cell_length_a 6.5499839723
_cell_length_b 12.5319693346
_cell_length_c 8.0379803312
_cell_angle_alpha 90.0000000000
_cell_angle_beta 127.7500000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'P 1 c 1'
_symmetry_Int_Tables_number 7

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
As1 As 2 a 0.67530 0.48280 0.33930 1.00000
As2 As 2 a 0.47110 0.64980 0.30670 1.00000
As3 As 2 a 0.41740 0.34330 0.08930 1.00000
As4 As 2 a 0.28830 0.15510 0.34320 1.00000
As5 As 2 a 0.14720 0.11120 0.55820 1.00000
As6 As 2 a 0.00000 0.07460 0.00000 1.00000
Ba1 Ba 2 a 0.56930 0.07852 0.09330 1.00000
Ba2 Ba 2 a 0.11840 0.41567 0.29380 1.00000
Ba3 Ba 2 a 0.84730 0.27155 0.66560 1.00000
```

As<sub>2</sub>Ba: A2B\_mP18\_7\_6a\_3a - POSCAR

```
A2B_mP18_7_6a_3a & a,b/a,c/a,beta,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8,x9,y9,z9 --params=
↳ 6.5499839723,1.91328244277,1.22717557252,127.75,0.6753,0.4828,0.3393,0.4711,0.6498,0.3067,0.4174,0.3433,0.0893,0.2883,0.1551,0.3432,0.1472,0.1112,0.5582,0.0,0.0746,0.0,0.5693,0.07852,0.0933,0.1184,0.41567,0.2938,0.8473,0.27155,0.6656 & Pc C_{s}^{2} #7 (a^9) & mP18 & None & As2Ba & F. Emmerling and D. Petri and C. R. Anorg. Allg. Chem. 630, 2490-2501 (2004)
1.0000000000000000
6.54998397230000 0.00000000000000 0.00000000000000
0.00000000000000 12.53196933460000 0.00000000000000
-4.92099045533766 0.00000000000000 6.35554724183793
As Ba
12 6
Direct
0.67530000000000 0.48280000000000 0.33930000000000 As (2a)
0.67530000000000 -0.48280000000000 0.83930000000000 As (2a)
0.47110000000000 0.64980000000000 0.30670000000000 As (2a)
0.47110000000000 -0.64980000000000 0.80670000000000 As (2a)
0.41740000000000 0.34330000000000 0.08930000000000 As (2a)
0.41740000000000 -0.34330000000000 0.58930000000000 As (2a)
0.28830000000000 0.15510000000000 0.34320000000000 As (2a)
0.28830000000000 -0.15510000000000 0.84320000000000 As (2a)
0.14720000000000 0.11120000000000 0.55820000000000 As (2a)
0.14720000000000 -0.11120000000000 1.05820000000000 As (2a)
0.00000000000000 0.07460000000000 0.00000000000000 As (2a)
0.00000000000000 -0.07460000000000 0.50000000000000 As (2a)
0.56930000000000 0.07852000000000 0.09330000000000 Ba (2a)
0.56930000000000 -0.07852000000000 0.59330000000000 Ba (2a)
0.11840000000000 0.41567000000000 0.29380000000000 Ba (2a)
0.11840000000000 -0.41567000000000 0.79380000000000 Ba (2a)
0.84730000000000 0.27155000000000 0.66560000000000 Ba (2a)
0.84730000000000 -0.27155000000000 1.16560000000000 Ba (2a)
```

e-WO<sub>3</sub> (Low-temperature): A3B\_mP16\_7\_6a\_2a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'epsilon-WO3'
_chemical_formula_sum 'O3 W'

loop_
_publ_author_name
'P. M. Woodward'
'A. W. Sleight'
'T. Vogt'
_journal_name_full_name
'Journal of Solid State Chemistry'
;
```

```
_journal_volume 131
_journal_year 1997
_journal_page_first 9
_journal_page_last 17
_publ_section_title
;
Ferroelectric tungsten trioxide
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title '$\epsilon$-WOS_{3}$ (Low-temperature) Structure'
_aflow_proto 'A3B_mP16_7_6a_2a'
_aflow_params 'a,b/a,c/a,\beta,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},y_{7},z_{7},x_{8},y_{8},z_{8}'
_aflow_params_values '5.2778002048,0.97690325515,1.45210125431,91.762,0.5044,0.292,0.01,0.5764,0.215,0.586,0.0,0.209,0.0,0.0864,0.29,0.58,0.2874,0.0717,0.287,0.7924,0.4201,0.301,0.2874,0.014,0.0012,0.7994,0.528,0.078'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mP16'

_cell_length_a 5.2778002048
_cell_length_b 5.1559002001
_cell_length_c 7.6639002974
_cell_angle_alpha 90.0000000000
_cell_angle_beta 91.7620000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'P 1 c 1'
_symmetry_Int_Tables_number 7

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 2 a 0.50440 0.29200 0.01000 1.00000
O2 O 2 a 0.57640 0.21500 0.58600 1.00000
O3 O 2 a 0.00000 0.20900 0.00000 1.00000
O4 O 2 a 0.08640 0.29000 0.58000 1.00000
O5 O 2 a 0.28740 0.07170 0.28700 1.00000
O6 O 2 a 0.79240 0.42010 0.30100 1.00000
W1 W 2 a 0.28740 0.01400 0.00120 1.00000
W2 W 2 a 0.79940 0.52800 0.07800 1.00000
```

e-WO<sub>3</sub> (Low-temperature): A3B\_mP16\_7\_6a\_2a - POSCAR

```
A3B_mP16_7_6a_2a & a,b/a,c/a,beta,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8 --params=5.2778002048,
↳ 0.97690325515,1.45210125431,91.762,0.5044,0.292,0.01,0.5764,0.215,0.586,0.0,0.209,0.0,0.0864,0.29,0.58,0.2874,0.0717,0.287,0.7924,0.4201,0.301,0.2874,0.014,0.0012,0.7994,0.528,0.078 & Pc C_{s}^{2} #7 (a^8) & mP16 & None & WO3 & epsilon & P. M. Woodward and A. W. Sleight and T. Vogt, J. Solid State Chem. 131, 9-17 (1997)
1.0000000000000000
5.27780020480000 0.00000000000000 0.00000000000000
0.00000000000000 5.15590020010000 0.00000000000000
-0.23564849020651 0.00000000000000 7.66027659797942
O W
12 4
Direct
0.50440000000000 0.29200000000000 0.01000000000000 O (2a)
0.50440000000000 -0.29200000000000 0.51000000000000 O (2a)
0.57640000000000 0.21500000000000 0.58600000000000 O (2a)
0.57640000000000 -0.21500000000000 1.08600000000000 O (2a)
0.00000000000000 0.20900000000000 0.00000000000000 O (2a)
0.00000000000000 -0.20900000000000 0.50000000000000 O (2a)
0.08640000000000 0.29000000000000 0.58000000000000 O (2a)
0.08640000000000 -0.29000000000000 1.08000000000000 O (2a)
0.28740000000000 0.07170000000000 0.28700000000000 O (2a)
0.28740000000000 -0.07170000000000 0.78700000000000 O (2a)
0.79240000000000 0.42010000000000 0.30100000000000 O (2a)
0.79240000000000 -0.42010000000000 0.80100000000000 O (2a)
0.28740000000000 0.01400000000000 0.00120000000000 W (2a)
0.28740000000000 -0.01400000000000 0.50120000000000 W (2a)
0.79940000000000 0.52800000000000 0.07800000000000 W (2a)
0.79940000000000 -0.52800000000000 0.07800000000000 W (2a)
```

Rh<sub>2</sub>Ga<sub>9</sub>: A9B2\_mP22\_7\_9a\_2a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Rh2Ga9'
_chemical_formula_sum 'Ga9 Rh2'

loop_
_publ_author_name
'M. Bostr{\o}m'
'H. Rosner'
```

```

'Y. Prots'
'U. Burkhardt'
'Y. Grin'
_journal_name_full_name
;
Zeitschrift fur Anorganische und Allgemeine Chemie
;
_journal_volume 631
_journal_year 2005
_journal_page_first 534
_journal_page_last 541
_publ_section_title
;
The CoS_{2}AlS_{9} structure type revisited
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013
_aflow_title 'Rh_{2}SGa_{9} Structure'
_aflow_proto 'A9B2_mP22_7_9a_2a'
_aflow_params 'a,b/a,c/a,\beta,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},y_{7},z_{7},x_{8},y_{8},z_{8},x_{9},y_{9},z_{9},x_{10},y_{10},z_{10},x_{11},y_{11},z_{11}'
_aflow_params_values '6.4165085102,0.999298672153,1.36910105356,93.39,0.4944,0.2369,0.0135,0.2965,0.2623,0.5568,0.4955,0.4453,0.2912,0.2817,0.0557,0.2805,0.8067,0.5491,0.0506,0.0,0.0309,0.0,0.6774,0.1539,0.7442,0.096,0.6343,0.3258,0.8638,0.2389,0.2526,0.6359,0.1217,0.4513,0.156,0.3761,0.11377'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mP22'
_cell_length_a 6.4165085102
_cell_length_b 6.4120084341
_cell_length_c 8.7848485615
_cell_angle_alpha 90.0000000000
_cell_angle_beta 93.3900000000
_cell_angle_gamma 90.0000000000
_symmetry_space_group_name_H-M "P 1 c 1"
_symmetry_Int_Tables_number 7
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,z+1/2
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ga1 Ga 2 a 0.49440 0.23690 0.01350 1.00000
Ga2 Ga 2 a 0.29650 0.26230 0.55680 1.00000
Ga3 Ga 2 a 0.49550 0.44530 0.29120 1.00000
Ga4 Ga 2 a 0.28170 0.05570 0.28050 1.00000
Ga5 Ga 2 a 0.80670 0.54910 0.05060 1.00000
Ga6 Ga 2 a 0.00000 0.03090 0.00000 1.00000
Ga7 Ga 2 a 0.67740 0.15390 0.74420 1.00000
Ga8 Ga 2 a 0.09600 0.63430 0.32580 1.00000
Ga9 Ga 2 a 0.86380 0.23890 0.25260 1.00000
Rh1 Rh 2 a 0.63590 0.12170 0.45130 1.00000
Rh2 Rh 2 a 0.15600 0.37610 0.11377 1.00000

```

Rh<sub>2</sub>Ga<sub>9</sub>: A9B2\_mP22\_7\_9a\_2a - POSCAR

```

A9B2_mP22_7_9a_2a & a,b/a,c/a,\beta,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,
↳ x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11,
↳ y11,z11 --params=6.4165085102,0.999298672153,1.36910105356,
↳ 93.39,0.4944,0.2369,0.0135,0.2965,0.2623,0.5568,0.4955,0.4453,
↳ 0.2912,0.2817,0.0557,0.2805,0.8067,0.5491,0.0506,0.0,0.0309,0.0
↳ 0.6774,0.1539,0.7442,0.096,0.6343,0.3258,0.8638,0.2389,0.2526,
↳ 0.6359,0.1217,0.4513,0.156,0.3761,0.11377 & Pc C_{s}^{2} #7 (a^
↳ 11) & mP22 & None & Rh2Ga9 & & M. Bostr{\"}ojm et al., Z.
↳ Anorg. Allg. Chem. 631, 534-541 (2005)
1.0000000000000000
6.41650851020000 0.00000000000000 0.00000000000000
0.00000000000000 6.41200843410000 0.00000000000000
-0.51946695612781 0.00000000000000 8.76947651402180
Ga Rh
18 4
Direct
0.49440000000000 0.23690000000000 0.01350000000000 Ga (2a)
0.49440000000000 -0.23690000000000 0.51350000000000 Ga (2a)
0.29650000000000 0.26230000000000 0.55680000000000 Ga (2a)
0.29650000000000 -0.26230000000000 1.05680000000000 Ga (2a)
0.49550000000000 0.44530000000000 0.29120000000000 Ga (2a)
0.49550000000000 -0.44530000000000 0.79120000000000 Ga (2a)
0.28170000000000 0.05570000000000 0.28050000000000 Ga (2a)
0.28170000000000 -0.05570000000000 0.78050000000000 Ga (2a)
0.80670000000000 0.54910000000000 0.05060000000000 Ga (2a)
0.80670000000000 -0.54910000000000 0.55060000000000 Ga (2a)
0.00000000000000 0.03090000000000 0.00000000000000 Ga (2a)
0.00000000000000 -0.03090000000000 0.50000000000000 Ga (2a)
0.67740000000000 0.15390000000000 0.74420000000000 Ga (2a)
0.67740000000000 -0.15390000000000 1.24420000000000 Ga (2a)
0.09600000000000 0.63430000000000 0.32580000000000 Ga (2a)
0.09600000000000 -0.63430000000000 0.82580000000000 Ga (2a)
0.86380000000000 0.23890000000000 0.25260000000000 Ga (2a)

```

```

0.86380000000000 -0.23890000000000 0.75260000000000 Ga (2a)
0.63590000000000 0.12170000000000 0.45130000000000 Rh (2a)
0.63590000000000 -0.12170000000000 0.95130000000000 Rh (2a)
0.15600000000000 0.37610000000000 0.11377000000000 Rh (2a)
0.15600000000000 -0.37610000000000 0.61377000000000 Rh (2a)

```

$\alpha$ -P<sub>3</sub>N<sub>5</sub>: ASB3\_mC32\_9\_5a\_3a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral '\alpha-P3N5'
_chemical_formula_sum 'N5 P3'
loop_
_publ_author_name
'S. Horstmann'
'E. Irran'
'W. Schnick'
_journal_name_full_name
;
Angewandte Chemie (International ed.)
;
_journal_volume 36
_journal_year 1997
_journal_page_first 1873
_journal_page_last 1875
_publ_section_title
;
Synthesis and Crystal Structure of Phosphorus(V) Nitride S\alpha-P3N5 (3
↳ )SNS_{5}S
;
_aflow_title '\alpha-P3NS5 Structure'
_aflow_proto 'ASB3_mC32_9_5a_3a'
_aflow_params 'a,b/a,c/a,\beta,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},y_{7},z_{7},x_{8},y_{8},z_{8}'
_aflow_params_values '8.12077,0.718445418353,1.12797801194,115.809,0.009
↳ ,-0.003,0.269,0.129,0.341,0.45,0.37,0.119,0.066,0.142,0.351,
↳ 0.147,0.356,0.135,0.348,0.0,0.5182,0.0,0.136,0.2,0.309,0.365,
↳ 0.2924,0.196'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mC32'
_symmetry_space_group_name_H-M "C 1 c 1"
_symmetry_Int_Tables_number 9
_cell_length_a 8.12077
_cell_length_b 5.83433
_cell_length_c 9.16005
_cell_angle_alpha 90.00000
_cell_angle_beta 115.80900
_cell_angle_gamma 90.00000
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,z+1/2
3 x+1/2,y+1/2,z
4 x+1/2,-y+1/2,z+1/2
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
N1 N 4 a 0.00900 -0.00300 0.26900 1.00000
N2 N 4 a 0.12900 0.34100 0.45000 1.00000
N3 N 4 a 0.37000 0.11900 0.06600 1.00000
N4 N 4 a 0.14200 0.35100 0.14700 1.00000
N5 N 4 a 0.35600 0.13500 0.34800 1.00000
P1 P 4 a 0.00000 0.51820 0.00000 1.00000
P2 P 4 a 0.13600 0.20000 0.30900 1.00000
P3 P 4 a 0.36500 0.29240 0.19600 1.00000

```

$\alpha$ -P<sub>3</sub>N<sub>5</sub>: ASB3\_mC32\_9\_5a\_3a - POSCAR

```

ASB3_mC32_9_5a_3a & a,b/a,c/a,\beta,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,
↳ x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8 --params=8.12077,
↳ 0.718445418353,1.12797801194,115.809,0.009,-0.003,0.269,0.129,
↳ 0.341,0.45,0.37,0.119,0.066,0.142,0.351,0.147,0.356,0.135,0.348
↳ ,0.0,0.5182,0.0,0.136,0.2,0.309,0.365,0.2924,0.196 & Cc C_{s}^{4}
↳ 4) #9 (a^8) & mC32 & None & P3N5 & S\alpha-P3N5 & S. Horstmann
↳ and E. Irran and W. Schnick, Angew. Chem. Int. Ed. 36,
↳ 1873-1875 (1997)
1.00000000000000
4.06038500000000 -2.91716500000000 0.00000000000000
4.06038500000000 2.91716500000000 0.00000000000000
-3.98803401284269 0.00000000000000 8.24633862480252
N P
10 6
Direct
0.01200000000000 0.00600000000000 0.26900000000000 N (4a)
0.06000000000000 0.01200000000000 0.76900000000000 N (4a)
-0.21200000000000 0.47000000000000 0.45000000000000 N (4a)
0.47000000000000 -0.21200000000000 0.95000000000000 N (4a)
0.25100000000000 0.48900000000000 0.06600000000000 N (4a)
0.48900000000000 0.25100000000000 0.56600000000000 N (4a)

```

-0.20900000000000	0.49300000000000	0.14700000000000	N	(4a)
0.49300000000000	-0.20900000000000	0.64700000000000	N	(4a)
0.22100000000000	0.49100000000000	0.34800000000000	N	(4a)
0.49100000000000	0.22100000000000	0.84800000000000	N	(4a)
-0.51820000000000	0.51820000000000	0.00000000000000	P	(4a)
0.51820000000000	-0.51820000000000	0.50000000000000	P	(4a)
-0.06400000000000	0.33600000000000	0.30900000000000	P	(4a)
0.33600000000000	-0.06400000000000	0.80900000000000	P	(4a)
0.07260000000000	0.65740000000000	0.19600000000000	P	(4a)
0.65740000000000	0.07260000000000	0.69600000000000	P	(4a)

0.55161000000000	0.02157000000000	0.77913000000000	H	(4a)
0.50820000000000	0.63332000000000	0.41996000000000	H	(4a)
0.63332000000000	0.50820000000000	0.91996000000000	H	(4a)
0.35136000000000	0.49210000000000	0.56036000000000	H	(4a)
0.49210000000000	0.35136000000000	1.06036000000000	H	(4a)

H<sub>3</sub>Cl (20 GPa): AB3\_mCl6\_9\_a\_3a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'H3Cl'
_chemical_formula_sum 'Cl H3'

loop_
  _publ_author_name
  'D. Duan'
  'X. Huang'
  'F. Tian'
  'Y. Liu'
  'Da Li'
  'H. Yu'
  'B. Liu'
  'W. Tian'
  'T. Cui'
_journal_name_full_name
;
Journal of Physical Chemistry A
;
_journal_volume 119
_journal_year 2015
_journal_page_first 11059
_journal_page_last 11065
_publ_section_title
;
Predicted Formation of HS_{3}^{+} in Solid Halogen Polyhydrides at
  ↳ High Pressures
;

_aflow_title 'HS_{3}Cl (20-GPa) Structure'
_aflow_proto 'AB3_mCl6_9_a_3a'
_aflow_params 'a,b/a,c/a,\beta,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4}'
↳ ',y_{3},z_{3},x_{4},y_{4},z_{4}'
_aflow_params_values '3.5367,2.67777872028,0.986823875364,93.018,0.50691
↳ 0.35551,0.49997,0.28659,0.26502,0.27913,0.57076,0.06256,
↳ 0.41996,0.42173,0.07037,0.56036'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mCl6'

_symmetry_space_group_name_H-M 'C 1 c 1'
_symmetry_Int_Tables_number 9

_cell_length_a 3.53670
_cell_length_b 9.47050
_cell_length_c 3.49010
_cell_angle_alpha 90.00000
_cell_angle_beta 93.01800
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x,-y,z+1/2
  3 x+1/2,y+1/2,z
  4 x+1/2,-y+1/2,z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Cl1 Cl 4 a 0.50691 0.35551 0.49997 1.00000
  H1 H 4 a 0.28659 0.26502 0.27913 1.00000
  H2 H 4 a 0.57076 0.06256 0.41996 1.00000
  H3 H 4 a 0.42173 0.07037 0.56036 1.00000
```

H<sub>3</sub>Cl (20 GPa): AB3\_mCl6\_9\_a\_3a - POSCAR

```
AB3_mCl6_9_a_3a & a,b/a,c/a,\beta,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4 --
↳ params=3.5367,2.67777872028,0.986823875364,93.018,0.50691,
↳ 0.35551,0.49997,0.28659,0.26502,0.27913,0.57076,0.06256,0.41996
↳ 0.42173,0.07037,0.56036 & Cc C_{s}^{4} #9 (a^4) & mCl6 & None
↳ & H3Cl & H3Cl & D. Duan et al., J. Phys. Chem. A 119,
↳ 11059-11065 (2015)
1.00000000000000
1.76835000000000 -4.73525000000000 0.00000000000000
1.76835000000000 4.73525000000000 0.00000000000000
-1.8375265646087 0.00000000000000 3.48525938363898
  Cl H
  2 6
Direct
0.15140000000000 0.86242000000000 0.49997000000000 Cl (4a)
0.86242000000000 0.15140000000000 0.99997000000000 Cl (4a)
0.02157000000000 0.55161000000000 0.77913000000000 H (4a)
```

δ-PdCl<sub>2</sub>: A2B\_mP6\_10\_mn\_bg - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '\delta$-PdCl2'
_chemical_formula_sum 'Cl2 Pd'

loop_
  _publ_author_name
  'J. Evers'
  'W. Beck'
  'M. G\{o}bel'
  'S. Jakob'
  'P. Mayer'
  'G. Oehlinger'
  'M. Rotter'
  'T. M. Klap\{o}tke'
_journal_name_full_name
;
Angewandte Chemie (International ed.)
;
_journal_volume 49
_journal_year 2010
_journal_page_first 5677
_journal_page_last 5682
_publ_section_title
;
The Structures of \delta$-PdCl_{2}$ and \gamma$-PdCl_{2}$: Phases
  ↳ with Negative Thermal Expansion in One Direction
;

_aflow_title '\delta$-PdCl_{2}$ Structure'
_aflow_proto 'A2B_mP6_10_mn_bg'
_aflow_params 'a,b/a,c/a,\beta,x_{3},z_{3},x_{4},z_{4}'
_aflow_params_values '4.012,0.819541375872,2.93668993021,97.03,0.843,
↳ 0.126,0.558,0.644'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mP6'

_symmetry_space_group_name_H-M 'P 1 2/m 1'
_symmetry_Int_Tables_number 10

_cell_length_a 4.01200
_cell_length_b 3.28800
_cell_length_c 11.78200
_cell_angle_alpha 90.00000
_cell_angle_beta 97.03000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 -x,y,-z
  3 -x,-y,-z
  4 x,-y,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Pd1 Pd 1 b 0.00000 0.50000 0.00000 1.00000
  Pd2 Pd 1 g 0.50000 0.00000 0.50000 1.00000
  Cl1 Cl 2 m 0.84300 0.00000 0.12600 1.00000
  Cl2 Cl 2 n 0.55800 0.50000 0.64400 1.00000
```

δ-PdCl<sub>2</sub>: A2B\_mP6\_10\_mn\_bg - POSCAR

```
A2B_mP6_10_mn_bg & a,b/a,c/a,\beta,x3,z3,x4,z4 --params=4.012,
↳ 0.819541375872,2.93668993021,97.03,0.843,0.126,0.558,0.644 & P2
↳ /m C_{2h}^{1} #10 (bgmn) & mP6 & None & PdCl2 & \delta$-PdCl2
↳ & J. Evers et al., Angew. Chem. Int. Ed. 49, 5677-5682 (2010)
1.00000000000000
4.01200000000000 0.00000000000000 0.00000000000000
0.00000000000000 3.28800000000000 0.00000000000000
-1.44198746457411 0.00000000000000 11.69342533871110
  Cl Pd
  4 2
Direct
0.84300000000000 0.00000000000000 0.12600000000000 Cl (2m)
-0.84300000000000 0.00000000000000 -0.12600000000000 Cl (2m)
0.55800000000000 0.50000000000000 0.64400000000000 Cl (2n)
-0.55800000000000 0.50000000000000 -0.64400000000000 Cl (2n)
0.00000000000000 0.50000000000000 0.00000000000000 Pd (1b)
0.50000000000000 0.00000000000000 0.50000000000000 Pd (1g)
```

H<sub>3</sub>Cl (400 GPa): AB3\_mP16\_10\_mn\_3m3n - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
```

```

_chemical_name_mineral 'H3Cl'
_chemical_formula_sum 'Cl H3'

loop_
  _publ_author_name
    'Q. Zeng'
    'S. Yu'
    'D. Li'
    'A. R. Oganov'
    'G. Frapper'
  _journal_name_full_name
  ;
  Physical Chemistry Chemical Physics
;
_journal_volume 19
_journal_year 2017
_journal_page_first 8236
_journal_page_last 8242
_publ_section_title
;
Emergence of novel hydrogen chlorides under high pressure
;

_aflow_title 'HS_{3}Cl (400-GPa) Structure'
_aflow_proto 'AB3_mP16_10_mn_3m3n'
_aflow_params 'a,b/a,c/a,\beta,x_{1},z_{1},x_{2},z_{2},x_{3},z_{3},x_{4},z_{4},x_{5},z_{5},x_{6},z_{6},x_{7},z_{7},x_{8},z_{8}'
_aflow_params_values '3.678,0.71098423056,1.23817292007,90.0,0.263,0.339,0.08,0.059,0.795,0.341,0.438,-0.069,0.763,0.161,0.705,0.841,0.58,0.441,0.062,0.431'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mP16'

_symmetry_space_group_name_H-M 'P 1 2/m 1'
_symmetry_Int_Tables_number 10

_cell_length_a 3.67800
_cell_length_b 2.61500
_cell_length_c 4.55400
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 -x,y,-z
3 -x,-y,-z
4 x,-y,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Cl1 Cl 2 m 0.26300 0.00000 0.33900 1.00000
H1 H 2 m 0.08000 0.00000 0.05900 1.00000
H2 H 2 m 0.79500 0.00000 0.34100 1.00000
H3 H 2 m 0.43800 0.00000 -0.06900 1.00000
Cl2 Cl 2 n 0.76300 0.50000 0.16100 1.00000
H4 H 2 n 0.70500 0.50000 0.84100 1.00000
H5 H 2 n 0.58000 0.50000 0.44100 1.00000
H6 H 2 n 0.06200 0.50000 0.43100 1.00000

```

H<sub>3</sub>Cl (400 GPa): AB<sub>3</sub>mP16\_10\_mn\_3m3n - POSCAR

```

AB3_mP16_10_mn_3m3n & a,b/a,c/a,\beta,x1,z1,x2,z2,x3,z3,x4,z4,x5,z5,x6,z6
_> x7,z7,x8,z8 --params=3.678,0.71098423056,1.23817292007,90.0,
_> 0.263,0.339,0.08,0.059,0.795,0.341,0.438,-0.069,0.763,0.161,
_> 0.705,0.841,0.58,0.441,0.062,0.431 & P2/m C_{2h}^{1} #10 (m^4n^4
_> 4) & mP16 & None & H3Cl & H3Cl & Q. Zeng et al., Phys. Chem.
_> Chem. Phys. 19, 8236-8242 (2017)
1.0000000000000000
3.6780000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 2.6150000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.5540000000000000
Cl H
4 12
Direct
0.2630000000000000 0.0000000000000000 0.3390000000000000 Cl (2m)
-0.2630000000000000 0.0000000000000000 -0.3390000000000000 Cl (2m)
0.7630000000000000 0.5000000000000000 0.1610000000000000 Cl (2n)
-0.7630000000000000 0.5000000000000000 -0.1610000000000000 Cl (2n)
0.0800000000000000 0.0000000000000000 0.0590000000000000 H (2m)
-0.0800000000000000 0.0000000000000000 -0.0590000000000000 H (2m)
0.7950000000000000 0.0000000000000000 0.3410000000000000 H (2m)
-0.7950000000000000 0.0000000000000000 -0.3410000000000000 H (2m)
0.4380000000000000 0.0000000000000000 -0.0690000000000000 H (2m)
-0.4380000000000000 0.0000000000000000 0.0690000000000000 H (2m)
0.7050000000000000 0.5000000000000000 0.8410000000000000 H (2n)
-0.7050000000000000 0.5000000000000000 -0.8410000000000000 H (2n)
0.5800000000000000 0.5000000000000000 0.4410000000000000 H (2n)
-0.5800000000000000 0.5000000000000000 -0.4410000000000000 H (2n)
0.0620000000000000 0.5000000000000000 0.4310000000000000 H (2n)
-0.0620000000000000 0.5000000000000000 -0.4310000000000000 H (2n)

```

Muthmannite (AuAgTe<sub>2</sub>): ABC<sub>2</sub>mP8\_10\_ac\_eh\_mn - CIF

# CIF file

```

data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'AuAgTe2'
_chemical_formula_sum 'Ag Au Te2'

loop_
  _publ_author_name
    'L. Bindi'
  _journal_name_full_name
  ;
  Philosophical Magazine Letters
;
_journal_volume 88
_journal_year 2008
_journal_page_first 533
_journal_page_last 541
_publ_section_title
;
Commensurate-incommensurate phase transition in muthmannite, AuAgTe2S
_> : first evidence of a modulated structure at low temperature
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
_> Inorganic Compounds, 2013

_aflow_title 'Muthmannite (AuAgTe2) Structure'
_aflow_proto 'ABC2_mP8_10_ac_eh_mn'
_aflow_params 'a,b/a,c/a,\beta,x_{5},z_{5},x_{6},z_{6}'
_aflow_params_values '5.1177434753,0.86107854631,1.45123094959,90.021,
_> 0.6089,0.24179,0.1277,0.24913'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mP8'

_cell_length_a 5.1177434753
_cell_length_b 4.4067791121
_cell_length_c 7.4270272734
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0210000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'P 1 2/m 1'
_symmetry_Int_Tables_number 10

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 -x,y,-z
3 -x,-y,-z
4 x,-y,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Ag1 Ag 1 a 0.00000 0.00000 1.00000
Ag2 Ag 1 c 0.00000 0.00000 0.50000 1.00000
Au1 Au 1 e 0.50000 0.50000 0.00000 1.00000
Au2 Au 1 h 0.50000 0.50000 0.50000 1.00000
Te1 Te 2 m 0.60890 0.00000 0.24179 1.00000
Te2 Te 2 n 0.12770 0.50000 0.24913 1.00000

```

Muthmannite (AuAgTe<sub>2</sub>): ABC<sub>2</sub>mP8\_10\_ac\_eh\_mn - POSCAR

```

ABC2_mP8_10_ac_eh_mn & a,b/a,c/a,\beta,x5,z5,x6,z6 --params=5.1177434753,
_> 0.86107854631,1.45123094959,90.021,0.6089,0.24179,0.1277,
_> 0.24913 & P2/m C_{2h}^{1} #10 (acehmn) & mP8 & None & AuAgTe2 &
_> & L. Bindi, Philos. Mag. Lett. 88, 533-541 (2008)
1.0000000000000000
5.1177434753000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 4.4067791121000000 0.0000000000000000
-0.00272214777467 0.0000000000000000 7.42702722454036
Ag Au Te
2 2 4
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 Ag (1a)
0.0000000000000000 0.0000000000000000 0.5000000000000000 Ag (1c)
0.5000000000000000 0.5000000000000000 0.0000000000000000 Au (1e)
0.5000000000000000 0.5000000000000000 0.5000000000000000 Au (1h)
0.6089000000000000 0.0000000000000000 0.2417900000000000 Te (2m)
-0.6089000000000000 0.0000000000000000 -0.2417900000000000 Te (2m)
0.1277000000000000 0.5000000000000000 0.2491300000000000 Te (2n)
-0.1277000000000000 0.5000000000000000 -0.2491300000000000 Te (2n)

```

LiSn: AB<sub>m</sub>P6\_10\_en\_am - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'LiSn'
_chemical_formula_sum 'Li Sn'

loop_
  _publ_author_name
    'W. Müller'
    'H. Schaffer'
  _journal_name_full_name
;

```

```

Zeitschrift f{"u}r Naturforschung B
;
_journal_volume 28
_journal_year 1973
_journal_page_first 246
_journal_page_last 248
_publ_section_title
;
Die Kristallstruktur der Phase LiSn
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title 'LiSn Structure'
_aflow_proto 'AB_mP6_10_en_am'
_aflow_params 'a,b/a,c/a,\beta,x_{3},z_{3},x_{4},z_{4}'
_aflow_params_values '5.1700416367,0.61508704062,1.49709864605,104.5,
  ↳ 0.234,0.66,0.263,0.336'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mP6'

_cell_length_a 5.1700416367
_cell_length_b 3.1800256102
_cell_length_c 7.7400623343
_cell_angle_alpha 90.0000000000
_cell_angle_beta 104.5000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 1 2/m 1"
_symmetry_Int_Tables_number 10

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,y,-z
3 -x,-y,-z
4 x,-y,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Sn1 Sn 1 a 0.00000 0.00000 1.00000
Li1 Li 1 e 0.50000 0.50000 0.00000 1.00000
Sn2 Sn 2 m 0.23400 0.00000 0.66000 1.00000
Li2 Li 2 n 0.26300 0.50000 0.33600 1.00000

```

LiSn: AB\_mP6\_10\_en\_am - POSCAR

```

AB_mP6_10_en_am & a,b/a,c/a,\beta,x3,z3,x4,z4 --params=5.1700416367,
  ↳ 0.61508704062,1.49709864605,104.5,0.234,0.66,0.263,0.336 & P2/m
  ↳ C_{2h}^{1} #10 (aem) & mP6 & None & LiSn & W. M{"u}ller
  ↳ and H. Sch{"a}fer, Z. Naturforsch. B 28, 246-248 (1973)
1.0000000000000000
5.17004163670000 0.00000000000000 0.00000000000000
0.00000000000000 3.18002561020000 0.00000000000000
-1.93795683864366 0.00000000000000 7.49352308533201
Li Sn
3 3
Direct
0.50000000000000 0.50000000000000 0.00000000000000 Li (1e)
0.26300000000000 0.50000000000000 0.33600000000000 Li (2n)
-0.26300000000000 0.50000000000000 -0.33600000000000 Li (2n)
0.00000000000000 0.00000000000000 0.00000000000000 Sn (1a)
0.23400000000000 0.00000000000000 0.66000000000000 Sn (2m)
-0.23400000000000 0.00000000000000 -0.66000000000000 Sn (2m)

```

S-carbon: A\_mP8\_10\_2m2n - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'S-carbon'
_chemical_formula_sum 'C'

loop_
_publ_author_name
'H. Niu'
'X.-Q. Chen'
'S. Wang'
'D. Li'
'W. L. Mao'
'Y. Li'
_journal_name_full_name
;
Physical Review Letters
;
_journal_volume 108
_journal_year 2012
_journal_page_first 135501
_journal_page_last 135501
_publ_section_title
;
Families of Superhard Crystalline Carbon Allotropes Constructed via
  ↳ Cold Compression of Graphite and Nanotubes
;

```

```

_aflow_title 'S-carbon Structure'
_aflow_proto 'A_mP8_10_2m2n'
_aflow_params 'a,b/a,c/a,\beta,x_{1},z_{1},x_{2},z_{2},x_{3},z_{3},x_{4},z_{4}'
_aflow_params_values '4.7302,0.527461840937,0.86332501797,106.1,0.1175,
  ↳ 0.6746,0.5344,0.3333,0.1131,0.8977,0.4209,0.1319'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mP8'

_symmetry_space_group_name_H-M "P 1 2/m 1"
_symmetry_Int_Tables_number 10

_cell_length_a 4.73020
_cell_length_b 2.49500
_cell_length_c 4.08370
_cell_angle_alpha 90.00000
_cell_angle_beta 106.10000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,y,-z
3 -x,-y,-z
4 x,-y,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
C1 C 2 m 0.11750 0.00000 0.67460 1.00000
C2 C 2 m 0.53440 0.00000 0.33330 1.00000
C3 C 2 n 0.11310 0.50000 0.89770 1.00000
C4 C 2 n 0.42090 0.50000 0.13190 1.00000

```

S-carbon: A\_mP8\_10\_2m2n - POSCAR

```

A_mP8_10_2m2n & a,b/a,c/a,\beta,x1,z1,x2,z2,x3,z3,x4,z4 --params=4.7302,
  ↳ 0.527461840937,0.86332501797,106.1,0.1175,0.6746,0.5344,0.3333,
  ↳ 0.1131,0.8977,0.4209,0.1319 & P2/m C_{2h}^{1} #10 (m^2n^2) &
  ↳ mP8 & None & C & S-carbon & H. Niu et al., Phys. Rev. Lett. 108
  ↳ , 135501 (2012)
1.0000000000000000
4.730200000000000 0.00000000000000 0.00000000000000
0.00000000000000 2.49500000000000 0.00000000000000
-1.13246984969092 0.00000000000000 3.92353383183337
C
8
Direct
0.11750000000000 0.00000000000000 0.67460000000000 C (2m)
-0.11750000000000 0.00000000000000 -0.67460000000000 C (2m)
0.53440000000000 0.00000000000000 0.33330000000000 C (2m)
-0.53440000000000 0.00000000000000 -0.33330000000000 C (2m)
0.11310000000000 0.50000000000000 0.89770000000000 C (2n)
-0.11310000000000 0.50000000000000 -0.89770000000000 C (2n)
0.42090000000000 0.50000000000000 0.13190000000000 C (2n)
-0.42090000000000 0.50000000000000 -0.13190000000000 C (2n)

```

Thortveitite ([Sc,Y]<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>, S<sub>2</sub>): A7B2C2\_mC22\_12\_aj\_h\_i - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Thortveitite'
_chemical_formula_sum 'O7 Sc2 Si2'

loop_
_publ_author_name
'R. Bianchi'
'T. Pilati'
'V. Diella'
'C. M. Gramaccioli'
'G. Mannucci'
_journal_name_full_name
;
American Mineralogist
;
_journal_volume 73
_journal_year 1988
_journal_page_first 601
_journal_page_last 607
_publ_section_title
;
A re-examination of thortveitite
;
# Found in The American Mineralogist Crystal Structure Database, 2003

_aflow_title 'Thortveitite ([Sc,Y]_2SSi_2SOS_7S, SS2_{1}S) Structure'
_aflow_proto 'A7B2C2_mC22_12_aj_h_i'
_aflow_params 'a,b/a,c/a,\beta,y_{2},x_{3},z_{3},x_{4},z_{4},x_{5},y_{5}'
_aflow_params_values '6.65,1.29563909774,0.704661654135,102.2,0.30503,
  ↳ 0.38654,0.22171,0.22108,-0.08762,0.23655,0.15499,0.71826'
_aflow_Strukturbericht 'SS2_{1}S'
_aflow_Pearson 'mC22'

_symmetry_space_group_name_H-M "C 1 2/m 1"

```



\_symmetry\_Int\_Tables\_number 12

\_cell\_length\_a 6.65000  
\_cell\_length\_b 8.61600  
\_cell\_length\_c 4.68600  
\_cell\_angle\_alpha 90.00000  
\_cell\_angle\_beta 102.20000  
\_cell\_angle\_gamma 90.00000

loop\_

\_space\_group\_symop\_id  
\_space\_group\_symop\_operation\_xyz  
1 x,y,z  
2 -x,y,-z  
3 -x,-y,-z  
4 x,-y,z  
5 x+1/2,y+1/2,z  
6 -x+1/2,y+1/2,-z  
7 -x+1/2,-y+1/2,-z  
8 x+1/2,-y+1/2,z

loop\_

\_atom\_site\_label  
\_atom\_site\_type\_symbol  
\_atom\_site\_symmetry\_multiplicity  
\_atom\_site\_Wyckoff\_label  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z  
\_atom\_site\_occupancy  
O1 O 2 a 0.00000 0.00000 1.00000  
Sc1 Sc 4 h 0.00000 0.30503 0.50000 1.00000  
O2 O 4 i 0.38654 0.00000 0.22171 1.00000  
Si1 Si 4 i 0.22108 0.00000 -0.08762 1.00000  
O3 O 8 j 0.23655 0.15499 0.71826 1.00000

Thortveitite ([Sc,Y]<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>, S<sub>2</sub>): A7B2C2\_mC22\_12\_aj\_h\_i - POSCAR

A7B2C2\_mC22\_12\_aj\_h\_i & a,b/a.c/a,beta,y2,x3,z3,x4,z4,x5,y5,z5 --params  
↪ =6.65, 1.29563909774, 0.704661654135, 102.2, 0.30503, 0.38654,  
↪ 0.22171, 0.22108, -0.08762, 0.23655, 0.15499, 0.71826 & C2/m C\_{2h}  
↪ ^{3} #12 (ahi^2j) & mC22 & SS\_{1}\$ & [Sc,Y]2Si2O7 &  
↪ Thortveitite & R. Bianchi et al., Am. Mineral. 73, 601-607 (  
↪ 1988)  
1.00000000000000  
3.32500000000000 -4.30800000000000 0.00000000000000  
3.32500000000000 4.30800000000000 0.00000000000000  
-0.99026799618995 0.00000000000000 4.58017088062465  
O Sc Si  
7 2 2  
Direct  
0.00000000000000 0.00000000000000 0.00000000000000 O (2a)  
0.38654000000000 0.38654000000000 0.22171000000000 O (4i)  
-0.38654000000000 -0.38654000000000 -0.22171000000000 O (4i)  
0.08156000000000 0.39154000000000 0.71826000000000 O (8j)  
-0.39154000000000 -0.08156000000000 -0.71826000000000 O (8j)  
-0.08156000000000 -0.39154000000000 -0.71826000000000 O (8j)  
0.39154000000000 0.08156000000000 0.71826000000000 O (8j)  
-0.30503000000000 0.30503000000000 0.50000000000000 Sc (4h)  
0.30503000000000 -0.30503000000000 0.50000000000000 Sc (4h)  
0.22108000000000 0.22108000000000 -0.08762000000000 Si (4i)  
-0.22108000000000 -0.22108000000000 0.08762000000000 Si (4i)

M-carbon: A\_mC16\_12\_4i - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'M-carbon'
_chemical_formula_sum 'C'

loop_
_publ_author_name
'Q. Li'
'Y. Ma'
'A. R. Oganov'
'H. Wang'
'H. Wang'
'Y. Xu'
'T. Cui'
'H.-K. Mao'
'G. Zou'
_journal_name_full_name
;
Physical Review Letters
;
_journal_volume 102
_journal_year 2009
_journal_page_first 175506
_journal_page_last 175506
_publ_section_title
;
Superhard Monoclinic Polymorph of Carbon
;

_aflow_title 'M-carbon Structure'
_aflow_proto 'A_mC16_12_4i'
_aflow_params 'a,b/a.c/a,\beta,x_{1},z_{1},x_{2},z_{2},x_{3},z_{3},x_{4},z_{4}'
↪ ,z_{4}'
_aflow_params_values '9.089,0.274617669711,0.451534822313,96.96,-0.0572,
↪ 0.1206,0.4419,0.3467,0.7858,-0.0594,0.2715,0.4149'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mC16'
```

\_symmetry\_space\_group\_name\_H-M "C 1 2/m 1"  
\_symmetry\_Int\_Tables\_number 12

\_cell\_length\_a 9.08900  
\_cell\_length\_b 2.49600  
\_cell\_length\_c 4.10400  
\_cell\_angle\_alpha 90.00000  
\_cell\_angle\_beta 96.96000  
\_cell\_angle\_gamma 90.00000

loop\_

\_space\_group\_symop\_id  
\_space\_group\_symop\_operation\_xyz  
1 x,y,z  
2 -x,y,-z  
3 -x,-y,-z  
4 x,-y,z  
5 x+1/2,y+1/2,z  
6 -x+1/2,y+1/2,-z  
7 -x+1/2,-y+1/2,-z  
8 x+1/2,-y+1/2,z

loop\_

\_atom\_site\_label  
\_atom\_site\_type\_symbol  
\_atom\_site\_symmetry\_multiplicity  
\_atom\_site\_Wyckoff\_label  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z  
\_atom\_site\_occupancy  
C1 C 4 i -0.05720 0.00000 0.12060 1.00000  
C2 C 4 i 0.44190 0.00000 0.34670 1.00000  
C3 C 4 i 0.78580 0.00000 -0.05940 1.00000  
C4 C 4 i 0.27150 0.00000 0.41490 1.00000

M-carbon: A\_mC16\_12\_4i - POSCAR

A\_mC16\_12\_4i & a,b/a.c/a,beta,x1,z1,x2,z2,x3,z3,x4,z4 --params=9.089,  
↪ 0.274617669711,0.451534822313,96.96,-0.0572,0.1206,0.4419,  
↪ 0.3467,0.7858,-0.0594,0.2715,0.4149 & C2/m C\_{2h}^{3} #12 (i^4)  
↪ & mC16 & None & C & M-carbon & Q. Li et al., Phys. Rev. Lett.  
↪ 102, 175506 (2009)  
1.00000000000000  
4.54450000000000 -1.24800000000000 0.00000000000000  
4.54450000000000 1.24800000000000 0.00000000000000  
-0.49730788744489 0.00000000000000 4.07375758545904  
C  
8  
Direct  
-0.05720000000000 -0.05720000000000 0.12060000000000 C (4i)  
0.05720000000000 0.05720000000000 -0.12060000000000 C (4i)  
0.44190000000000 0.44190000000000 0.34670000000000 C (4i)  
-0.44190000000000 -0.44190000000000 -0.34670000000000 C (4i)  
0.78580000000000 0.78580000000000 -0.05940000000000 C (4i)  
-0.78580000000000 -0.78580000000000 0.05940000000000 C (4i)  
0.27150000000000 0.27150000000000 0.41490000000000 C (4i)  
-0.27150000000000 -0.27150000000000 -0.41490000000000 C (4i)

H<sub>2</sub>S (15 GPa): A2B\_mP12\_13\_2g\_ef - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'H2S'
_chemical_formula_sum 'H2 S'

loop_
_publ_author_name
'Y. Li'
'J. Hao'
'H. Liu'
'Y. Li'
'Y. Ma'
_journal_name_full_name
;
Journal of Chemical Physics
;
_journal_volume 140
_journal_year 2014
_journal_page_first 174712
_journal_page_last 174712
_publ_section_title
;
The metallization and superconductivity of dense hydrogen sulfide
;

_aflow_title 'HS_{2}$S (15-GPa) Structure'
_aflow_proto 'A2B_mP12_13_2g_ef'
_aflow_params 'a,b/a.c/a,\beta,y_{1},y_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4}'
↪ ,z_{4}'
_aflow_params_values '5.6255,0.61198115723,1.23780997245,127.44,0.1808,-
↪ 0.004,0.155,0.346,0.225,0.345,0.273,0.573'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mP12'

_symmetry_space_group_name_H-M "P 1 2/c 1"
_symmetry_Int_Tables_number 13

_cell_length_a 5.62550
_cell_length_b 3.44270
_cell_length_c 6.96330
_cell_angle_alpha 90.00000
_cell_angle_beta 127.44000
```

```

_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,y,-z+1/2
3 -x,-y,-z
4 x,-y,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
S1 S 2 e 0.00000 0.18080 0.25000 1.00000
S2 S 2 f 0.50000 -0.00400 0.25000 1.00000
H1 H 4 g 0.15500 0.34600 0.22500 1.00000
H2 H 4 g 0.34500 0.27300 0.57300 1.00000

```

H<sub>2</sub>S (15 GPa): A2B\_mP12\_13\_2g\_ef - POSCAR

```

A2B_mP12_13_2g_ef & a,b/a,c/a,beta,y1,y2,x3,y3,z3,x4,y4,z4 --params=
↪ 5.6255, 0.61198115723, 1.23780997245, 127.44, 0.1808, -0.004, 0.155,
↪ 0.346, 0.225, 0.345, 0.273, 0.573 & P2/c C_{2h}^{4} #13 (efg^2) &
↪ mP12 & None & H2S & H2S & Y. Li et al., J. Chem. Phys. 140,
↪ 174712 (2014)
1.0000000000000000
5.6255000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 3.4427000000000000 0.0000000000000000
-4.23320104193685 0.0000000000000000 5.52879334290447
H S
8 4
Direct
0.1550000000000000 0.3460000000000000 0.2250000000000000 H (4g)
-0.1550000000000000 0.3460000000000000 0.2750000000000000 H (4g)
-0.1550000000000000 -0.3460000000000000 -0.2250000000000000 H (4g)
0.1550000000000000 -0.3460000000000000 0.7250000000000000 H (4g)
0.3450000000000000 0.2730000000000000 0.5730000000000000 H (4g)
-0.3450000000000000 0.2730000000000000 -0.0730000000000000 H (4g)
-0.3450000000000000 -0.2730000000000000 -0.5730000000000000 H (4g)
0.3450000000000000 -0.2730000000000000 1.0730000000000000 H (4g)
0.0000000000000000 0.1808000000000000 0.2500000000000000 S (2e)
0.0000000000000000 -0.1808000000000000 0.7500000000000000 S (2e)
0.5000000000000000 -0.0040000000000000 0.2500000000000000 S (2f)
0.5000000000000000 0.0040000000000000 0.7500000000000000 S (2f)

```

γ-PdCl<sub>2</sub>: A2B\_mP6\_14\_e\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '$\gamma$-PdCl2'
_chemical_formula_sum 'Cl2 Pd'

loop_
_publ_author_name
'J. Evers'
'W. Beck'
'M. G\{o}bel'
'S. Jakob'
'P. Mayer'
'G. Oehlinger'
'M. Rotter'
'T. M. Klap\{o}tke'
_journal_name_full_name
;
Angewandte Chemie (International ed.)
;
_journal_volume 49
_journal_year 2010
_journal_page_first 5677
_journal_page_last 5682
_publ_section_title
;
The Structures of $\delta$-PdClS_{2}$ and $\gamma$-PdClS_{2}$: Phases
↪ with Negative Thermal Expansion in One Direction
;
_aflow_title '$\gamma$-PdClS_{2}$ Structure'
_aflow_proto 'A2B_mP6_14_e_a'
_aflow_params 'a,b/a,c/a,\beta,x_{2},y_{2},z_{2}'
_aflow_params_values '5.5496, 0.695689779444, 1.15512829753, 107.151, 0.255,
↪ 0.2573, 0.3141'
_aflow_strukturbericht 'None'
_aflow_pearson 'mP6'

_symmetry_space_group_name_H-M 'P 1 21/c 1'
_symmetry_Int_Tables_number 14

_cell_length_a 5.54960
_cell_length_b 3.86080
_cell_length_c 6.41050
_cell_angle_alpha 90.00000
_cell_angle_beta 107.15100
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz

```

```

1 x,y,z
2 -x,y+1/2,-z+1/2
3 -x,-y,-z
4 x,-y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Pd1 Pd 2 a 0.00000 0.00000 0.00000 1.00000
Cl1 Cl 4 e 0.25500 0.25730 0.31410 1.00000

```

γ-PdCl<sub>2</sub>: A2B\_mP6\_14\_e\_a - POSCAR

```

A2B_mP6_14_e_a & a,b/a,c/a,beta,x2,y2,z2 --params=5.5496, 0.695689779444,
↪ 1.15512829753, 107.151, 0.255, 0.2573, 0.3141 & P2_{1}/c C_{2h}^{5}
↪ #14 (ae) & mP6 & None & PdCl2 & $\gamma$-PdCl2 & J. Evers et
↪ al., Angew. Chem. Int. Ed. 49, 5677-5682 (2010)
1.0000000000000000
5.5496000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 3.8608000000000000 0.0000000000000000
-1.89039860884891 0.0000000000000000 6.12543087053165
Cl Pd
4 2
Direct
0.2550000000000000 0.2573000000000000 0.3141000000000000 Cl (4e)
-0.2550000000000000 0.7573000000000000 0.1859000000000000 Cl (4e)
-0.2550000000000000 -0.2573000000000000 -0.3141000000000000 Cl (4e)
0.2550000000000000 0.2427000000000000 0.8141000000000000 Cl (4e)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Pd (2a)
0.0000000000000000 0.5000000000000000 0.5000000000000000 Pd (2a)

```

α-Toluene: A7B8\_mP120\_14\_14e\_16e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'alpha-Toluene'
_chemical_formula_sum 'C7 H8'

loop_
_publ_author_name
'S. K Nayak'
'R. Sathishkumar'
'T. N. {Guru Row}'
_journal_name_full_name
;
CrystEngComm
;
_journal_volume 12
_journal_year 2010
_journal_page_first 3112
_journal_page_last 3118
_publ_section_title
;
Directing role of functional groups in selective generation of C-H-$\pi$
↪ interactions: In situ cryo-crystallographic studies on
↪ benzyl derivatives
;

# Found in Cambridge Structural Database, {CSD Entry: TOLUEN03},

_aflow_title '$\alpha$-Toluene Structure'
_aflow_proto 'A7B8_mP120_14_14e_16e'
_aflow_params 'a,b/a,c/a,\beta,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},y_{7},z_{7},x_{8},y_{8},z_{8},x_{9},y_{9},z_{9},x_{10},y_{10},z_{10},x_{11},y_{11},z_{11},x_{12},y_{12},z_{12},x_{13},y_{13},z_{13},x_{14},y_{14},z_{14},x_{15},y_{15},z_{15},x_{16},y_{16},z_{16},x_{17},y_{17},z_{17},x_{18},y_{18},z_{18},x_{19},y_{19},z_{19},x_{20},y_{20},z_{20},x_{21},y_{21},z_{21},x_{22},y_{22},z_{22},x_{23},y_{23},z_{23},x_{24},y_{24},z_{24},x_{25},y_{25},z_{25},x_{26},y_{26},z_{26},x_{27},y_{27},z_{27},x_{28},y_{28},z_{28},x_{29},y_{29},z_{29},x_{30},y_{30},z_{30}'
_aflow_params_values '7.5889, 0.766725085322, 3.55545599494, 106.136,
↪ 0.25252, 0.5751, 0.3402, 0.76924, 0.888, 0.47034, 0.13489, 0.3866,
↪ 0.33222, 0.8218, 0.8146, 0.42747, 0.12506, 0.2343, 0.29191, 0.78423,
↪ 0.9464, 0.38285, 0.23276, 0.2673, 0.25885, 0.69189, 0.1533, 0.38027,
↪ 0.34844, 0.4547, 0.26591, 0.63874, 0.2281, 0.42248, 0.35819, 0.6069,
↪ 0.3061, 0.67752, 0.0969, 0.46714, 0.26777, 0.7386, 0.3843, 0.8119,
↪ 0.7461, 0.51889, 0.0602, 0.3617, 0.3547, 0.8843, 0.6723, 0.4287, 0.0438
↪ 0.1068, 0.2871, 0.822, 0.8945, 0.354, 0.2273, 0.1621, 0.2315, 0.6653,
↪ 0.243, 0.3497, 0.4219, 0.4796, 0.2431, 0.5754, 0.3699, 0.4209, 0.4385,
↪ 0.7352, 0.3104, 0.6409, 0.1506, 0.496, 0.9409, 0.7672, 0.5381, 0.7891,
↪ 0.5835, 0.5099, 0.7334, 0.7952, 0.5403, 0.2081, 0.8842, 0.3711, 0.3975,
↪ 0.7664, 0.4019, 0.2077, 0.6717, 0.4087'
_aflow_strukturbericht 'None'
_aflow_pearson 'mP120'

_symmetry_space_group_name_H-M 'P 1 21/c 1'
_symmetry_Int_Tables_number 14

_cell_length_a 7.58890
_cell_length_b 5.81860
_cell_length_c 26.98200
_cell_angle_alpha 90.00000
_cell_angle_beta 106.13600
_cell_angle_gamma 90.00000

```

```

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 -x,y+1/2,-z+1/2
3 -x,-y,-z
4 x,-y+1/2,z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
C1 C 4 e 0.25252 0.57510 0.34020 1.00000
C2 C 4 e 0.76924 0.88800 0.47034 1.00000
C3 C 4 e 0.13489 0.38660 0.33222 1.00000
C4 C 4 e 0.82180 0.81460 0.42747 1.00000
C5 C 4 e 0.12506 0.23430 0.29191 1.00000
C6 C 4 e 0.78423 0.94640 0.38285 1.00000
C7 C 4 e 0.23276 0.26730 0.25885 1.00000
C8 C 4 e 0.69189 0.15330 0.38027 1.00000
C9 C 4 e 0.34844 0.45470 0.26591 1.00000
C10 C 4 e 0.63874 0.22810 0.42248 1.00000
C11 C 4 e 0.35819 0.60690 0.30610 1.00000
C12 C 4 e 0.67752 0.09690 0.46714 1.00000
C13 C 4 e 0.26777 0.73860 0.38430 1.00000
C14 C 4 e 0.81190 0.74610 0.51889 1.00000
H1 H 4 e 0.06020 0.36170 0.35470 1.00000
H2 H 4 e 0.88430 0.67230 0.42870 1.00000
H3 H 4 e 0.04380 0.10680 0.28710 1.00000
H4 H 4 e 0.82200 0.89450 0.35400 1.00000
H5 H 4 e 0.22730 0.16210 0.23150 1.00000
H6 H 4 e 0.66530 0.24300 0.34970 1.00000
H7 H 4 e 0.42190 0.47960 0.24310 1.00000
H8 H 4 e 0.57540 0.36990 0.42090 1.00000
H9 H 4 e 0.43850 0.73520 0.31040 1.00000
H10 H 4 e 0.64090 0.15060 0.49600 1.00000
H11 H 4 e 0.94090 0.76720 0.53810 1.00000
H12 H 4 e 0.78910 0.58350 0.50990 1.00000
H13 H 4 e 0.73340 0.79520 0.54030 1.00000
H14 H 4 e 0.20810 0.88420 0.37110 1.00000
H15 H 4 e 0.39750 0.76640 0.40190 1.00000
H16 H 4 e 0.20770 0.67170 0.40870 1.00000

```

***o*-Toluene: A7B8\_mP120\_14\_14e\_16e - POSCAR**

```

A7B8_mP120_14_14e_16e & a,b/a,c/a,beta,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,
↳ z4,x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11
↳ ,y11,z11,x12,y12,z12,x13,y13,z13,x14,y14,z14,x15,y15,z15,x16,
↳ y16,z16,x17,y17,z17,x18,y18,z18,x19,y19,z19,x20,y20,z20,x21,y21
↳ ,z21,x22,y22,z22,x23,y23,z23,x24,y24,z24,x25,y25,z25,x26,y26,
↳ z26,x27,y27,z27,x28,y28,z28,x29,y29,z29,x30,y30,z30 --params=
↳ 7.5889,0.766725085322,3.55545599494,106.136,0.25252,0.5751,
↳ 0.3402,0.76924,0.888,0.47034,0.13489,0.3866,0.33222,0.8218,
↳ 0.8146,0.42747,0.12506,0.2343,0.29191,0.78423,0.9464,0.38285,
↳ 0.23276,0.2673,0.25885,0.69189,0.1533,0.38027,0.34844,0.4547,
↳ 0.26591,0.63874,0.2281,0.42248,0.35819,0.6069,0.3061,0.67752,
↳ 0.0969,0.46714,0.26777,0.7386,0.3843,0.8119,0.7461,0.51889,
↳ 0.0602,0.3617,0.3547,0.8843,0.6723,0.4287,0.0438,0.1068,0.2871,
↳ 0.822,0.8945,0.354,0.2273,0.1621,0.2315,0.6653,0.243,0.3497,
↳ 0.4219,0.4796,0.2431,0.5754,0.3699,0.4209,0.4385,0.7352,0.3104,
↳ 0.6409,0.1506,0.496,0.9409,0.7672,0.5381,0.7891,0.5835,0.5099,
↳ 0.7334,0.7952,0.5403,0.2081,0.8842,0.3711,0.3975,0.7664,0.4019,
↳ 0.2077,0.6717,0.4087 & P2_[1]/c_C_[2h]^5 #14 (e^30) & mP120 &
↳ None & C7H8 & alpha-Toluene & S. K Nayak and R. Sathishkumar
↳ and T. N. {Guru Row}, CrystEngComm 12, 3112-3118 (2010)
1.0000000000000000
7.588900000000000 0.000000000000000 0.000000000000000
0.000000000000000 5.818600000000000 0.000000000000000
-7.49879086554484 0.000000000000000 25.91903662474400
C H
56 64
Direct
0.252520000000000 0.575100000000000 0.340200000000000 C (4e)
-0.252520000000000 0.075100000000000 0.159800000000000 C (4e)
-0.252520000000000 -0.575100000000000 -0.340200000000000 C (4e)
0.252520000000000 -0.075100000000000 0.840200000000000 C (4e)
0.769240000000000 0.888000000000000 0.470340000000000 C (4e)
-0.769240000000000 1.388000000000000 0.029660000000000 C (4e)
-0.769240000000000 -0.888000000000000 -0.470340000000000 C (4e)
0.769240000000000 -0.388000000000000 0.970340000000000 C (4e)
0.134890000000000 0.386600000000000 0.332220000000000 C (4e)
-0.134890000000000 0.886600000000000 0.167780000000000 C (4e)
-0.134890000000000 -0.386600000000000 -0.332220000000000 C (4e)
0.134890000000000 0.113400000000000 0.832220000000000 C (4e)
0.821800000000000 0.814600000000000 0.427470000000000 C (4e)
-0.821800000000000 1.314600000000000 0.072530000000000 C (4e)
-0.821800000000000 -0.814600000000000 -0.427470000000000 C (4e)
0.821800000000000 -0.314600000000000 0.927470000000000 C (4e)
0.125060000000000 0.234300000000000 0.291910000000000 C (4e)
-0.125060000000000 0.734300000000000 0.208090000000000 C (4e)
-0.125060000000000 -0.234300000000000 -0.291910000000000 C (4e)
0.125060000000000 0.265700000000000 0.791910000000000 C (4e)
0.784230000000000 0.946400000000000 0.382850000000000 C (4e)
-0.784230000000000 1.446400000000000 0.117150000000000 C (4e)
-0.784230000000000 -0.946400000000000 -0.382850000000000 C (4e)
0.784230000000000 -0.446400000000000 0.882850000000000 C (4e)
0.232760000000000 0.267300000000000 0.258850000000000 C (4e)
-0.232760000000000 0.767300000000000 0.241150000000000 C (4e)
-0.232760000000000 -0.267300000000000 -0.258850000000000 C (4e)
0.232760000000000 0.232700000000000 0.758850000000000 C (4e)

```

```

0.691890000000000 0.153300000000000 0.380270000000000 C (4e)
-0.691890000000000 0.653300000000000 0.119730000000000 C (4e)
-0.691890000000000 -0.153300000000000 -0.380270000000000 C (4e)
0.691890000000000 0.346700000000000 0.880270000000000 C (4e)
0.348440000000000 0.454700000000000 0.265910000000000 C (4e)
-0.348440000000000 0.954700000000000 0.234090000000000 C (4e)
-0.348440000000000 -0.454700000000000 -0.265910000000000 C (4e)
0.348440000000000 0.045300000000000 0.765910000000000 C (4e)
0.638740000000000 0.228100000000000 0.422480000000000 C (4e)
-0.638740000000000 0.728100000000000 0.077520000000000 C (4e)
-0.638740000000000 -0.228100000000000 -0.422480000000000 C (4e)
0.638740000000000 0.271900000000000 0.922480000000000 C (4e)
0.358190000000000 0.606900000000000 0.306100000000000 C (4e)
-0.358190000000000 1.106900000000000 0.193900000000000 C (4e)
-0.358190000000000 -0.606900000000000 -0.306100000000000 C (4e)
0.358190000000000 -0.106900000000000 0.806100000000000 C (4e)
0.677520000000000 0.096900000000000 0.467140000000000 C (4e)
-0.677520000000000 0.596900000000000 0.032860000000000 C (4e)
-0.677520000000000 -0.096900000000000 -0.467140000000000 C (4e)
0.677520000000000 0.403100000000000 0.967140000000000 C (4e)
0.267770000000000 0.738600000000000 0.384300000000000 C (4e)
-0.267770000000000 1.238600000000000 0.115700000000000 C (4e)
-0.267770000000000 -0.738600000000000 -0.384300000000000 C (4e)
0.267770000000000 -0.238600000000000 0.884300000000000 C (4e)
0.811900000000000 0.746100000000000 0.518890000000000 C (4e)
-0.811900000000000 1.246100000000000 -0.018890000000000 C (4e)
-0.811900000000000 -0.746100000000000 -0.518890000000000 C (4e)
0.811900000000000 -0.246100000000000 1.018890000000000 C (4e)
0.060200000000000 0.361700000000000 0.354700000000000 H (4e)
-0.060200000000000 0.861700000000000 0.145300000000000 H (4e)
-0.060200000000000 -0.361700000000000 -0.354700000000000 H (4e)
0.060200000000000 0.138300000000000 0.854700000000000 H (4e)
0.884300000000000 0.672300000000000 0.428700000000000 H (4e)
-0.884300000000000 1.172300000000000 0.071300000000000 H (4e)
-0.884300000000000 -0.672300000000000 -0.428700000000000 H (4e)
0.884300000000000 -0.172300000000000 0.928700000000000 H (4e)
0.043800000000000 0.106800000000000 0.287100000000000 H (4e)
-0.043800000000000 0.606800000000000 0.212900000000000 H (4e)
0.043800000000000 -0.106800000000000 -0.287100000000000 H (4e)
0.043800000000000 0.393200000000000 0.787100000000000 H (4e)
0.822000000000000 0.894500000000000 0.354000000000000 H (4e)
-0.822000000000000 1.394500000000000 0.146000000000000 H (4e)
-0.822000000000000 -0.894500000000000 -0.354000000000000 H (4e)
0.822000000000000 -0.394500000000000 0.854000000000000 H (4e)
0.227300000000000 0.162100000000000 0.231500000000000 H (4e)
-0.227300000000000 0.662100000000000 0.268500000000000 H (4e)
-0.227300000000000 -0.162100000000000 -0.231500000000000 H (4e)
0.227300000000000 0.337900000000000 0.731500000000000 H (4e)
0.665300000000000 0.243000000000000 0.349700000000000 H (4e)
-0.665300000000000 0.743000000000000 0.150300000000000 H (4e)
-0.665300000000000 -0.243000000000000 -0.349700000000000 H (4e)
0.665300000000000 0.257000000000000 0.849700000000000 H (4e)
0.421900000000000 0.479600000000000 0.243100000000000 H (4e)
-0.421900000000000 0.979600000000000 0.256900000000000 H (4e)
-0.421900000000000 -0.479600000000000 -0.243100000000000 H (4e)
0.421900000000000 0.020400000000000 0.743100000000000 H (4e)
0.575400000000000 0.369900000000000 0.420900000000000 H (4e)
-0.575400000000000 0.869900000000000 0.079100000000000 H (4e)
-0.575400000000000 -0.369900000000000 -0.420900000000000 H (4e)
0.575400000000000 0.130100000000000 0.920900000000000 H (4e)
0.438500000000000 0.735200000000000 0.310400000000000 H (4e)
-0.438500000000000 1.235200000000000 0.189600000000000 H (4e)
-0.438500000000000 -0.735200000000000 -0.310400000000000 H (4e)
0.438500000000000 -0.235200000000000 0.810400000000000 H (4e)
0.640900000000000 0.150600000000000 0.496000000000000 H (4e)
-0.640900000000000 0.650600000000000 0.004000000000000 H (4e)
-0.640900000000000 -0.150600000000000 -0.496000000000000 H (4e)
0.640900000000000 0.349400000000000 0.996000000000000 H (4e)
0.940900000000000 0.767200000000000 0.538100000000000 H (4e)
-0.940900000000000 1.267200000000000 -0.038100000000000 H (4e)
-0.940900000000000 -0.767200000000000 -0.538100000000000 H (4e)
0.940900000000000 -0.267200000000000 1.038100000000000 H (4e)
0.789100000000000 0.583500000000000 0.509900000000000 H (4e)
-0.789100000000000 1.083500000000000 -0.009900000000000 H (4e)
-0.789100000000000 -0.583500000000000 -0.509900000000000 H (4e)
0.789100000000000 -0.083500000000000 1.009900000000000 H (4e)
0.733400000000000 0.795200000000000 0.540300000000000 H (4e)
-0.733400000000000 1.295200000000000 -0.040300000000000 H (4e)
-0.733400000000000 -0.795200000000000 -0.540300000000000 H (4e)
0.733400000000000 -0.295200000000000 1.040300000000000 H (4e)
0.208100000000000 0.884200000000000 0.371100000000000 H (4e)
-0.208100000000000 1.384200000000000 0.128900000000000 H (4e)
-0.208100000000000 -0.884200000000000 -0.371100000000000 H (4e)
0.208100000000000 -0.384200000000000 0.871100000000000 H (4e)
0.397500000000000 0.766400000000000 0.401900000000000 H (4e)
-0.397500000000000 1.266400000000000 0.098100000000000 H (4e)
-0.397500000000000 -0.766400000000000 -0.401900000000000 H (4e)
0.397500000000000 -0.266400000000000 0.901900000000000 H (4e)
0.207700000000000 0.671700000000000 0.408700000000000 H (4e)
-0.207700000000000 1.171700000000000 0.091300000000000 H (4e)
-0.207700000000000 -0.671700000000000 -0.408700000000000 H (4e)
0.207700000000000 -0.171700000000000 0.908700000000000 H (4e)

```

**H<sub>3</sub>Cl (50 GPa): AB3\_mCl16\_15\_e\_cf - CIF**

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'H3Cl'
_chemical_formula_sum 'Cl H3'

loop_
  _publ_author_name
'D. Duan'

```

```
'X. Huang'
'F. Tian'
'Y. Liu'
'Da Li'
'H. Yu'
'B. Liu'
'W. Tian'
'T. Cui'
_journal_name_full_name
;
Journal of Physical Chemistry A
;
_journal_volume 119
_journal_year 2015
_journal_page_first 11059
_journal_page_last 11065
_publ_section_title
;
Predicted Formation of HS_{3}^{+} in Solid Halogen Polyhydrides at
↪ High Pressures
;
_aflow_title 'HS_{3}Cl (50-GPa) Structure'
_aflow_proto 'AB3_mC16_15_e_cf'
_aflow_params 'a,b/a,c/a,\beta,y_{2},x_{3},y_{3},z_{3}'
_aflow_params_values '3.282,2.64137720902,0.970749542962,91.9,0.86,0.577
↪ ,0.068,0.169'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mC16'

_symmetry_space_group_name_H-M "C 1 2/c 1"
_symmetry_Int_Tables_number 15

_cell_length_a 3.28200
_cell_length_b 8.66900
_cell_length_c 3.18600
_cell_angle_alpha 90.00000
_cell_angle_beta 91.90000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,y,-z+1/2
3 -x,-y,-z
4 x,-y,z+1/2
5 x+1/2,y+1/2,z
6 -x+1/2,y+1/2,-z+1/2
7 -x+1/2,-y+1/2,-z
8 x+1/2,-y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 e 0.00000 0.25000 1.00000
H2 H 4 e 0.00000 0.86000 0.25000 1.00000
H3 H 8 f 0.57700 0.06800 0.16900 1.00000
```

H<sub>3</sub>Cl (50 GPa): AB<sub>3</sub>mC16\_15\_e\_cf - POSCAR

```
AB3_mC16_15_e_cf & a,b/a,c/a,\beta,y_2,x_3,y_3,z_3 --params=3.282,
↪ 2.64137720902,0.970749542962,91.9,0.86,0.577,0.068,0.169 & C2/c
↪ C_{2h}^{6} #15 (cef) & mC16 & None & H3Cl & H3Cl & D. Duan et
↪ al., J. Phys. Chem. A 119, 11059-11065 (2015)
1.0000000000000000
1.6410000000000000 -4.3345000000000000 0.0000000000000000
1.6410000000000000 4.3345000000000000 0.0000000000000000
-0.10563239834584 0.0000000000000000 3.18424838799044
Cl H
2 6
Direct
-0.8600000000000000 0.8600000000000000 0.2500000000000000 Cl (4e)
0.8600000000000000 -0.8600000000000000 0.7500000000000000 Cl (4e)
0.0000000000000000 0.5000000000000000 0.0000000000000000 H (4c)
0.5000000000000000 0.0000000000000000 0.5000000000000000 H (4c)
0.5090000000000000 0.6450000000000000 0.1690000000000000 H (8f)
-0.6450000000000000 -0.5090000000000000 0.3310000000000000 H (8f)
-0.5090000000000000 -0.6450000000000000 -0.1690000000000000 H (8f)
0.6450000000000000 0.5090000000000000 0.6690000000000000 H (8f)
```

H-III (300 GPa): A\_mC24\_15\_2e2f - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'H'
_chemical_formula_sum 'H'

loop_
_publ_author_name
'C. J. Pickard'
'R. J. Needs'
_journal_name_full_name
;
Nature Physics
;
_journal_volume 3
```

```
_journal_year 2007
_journal_page_first 473
_journal_page_last 476
_publ_section_title
;
Structure of phase III of solid hydrogen
;

_aflow_title 'H-III (300-GPa) Structure'
_aflow_proto 'A_mC24_15_2e2f'
_aflow_params 'a,b/a,c/a,\beta,y_{1},y_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4}'
↪ ,z_{4}'
_aflow_params_values '4.939,0.569143551326,0.838023891476,142.47,0.1012,
↪ 0.3684,0.226,0.0672,0.2464,0.3443,0.1958,0.2227'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'mC24'

_symmetry_space_group_name_H-M "C 1 2/c 1"
_symmetry_Int_Tables_number 15

_cell_length_a 4.93900
_cell_length_b 2.81100
_cell_length_c 4.13900
_cell_angle_alpha 90.00000
_cell_angle_beta 142.47000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,y,-z+1/2
3 -x,-y,-z
4 x,-y,z+1/2
5 x+1/2,y+1/2,z
6 -x+1/2,y+1/2,-z+1/2
7 -x+1/2,-y+1/2,-z
8 x+1/2,-y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 e 0.00000 0.10120 0.25000 1.00000
H2 H 4 e 0.00000 0.36840 0.25000 1.00000
H3 H 8 f 0.22600 0.06720 0.24640 1.00000
H4 H 8 f 0.34430 0.19580 0.22270 1.00000
```

H-III (300 GPa): A\_mC24\_15\_2e2f - POSCAR

```
A_mC24_15_2e2f & a,b/a,c/a,\beta,y_1,y_2,x_3,y_3,z_3,x_4,y_4,z_4 --params=4.939,
↪ 0.569143551326,0.838023891476,142.47,0.1012,0.3684,0.226,0.0672
↪ ,0.2464,0.3443,0.1958,0.2227 & C2/c C_{2h}^{6} #15 (e^2f^2) &
↪ mC24 & None & H & H & C. J. Pickard and R. J. Needs, Nat. Phys.
↪ 3, 473-476 (2007)
1.0000000000000000
2.4695000000000000 -1.4055000000000000 0.0000000000000000
2.4695000000000000 1.4055000000000000 0.0000000000000000
-3.28236973265251 0.0000000000000000 2.52138254498731
H
12
Direct
-0.1012000000000000 0.1012000000000000 0.2500000000000000 H (4e)
0.1012000000000000 -0.1012000000000000 0.7500000000000000 H (4e)
-0.3684000000000000 0.3684000000000000 0.2500000000000000 H (4e)
0.3684000000000000 -0.3684000000000000 0.7500000000000000 H (4e)
0.1588000000000000 0.2932000000000000 0.2464000000000000 H (8f)
-0.2932000000000000 -0.1588000000000000 0.2536000000000000 H (8f)
-0.1588000000000000 -0.2932000000000000 -0.2464000000000000 H (8f)
0.2932000000000000 0.1588000000000000 0.7464000000000000 H (8f)
0.1485000000000000 0.5401000000000000 0.2227000000000000 H (8f)
-0.5401000000000000 -0.1485000000000000 0.2773000000000000 H (8f)
-0.1485000000000000 -0.5401000000000000 -0.2227000000000000 H (8f)
0.5401000000000000 0.1485000000000000 0.7227000000000000 H (8f)
```

$\alpha$ -Naumannite (Ag<sub>2</sub>Se): A2B\_oP12\_17\_abe\_e - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'alpha-Ag2Se'
_chemical_formula_sum 'Ag2 Se'

loop_
_publ_author_name
'Z. G. Pinsker'
'C. {Ching-liang}'
'R. M. Imamov'
'E. L. Lapidus'
_journal_name_full_name
;
Soviet Physics Crystallography
;
_journal_volume 10
_journal_year 1965
_journal_page_first 225
_journal_page_last 231
_publ_section_title
;
```

```

Determination of the crystal structure of the low-temperature phase  $\alpha$ 
   $\rightarrow$  alpha-Ag2Se
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
   $\rightarrow$  Inorganic Compounds, 2013

_aflow_title '$\alpha$-Naumannite (Ag2)Se Structure'
_aflow_proto 'A2B_oP12_17_abe_e'
_aflow_params 'a,b/a,c/a,x_{1},x_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4}'
   $\rightarrow$  )
_aflow_params_values '7.0499703347,1.11347517732,0.614184397158,0.893,
   $\rightarrow$  0.878,0.379,0.225,0.522,0.202,0.275,0.022'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP12'

_cell_length_a 7.0499703347
_cell_length_b 7.8499669685
_cell_length_c 4.3299817800
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2 2 21"
_symmetry_Int_Tables_number 17

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z+1/2
4 -x,-y,z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Ag1 Ag 2 a 0.89300 0.00000 0.00000 1.00000
Ag2 Ag 2 b 0.87800 0.50000 0.00000 1.00000
Ag3 Ag 4 e 0.37900 0.22500 0.52200 1.00000
Se1 Se 4 e 0.20200 0.27500 0.02200 1.00000

```

$\alpha$ -Naumannite (Ag<sub>2</sub>Se): A2B\_oP12\_17\_abe\_e - POSCAR

```

A2B_oP12_17_abe_e & a,b/a,c/a,x1,x2,x3,y3,z3,x4,y4,z4 --params=
   $\rightarrow$  7.0499703347,1.11347517732,0.614184397158,0.893,0.878,0.379,
   $\rightarrow$  0.225,0.522,0.202,0.275,0.022 & P222_{1} D_{2}^{2} #17 (abe^2)
   $\rightarrow$  & oP12 & None & Ag2Se & alpha & Z. G. Pinsker et al., Sov.
   $\rightarrow$  Phys. Crystallogr. 10, 225-231 (1965)
1.0000000000000000
7.04997033470000 0.00000000000000 0.00000000000000
0.00000000000000 7.84996696850000 0.00000000000000
0.00000000000000 0.00000000000000 4.32998178000000
Ag Se
8 4
Direct
0.89300000000000 0.00000000000000 0.00000000000000 Ag (2a)
-0.89300000000000 0.00000000000000 0.50000000000000 Ag (2a)
0.87800000000000 0.50000000000000 0.00000000000000 Ag (2b)
-0.87800000000000 0.50000000000000 0.50000000000000 Ag (2b)
0.37900000000000 0.22500000000000 0.52200000000000 Ag (4e)
-0.37900000000000 -0.22500000000000 1.02200000000000 Ag (4e)
-0.37900000000000 -0.22500000000000 -0.02200000000000 Ag (4e)
0.37900000000000 -0.22500000000000 -0.52200000000000 Ag (4e)
0.20200000000000 0.27500000000000 0.02200000000000 Se (4e)
-0.20200000000000 -0.27500000000000 0.52200000000000 Se (4e)
-0.20200000000000 0.27500000000000 0.47800000000000 Se (4e)
0.20200000000000 -0.27500000000000 -0.02200000000000 Se (4e)

```

H<sub>3</sub>Cl (100 GPa): AB<sub>3</sub>\_oP16\_19\_a\_3a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'H3Cl'
_chemical_formula_sum 'Cl H3'

loop_
  _publ_author_name
'D. Duan'
'X. Huang'
'F. Tian'
'Y. Liu'
'Da Li'
'H. Yu'
'B. Liu'
'W. Tian'
'T. Cui'
_journal_name_full_name
;
Journal of Physical Chemistry A
;
_journal_volume 119
_journal_year 2015
_journal_page_first 11059
_journal_page_last 11065
_publ_section_title
;

```

```

Predicted Formation of HS3^{+} in Solid Halogen Polyhydrides at
   $\rightarrow$  High Pressures
;

_aflow_title 'HS3Cl (100-GPa) Structure'
_aflow_proto 'AB3_oP16_19_a_3a'
_aflow_params 'a,b/a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4}'
   $\rightarrow$  )
_aflow_params_values '5.668,0.758997882851,0.528757939308,0.584,0.123,
   $\rightarrow$  0.027,0.31,0.159,0.417,0.257,0.073,0.603,0.983,0.124,0.227'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP16'

_symmetry_space_group_name_H-M "P 21 21 21"
_symmetry_Int_Tables_number 19

_cell_length_a 5.66800
_cell_length_b 4.30200
_cell_length_c 2.99700
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z
3 -x,y+1/2,-z+1/2
4 -x+1/2,-y,z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Cl1 Cl 4 a 0.58400 0.12300 0.02700 1.00000
H1 H 4 a 0.31000 0.15900 0.41700 1.00000
H2 H 4 a 0.25700 0.07300 0.60300 1.00000
H3 H 4 a 0.98300 0.12400 0.22700 1.00000

```

H<sub>3</sub>Cl (100 GPa): AB<sub>3</sub>\_oP16\_19\_a\_3a - POSCAR

```

AB3_oP16_19_a_3a & a,b/a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4 --
   $\rightarrow$  params=5.668,0.758997882851,0.528757939308,0.584,0.123,0.027,
   $\rightarrow$  0.31,0.159,0.417,0.257,0.073,0.603,0.983,0.124,0.227 & P2_{1}2_{1}2_{1}
   $\rightarrow$  {1}2_{1} D_{2}^{2} #19 (a^4) & oP16 & None & H3Cl & H3Cl & D.
   $\rightarrow$  Duan et al., J. Phys. Chem. A 119, 11059-11065 (2015)
1.0000000000000000
5.66800000000000 0.00000000000000 0.00000000000000
0.00000000000000 4.30200000000000 0.00000000000000
0.00000000000000 0.00000000000000 2.99700000000000
Cl H
4 12
Direct
0.58400000000000 0.12300000000000 0.02700000000000 Cl (4a)
-0.08400000000000 -0.12300000000000 0.52700000000000 Cl (4a)
-0.58400000000000 0.62300000000000 0.47300000000000 Cl (4a)
1.08400000000000 0.37700000000000 -0.02700000000000 Cl (4a)
0.31000000000000 0.15900000000000 0.41700000000000 H (4a)
0.19000000000000 -0.15900000000000 0.91700000000000 H (4a)
-0.31000000000000 0.65900000000000 0.08300000000000 H (4a)
0.81000000000000 0.34100000000000 -0.41700000000000 H (4a)
0.25700000000000 0.07300000000000 0.60300000000000 H (4a)
0.24300000000000 -0.07300000000000 1.10300000000000 H (4a)
-0.25700000000000 0.57300000000000 -0.10300000000000 H (4a)
0.75700000000000 0.42700000000000 -0.60300000000000 H (4a)
0.98300000000000 0.12400000000000 0.22700000000000 H (4a)
-0.48300000000000 -0.12400000000000 0.72700000000000 H (4a)
-0.98300000000000 0.62400000000000 0.27300000000000 H (4a)
1.48300000000000 0.37600000000000 -0.22700000000000 H (4a)

```

Ta<sub>2</sub>H: AB<sub>2</sub>\_oC6\_21\_a\_k - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ta2H'
_chemical_formula_sum 'H Ta2'

loop_
  _publ_author_name
'H. Asano'
'Y. Ishikawa'
'M. Hirabayashi'
_journal_name_full_name
;
Journal of Applied Crystallography
;
_journal_volume 11
_journal_year 1978
_journal_page_first 681
_journal_page_last 683
_publ_section_title
;
Single-crystal X-ray diffraction study on the hydrogen ordering in Ta$_{2}$H
   $\rightarrow$  {2}$H
;

```

# Found in Pearson's Crystal Data - Crystal Structure Database for  
↳ Inorganic Compounds, 2013

\_aflow\_title 'TaS<sub>2</sub>(2)SH Structure'  
\_aflow\_proto 'AB<sub>2</sub>oC6\_21\_a\_k'  
\_aflow\_params 'a,b/a,c/a,z<sub>2</sub>{2}'  
\_aflow\_params\_values '3.3982513,1.3943496174,1.40170688639,0.268'  
\_aflow\_Strukturbericht 'None'  
\_aflow\_Pearson 'oC6'

\_cell\_length\_a 3.3982513000  
\_cell\_length\_b 4.7383504000  
\_cell\_length\_c 4.7633522489  
\_cell\_angle\_alpha 90.0000000000  
\_cell\_angle\_beta 90.0000000000  
\_cell\_angle\_gamma 90.0000000000

\_symmetry\_space\_group\_name\_H-M "C 2 2 2"  
\_symmetry\_Int\_Tables\_number 21

loop\_  
\_space\_group\_symop\_id  
\_space\_group\_symop\_operation\_xyz  
1 x,y,z  
2 x,-y,-z  
3 -x,y,-z  
4 -x,-y,z  
5 x+1/2,y+1/2,z  
6 x+1/2,-y+1/2,-z  
7 -x+1/2,y+1/2,-z  
8 -x+1/2,-y+1/2,z

loop\_  
\_atom\_site\_label  
\_atom\_site\_type\_symbol  
\_atom\_site\_symmetry\_multiplicity  
\_atom\_site\_Wyckoff\_label  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z  
\_atom\_site\_occupancy  
H1 H 2 a 0.00000 0.00000 0.00000 1.00000  
Ta1 Ta 4 k 0.25000 0.25000 0.26800 1.00000

Ta<sub>2</sub>H: AB<sub>2</sub>oC6\_21\_a\_k - POSCAR

AB<sub>2</sub>oC6\_21\_a\_k & a,b/a,c/a,z<sub>2</sub> --params=3.3982513,1.3943496174,  
↳ 1.40170688639,0.268 & C222 D<sub>2</sub>{2}<sup>6</sup> #21 (ak) & oC6 & None &  
↳ Ta<sub>2</sub>H & H. Asano and Y. Ishikawa and M. Hirabayashi, J. Appl.  
↳ Crystallogr. 11, 681-683 (1978)  
1.0000000000000000  
1.69912565000000 -2.36917520000000 0.00000000000000  
1.69912565000000 2.36917520000000 0.00000000000000  
0.00000000000000 0.00000000000000 4.76335224890000  
H Ta  
1 2  
Direct  
0.00000000000000 0.00000000000000 0.00000000000000 H (2a)  
0.00000000000000 0.50000000000000 0.26800000000000 Ta (4k)  
0.50000000000000 0.00000000000000 -0.26800000000000 Ta (4k)

CeRu<sub>2</sub>B<sub>2</sub>: A2BC2\_oF40\_22\_fi\_ad\_gh - CIF

# CIF file  
data\_findsym-output  
\_audit\_creation\_method FINDSYM  
\_chemical\_name\_mineral 'CeRu<sub>2</sub>B<sub>2</sub>'  
\_chemical\_formula\_sum 'B2 Ce Ru2'

loop\_  
\_publ\_author\_name  
'P. Rogl'  
\_journal\_name\_full\_name  
; Journal of the Less-Common Metals  
;  
\_journal\_volume 110  
\_journal\_year 1985  
\_journal\_page\_first 283  
\_journal\_page\_last 294  
\_publ\_section\_title  
; Structural chemistry and phase equilibria of ternary rare  
↳ earth-platinum metal borides  
;

# Found in Pearson's Crystal Data - Crystal Structure Database for  
↳ Inorganic Compounds, 2013

\_aflow\_title 'CeRu<sub>2</sub>(2)SB<sub>2</sub>(2)S Structure'  
\_aflow\_proto 'A2BC2\_oF40\_22\_fi\_ad\_gh'  
\_aflow\_params 'a,b/a,c/a,y<sub>3</sub>,z<sub>4</sub>{4},z<sub>5</sub>{5},y<sub>6</sub>{6}'  
\_aflow\_params\_values '6.4793068924,1.3977127159,1.54737394473,0.3134,  
↳ 0.3627,0.1144,0.0719'  
\_aflow\_Strukturbericht 'None'  
\_aflow\_Pearson 'oF40'

\_cell\_length\_a 6.4793068924  
\_cell\_length\_b 9.0562096337  
\_cell\_length\_c 10.0259106652  
\_cell\_angle\_alpha 90.0000000000  
\_cell\_angle\_beta 90.0000000000  
\_cell\_angle\_gamma 90.0000000000

\_symmetry\_space\_group\_name\_H-M "F 2 2 2"  
\_symmetry\_Int\_Tables\_number 22

loop\_  
\_space\_group\_symop\_id  
\_space\_group\_symop\_operation\_xyz  
1 x,y,z  
2 x,-y,-z  
3 -x,y,-z  
4 -x,-y,z  
5 x,y+1/2,z+1/2  
6 x,-y+1/2,-z+1/2  
7 -x,y+1/2,-z+1/2  
8 -x,-y+1/2,z+1/2  
9 x+1/2,y,z+1/2  
10 x+1/2,-y,-z+1/2  
11 -x+1/2,y,-z+1/2  
12 -x+1/2,-y,z+1/2  
13 x+1/2,y+1/2,z  
14 x+1/2,-y+1/2,-z  
15 -x+1/2,y+1/2,-z  
16 -x+1/2,-y+1/2,z

loop\_  
\_atom\_site\_label  
\_atom\_site\_type\_symbol  
\_atom\_site\_symmetry\_multiplicity  
\_atom\_site\_Wyckoff\_label  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z  
\_atom\_site\_occupancy  
Ce1 Ce 4 a 0.00000 0.00000 0.00000 1.00000  
Ce2 Ce 4 d 0.25000 0.25000 0.75000 1.00000  
B1 B 8 f 0.00000 0.31340 0.00000 1.00000  
Ru1 Ru 8 g 0.00000 0.00000 0.36270 1.00000  
Ru2 Ru 8 h 0.25000 0.25000 0.11440 1.00000  
B2 B 8 i 0.25000 0.07190 0.25000 1.00000

CeRu<sub>2</sub>B<sub>2</sub>: A2BC2\_oF40\_22\_fi\_ad\_gh - POSCAR

A2BC2\_oF40\_22\_fi\_ad\_gh & a,b/a,c/a,y<sub>3</sub>,z<sub>4</sub>,z<sub>5</sub>,y<sub>6</sub> --params=6.4793068924,  
↳ 1.3977127159,1.54737394473,0.3134,0.3627,0.1144,0.0719 & F222  
↳ D<sub>2</sub>{2}<sup>7</sup> #22 (adfgih) & oF40 & None & CeRu<sub>2</sub>B<sub>2</sub> & P. Rogl, J.  
↳ Less-Common Met. 110, 283-294 (1985)  
1.0000000000000000  
0.0000000000000000 4.52810481685000 5.01295533260000  
3.23965344620000 0.00000000000000 5.01295533260000  
3.23965344620000 4.52810481685000 0.00000000000000  
B Ce Ru  
4 2 4  
Direct  
0.31340000000000 -0.31340000000000 0.31340000000000 B (8f)  
-0.31340000000000 0.31340000000000 -0.31340000000000 B (8f)  
0.07190000000000 0.42810000000000 0.07190000000000 B (8i)  
0.42810000000000 0.07190000000000 0.42810000000000 B (8i)  
0.00000000000000 0.00000000000000 0.00000000000000 Ce (4a)  
0.75000000000000 0.75000000000000 0.75000000000000 Ce (4d)  
0.36270000000000 0.36270000000000 -0.36270000000000 Ru (8g)  
-0.36270000000000 -0.36270000000000 0.36270000000000 Ru (8g)  
0.11440000000000 0.11440000000000 0.38560000000000 Ru (8h)  
0.38560000000000 0.38560000000000 0.11440000000000 Ru (8h)

FeS (Low-temperature): AB\_oF8\_22\_a\_c - CIF

# CIF file  
data\_findsym-output  
\_audit\_creation\_method FINDSYM

\_chemical\_name\_mineral 'FeS'  
\_chemical\_formula\_sum 'Fe S'

loop\_  
\_publ\_author\_name  
'M. Wintenberger'  
'B. Srouf'  
'C. Meyer'  
'F. Hartmannboutron'  
'Y. Gros'  
'J. L. Buevoz'  
\_journal\_name\_full\_name  
; Acta Crystallographica Section A: Foundations and Advances  
;  
\_journal\_volume 34  
\_journal\_year 1978  
\_journal\_page\_first S318  
\_journal\_page\_last S318  
\_publ\_section\_title

↳ First order transitions and magnetic-structure of zinblende-type iron  
↳ sulfide

# Found in Pearson's Crystal Data - Crystal Structure Database for  
↳ Inorganic Compounds, 2013

\_aflow\_title 'FeS (Low-temperature) Structure'  
\_aflow\_proto 'AB\_oF8\_22\_a\_c'  
\_aflow\_params 'a,b/a,c/a'  
\_aflow\_params\_values '5.5400291632,0.990433212996,0.937725631773'  
\_aflow\_Strukturbericht 'None'  
\_aflow\_Pearson 'oF8'

\_cell\_length\_a 5.5400291632

```

_cell_length_b 5.4870288842
_cell_length_c 5.1950273471
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "F 2 2 2"
_symmetry_Int_Tables_number 22

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y, -z
4 -x, -y, z
5 x, y+1/2, z+1/2
6 x, -y+1/2, -z+1/2
7 -x, y+1/2, -z+1/2
8 -x, -y+1/2, z+1/2
9 x+1/2, y, z+1/2
10 x+1/2, -y, -z+1/2
11 -x+1/2, y, -z+1/2
12 -x+1/2, -y, z+1/2
13 x+1/2, y+1/2, z
14 x+1/2, -y+1/2, -z
15 -x+1/2, y+1/2, -z
16 -x+1/2, -y+1/2, z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Fe1 Fe 4 a 0.00000 0.00000 0.00000 1.00000
S1 S 4 c 0.25000 0.25000 0.25000 1.00000

```

FeS (Low-temperature): AB\_oF8\_22\_a\_c - POSCAR

```

AB_oF8_22_a_c & a, b/a, c/a --params=5.5400291632, 0.990433212996,
↪ 0.937725631773 & F222 D_{2}^{17} #22 (ac) & oF8 & None & FeS &
↪ & M. Wintenberger et al., Acta Crystallogr. Sect. A 34,
↪ S318-S318 (1978)
1.0000000000000000
0.0000000000000000 2.74351444210000 2.59751367355000
2.77001458160000 0.0000000000000000 2.59751367355000
2.77001458160000 2.74351444210000 0.0000000000000000
Fe S
1 1
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 Fe (4a)
0.2500000000000000 0.2500000000000000 0.2500000000000000 S (4c)

```

H<sub>3</sub>S (5 GPa): A3B\_oI32\_23\_ij2k\_k - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'H3S'
_chemical_formula_sum 'H3 S'

loop_
_publ_author_name
'T. A. Strobel'
'P. Ganesh'
'M. Somayazulu'
'P. R. C. Kent'
'R. J. Hemley'
_journal_name_full_name
;
Physical Review Letters
;
_journal_volume 107
_journal_year 2011
_journal_page_first 255503
_journal_page_last 255503
_publ_section_title
;
Novel Cooperative Interactions and Structural Ordering in HS_{2}SS-HS_{2}S
↪ 2)S
;

_aflow_title 'HS_{3}SS (5-GPa) Structure'
_aflow_proto 'A3B_oI32_23_ij2k_k'
_aflow_params 'a, b/a, c/a, z_{1}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}
↪ , x_{5}, y_{5}, z_{5}'
↪ 0.8216, 0.36488'
_aflow_Structurbericht 'None'
_aflow_Pearson 'oI32'

_symmetry_space_group_name_H-M "I 2 2 2"
_symmetry_Int_Tables_number 23

_cell_length_a 5.82463
_cell_length_b 7.24404
_cell_length_c 7.70331
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000

```

```

_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y, -z
4 -x, -y, z
5 x+1/2, y+1/2, z+1/2
6 x+1/2, -y+1/2, -z+1/2
7 -x+1/2, y+1/2, -z+1/2
8 -x+1/2, -y+1/2, z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 i 0.00000 0.00000 0.04851 1.00000
H2 H 4 j 0.00000 0.50000 0.45153 1.00000
H3 H 8 k 0.75475 0.49255 0.20405 1.00000
H4 H 8 k 0.44210 0.23223 0.28616 1.00000
S1 S 8 k 0.76005 0.82160 0.36488 1.00000

```

H<sub>3</sub>S (5 GPa): A3B\_oI32\_23\_ij2k\_k - POSCAR

```

A3B_oI32_23_ij2k_k & a, b/a, c/a, z1, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5 --params
↪ =5.82463, 1.24369101557, 1.32254065924, 0.04851, 0.45153, 0.75475,
↪ 0.49255, 0.20405, 0.4421, 0.23223, 0.28616, 0.76005, 0.8216, 0.36488 &
↪ I222 D_{2}^{17} #23 (ijk^3) & oI32 & None & H3S & H3S & T. A.
↪ Strobel et al., Phys. Rev. Lett. 107, 255503 (2011)
1.0000000000000000
-2.9123150000000000 3.6220200000000000 3.8516550000000000
2.9123150000000000 -3.6220200000000000 3.8516550000000000
2.9123150000000000 3.6220200000000000 -3.8516550000000000
H S
12 4
Direct
0.0485100000000000 0.0485100000000000 0.0000000000000000 H (4i)
-0.0485100000000000 -0.0485100000000000 0.0000000000000000 H (4i)
0.9515300000000000 0.4515300000000000 0.5000000000000000 H (4j)
0.0484700000000000 -0.4515300000000000 0.5000000000000000 H (4j)
0.6966000000000000 0.9588000000000000 1.2473000000000000 H (8k)
-0.2885000000000000 -0.5507000000000000 -1.2473000000000000 H (8k)
0.2885000000000000 -0.9588000000000000 -0.2622000000000000 H (8k)
-0.6966000000000000 0.5507000000000000 0.2622000000000000 H (8k)
0.5183900000000000 0.7282600000000000 0.6743300000000000 H (8k)
0.0539300000000000 -0.1559400000000000 -0.6743300000000000 H (8k)
-0.0539300000000000 -0.7282600000000000 -0.2098700000000000 H (8k)
-0.5183900000000000 0.1559400000000000 0.2098700000000000 H (8k)
1.1864800000000000 1.1249300000000000 1.5816500000000000 S (8k)
-0.4567200000000000 -0.3951700000000000 -1.5816500000000000 S (8k)
0.4567200000000000 -1.1249300000000000 0.0615500000000000 S (8k)
-1.1864800000000000 0.3951700000000000 -0.0615500000000000 S (8k)

```

Stannoidite (Cu<sub>8</sub>(Fe,Zn)<sub>3</sub>Sn<sub>2</sub>S<sub>12</sub>): A8B2C12D2E\_oI50\_23\_bcfk\_i\_3k\_j\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Stannoidite'
_chemical_formula_sum 'Cu8 Fe2 S12 Sn2 Zn'

loop_
_publ_author_name
'Y. Kudoh'
'Y. Tak\{e\}uchi'
_journal_name_full_name
;
Zeitschrift f{\u}r Kristallographie - Crystalline Materials
;
_journal_volume 144
_journal_year 1976
_journal_page_first 145
_journal_page_last 160
_publ_section_title
;
The superstructure of stannoidite

_aflow_title 'Stannoidite (Cu_{8})(Fe,Zn)_{3}Sn_{2}S_{12}S_{12})
↪ Structure'
_aflow_proto 'A8B2C12D2E_oI50_23_bcfk_i_3k_j_a'
_aflow_params 'a, b/a, c/a, x_{4}, z_{5}, z_{6}, z_{7}, y_{7}, z_{7}, x_{8}, y_{8}
↪ , z_{8}, x_{9}, y_{9}, z_{9}, x_{10}, y_{10}, z_{10}'
↪ 0.1693, 0.2465, 0.0107, 0.1695, 0.1308, 0.2443, 0.0826, 0.3792, 0.7558,
↪ 0.0801, 0.1294, 0.7488, 0.2546'
_aflow_Structurbericht 'None'
_aflow_Pearson 'oI50'

_symmetry_space_group_name_H-M "I 2 2 2"
_symmetry_Int_Tables_number 23

_cell_length_a 10.76700
_cell_length_b 5.41100
_cell_length_c 16.11800
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000

```

```

_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 x+1/2,y+1/2,z+1/2
6 x+1/2,-y+1/2,-z+1/2
7 -x+1/2,y+1/2,-z+1/2
8 -x+1/2,-y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Zn1 Zn 2 a 0.00000 0.00000 1.00000
Cu1 Cu 2 b 0.50000 0.00000 0.00000 1.00000
Cu2 Cu 2 c 0.00000 0.00000 0.50000 1.00000
Cu3 Cu 4 f 0.25110 0.00000 0.50000 1.00000
Fe1 Fe 4 i 0.00000 0.00000 0.32980 1.00000
Sn1 Sn 4 j 0.00000 0.50000 0.16930 1.00000
Cu4 Cu 8 k 0.24650 0.01070 0.16950 1.00000
S1 S 8 k 0.13080 0.24430 0.08260 1.00000
S2 S 8 k 0.37920 0.75580 0.08010 1.00000
S3 S 8 k 0.12940 0.74880 0.25460 1.00000

```

Stannoidite (Cu<sub>8</sub>(Fe,Zn)<sub>3</sub>Sn<sub>2</sub>S<sub>12</sub>): A8B2C12D2E\_oI50\_23\_bcfk\_i\_3k\_j\_a - POSCAR

```

A8B2C12D2E_oI50_23_bcfk_i_3k_j_a & a, b/a, c/a, x4, z5, z6, x7, y7, z7, x8, y8, z8,
↪ x9, y9, z9, x10, y10, z10 --params=10.767, 0.502554100492,
↪ 1.4969815176, 0.2511, 0.3298, 0.1693, 0.2465, 0.0107, 0.1695, 0.1308,
↪ 0.2443, 0.0826, 0.3792, 0.7558, 0.0801, 0.1294, 0.7488, 0.2546 & 1222
↪ D_{2}^{18} #23 (abcfijk^4) & oI50 & None & Cu8(Fe,Zn)3Sn2S12 &
↪ Stannoidite & Y. Kudoh and Y. Tak\{e\}uchi, Zeitschrift f\{u\}r
↪ Kristallographie - Crystalline Materials 144, 145-160 (1976)
1.0000000000000000
-5.3835000000000000 2.7055000000000000 8.0590000000000000
5.3835000000000000 -2.7055000000000000 8.0590000000000000
5.3835000000000000 2.7055000000000000 -8.0590000000000000
Cu Fe S Sn Zn
8 2 12 2 1
Direct
0.0000000000000000 0.5000000000000000 0.5000000000000000 Cu (2b)
0.5000000000000000 0.5000000000000000 0.0000000000000000 Cu (2c)
0.5000000000000000 0.7511000000000000 0.2511000000000000 Cu (4f)
0.5000000000000000 0.2489000000000000 -0.2511000000000000 Cu (4f)
0.1802000000000000 0.4160000000000000 0.2572000000000000 Cu (8k)
0.1588000000000000 -0.0770000000000000 -0.2572000000000000 Cu (8k)
-0.1588000000000000 -0.4160000000000000 -0.2358000000000000 Cu (8k)
-0.1802000000000000 0.0770000000000000 0.2358000000000000 Cu (8k)
0.3298000000000000 0.3298000000000000 0.0000000000000000 Fe (4i)
-0.3298000000000000 -0.3298000000000000 0.0000000000000000 Fe (4i)
0.3269000000000000 0.2134000000000000 0.3751000000000000 S (8k)
-0.1617000000000000 -0.0482000000000000 -0.3751000000000000 S (8k)
0.1617000000000000 -0.2134000000000000 0.1135000000000000 S (8k)
-0.3269000000000000 0.0482000000000000 -0.1135000000000000 S (8k)
0.8359000000000000 0.4593000000000000 1.1350000000000000 S (8k)
-0.6757000000000000 -0.2991000000000000 -1.1350000000000000 S (8k)
0.6757000000000000 -0.4593000000000000 0.3766000000000000 S (8k)
-0.8359000000000000 0.2991000000000000 -0.3766000000000000 S (8k)
1.0034000000000000 0.3840000000000000 0.8782000000000000 S (8k)
-0.4942000000000000 0.1252000000000000 -0.8782000000000000 S (8k)
0.4942000000000000 -0.3840000000000000 0.6194000000000000 S (8k)
-1.0034000000000000 -0.1252000000000000 -0.6194000000000000 S (8k)
0.6693000000000000 0.1693000000000000 0.5000000000000000 Sn (4j)
0.3307000000000000 -0.1693000000000000 0.5000000000000000 Sn (4j)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Zn (2a)

```

NaFeS<sub>2</sub>: ABC2\_oI16\_23\_ab\_i\_k - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'NaFeS2'
_chemical_formula_sum 'Fe Na S2'

loop_
_publ_author_name
'H. Boller'
'H. Blaha'
_journal_name_full_name
;
Monatshefte f\{u\}r Chemie - Chemical Monthly
;
_journal_volume 114
_journal_year 1983
_journal_page_first 145
_journal_page_last 154
_publ_section_title
;
Zur Kenntnis des Natriumthioferates (III)
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

```

```

_aflow_title 'NaFeS_{2}$ Structure '
_aflow_proto 'ABC2_oI16_23_ab_i_k'
_aflow_params 'a, b/a, c/a, z_{3}, x_{4}, y_{4}, z_{4}'
_aflow_params_values '5.3999384419, 1.15740740741, 2.00555555555, 0.28, 0.25,
↪ 0.2, 0.115'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oI16'

_cell_length_a 5.3999384419
_cell_length_b 6.2499287522
_cell_length_c 10.8298765418
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'I 2 2 2'
_symmetry_Int_Tables_number 23

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 x+1/2,y+1/2,z+1/2
6 x+1/2,-y+1/2,-z+1/2
7 -x+1/2,y+1/2,-z+1/2
8 -x+1/2,-y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Fe1 Fe 2 a 0.00000 0.00000 0.00000 1.00000
Fe2 Fe 2 b 0.50000 0.00000 0.00000 1.00000
Na1 Na 4 i 0.00000 0.00000 0.28000 1.00000
S1 S 8 k 0.25000 0.20000 0.11500 1.00000

```

NaFeS<sub>2</sub>: ABC2\_oI16\_23\_ab\_i\_k - POSCAR

```

ABC2_oI16_23_ab_i_k & a, b/a, c/a, z3, x4, y4, z4 --params=5.3999384419,
↪ 1.15740740741, 2.00555555555, 0.28, 0.25, 0.2, 0.115 & 1222 D_{2}^{18}
↪ #23 (abik) & oI16 & None & NaFeS2 & H. Boller and H. Blaha
↪ , Monatsh. Chem. 114, 145-154 (1983)
1.0000000000000000
-2.69996922095000 3.12496437610000 5.41493827090000
2.69996922095000 -3.12496437610000 5.41493827090000
2.69996922095000 3.12496437610000 -5.41493827090000
Fe Na S
2 2 4
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 Fe (2a)
0.0000000000000000 0.5000000000000000 0.5000000000000000 Fe (2b)
0.2800000000000000 0.2800000000000000 0.0000000000000000 Na (4i)
-0.2800000000000000 -0.2800000000000000 0.0000000000000000 Na (4i)
0.3150000000000000 0.3650000000000000 0.4500000000000000 S (8k)
-0.0850000000000000 -0.1350000000000000 -0.4500000000000000 S (8k)
0.0850000000000000 -0.3650000000000000 -0.0500000000000000 S (8k)
-0.3150000000000000 0.1350000000000000 0.0500000000000000 S (8k)

```

BPS<sub>4</sub>: ABC4\_oI12\_23\_a\_b\_k - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'BPS4'
_chemical_formula_sum 'B P S4'

loop_
_publ_author_name
'A. Weiss'
'H. Sch\{a\}fer'
_journal_name_full_name
;
Zeitschrift f\{u\}r Naturforschung B
;
_journal_volume 18
_journal_year 1963
_journal_page_first 81
_journal_page_last 82
_publ_section_title
;
Zur Kenntnis von Bortetrathiofosphat BPS_{4}$
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'BPS_{4}$ Structure '
_aflow_proto 'ABC4_oI12_23_a_b_k'
_aflow_params 'a, b/a, c/a, x_{3}, y_{3}, z_{3}'
_aflow_params_values '5.2501580231, 1.06666666665, 1.7219047619, 0.21, 0.2,
↪ 0.115'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oI12'

_cell_length_a 5.2501580231
_cell_length_b 5.6001685579

```



```

_cell_length_c 9.0402721007
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 2 2 2"
_symmetry_Int_Tables_number 23

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 x+1/2,y+1/2,z+1/2
6 x+1/2,-y+1/2,-z+1/2
7 -x+1/2,y+1/2,-z+1/2
8 -x+1/2,-y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
B1 B 2 a 0.00000 0.00000 0.00000 1.00000
P1 P 2 b 0.50000 0.00000 0.00000 1.00000
S1 S 8 k 0.21000 0.20000 0.11500 1.00000

```

BPS4: ABC4\_oI12\_23\_a\_b\_k - POSCAR

```

ABC4_oI12_23_a_b_k & a,b/a,c/a,x3,y3,z3 --params=5.2501580231,
↪ 1.06666666665,1.7219047619,0.21,0.2,0.115 & I222 D_{2}^{14} #23
↪ (abk) & oI12 & None & BPS4 & A. Weiss and H. Sch{\a}fer, Z.
↪ Naturforsch. B 18, 81-82 (1963)
1.0000000000000000
-2.62507901155000 2.80008427895000 4.52013605035000
2.62507901155000 -2.80008427895000 4.52013605035000
2.62507901155000 2.80008427895000 -4.52013605035000
B P S
1 1 4
Direct
0.00000000000000 0.00000000000000 0.00000000000000 B (2a)
0.00000000000000 0.50000000000000 0.50000000000000 P (2b)
0.31500000000000 0.32500000000000 0.41000000000000 S (8k)
-0.08500000000000 -0.09500000000000 -0.41000000000000 S (8k)
0.08500000000000 -0.32500000000000 -0.01000000000000 S (8k)
-0.31500000000000 0.09500000000000 0.01000000000000 S (8k)

```

Weberite (Na<sub>2</sub>MgAlF<sub>7</sub>): AB7CD2\_oI44\_24\_a\_b3d\_c\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Na2MgAlF7'
_chemical_formula_sum 'Al F7 Mg Na2'

loop_
_publ_author_name
'O. Knop'
'T. S. Cameron'
'K. Jochem'
_journal_name_full_name
;
Journal of Solid State Chemistry
;
_journal_volume 43
_journal_year 1982
_journal_page_first 213
_journal_page_last 221
_publ_section_title
;
What is the true space group of weberite?
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'Weberite (NaS_{2}SMgAlF_{7})$ Structure'
_aflow_proto 'AB7CD2_oI44_24_a_b3d_c_c'
_aflow_params 'a,b/a,c/a,x_{1},x_{2},y_{3},z_{4},z_{5},x_{6},y_{6},z_{6}
↪ ,x_{7},y_{7},z_{7},x_{8},y_{8},z_{8}'
_aflow_params_values '7.0501914381,1.035035461,1.41546099291,0.7511,
↪ 0.2496,0.1361,-0.0003,0.5002,0.7501,0.2213,0.3356,0.5662,0.0681
↪ ,0.1362,-0.0648,0.0709,0.1385'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oI44'

_cell_length_a 7.0501914381
_cell_length_b 7.2971981453
_cell_length_c 9.9792709732
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 21 21 21"
_symmetry_Int_Tables_number 24

loop_
_space_group_symop_id

```

```

_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z+1/2
3 -x+1/2,y,-z
4 -x,-y+1/2,z
5 x+1/2,y+1/2,z+1/2
6 x+1/2,-y+1/2,-z
7 -x,y+1/2,-z+1/2
8 -x+1/2,-y,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 4 a 0.75110 0.00000 0.25000 1.00000
Na1 Na 4 a 0.24960 0.00000 0.25000 1.00000
F1 F 4 b 0.25000 0.13610 0.00000 1.00000
Mg1 Mg 4 c 0.00000 0.25000 -0.00030 1.00000
Na2 Na 4 c 0.00000 0.25000 0.50020 1.00000
F2 F 8 d 0.75010 0.22130 0.33560 1.00000
F3 F 8 d 0.56620 0.06810 0.13620 1.00000
F4 F 8 d -0.06480 0.07090 0.13850 1.00000

```

Weberite (Na<sub>2</sub>MgAlF<sub>7</sub>): AB7CD2\_oI44\_24\_a\_b3d\_c\_c - POSCAR

```

AB7CD2_oI44_24_a_b3d_c_c & a,b/a,c/a,x1,x2,y3,z4,z5,x6,y6,z6,x7,y7,z7,
↪ x8,y8,z8 --params=7.0501914381,1.035035461,1.41546099291,0.7511
↪ ,0.2496,0.1361,-0.0003,0.5002,0.7501,0.2213,0.3356,0.5662,
↪ 0.0681,0.1362,-0.0648,0.0709,0.1385 & I2_{1}2_{1}2_{1} D_{2}^{14} #19
↪ #24 (a^2bc^2d^3) & oI44 & None & Na2MgAlF7 & O. Knop and
↪ T. S. Cameron and K. Jochem, J. Solid State Chem. 43, 213-221 (
↪ 1982)
1.0000000000000000 3.64859907265000 4.98963548660000
-3.52509571905000 3.64859907265000 4.98963548660000
3.52509571905000 -3.64859907265000 4.98963548660000
3.52509571905000 3.64859907265000 -4.98963548660000
Al F Mg Na
2 14 2 4
Direct
0.25000000000000 1.00110000000000 0.75110000000000 Al (4a)
0.75000000000000 -0.50110000000000 -0.25110000000000 Al (4a)
0.13610000000000 0.25000000000000 0.38610000000000 F (4b)
0.36390000000000 0.75000000000000 0.11390000000000 F (4b)
0.55690000000000 1.08570000000000 0.97140000000000 F (8d)
0.61430000000000 -0.41450000000000 -0.47140000000000 F (8d)
-0.11430000000000 -0.58570000000000 -0.02880000000000 F (8d)
-0.05690000000000 0.91450000000000 0.52880000000000 F (8d)
0.20430000000000 0.70240000000000 0.63430000000000 F (8d)
0.56810000000000 -0.43000000000000 -0.13430000000000 F (8d)
-0.06810000000000 -0.20240000000000 0.00190000000000 F (8d)
0.29570000000000 0.93000000000000 0.49810000000000 F (8d)
0.20940000000000 0.07370000000000 0.00610000000000 F (8d)
0.56760000000000 0.20330000000000 0.49390000000000 F (8d)
-0.06760000000000 0.42630000000000 0.63570000000000 F (8d)
0.29060000000000 0.29670000000000 -0.13570000000000 F (8d)
0.24970000000000 -0.00030000000000 0.25000000000000 Mg (4c)
0.25030000000000 0.50030000000000 0.75000000000000 Mg (4c)
0.25000000000000 0.49960000000000 0.24960000000000 Na (4a)
0.75000000000000 0.00040000000000 0.25040000000000 Na (4a)
0.75020000000000 0.50020000000000 0.25000000000000 Na (4c)
-0.25020000000000 -0.00020000000000 0.75000000000000 Na (4c)

```

H<sub>2</sub>S (70 GPa): A2B\_oP12\_26\_abc\_ab - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'H2S'
_chemical_formula_sum 'H2 S'

loop_
_publ_author_name
'Y. Li'
'J. Hao'
'H. Liu'
'Y. Li'
'Y. Ma'
_journal_name_full_name
;
Journal of Chemical Physics
;
_journal_volume 140
_journal_year 2014
_journal_page_first 174712
_journal_page_last 174712
_publ_section_title
;
The metallization and superconductivity of dense hydrogen sulfide

_aflow_title 'HS_{2}SS (70-GPa) Structure'
_aflow_proto 'A2B_oP12_26_abc_ab'
_aflow_params 'a,b/a,c/a,y_{1},y_{2},z_{2},y_{3},z_{3},y_{4},z_{4}
↪ ,x_{5},y_{5},z_{5}'
_aflow_params_values '4.6806,0.627034995513,1.05710806307,0.455,0.858,
↪ 0.179,0.623,0.048,0.545,0.375,0.355,0.751,0.119,0.213'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP12'

```

```

_symmetry_space_group_name_H-M "P m c 21"
_symmetry_Int_Tables_number 26

_cell_length_a 4.68060
_cell_length_b 2.93490
_cell_length_c 4.94790
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z+1/2
3 -x,y,z
4 x,-y,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 2 a 0.00000 0.45500 0.85800 1.00000
S1 S 2 a 0.00000 0.17900 0.62300 1.00000
H2 H 2 b 0.50000 0.04800 0.54500 1.00000
S2 S 2 b 0.50000 0.37500 0.35500 1.00000
H3 H 4 c 0.75100 0.11900 0.21300 1.00000

```

H<sub>2</sub>S (70 GPa): A2B\_oP12\_26\_abc\_ab - POSCAR

```

A2B_oP12_26_abc_ab & a,b/a,c/a,y1,z1,y2,z2,y3,z3,y4,z4,x5,y5,z5 --params
↪ =4.6806,0.627034995513,1.05710806307,0.455,0.858,0.179,0.623,
↪ 0.048,0.545,0.375,0.355,0.751,0.119,0.213 & Pmc2_1 C_{2v}^{2}
↪ #26 (a^2b^2c) & oP12 & None & H2S & H2S & Y. Li et al., J.
↪ Chem. Phys. 140, 174712(2014)
1.0000000000000000
4.680600000000000 0.000000000000000 0.000000000000000
0.000000000000000 2.934900000000000 0.000000000000000
0.000000000000000 0.000000000000000 4.947900000000000
H S
8 4
Direct
0.000000000000000 0.455000000000000 0.858000000000000 H (2a)
0.000000000000000 -0.455000000000000 1.358000000000000 H (2a)
0.500000000000000 0.048000000000000 0.545000000000000 H (2b)
0.500000000000000 -0.048000000000000 1.045000000000000 H (2b)
0.751000000000000 0.119000000000000 0.213000000000000 H (4c)
-0.751000000000000 -0.119000000000000 0.713000000000000 H (4c)
0.751000000000000 -0.119000000000000 0.713000000000000 H (4c)
-0.751000000000000 0.119000000000000 0.213000000000000 H (4c)
0.000000000000000 0.179000000000000 0.623000000000000 S (2a)
0.000000000000000 -0.179000000000000 1.123000000000000 S (2a)
0.500000000000000 0.375000000000000 0.355000000000000 S (2b)
0.500000000000000 -0.375000000000000 0.855000000000000 S (2b)

```

β-SeO<sub>2</sub>: A2B\_oP12\_26\_abc\_ab - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'beta-SeO2'
_chemical_formula_sum 'O2 Se'

loop_
_publ_author_name
'D. Orosel'
'O. Leynaud'
'P. Balog'
'M. Jansen'
_journal_name_full_name
:
Journal of Solid State Chemistry
;
_journal_volume 177
_journal_year 2004
_journal_page_first 1631
_journal_page_last 1638
_publ_section_title
:
Pressure-temperature phase diagram of SeO_{2}$. Characterization of
↪ new phases
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title '$\beta$SeO_{2}$ Structure'
_aflow_proto 'A2B_oP12_26_abc_ab'
_aflow_params 'a,b/a,c/a,y_{1},z_{1},y_{2},z_{2},y_{3},z_{3},y_{4},z_{4},z_{4}
↪ ,x_{5},y_{5},z_{5}'
_aflow_params_values '5.0725824349,0.881353258932,1.48474034935,0.12,0.0
↪ ,0.2484,0.461,0.246,0.289,0.3781,0.0862,0.253,0.652,0.12'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP12'

_cell_length_a 5.0725824349
_cell_length_b 4.4707370602
_cell_length_c 7.5314678165
_cell_angle_alpha 90.0000000000

```

```

_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P m c 21"
_symmetry_Int_Tables_number 26

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z+1/2
3 -x,y,z
4 x,-y,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 2 a 0.00000 0.12000 0.00000 1.00000
Se1 Se 2 a 0.00000 0.24840 0.46100 1.00000
O2 O 2 b 0.50000 0.24600 0.28900 1.00000
Se2 Se 2 b 0.50000 0.37810 0.08620 1.00000
O3 O 4 c 0.25300 0.65200 0.12000 1.00000

```

β-SeO<sub>2</sub>: A2B\_oP12\_26\_abc\_ab - POSCAR

```

A2B_oP12_26_abc_ab & a,b/a,c/a,y1,z1,y2,z2,y3,z3,y4,z4,x5,y5,z5 --params
↪ =5.0725824349,0.881353258932,1.48474034935,0.12,0.0,0.2484,
↪ 0.461,0.246,0.289,0.3781,0.0862,0.253,0.652,0.12 & Pmc2_1 C_{
↪ 2v}^{2} #26 (a^2b^2c) & oP12 & None & SeO2 & beta & D. Orosel
↪ et al., J. Solid State Chem. 177, 1631-1638 (2004)
1.0000000000000000
5.072582434900000 0.000000000000000 0.000000000000000
0.000000000000000 4.470737060200000 0.000000000000000
0.000000000000000 0.000000000000000 7.531467816500000
O Se
8 4
Direct
0.000000000000000 0.120000000000000 0.000000000000000 O (2a)
0.000000000000000 -0.120000000000000 0.500000000000000 O (2a)
0.500000000000000 0.246000000000000 0.289000000000000 O (2b)
0.500000000000000 -0.246000000000000 0.789000000000000 O (2b)
0.253000000000000 0.652000000000000 0.120000000000000 O (4c)
-0.253000000000000 -0.652000000000000 0.620000000000000 O (4c)
0.253000000000000 0.652000000000000 0.120000000000000 O (4c)
-0.253000000000000 -0.652000000000000 0.620000000000000 O (4c)
0.000000000000000 0.248400000000000 0.461000000000000 Se (2a)
0.000000000000000 -0.248400000000000 0.961000000000000 Se (2a)
0.500000000000000 0.378100000000000 0.086200000000000 Se (2b)
0.500000000000000 -0.378100000000000 0.586200000000000 Se (2b)

```

TIP<sub>5</sub>: A5B\_oP24\_26\_3a3b2c\_ab - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'TIP5'
_chemical_formula_sum 'P5 Tl'

loop_
_publ_author_name
'O. Olofsson'
'J. Gullman'
_journal_name_full_name
:
Acta Chemica Scandinavica
;
_journal_volume 25
_journal_year 1971
_journal_page_first 1327
_journal_page_last 1337
_publ_section_title
:
The crystal structure of TIP5_{5}$
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'TIP5_{5}$ Structure'
_aflow_proto 'A5B_oP24_26_3a3b2c_ab'
_aflow_params 'a,b/a,c/a,y_{1},z_{1},y_{2},z_{2},y_{3},z_{3},y_{4},z_{4},z_{4}
↪ ,y_{5},z_{5},y_{6},z_{6},y_{7},z_{7},y_{8},z_{8},x_{9},y_{9},z_{9}
↪ ,x_{10},y_{10},z_{10}'
_aflow_params_values '6.465013742,1.07113689096,1.87440061873,0.1628,
↪ 0.2907,0.112,0.0,0.1452,0.8256,0.4859,0.1227,0.1146,0.0096,
↪ 0.249,0.0963,0.5436'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP24'

_cell_length_a 6.4650137420
_cell_length_b 6.9249147196
_cell_length_c 12.1180257581
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P m c 21"

```

```

_symmetry_Int_Tables_number 26

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 -x,-y,z+1/2
  3 -x,y,z
  4 x,-y,z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
P1 P 2 a 0.00000 0.16280 0.29070 1.00000
P2 P 2 a 0.00000 0.11200 0.00000 1.00000
P3 P 2 a 0.00000 0.14520 0.82560 1.00000
T11 Tl 2 a 0.00000 0.48590 0.12270 1.00000
P4 P 2 b 0.50000 0.11460 0.00960 1.00000
P5 P 2 b 0.50000 0.32860 0.13580 1.00000
P6 P 2 b 0.50000 0.15650 0.29050 1.00000
T12 Tl 2 b 0.50000 0.72140 0.28180 1.00000
P7 P 4 c 0.24890 0.28540 0.39470 1.00000
P8 P 4 c 0.24900 0.09630 0.54360 1.00000

```

TIPs: A5B\_oP24\_26\_3a3b2c\_ab - POSCAR

```

A5B_oP24_26_3a3b2c_ab & a,b/a,c/a,y1,z1,y2,z2,y3,z3,y4,z4,y5,z5,y6,z6,y7
↪ z7,y8,z8,x9,y9,z9,x10,y10,z10 --params=6.465013742,
↪ 1.07113689096,1.87440061873,0.1628,0.2907,0.112,0.0,0.1452,
↪ 0.8256,0.4859,0.1227,0.1146,0.0096,0.3286,0.1358,0.1565,0.2905,
↪ 0.7214,0.2818,0.2489,0.2854,0.3947,0.249,0.0963,0.5436 & Pmc2_1]
↪ C_{2v}^{[2]} #26 (a^4b^4c^2) & oP24 & None & TIP5 & O.
↪ Olafsson and J. Gullman, Acta Chem. Scand. 25, 1327-1337 (1971)
1.00000000000000
6.46501374200000 0.00000000000000 0.00000000000000
0.00000000000000 6.92491471960000 0.00000000000000
0.00000000000000 0.00000000000000 12.11802575810000
P Tl
20 4
Direct
0.00000000000000 0.16280000000000 0.29070000000000 P (2a)
0.00000000000000 -0.16280000000000 0.79070000000000 P (2a)
0.00000000000000 0.11200000000000 0.00000000000000 P (2a)
0.00000000000000 -0.11200000000000 0.50000000000000 P (2a)
0.00000000000000 0.14520000000000 0.82560000000000 P (2a)
0.00000000000000 -0.14520000000000 1.32560000000000 P (2a)
0.50000000000000 0.11460000000000 0.00960000000000 P (2b)
0.50000000000000 -0.11460000000000 0.50960000000000 P (2b)
0.50000000000000 0.32860000000000 0.13580000000000 P (2b)
0.50000000000000 -0.32860000000000 0.63580000000000 P (2b)
0.50000000000000 0.15650000000000 0.29050000000000 P (2b)
0.50000000000000 -0.15650000000000 0.79050000000000 P (2b)
0.24890000000000 0.28540000000000 0.39470000000000 P (4c)
-0.24890000000000 0.28540000000000 0.89470000000000 P (4c)
0.24890000000000 -0.28540000000000 0.89470000000000 P (4c)
-0.24890000000000 0.28540000000000 0.39470000000000 P (4c)
0.24900000000000 0.09630000000000 0.54360000000000 P (4c)
-0.24900000000000 -0.09630000000000 1.04360000000000 P (4c)
0.24900000000000 -0.09630000000000 1.04360000000000 P (4c)
-0.24900000000000 0.09630000000000 0.54360000000000 P (4c)
0.00000000000000 0.48590000000000 0.12270000000000 Tl (2a)
0.00000000000000 -0.48590000000000 0.62270000000000 Tl (2a)
0.50000000000000 0.72140000000000 0.28180000000000 Tl (2b)
0.50000000000000 -0.72140000000000 0.78180000000000 Tl (2b)

```

Ca<sub>4</sub>Al<sub>6</sub>O<sub>16</sub>S: A6B4C16D\_oP108\_27\_abcd4e\_4e\_16e\_e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ca4Al6O16S'
_chemical_formula_sum 'Al6 Ca4 O16 S'

loop_
  _publ_author_name
  'N. J. Calos'
  'C. H. L. Kennard'
  'A. K. Whittaker'
  'R. L. Davis'
  _journal_name_full_name
  'Journal of Solid State Chemistry'
  _journal_volume 119
  _journal_year 1995
  _journal_page_first 1
  _journal_page_last 7
  _publ_section_title
  'Structure of calcium aluminate sulfate Ca4{4}Al6{6}SO4{16}SS'
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'CaS_{4}AlS_{6}SO_{16}S Structure'
_aflow_proto 'A6B4C16D_oP108_27_abcd4e_4e_16e_e'

```

```

_aflow_params 'a,b/a,c/a,z_{1},z_{2},z_{3},z_{4},x_{5},y_{5},z_{5},x_{6}
↪ ,y_{6},z_{6},x_{7},y_{7},z_{7},x_{8},y_{8},z_{8},x_{9},y_{9},
↪ z_{9},x_{10},y_{10},z_{10},x_{11},y_{11},z_{11},x_{12},y_{12},
↪ z_{12},x_{13},y_{13},z_{13},x_{14},y_{14},z_{14},x_{15},y_{15},
↪ z_{15},x_{16},y_{16},z_{16},x_{17},y_{17},z_{17},x_{18},y_{18},
↪ z_{18},x_{19},y_{19},z_{19},x_{20},y_{20},z_{20},x_{21},y_{21},
↪ z_{21},x_{22},y_{22},z_{22},x_{23},y_{23},z_{23},x_{24},y_{24},
↪ z_{24},x_{25},y_{25},z_{25},x_{26},y_{26},z_{26},x_{27},y_{27},
↪ z_{27},x_{28},y_{28},z_{28},x_{29},y_{29},z_{29}'
_aflow_params_values '13.0409854622,0.999877309088,0.703110981603,0.0,
↪ 0.005,0.03,0.05,0.373,0.379,0.296,0.122,0.125,0.249,0.369,0.129
↪ ,0.28,0.122,0.376,0.26,0.058,0.751,0.449,0.237,0.574,0.086,
↪ 0.257,0.012,0.554,0.483,0.247,0.028,0.729,0.183,0.412,0.162,
↪ 0.684,0.26,0.23,0.164,0.679,0.651,0.299,0.6217,0.4,0.254,0.238,
↪ 0.433,0.091,0.44,0.445,0.395,0.455,0.245,0.09,0.304,0.404,0.057
↪ ,0.126,0.093,0.054,0.102,0.243,0.402,0.336,0.099,0.466,0.124,
↪ 0.392,0.467,0.154,0.103,0.253,0.191,0.047,0.385,0.425,0.052,
↪ 0.111,0.41,0.74634,0.2513,0.28218'
_aflow_strukturbericht 'None'
_aflow_pearson 'oP108'

_cell_length_a 13.0409854622
_cell_length_b 13.0393854518
_cell_length_c 9.1692600894
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P c c 2"
_symmetry_Int_Tables_number 27

```

```

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 -x,-y,z
  3 -x,y,z+1/2
  4 x,-y,z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
A11 Al 2 a 0.00000 0.00000 0.00000 1.00000
A12 Al 2 b 0.00000 0.50000 0.00500 1.00000
A13 Al 2 c 0.50000 0.00000 0.03000 1.00000
A14 Al 2 d 0.50000 0.50000 0.05000 1.00000
A15 Al 4 e 0.37300 0.37900 0.29600 1.00000
A16 Al 4 e 0.12200 0.12500 0.24900 1.00000
A17 Al 4 e 0.36900 0.12900 0.28000 1.00000
A18 Al 4 e 0.12200 0.37600 0.26000 1.00000
Ca1 Ca 4 e 0.05800 0.75100 0.44900 1.00000
Ca2 Ca 4 e 0.23700 0.57400 0.08600 1.00000
Ca3 Ca 4 e 0.25700 0.01200 0.55400 1.00000
Ca4 Ca 4 e 0.48300 0.24700 0.02800 1.00000
O1 O 4 e 0.72900 0.18300 0.41200 1.00000
O2 O 4 e 0.16200 0.68400 0.26000 1.00000
O3 O 4 e 0.23000 0.16400 0.67900 1.00000
O4 O 4 e 0.65100 0.29900 0.62170 1.00000
O5 O 4 e 0.40000 0.25400 0.23800 1.00000
O6 O 4 e 0.43300 0.09100 0.44000 1.00000
O7 O 4 e 0.44500 0.39500 0.45500 1.00000
O8 O 4 e 0.24500 0.09000 0.30400 1.00000
O9 O 4 e 0.40400 0.05700 0.12600 1.00000
O10 O 4 e 0.09300 0.05400 0.10200 1.00000
O11 O 4 e 0.24300 0.40200 0.33600 1.00000
O12 O 4 e 0.09900 0.46600 0.12400 1.00000
O13 O 4 e 0.39200 0.46700 0.15400 1.00000
O14 O 4 e 0.10300 0.25300 0.19100 1.00000
O15 O 4 e 0.04700 0.38500 0.42500 1.00000
O16 O 4 e 0.05200 0.11100 0.41000 1.00000
S1 S 4 e 0.74634 0.25130 0.28218 1.00000

```

Ca<sub>4</sub>Al<sub>6</sub>O<sub>16</sub>S: A6B4C16D\_oP108\_27\_abcd4e\_4e\_16e\_e - POSCAR

```

A6B4C16D_oP108_27_abcd4e_4e_16e_e & a,b/a,c/a,z1,z2,z3,z4,x5,y5,z5,x6,y6
↪ z6,x7,y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11,y11,z11,x12,y12,
↪ z12,x13,y13,z13,x14,y14,z14,x15,y15,z15,x16,y16,z16,x17,y17,z17,
↪ x18,y18,z18,x19,y19,z19,x20,y20,z20,x21,y21,z21,x22,y22,z22,
↪ x23,y23,z23,x24,y24,z24,x25,y25,z25,x26,y26,z26,x27,y27,z27,x28,
↪ y28,z28,x29,y29,z29 --params=13.0409854622,0.999877309088,
↪ 0.703110981603,0.0,0.005,0.03,0.05,0.373,0.379,0.296,0.122,
↪ 0.125,0.249,0.369,0.129,0.28,0.122,0.376,0.26,0.058,0.751,0.449
↪ ,0.237,0.574,0.086,0.257,0.012,0.554,0.483,0.247,0.028,0.729,
↪ 0.183,0.412,0.162,0.684,0.26,0.23,0.164,0.679,0.651,0.299,
↪ 0.6217,0.4,0.254,0.238,0.433,0.091,0.44,0.445,0.395,0.455,0.245
↪ ,0.09,0.304,0.404,0.057,0.126,0.093,0.054,0.102,0.243,0.402,
↪ 0.336,0.099,0.466,0.124,0.392,0.467,0.154,0.103,0.253,0.191,
↪ 0.047,0.385,0.425,0.052,0.111,0.41,0.74634,0.2513,0.28218 &
↪ Pcc2 C_{2v}^{[3]} #27 (abcde^25) & oP108 & None & Ca4Al6O16S & &
↪ N. J. Calos et al., J. Solid State Chem. 119, 1-7 (1995)
1.00000000000000
13.04098546220000 0.00000000000000 0.00000000000000
0.00000000000000 13.03938545180000 0.00000000000000
0.00000000000000 0.00000000000000 9.16926008940000
Al Ca O S
24 16 64 4
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Al (2a)
0.00000000000000 0.00000000000000 0.50000000000000 Al (2a)

```

0.000000000000	0.500000000000	0.005000000000	Al	(2b)
0.000000000000	0.500000000000	0.505000000000	Al	(2b)
0.500000000000	0.000000000000	0.030000000000	Al	(2c)
0.500000000000	0.000000000000	0.530000000000	Al	(2c)
0.500000000000	0.500000000000	0.050000000000	Al	(2d)
0.500000000000	0.500000000000	0.550000000000	Al	(2d)
0.373000000000	0.379000000000	0.296000000000	Al	(4e)
-0.373000000000	-0.379000000000	0.296000000000	Al	(4e)
0.373000000000	0.379000000000	0.796000000000	Al	(4e)
-0.373000000000	-0.379000000000	0.796000000000	Al	(4e)
0.122000000000	0.125000000000	0.249000000000	Al	(4e)
-0.122000000000	-0.125000000000	0.249000000000	Al	(4e)
0.122000000000	0.125000000000	0.749000000000	Al	(4e)
-0.122000000000	-0.125000000000	0.749000000000	Al	(4e)
0.369000000000	0.129000000000	0.280000000000	Al	(4e)
-0.369000000000	-0.129000000000	0.280000000000	Al	(4e)
0.369000000000	0.129000000000	0.780000000000	Al	(4e)
-0.369000000000	-0.129000000000	0.780000000000	Al	(4e)
0.122000000000	0.376000000000	0.260000000000	Al	(4e)
-0.122000000000	-0.376000000000	0.260000000000	Al	(4e)
0.122000000000	0.376000000000	0.760000000000	Al	(4e)
-0.122000000000	-0.376000000000	0.760000000000	Al	(4e)
0.058000000000	0.751000000000	0.449000000000	Ca	(4e)
-0.058000000000	-0.751000000000	0.449000000000	Ca	(4e)
0.058000000000	0.751000000000	0.949000000000	Ca	(4e)
-0.058000000000	-0.751000000000	0.949000000000	Ca	(4e)
0.237000000000	0.574000000000	0.086000000000	Ca	(4e)
-0.237000000000	-0.574000000000	0.086000000000	Ca	(4e)
0.237000000000	0.574000000000	0.586000000000	Ca	(4e)
-0.237000000000	-0.574000000000	0.586000000000	Ca	(4e)
0.257000000000	0.012000000000	0.554000000000	Ca	(4e)
-0.257000000000	-0.012000000000	0.554000000000	Ca	(4e)
0.257000000000	0.012000000000	1.054000000000	Ca	(4e)
-0.257000000000	-0.012000000000	1.054000000000	Ca	(4e)
0.483000000000	0.247000000000	0.028000000000	Ca	(4e)
-0.483000000000	-0.247000000000	0.028000000000	Ca	(4e)
0.483000000000	0.247000000000	0.528000000000	Ca	(4e)
-0.483000000000	-0.247000000000	0.528000000000	Ca	(4e)
0.729000000000	0.183000000000	0.412000000000	O	(4e)
-0.729000000000	-0.183000000000	0.412000000000	O	(4e)
0.729000000000	0.183000000000	0.912000000000	O	(4e)
-0.729000000000	-0.183000000000	0.912000000000	O	(4e)
0.162000000000	0.684000000000	0.260000000000	O	(4e)
-0.162000000000	-0.684000000000	0.260000000000	O	(4e)
0.162000000000	0.684000000000	0.760000000000	O	(4e)
-0.162000000000	-0.684000000000	0.760000000000	O	(4e)
0.230000000000	0.164000000000	0.679000000000	O	(4e)
-0.230000000000	-0.164000000000	0.679000000000	O	(4e)
0.230000000000	0.164000000000	1.179000000000	O	(4e)
-0.230000000000	-0.164000000000	1.179000000000	O	(4e)
0.651000000000	0.299000000000	0.621700000000	O	(4e)
-0.651000000000	-0.299000000000	0.621700000000	O	(4e)
0.651000000000	0.299000000000	1.121700000000	O	(4e)
-0.651000000000	-0.299000000000	1.121700000000	O	(4e)
0.400000000000	0.254000000000	0.238000000000	O	(4e)
-0.400000000000	-0.254000000000	0.238000000000	O	(4e)
0.400000000000	0.254000000000	0.738000000000	O	(4e)
-0.400000000000	-0.254000000000	0.738000000000	O	(4e)
0.433000000000	0.091000000000	0.440000000000	O	(4e)
-0.433000000000	-0.091000000000	0.440000000000	O	(4e)
0.433000000000	0.091000000000	0.940000000000	O	(4e)
-0.433000000000	-0.091000000000	0.940000000000	O	(4e)
0.445000000000	0.395000000000	0.455000000000	O	(4e)
-0.445000000000	-0.395000000000	0.455000000000	O	(4e)
0.445000000000	0.395000000000	0.955000000000	O	(4e)
-0.445000000000	-0.395000000000	0.955000000000	O	(4e)
0.245000000000	0.090000000000	0.304000000000	O	(4e)
-0.245000000000	-0.090000000000	0.304000000000	O	(4e)
0.245000000000	0.090000000000	0.804000000000	O	(4e)
-0.245000000000	-0.090000000000	0.804000000000	O	(4e)
0.404000000000	0.057000000000	0.126000000000	O	(4e)
-0.404000000000	-0.057000000000	0.126000000000	O	(4e)
0.404000000000	0.057000000000	0.626000000000	O	(4e)
-0.404000000000	-0.057000000000	0.626000000000	O	(4e)
0.093000000000	0.054000000000	0.102000000000	O	(4e)
-0.093000000000	-0.054000000000	0.102000000000	O	(4e)
0.093000000000	0.054000000000	0.602000000000	O	(4e)
-0.093000000000	-0.054000000000	0.602000000000	O	(4e)
0.243000000000	0.402000000000	0.336000000000	O	(4e)
-0.243000000000	-0.402000000000	0.336000000000	O	(4e)
0.243000000000	0.402000000000	0.836000000000	O	(4e)
-0.243000000000	-0.402000000000	0.836000000000	O	(4e)
0.099000000000	0.466000000000	0.124000000000	O	(4e)
-0.099000000000	-0.466000000000	0.124000000000	O	(4e)
0.099000000000	0.466000000000	0.624000000000	O	(4e)
-0.099000000000	-0.466000000000	0.624000000000	O	(4e)
0.392000000000	0.467000000000	0.154000000000	O	(4e)
-0.392000000000	-0.467000000000	0.154000000000	O	(4e)
0.392000000000	0.467000000000	0.654000000000	O	(4e)
-0.392000000000	-0.467000000000	0.654000000000	O	(4e)
0.103000000000	0.253000000000	0.191000000000	O	(4e)
-0.103000000000	-0.253000000000	0.191000000000	O	(4e)
0.103000000000	0.253000000000	0.691000000000	O	(4e)
-0.103000000000	-0.253000000000	0.691000000000	O	(4e)
0.047000000000	0.385000000000	0.425000000000	O	(4e)
-0.047000000000	-0.385000000000	0.425000000000	O	(4e)
0.047000000000	0.385000000000	0.925000000000	O	(4e)
-0.047000000000	-0.385000000000	0.925000000000	O	(4e)
0.052000000000	0.111000000000	0.410000000000	O	(4e)
-0.052000000000	-0.111000000000	0.410000000000	O	(4e)
0.052000000000	0.111000000000	0.910000000000	O	(4e)
-0.052000000000	-0.111000000000	0.910000000000	O	(4e)
0.746340000000	0.251300000000	0.782180000000	S	(4e)
-0.746340000000	-0.251300000000	0.782180000000	S	(4e)
0.746340000000	0.251300000000	0.782180000000	S	(4e)
-0.746340000000	-0.251300000000	0.782180000000	S	(4e)

-0.746340000000 0.251300000000 0.782180000000 S (4e)

ZrO<sub>2</sub>: A2B\_oP12\_29\_2a\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'ZrO2'
_chemical_formula_sum 'O2 Zr'

loop_
  _publ_author_name
  'J. Grins',
  'P.-O. K{\a}ll',
  'G. Svensson'
_journal_name_full_name
;
  Journal of Materials Chemistry
_journal_volume 4
_journal_year 1994
_journal_page_first 1293
_journal_page_last 1301
_publ_section_title
;
  Phases in the ZrS_{x}Ta_{1-x}(O,N)_y system, formed by
  → ammonolysis of Zr-Ta gels: Preparation of a baddeleyite-type
  → solid solution phase ZrS_{x}Ta_{1-x}S_{1+x}NS_{1-x}S, $O
  → \l e x \l e 1$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  → Inorganic Compounds, 2013

_aflow_title 'ZrO_{2} Structure'
_aflow_proto 'A2B_oP12_29_2a_a'
_aflow_params 'a,b/a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3}'
_aflow_params_values '5.2594682584,0.963498098863,0.965209125484,0.639,
  → 0.068,0.0,0.771,0.537,0.106,0.53,0.267,0.356'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP12'

_cell_length_a 5.2594682584
_cell_length_b 5.0674876680
_cell_length_c 5.0764867582
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'P c a 21'
_symmetry_Int_Tables_number 29

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 -x,-y,z+1/2
  3 -x+1/2,y,z+1/2
  4 x+1/2,-y,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  O1 O 4 a 0.63900 0.06800 0.00000 1.00000
  O2 O 4 a 0.77100 0.53700 0.10600 1.00000
  Zr1 Zr 4 a 0.53000 0.26700 0.35600 1.00000
```

ZrO<sub>2</sub>: A2B\_oP12\_29\_2a\_a - POSCAR

```
A2B_oP12_29_2a_a & a,b/a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3 --params=
  → 5.2594682584,0.963498098863,0.965209125484,0.639,0.068,0.0,
  → 0.771,0.537,0.106,0.53,0.267,0.356 & Pca2_{1} C_{2v}^{5} #29 (a
  → ^3) & oP12 & None & ZrO2 & J. Grins and P.-O. K{\a}ll and
  → G. Svensson, J. Mater. Chem. 4, 1293-1301 (1994)
1.000000000000
5.25946825840000 0.000000000000 0.000000000000
0.000000000000 5.06748766800000 0.000000000000
0.000000000000 0.000000000000 5.07648675820000
O Zr
8 4
Direct
0.639000000000 0.068000000000 0.000000000000 O (4a)
-0.639000000000 -0.068000000000 0.500000000000 O (4a)
1.139000000000 -0.068000000000 0.000000000000 O (4a)
-0.139000000000 0.068000000000 0.500000000000 O (4a)
0.771000000000 0.537000000000 0.106000000000 O (4a)
-0.771000000000 -0.537000000000 0.606000000000 O (4a)
1.271000000000 -0.537000000000 0.106000000000 O (4a)
-0.271000000000 0.537000000000 0.606000000000 O (4a)
0.530000000000 0.267000000000 0.356000000000 Zr (4a)
-0.530000000000 -0.267000000000 0.856000000000 Zr (4a)
1.030000000000 -0.267000000000 0.356000000000 Zr (4a)
-0.030000000000 0.267000000000 0.856000000000 Zr (4a)
```

Pyrite (FeS<sub>2</sub>, Low-temperature): AB2\_oP12\_29\_2a\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'FeS2'
_chemical_formula_sum 'Fe S2'

loop_
_publ_author_name
'P. Bayliss'
_journal_name_full_name
;
American Mineralogist
;
_journal_volume 74
_journal_year 1989
_journal_page_first 1168
_journal_page_last 1176
_publ_section_title
;
Crystal chemistry and crystallography of some minerals within the
↳ pyrite group
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'Pyrite (FeSS_{2})$, Low-temperature) Structure'
_aflow_proto 'AB2_oP12_29_a_2a'
_aflow_params 'a,b/a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3}'
↳ ',z_{3}'
_aflow_params_values '5.4179557747,1.0,1.0,0.5049,0.2419,0.0,0.615,0.135'
↳ ',0.3834,0.615,0.635,0.1134'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP12'

_cell_length_a 5.4179557747
_cell_length_b 5.4179557747
_cell_length_c 5.4179557747
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P c a 21"
_symmetry_Int_Tables_number 29

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z+1/2
3 -x+1/2,y,z+1/2
4 x+1/2,-y,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
As1 As 4 a 0.61885 0.63065 0.11668 1.00000
Co1 Co 4 a 0.50496 0.24091 0.00000 1.00000
S1 S 4 a 0.61734 0.13129 0.37996 1.00000
```

Pyrite (FeS<sub>2</sub>, Low-temperature): AB2\_oP12\_29\_a\_2a - POSCAR

```
AB2_oP12_29_a_2a & a,b/a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3 --params=
↳ 5.4179557747,1.0,1.0,0.5049,0.2419,0.0,0.615,0.135,0.3834,0.615
↳ ',0.635,0.1134 & Pca2_{1} C_{2v}^{5} #29 (a^3) & oP12 & None &
↳ FeS2 & P. Bayliss, Am. Mineral. 74, 1168-1176 (1989)

1.0000000000000000
5.41795577470000 0.00000000000000 0.00000000000000
0.00000000000000 5.41795577470000 0.00000000000000
0.00000000000000 0.00000000000000 5.41795577470000
Fe S
4 8
Direct
0.50490000000000 0.24190000000000 0.00000000000000 Fe (4a)
-0.50490000000000 -0.24190000000000 0.50000000000000 Fe (4a)
1.00490000000000 -0.24190000000000 0.00000000000000 Fe (4a)
-0.00490000000000 0.24190000000000 0.50000000000000 Fe (4a)
0.61500000000000 0.13500000000000 0.38340000000000 S (4a)
-0.61500000000000 -0.13500000000000 0.88340000000000 S (4a)
1.11500000000000 -0.13500000000000 0.38340000000000 S (4a)
-0.11500000000000 0.13500000000000 0.88340000000000 S (4a)
0.61500000000000 0.63500000000000 0.11340000000000 S (4a)
-0.61500000000000 -0.63500000000000 0.61340000000000 S (4a)
1.11500000000000 -0.63500000000000 0.11340000000000 S (4a)
-0.11500000000000 0.63500000000000 0.61340000000000 S (4a)
```

Cobaltite (CoAsS): ABC\_oP12\_29\_a\_a\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'CoAsS'
_chemical_formula_sum 'As Co S'

loop_
_publ_author_name
'S. Tahara'
'A. Shimada'
'N. Kumada'
'Y. Sugahara'
_journal_name_full_name
;
Journal of Solid State Chemistry
;
_journal_volume 180
```

```
'M. E. Fleet'
'P. C. Burns'
_journal_name_full_name
;
Canadian Mineralogist
;
_journal_volume 28
_journal_year 1990
_journal_page_first 719
_journal_page_last 723
_publ_section_title
;
Structure and twinning of cobaltite
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'Cobaltite (CoAsS) Structure'
_aflow_proto 'ABC_oP12_29_a_a_a'
_aflow_params 'a,b/a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3}'
↳ ',z_{3}'
_aflow_params_values '5.2594682584,0.963498098863,0.965209125484,0.61885'
↳ ',0.63065,0.11668,0.50496,0.24091,0.0,0.61734,0.13129,0.37996'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP12'

_cell_length_a 5.2594682584
_cell_length_b 5.0674876680
_cell_length_c 5.0764867582
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P c a 21"
_symmetry_Int_Tables_number 29

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z+1/2
3 -x+1/2,y,z+1/2
4 x+1/2,-y,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
As1 As 4 a 0.61885 0.63065 0.11668 1.00000
Co1 Co 4 a 0.50496 0.24091 0.00000 1.00000
S1 S 4 a 0.61734 0.13129 0.37996 1.00000
```

Cobaltite (CoAsS): ABC\_oP12\_29\_a\_a\_a - POSCAR

```
ABC_oP12_29_a_a_a & a,b/a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3 --params=
↳ 5.2594682584,0.963498098863,0.965209125484,0.61885,0.63065,
↳ 0.11668,0.50496,0.24091,0.0,0.61734,0.13129,0.37996 & Pca2_{1}
↳ C_{2v}^{5} #29 (a^3) & oP12 & None & CoAsS & M. E. Fleet and
↳ P. C. Burns, Can. Mineral. 28, 719-723 (1990)

1.0000000000000000
5.25946825840000 0.00000000000000 0.00000000000000
0.00000000000000 5.06748766800000 0.00000000000000
0.00000000000000 0.00000000000000 5.07648675820000
As Co S
4 4 4
Direct
0.61885000000000 0.63065000000000 0.11668000000000 As (4a)
-0.61885000000000 -0.63065000000000 0.61668000000000 As (4a)
1.11885000000000 -0.63065000000000 0.11668000000000 As (4a)
-0.11885000000000 0.63065000000000 0.61668000000000 As (4a)
0.50496000000000 0.24091000000000 0.00000000000000 Co (4a)
-0.50496000000000 -0.24091000000000 0.50000000000000 Co (4a)
1.00496000000000 -0.24091000000000 0.00000000000000 Co (4a)
-0.00496000000000 0.24091000000000 0.50000000000000 Co (4a)
0.61734000000000 0.13129000000000 0.37996000000000 S (4a)
-0.61734000000000 -0.13129000000000 0.87996000000000 S (4a)
1.11734000000000 -0.13129000000000 0.37996000000000 S (4a)
-0.11734000000000 0.13129000000000 0.87996000000000 S (4a)
```

Bi<sub>5</sub>Nb<sub>3</sub>O<sub>15</sub>: ASB3C15\_oP46\_30\_a2c\_bc\_a7c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Bi5Nb3O15'
_chemical_formula_sum 'Bi5 Nb3 O15'

loop_
_publ_author_name
'S. Tahara'
'A. Shimada'
'N. Kumada'
'Y. Sugahara'
_journal_name_full_name
;
Journal of Solid State Chemistry
;
_journal_volume 180
```

```

_journal_year 2007
_journal_page_first 2517
_journal_page_last 2524
_publ_Section_title
;
Characterization of Bi5Nb3O15 by refinement of neutron
  ↳ diffraction pattern, acid treatment and reaction of the
  ↳ acid-treated product with Sn4-alkylamines
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title 'Bi5Nb3O15 Structure'
_aflow_proto 'A5B3C15_oP46_30_a2c_bc_a7c'
_aflow_params 'a,b/a,c/a,z_{1},z_{2},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},y_{7},z_{7},x_{8},y_{8},z_{8},x_{9},y_{9},z_{9},x_{10},y_{10},z_{10},x_{11},y_{11},z_{11},x_{12},y_{12},z_{12},x_{13},y_{13},z_{13}'
_aflow_params_values '5.4630061801,1.00183049606,3.84605528098,0.5,0.107,0.523,0.2442,0.513,0.019,0.3675,0.026,0.016,0.1074,0.003,0.02,0.1949,0.05,0.074,0.097,0.687,0.22,0.0844,0.254,0.226,0.413,0.52,0.105,0.505,0.718,0.31,0.305,0.763,0.271,0.695,0.752,0.289'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP46'

_cell_length_a 5.4630061801
_cell_length_b 5.4730061914
_cell_length_c 21.0110237690
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P n c 2"
_symmetry_Int_Tables_number 30

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x,y+1/2,z+1/2
4 x,-y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Bi1 Bi 2 a 0.00000 0.00000 0.50000 1.00000
O1 O 2 a 0.00000 0.00000 0.10700 1.00000
Nb1 Nb 2 b 0.50000 0.00000 0.52300 1.00000
Bi2 Bi 4 c 0.24420 0.51300 0.01900 1.00000
Bi3 Bi 4 c 0.36750 0.02600 0.01600 1.00000
Nb2 Nb 4 c 0.10740 0.00300 0.02000 1.00000
O2 O 4 c 0.19490 0.05000 0.07400 1.00000
O3 O 4 c 0.09700 0.68700 0.22000 1.00000
O4 O 4 c 0.08440 0.25400 0.22600 1.00000
O5 O 4 c 0.41300 0.52000 0.10500 1.00000
O6 O 4 c 0.50500 0.71800 0.31000 1.00000
O7 O 4 c 0.30500 0.76300 0.27100 1.00000
O8 O 4 c 0.69500 0.75200 0.28900 1.00000

```

Bi<sub>5</sub>Nb<sub>3</sub>O<sub>15</sub>: A5B3C15\_oP46\_30\_a2c\_bc\_a7c - POSCAR

```

A5B3C15_oP46_30_a2c_bc_a7c & a,b/a,c/a,z1,z2,z3,x4,y4,z4,x5,y5,z5,x6,y6,
  ↳ z6,x7,y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11,y11,z11,x12,y12,
  ↳ z12,x13,y13,z13 --params=5.4630061801,1.00183049606,
  ↳ 3.84605528098,0.5,0.107,0.523,0.2442,0.513,0.019,0.3675,0.026,
  ↳ 0.016,0.1074,0.003,0.02,0.1949,0.05,0.074,0.097,0.687,0.22,
  ↳ 0.0844,0.254,0.226,0.413,0.52,0.105,0.505,0.718,0.31,0.305,
  ↳ 0.763,0.271,0.695,0.752,0.289 & Pnc2 C_{2v}^{6} #30 (a^2bc^10)
  ↳ & oP46 & None & Bi5Nb3O15 & S. Tahara et al., J. Solid State
  ↳ Chem. 180, 2517-2524 (2007)
1.0000000000000000
5.46300618010000 0.000000000000000 0.000000000000000
0.000000000000000 5.47300619140000 0.000000000000000
0.000000000000000 0.000000000000000 21.01102376900000
Bi Nb O
10 6 30
Direct
0.000000000000000 0.000000000000000 0.500000000000000 Bi (2a)
0.000000000000000 0.500000000000000 1.000000000000000 Bi (2a)
0.244200000000000 0.513000000000000 0.019000000000000 Bi (4c)
-0.244200000000000 -0.513000000000000 0.019000000000000 Bi (4c)
0.244200000000000 -0.013000000000000 0.519000000000000 Bi (4c)
-0.244200000000000 1.013000000000000 0.519000000000000 Bi (4c)
0.367500000000000 0.026000000000000 0.016000000000000 Bi (4c)
-0.367500000000000 -0.026000000000000 0.016000000000000 Bi (4c)
0.367500000000000 0.474000000000000 0.516000000000000 Bi (4c)
-0.367500000000000 0.526000000000000 0.516000000000000 Bi (4c)
0.500000000000000 0.000000000000000 0.523000000000000 Nb (2b)
0.500000000000000 0.500000000000000 1.023000000000000 Nb (2b)
0.107400000000000 0.003000000000000 0.020000000000000 Nb (4c)
-0.107400000000000 -0.003000000000000 0.020000000000000 Nb (4c)
0.107400000000000 0.497000000000000 0.520000000000000 Nb (4c)
-0.107400000000000 0.503000000000000 0.520000000000000 Nb (4c)
0.000000000000000 0.000000000000000 0.107000000000000 O (2a)
0.000000000000000 0.500000000000000 0.607000000000000 O (2a)
0.194900000000000 0.050000000000000 0.074000000000000 O (4c)

```

```

-0.194900000000000 -0.050000000000000 0.074000000000000 O (4c)
0.194900000000000 0.450000000000000 0.574000000000000 O (4c)
-0.194900000000000 0.550000000000000 0.574000000000000 O (4c)
0.097000000000000 0.687000000000000 0.220000000000000 O (4c)
-0.097000000000000 -0.687000000000000 0.220000000000000 O (4c)
0.097000000000000 -0.187000000000000 0.720000000000000 O (4c)
-0.097000000000000 1.187000000000000 0.720000000000000 O (4c)
0.084400000000000 0.254000000000000 0.226000000000000 O (4c)
-0.084400000000000 -0.254000000000000 0.226000000000000 O (4c)
0.084400000000000 0.246000000000000 0.726000000000000 O (4c)
-0.084400000000000 0.754000000000000 0.726000000000000 O (4c)
0.413000000000000 0.520000000000000 0.105000000000000 O (4c)
-0.413000000000000 -0.520000000000000 0.105000000000000 O (4c)
0.413000000000000 -0.020000000000000 0.605000000000000 O (4c)
-0.413000000000000 1.020000000000000 0.605000000000000 O (4c)
0.505000000000000 0.718000000000000 0.310000000000000 O (4c)
-0.505000000000000 -0.718000000000000 0.310000000000000 O (4c)
0.505000000000000 -0.218000000000000 0.810000000000000 O (4c)
-0.505000000000000 1.218000000000000 0.810000000000000 O (4c)
0.305000000000000 0.763000000000000 0.271000000000000 O (4c)
-0.305000000000000 -0.763000000000000 0.271000000000000 O (4c)
0.305000000000000 -0.263000000000000 0.771000000000000 O (4c)
-0.305000000000000 1.263000000000000 0.771000000000000 O (4c)
0.695000000000000 0.752000000000000 0.289000000000000 O (4c)
-0.695000000000000 -0.752000000000000 0.289000000000000 O (4c)
0.695000000000000 -0.252000000000000 0.789000000000000 O (4c)
-0.695000000000000 1.252000000000000 0.789000000000000 O (4c)

```

CuBrSe<sub>3</sub>: ABC3\_oP20\_30\_2a\_c\_3c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'CuBrSe3'
_chemical_formula_sum 'Br Cu Se3'

loop_
_publ_author_name
'T. Sakuma'
'T. Kaneko'
'T. Kurita'
'H. Takahashi'
_journal_name_full_name
;
Journal of the Physical Society of Japan
;
_journal_volume 60
_journal_year 1991
_journal_page_first 1608
_journal_page_last 1611
_publ_Section_title
;
Crystal structure of CuBrSe3
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title 'CuBrSe3 Structure'
_aflow_proto 'ABC3_oP20_30_2a_c_3c'
_aflow_params 'a,b/a,c/a,z_{1},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6}'
_aflow_params_values '4.480982758,1.71211783083,3.19772372237,0.8543,0.5,0.3011,0.721,0.4096,0.3607,0.7305,0.1733,0.5847,0.8629,0.0496,0.6302,0.8523,0.2991'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP20'

_cell_length_a 4.4809827580
_cell_length_b 7.6719704796
_cell_length_c 14.3289448648
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P n c 2"
_symmetry_Int_Tables_number 30

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x,y+1/2,z+1/2
4 x,-y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Br1 Br 2 a 0.00000 0.00000 0.85430 1.00000
Br2 Br 2 a 0.00000 0.00000 0.50000 1.00000
Cu1 Cu 4 c 0.30110 0.72100 0.40960 1.00000
Se1 Se 4 c 0.36070 0.73050 0.17330 1.00000
Se2 Se 4 c 0.58470 0.86290 0.04960 1.00000
Se3 Se 4 c 0.63020 0.85230 0.29910 1.00000

```

CuBrSe<sub>3</sub>: ABC3\_oP20\_30\_2a\_c\_3c - POSCAR

```

ABC3_oP20_30_2a_c_3c & a ,b/a ,c/a ,z1 ,z2 ,x3 ,y3 ,z3 ,x4 ,y4 ,z4 ,x5 ,y5 ,z5 ,x6 ,y6 ,
↪ z6 --params=4.480982758 , 1.71211783083 , 3.19772372237 , 0.8543 , 0.5 ,
↪ 0.3011 , 0.721 , 0.4096 , 0.3607 , 0.7305 , 0.1733 , 0.5847 , 0.8629 , 0.0496 ,
↪ 0.6302 , 0.8523 , 0.2991 & Pnc2 C_[2v]^6 #30 (a^2c^4) & oP20 &
↪ None & CuBrSe3 & T. Sakuma et al. , J. Phys. Soc. Jpn. 60 ,
↪ 1608-1611 (1991)
1.0000000000000000
4.480982758000000 0.000000000000000 0.000000000000000
0.000000000000000 7.671970479600000 0.000000000000000
0.000000000000000 0.000000000000000 14.328944864800000
Br Cu Se
4 4 12
Direct
0.000000000000000 0.000000000000000 0.854300000000000 Br (2a)
0.000000000000000 0.500000000000000 1.354300000000000 Br (2a)
0.000000000000000 0.000000000000000 0.500000000000000 Br (2a)
0.000000000000000 0.500000000000000 1.000000000000000 Br (2a)
0.301100000000000 0.721000000000000 0.409600000000000 Cu (4c)
-0.301100000000000 -0.721000000000000 0.409600000000000 Cu (4c)
0.301100000000000 -0.221000000000000 0.909600000000000 Cu (4c)
-0.301100000000000 1.221000000000000 0.909600000000000 Cu (4c)
0.360700000000000 0.730500000000000 0.173300000000000 Se (4c)
-0.360700000000000 -0.730500000000000 0.173300000000000 Se (4c)
0.360700000000000 -0.230500000000000 0.673300000000000 Se (4c)
-0.360700000000000 1.230500000000000 0.673300000000000 Se (4c)
0.584700000000000 0.862900000000000 0.049600000000000 Se (4c)
-0.584700000000000 -0.862900000000000 0.049600000000000 Se (4c)
0.584700000000000 -0.362900000000000 0.549600000000000 Se (4c)
-0.584700000000000 1.362900000000000 0.549600000000000 Se (4c)
0.630200000000000 0.852300000000000 0.299100000000000 Se (4c)
-0.630200000000000 -0.852300000000000 0.299100000000000 Se (4c)
0.630200000000000 -0.352300000000000 0.799100000000000 Se (4c)
-0.630200000000000 1.352300000000000 0.799100000000000 Se (4c)

```

Re<sub>2</sub>O<sub>5</sub>[SO<sub>4</sub>]<sub>2</sub>: A13B2C<sub>2</sub>oP34\_32\_a6c\_c\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Re2O5[SO4]2'
_chemical_formula_sum 'O13 Re2 S2'

loop_
  _publ_author_name
  'U. Betke'
  'M. S. Wickleder'
  _journal_name_full_name
  ;
Inorganic Chemistry
;
_journal_volume 50
_journal_year 2011
_journal_page_first 858
_journal_page_last 872
_publ_section_title
;
Sulfates of the Refractory Metals: Crystal Structure and Thermal
↪ Behavior of NbS2(SO4)2, MoOS2(SO4)2,
↪ WO(SO4)2, and Two Modifications of ReS2(SO4)2
↪ (SO4)2
;

```

# Found in Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds, 2013

```

_aware_title 'ReS2(SO4)2 Structure'
_aware_proto 'A13B2C2oP34_32_a6c_c_c'
_aware_params 'a ,b/a ,c/a ,z1 ,x2 ,y2 ,z2 ,x3 ,y3 ,z3 ,x4 ,y4 ,z4 ,x5 ,y5 ,z5 ,x6 ,y6 ,z6 ,x7 ,y7 ,z7 ,x8 ,y8 ,z8 ,x9 ,y9 ,z9 ,x10 ,y10 ,z10 ,x11 ,y11 ,z11 ,x12 ,y12 ,z12 ,x13 ,y13 ,z13 ,x14 ,y14 ,z14 ,x15 ,y15 ,z15 ,x16 ,y16 ,z16 ,x17 ,y17 ,z17 ,x18 ,y18 ,z18 ,x19 ,y19 ,z19 ,x20 ,y20 ,z20 ,x21 ,y21 ,z21 ,x22 ,y22 ,z22 ,x23 ,y23 ,z23 ,x24 ,y24 ,z24 ,x25 ,y25 ,z25 ,x26 ,y26 ,z26 ,x27 ,y27 ,z27 ,x28 ,y28 ,z28 ,x29 ,y29 ,z29 ,x30 ,y30 ,z30 ,x31 ,y31 ,z31 ,x32 ,y32 ,z32 ,x33 ,y33 ,z33 ,x34 ,y34 ,z34 ,x35 ,y35 ,z35 ,x36 ,y36 ,z36 ,x37 ,y37 ,z37 ,x38 ,y38 ,z38 ,x39 ,y39 ,z39 ,x40 ,y40 ,z40 ,x41 ,y41 ,z41 ,x42 ,y42 ,z42 ,x43 ,y43 ,z43 ,x44 ,y44 ,z44 ,x45 ,y45 ,z45 ,x46 ,y46 ,z46 ,x47 ,y47 ,z47 ,x48 ,y48 ,z48 ,x49 ,y49 ,z49 ,x50 ,y50 ,z50 ,x51 ,y51 ,z51 ,x52 ,y52 ,z52 ,x53 ,y53 ,z53 ,x54 ,y54 ,z54 ,x55 ,y55 ,z55 ,x56 ,y56 ,z56 ,x57 ,y57 ,z57 ,x58 ,y58 ,z58 ,x59 ,y59 ,z59 ,x60 ,y60 ,z60 ,x61 ,y61 ,z61 ,x62 ,y62 ,z62 ,x63 ,y63 ,z63 ,x64 ,y64 ,z64 ,x65 ,y65 ,z65 ,x66 ,y66 ,z66 ,x67 ,y67 ,z67 ,x68 ,y68 ,z68 ,x69 ,y69 ,z69 ,x70 ,y70 ,z70 ,x71 ,y71 ,z71 ,x72 ,y72 ,z72 ,x73 ,y73 ,z73 ,x74 ,y74 ,z74 ,x75 ,y75 ,z75 ,x76 ,y76 ,z76 ,x77 ,y77 ,z77 ,x78 ,y78 ,z78 ,x79 ,y79 ,z79 ,x80 ,y80 ,z80 ,x81 ,y81 ,z81 ,x82 ,y82 ,z82 ,x83 ,y83 ,z83 ,x84 ,y84 ,z84 ,x85 ,y85 ,z85 ,x86 ,y86 ,z86 ,x87 ,y87 ,z87 ,x88 ,y88 ,z88 ,x89 ,y89 ,z89 ,x90 ,y90 ,z90 ,x91 ,y91 ,z91 ,x92 ,y92 ,z92 ,x93 ,y93 ,z93 ,x94 ,y94 ,z94 ,x95 ,y95 ,z95 ,x96 ,y96 ,z96 ,x97 ,y97 ,z97 ,x98 ,y98 ,z98 ,x99 ,y99 ,z99 ,x100 ,y100 ,z100 ,x101 ,y101 ,z101 ,x102 ,y102 ,z102 ,x103 ,y103 ,z103 ,x104 ,y104 ,z104 ,x105 ,y105 ,z105 ,x106 ,y106 ,z106 ,x107 ,y107 ,z107 ,x108 ,y108 ,z108 ,x109 ,y109 ,z109 ,x110 ,y110 ,z110 ,x111 ,y111 ,z111 ,x112 ,y112 ,z112 ,x113 ,y113 ,z113 ,x114 ,y114 ,z114 ,x115 ,y115 ,z115 ,x116 ,y116 ,z116 ,x117 ,y117 ,z117 ,x118 ,y118 ,z118 ,x119 ,y119 ,z119 ,x120 ,y120 ,z120 ,x121 ,y121 ,z121 ,x122 ,y122 ,z122 ,x123 ,y123 ,z123 ,x124 ,y124 ,z124 ,x125 ,y125 ,z125 ,x126 ,y126 ,z126 ,x127 ,y127 ,z127 ,x128 ,y128 ,z128 ,x129 ,y129 ,z129 ,x130 ,y130 ,z130 ,x131 ,y131 ,z131 ,x132 ,y132 ,z132 ,x133 ,y133 ,z133 ,x134 ,y134 ,z134 ,x135 ,y135 ,z135 ,x136 ,y136 ,z136 ,x137 ,y137 ,z137 ,x138 ,y138 ,z138 ,x139 ,y139 ,z139 ,x140 ,y140 ,z140 ,x141 ,y141 ,z141 ,x142 ,y142 ,z142 ,x143 ,y143 ,z143 ,x144 ,y144 ,z144 ,x145 ,y145 ,z145 ,x146 ,y146 ,z146 ,x147 ,y147 ,z147 ,x148 ,y148 ,z148 ,x149 ,y149 ,z149 ,x150 ,y150 ,z150 ,x151 ,y151 ,z151 ,x152 ,y152 ,z152 ,x153 ,y153 ,z153 ,x154 ,y154 ,z154 ,x155 ,y155 ,z155 ,x156 ,y156 ,z156 ,x157 ,y157 ,z157 ,x158 ,y158 ,z158 ,x159 ,y159 ,z159 ,x160 ,y160 ,z160 ,x161 ,y161 ,z161 ,x162 ,y162 ,z162 ,x163 ,y163 ,z163 ,x164 ,y164 ,z164 ,x165 ,y165 ,z165 ,x166 ,y166 ,z166 ,x167 ,y167 ,z167 ,x168 ,y168 ,z168 ,x169 ,y169 ,z169 ,x170 ,y170 ,z170 ,x171 ,y171 ,z171 ,x172 ,y172 ,z172 ,x173 ,y173 ,z173 ,x174 ,y174 ,z174 ,x175 ,y175 ,z175 ,x176 ,y176 ,z176 ,x177 ,y177 ,z177 ,x178 ,y178 ,z178 ,x179 ,y179 ,z179 ,x180 ,y180 ,z180 ,x181 ,y181 ,z181 ,x182 ,y182 ,z182 ,x183 ,y183 ,z183 ,x184 ,y184 ,z184 ,x185 ,y185 ,z185 ,x186 ,y186 ,z186 ,x187 ,y187 ,z187 ,x188 ,y188 ,z188 ,x189 ,y189 ,z189 ,x190 ,y190 ,z190 ,x191 ,y191 ,z191 ,x192 ,y192 ,z192 ,x193 ,y193 ,z193 ,x194 ,y194 ,z194 ,x195 ,y195 ,z195 ,x196 ,y196 ,z196 ,x197 ,y197 ,z197 ,x198 ,y198 ,z198 ,x199 ,y199 ,z199 ,x200 ,y200 ,z200 ,x201 ,y201 ,z201 ,x202 ,y202 ,z202 ,x203 ,y203 ,z203 ,x204 ,y204 ,z204 ,x205 ,y205 ,z205 ,x206 ,y206 ,z206 ,x207 ,y207 ,z207 ,x208 ,y208 ,z208 ,x209 ,y209 ,z209 ,x210 ,y210 ,z210 ,x211 ,y211 ,z211 ,x212 ,y212 ,z212 ,x213 ,y213 ,z213 ,x214 ,y214 ,z214 ,x215 ,y215 ,z215 ,x216 ,y216 ,z216 ,x217 ,y217 ,z217 ,x218 ,y218 ,z218 ,x219 ,y219 ,z219 ,x220 ,y220 ,z220 ,x221 ,y221 ,z221 ,x222 ,y222 ,z222 ,x223 ,y223 ,z223 ,x224 ,y224 ,z224 ,x225 ,y225 ,z225 ,x226 ,y226 ,z226 ,x227 ,y227 ,z227 ,x228 ,y228 ,z228 ,x229 ,y229 ,z229 ,x230 ,y230 ,z230 ,x231 ,y231 ,z231 ,x232 ,y232 ,z232 ,x233 ,y233 ,z233 ,x234 ,y234 ,z234 ,x235 ,y235 ,z235 ,x236 ,y236 ,z236 ,x237 ,y237 ,z237 ,x238 ,y238 ,z238 ,x239 ,y239 ,z239 ,x240 ,y240 ,z240 ,x241 ,y241 ,z241 ,x242 ,y242 ,z242 ,x243 ,y243 ,z243 ,x244 ,y244 ,z244 ,x245 ,y245 ,z245 ,x246 ,y246 ,z246 ,x247 ,y247 ,z247 ,x248 ,y248 ,z248 ,x249 ,y249 ,z249 ,x250 ,y250 ,z250 ,x251 ,y251 ,z251 ,x252 ,y252 ,z252 ,x253 ,y253 ,z253 ,x254 ,y254 ,z254 ,x255 ,y255 ,z255 ,x256 ,y256 ,z256 ,x257 ,y257 ,z257 ,x258 ,y258 ,z258 ,x259 ,y259 ,z259 ,x260 ,y260 ,z260 ,x261 ,y261 ,z261 ,x262 ,y262 ,z262 ,x263 ,y263 ,z263 ,x264 ,y264 ,z264 ,x265 ,y265 ,z265 ,x266 ,y266 ,z266 ,x267 ,y267 ,z267 ,x268 ,y268 ,z268 ,x269 ,y269 ,z269 ,x270 ,y270 ,z270 ,x271 ,y271 ,z271 ,x272 ,y272 ,z272 ,x273 ,y273 ,z273 ,x274 ,y274 ,z274 ,x275 ,y275 ,z275 ,x276 ,y276 ,z276 ,x277 ,y277 ,z277 ,x278 ,y278 ,z278 ,x279 ,y279 ,z279 ,x280 ,y280 ,z280 ,x281 ,y281 ,z281 ,x282 ,y282 ,z282 ,x283 ,y283 ,z283 ,x284 ,y284 ,z284 ,x285 ,y285 ,z285 ,x286 ,y286 ,z286 ,x287 ,y287 ,z287 ,x288 ,y288 ,z288 ,x289 ,y289 ,z289 ,x290 ,y290 ,z290 ,x291 ,y291 ,z291 ,x292 ,y292 ,z292 ,x293 ,y293 ,z293 ,x294 ,y294 ,z294 ,x295 ,y295 ,z295 ,x296 ,y296 ,z296 ,x297 ,y297 ,z297 ,x298 ,y298 ,z298 ,x299 ,y299 ,z299 ,x300 ,y300 ,z300 ,x301 ,y301 ,z301 ,x302 ,y302 ,z302 ,x303 ,y303 ,z303 ,x304 ,y304 ,z304 ,x305 ,y305 ,z305 ,x306 ,y306 ,z306 ,x307 ,y307 ,z307 ,x308 ,y308 ,z308 ,x309 ,y309 ,z309 ,x310 ,y310 ,z310 ,x311 ,y311 ,z311 ,x312 ,y312 ,z312 ,x313 ,y313 ,z313 ,x314 ,y314 ,z314 ,x315 ,y315 ,z315 ,x316 ,y316 ,z316 ,x317 ,y317 ,z317 ,x318 ,y318 ,z318 ,x319 ,y319 ,z319 ,x320 ,y320 ,z320 ,x321 ,y321 ,z321 ,x322 ,y322 ,z322 ,x323 ,y323 ,z323 ,x324 ,y324 ,z324 ,x325 ,y325 ,z325 ,x326 ,y326 ,z326 ,x327 ,y327 ,z327 ,x328 ,y328 ,z328 ,x329 ,y329 ,z329 ,x330 ,y330 ,z330 ,x331 ,y331 ,z331 ,x332 ,y332 ,z332 ,x333 ,y333 ,z333 ,x334 ,y334 ,z334 ,x335 ,y335 ,z335 ,x336 ,y336 ,z336 ,x337 ,y337 ,z337 ,x338 ,y338 ,z338 ,x339 ,y339 ,z339 ,x340 ,y340 ,z340 ,x341 ,y341 ,z341 ,x342 ,y342 ,z342 ,x343 ,y343 ,z343 ,x344 ,y344 ,z344 ,x345 ,y345 ,z345 ,x346 ,y346 ,z346 ,x347 ,y347 ,z347 ,x348 ,y348 ,z348 ,x349 ,y349 ,z349 ,x350 ,y350 ,z350 ,x351 ,y351 ,z351 ,x352 ,y352 ,z352 ,x353 ,y353 ,z353 ,x354 ,y354 ,z354 ,x355 ,y355 ,z355 ,x356 ,y356 ,z356 ,x357 ,y357 ,z357 ,x358 ,y358 ,z358 ,x359 ,y359 ,z359 ,x360 ,y360 ,z360 ,x361 ,y361 ,z361 ,x362 ,y362 ,z362 ,x363 ,y363 ,z363 ,x364 ,y364 ,z364 ,x365 ,y365 ,z365 ,x366 ,y366 ,z366 ,x367 ,y367 ,z367 ,x368 ,y368 ,z368 ,x369 ,y369 ,z369 ,x370 ,y370 ,z370 ,x371 ,y371 ,z371 ,x372 ,y372 ,z372 ,x373 ,y373 ,z373 ,x374 ,y374 ,z374 ,x375 ,y375 ,z375 ,x376 ,y376 ,z376 ,x377 ,y377 ,z377 ,x378 ,y378 ,z378 ,x379 ,y379 ,z379 ,x380 ,y380 ,z380 ,x381 ,y381 ,z381 ,x382 ,y382 ,z382 ,x383 ,y383 ,z383 ,x384 ,y384 ,z384 ,x385 ,y385 ,z385 ,x386 ,y386 ,z386 ,x387 ,y387 ,z387 ,x388 ,y388 ,z388 ,x389 ,y389 ,z389 ,x390 ,y390 ,z390 ,x391 ,y391 ,z391 ,x392 ,y392 ,z392 ,x393 ,y393 ,z393 ,x394 ,y394 ,z394 ,x395 ,y395 ,z395 ,x396 ,y396 ,z396 ,x397 ,y397 ,z397 ,x398 ,y398 ,z398 ,x399 ,y399 ,z399 ,x400 ,y400 ,z400 ,x401 ,y401 ,z401 ,x402 ,y402 ,z402 ,x403 ,y403 ,z403 ,x404 ,y404 ,z404 ,x405 ,y405 ,z405 ,x406 ,y406 ,z406 ,x407 ,y407 ,z407 ,x408 ,y408 ,z408 ,x409 ,y409 ,z409 ,x410 ,y410 ,z410 ,x411 ,y411 ,z411 ,x412 ,y412 ,z412 ,x413 ,y413 ,z413 ,x414 ,y414 ,z414 ,x415 ,y415 ,z415 ,x416 ,y416 ,z416 ,x417 ,y417 ,z417 ,x418 ,y418 ,z418 ,x419 ,y419 ,z419 ,x420 ,y420 ,z420 ,x421 ,y421 ,z421 ,x422 ,y422 ,z422 ,x423 ,y423 ,z423 ,x424 ,y424 ,z424 ,x425 ,y425 ,z425 ,x426 ,y426 ,z426 ,x427 ,y427 ,z427 ,x428 ,y428 ,z428 ,x429 ,y429 ,z429 ,x430 ,y430 ,z430 ,x431 ,y431 ,z431 ,x432 ,y432 ,z432 ,x433 ,y433 ,z433 ,x434 ,y434 ,z434 ,x435 ,y435 ,z435 ,x436 ,y436 ,z436 ,x437 ,y437 ,z437 ,x438 ,y438 ,z438 ,x439 ,y439 ,z439 ,x440 ,y440 ,z440 ,x441 ,y441 ,z441 ,x442 ,y442 ,z442 ,x443 ,y443 ,z443 ,x444 ,y444 ,z444 ,x445 ,y445 ,z445 ,x446 ,y446 ,z446 ,x447 ,y447 ,z447 ,x448 ,y448 ,z448 ,x449 ,y449 ,z449 ,x450 ,y450 ,z450 ,x451 ,y451 ,z451 ,x452 ,y452 ,z452 ,x453 ,y453 ,z453 ,x454 ,y454 ,z454 ,x455 ,y455 ,z455 ,x456 ,y456 ,z456 ,x457 ,y457 ,z457 ,x458 ,y458 ,z458 ,x459 ,y459 ,z459 ,x460 ,y460 ,z460 ,x461 ,y461 ,z461 ,x462 ,y462 ,z462 ,x463 ,y463 ,z463 ,x464 ,y464 ,z464 ,x465 ,y465 ,z465 ,x466 ,y466 ,z466 ,x467 ,y467 ,z467 ,x468 ,y468 ,z468 ,x469 ,y469 ,z469 ,x470 ,y470 ,z470 ,x471 ,y471 ,z471 ,x472 ,y472 ,z472 ,x473 ,y473 ,z473 ,x474 ,y474 ,z474 ,x475 ,y475 ,z475 ,x476 ,y476 ,z476 ,x477 ,y477 ,z477 ,x478 ,y478 ,z478 ,x479 ,y479 ,z479 ,x480 ,y480 ,z480 ,x481 ,y481 ,z481 ,x482 ,y482 ,z482 ,x483 ,y483 ,z483 ,x484 ,y484 ,z484 ,x485 ,y485 ,z485 ,x486 ,y486 ,z486 ,x487 ,y487 ,z487 ,x488 ,y488 ,z488 ,x489 ,y489 ,z489 ,x490 ,y490 ,z490 ,x491 ,y491 ,z491 ,x492 ,y492 ,z492 ,x493 ,y493 ,z493 ,x494 ,y494 ,z494 ,x495 ,y495 ,z495 ,x496 ,y496 ,z496 ,x497 ,y497 ,z497 ,x498 ,y498 ,z498 ,x499 ,y499 ,z499 ,x500 ,y500 ,z500 ,x501 ,y501 ,z501 ,x502 ,y502 ,z502 ,x503 ,y503 ,z503 ,x504 ,y504 ,z504 ,x505 ,y505 ,z505 ,x506 ,y506 ,z506 ,x507 ,y507 ,z507 ,x508 ,y508 ,z508 ,x509 ,y509 ,z509 ,x510 ,y510 ,z510 ,x511 ,y511 ,z511 ,x512 ,y512 ,z512 ,x513 ,y513 ,z513 ,x514 ,y514 ,z514 ,x515 ,y515 ,z515 ,x516 ,y516 ,z516 ,x517 ,y517 ,z517 ,x518 ,y518 ,z518 ,x519 ,y519 ,z519 ,x520 ,y520 ,z520 ,x521 ,y521 ,z521 ,x522 ,y522 ,z522 ,x523 ,y523 ,z523 ,x524 ,y524 ,z524 ,x525 ,y525 ,z525 ,x526 ,y526 ,z526 ,x527 ,y527 ,z527 ,x528 ,y528 ,z528 ,x529 ,y529 ,z529 ,x530 ,y530 ,z530 ,x531 ,y531 ,z531 ,x532 ,y532 ,z532 ,x533 ,y533 ,z533 ,x534 ,y534 ,z534 ,x535 ,y535 ,z535 ,x536 ,y536 ,z536 ,x537 ,y537 ,z537 ,x538 ,y538 ,z538 ,x539 ,y539 ,z539 ,x540 ,y540 ,z540 ,x541 ,y541 ,z541 ,x542 ,y542 ,z542 ,x543 ,y543 ,z543 ,x544 ,y544 ,z544 ,x545 ,y545 ,z545 ,x546 ,y546 ,z546 ,x547 ,y547 ,z547 ,x548 ,y548 ,z548 ,x549 ,y549 ,z549 ,x550 ,y550 ,z550 ,x551 ,y551 ,z551 ,x552 ,y552 ,z552 ,x553 ,y553 ,z553 ,x554 ,y554 ,z554 ,x555 ,y555 ,z555 ,x556 ,y556 ,z556 ,x557 ,y557 ,z557 ,x558 ,y558 ,z558 ,x559 ,y559 ,z559 ,x560 ,y560 ,z560 ,x561 ,y561 ,z561 ,x562 ,y562 ,z562 ,x563 ,y563 ,z563 ,x564 ,y564 ,z564 ,x565 ,y565 ,z565 ,x566 ,y566 ,z566 ,x567 ,y567 ,z567 ,x568 ,y568 ,z568 ,x569 ,y569 ,z569 ,x570 ,y570 ,z570 ,x571 ,y571 ,z571 ,x572 ,y572 ,z572 ,x573 ,y573 ,z573 ,x574 ,y574 ,z574 ,x575 ,y575 ,z575 ,x576 ,y576 ,z576 ,x577 ,y577 ,z577 ,x578 ,y578 ,z578 ,x579 ,y579 ,z579 ,x580 ,y580 ,z580 ,x581 ,y581 ,z581 ,x582 ,y582 ,z582 ,x583 ,y583 ,z583 ,x584 ,y584 ,z584 ,x585 ,y585 ,z585 ,x586 ,y586 ,z586 ,x587 ,y587 ,z587 ,x588 ,y588 ,z588 ,x589 ,y589 ,z589 ,x590 ,y590 ,z590 ,x591 ,y591 ,z591 ,x592 ,y592 ,z592 ,x593 ,y593 ,z593 ,x594 ,y594 ,z594 ,x595 ,y595 ,z595 ,x596 ,y596 ,z596 ,x597 ,y597 ,z597 ,x598 ,y598 ,z598 ,x599 ,y599 ,z599 ,x600 ,y600 ,z600 ,x601 ,y601 ,z601 ,x602 ,y602 ,z602 ,x603 ,y603 ,z603 ,x604 ,y604 ,z604 ,x605 ,y605 ,z605 ,x606 ,y606 ,z606 ,x607 ,y607 ,z607 ,x608 ,y608 ,z608 ,x609 ,y609 ,z609 ,x610 ,y610 ,z610 ,x611 ,y611 ,z611 ,x612 ,y612 ,z612 ,x613 ,y613 ,z613 ,x614 ,y614 ,z614 ,x615 ,y615 ,z615 ,x616 ,y616 ,z616 ,x617 ,y617 ,z617 ,x618 ,y618 ,z618 ,x619 ,y619 ,z619 ,x620 ,y620 ,z620 ,x621 ,y621 ,z621 ,x622 ,y622 ,z622 ,x623 ,y623 ,z623 ,x624 ,y624 ,z624 ,x625 ,y625 ,z625 ,x626 ,y626 ,z626 ,x627 ,y627 ,z627 ,x628 ,y628 ,z628 ,x629 ,y629 ,z629 ,x630 ,y630 ,z630 ,x631 ,y631 ,z631 ,x632 ,y632 ,z632 ,x633 ,y633 ,z633 ,x634 ,y634 ,z634 ,x635 ,y635 ,z635 ,x636 ,y636 ,z636 ,x637 ,y637 ,z637 ,x638 ,y638 ,z638 ,x639 ,y639 ,z639 ,x640 ,y640 ,z640 ,x641 ,y641 ,z641 ,x642 ,y642 ,z642 ,x643 ,y643 ,z643 ,x644 ,y644 ,z644 ,x645 ,y645 ,z645 ,x646 ,y646 ,z646 ,x647 ,y647 ,z647 ,x648 ,y648 ,z648 ,x649 ,y649 ,z649 ,x650 ,y650 ,z650 ,x651 ,y651 ,z651 ,x652 ,y652 ,z652 ,x653 ,y653 ,z653 ,x654 ,y654 ,z654 ,x655 ,y655 ,z655 ,x656 ,y656 ,z656 ,x657 ,y657 ,z657 ,x658 ,y658 ,z658 ,x659 ,y659 ,z659 ,x660 ,y660 ,z660 ,x661 ,y661 ,z661 ,x662 ,y662 ,z662 ,x663 ,y663 ,z663 ,x664 ,y664 ,z664 ,x665 ,y665 ,z665 ,x666 ,y666 ,z666 ,x667 ,y667 ,z667 ,x668 ,y668 ,z668 ,x669 ,y669 ,z669 ,x670 ,y670 ,z670 ,x671 ,y671 ,z671 ,x672 ,y672 ,z672 ,x673 ,y673 ,z673 ,x674 ,y674 ,z674 ,x675 ,y675 ,z675 ,x676 ,y676 ,z676 ,x677 ,y677 ,z677 ,x678 ,y678 ,z678 ,x679 ,y679 ,z679 ,x680 ,y680 ,z680 ,x681 ,y681 ,z681 ,x682 ,y682 ,z682 ,x683 ,y683 ,z683 ,x684 ,y684 ,z684 ,x685 ,y685 ,z685 ,x686 ,y686 ,z686 ,x687 ,y687 ,z687 ,x688 ,y688 ,z688 ,x689 ,y689 ,z689 ,x690 ,y690 ,z690 ,x691 ,y691 ,z691 ,x692 ,y692 ,z692 ,x693 ,y693 ,z693 ,x694 ,y694 ,z694 ,x695 ,y
```

```

↪ 0.6381 , 0.5145 , 0.6728 , 0.1212 , 0.8608 , 0.3301 , 0.8662 , 0.336 , 0.4992 ,
↪ 0.9
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP40'

_symmetry_space_group_name_H-M "P n n 21"
_symmetry_Int_Tables_number 33

_cell_length_a 4.84370
_cell_length_b 8.33000
_cell_length_c 8.95470
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z+1/2
3 -x+1/2,y+1/2,z+1/2
4 x+1/2,-y+1/2,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 4 a 0.67870 0.84160 0.00000 1.00000
Al2 Al 4 a 0.18460 0.34320 0.78680 1.00000
Al3 Al 4 a 0.81150 0.64890 0.69720 1.00000
Al4 Al 4 a 0.66770 0.46960 0.99930 1.00000
O1 O 4 a 0.32900 0.83130 0.89270 1.00000
O2 O 4 a 0.02480 0.49080 0.62920 1.00000
O3 O 4 a 0.47170 0.66470 0.63810 1.00000
O4 O 4 a 0.51450 0.67280 0.12120 1.00000
O5 O 4 a 0.86080 0.33010 0.86620 1.00000
O6 O 4 a 0.33600 0.49920 0.90000 1.00000

```

**κ-alumina (Al<sub>2</sub>O<sub>3</sub>): A2B3\_oP40\_33\_4a\_6a - POSCAR**

```

A2B3_oP40_33_4a_6a & a,b/a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5
↪ z5,x6,y6,z6,x7,y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10 --params=
↪ 4.8437 , 1.71975968784 , 1.84873134174 , 0.6787 , 0.8416 , 0.0 , 0.1846 ,
↪ 0.3432 , 0.7868 , 0.8115 , 0.6489 , 0.6972 , 0.6677 , 0.4696 , 0.9993 , 0.329 ,
↪ 0.8313 , 0.8927 , 0.0248 , 0.4908 , 0.6292 , 0.4717 , 0.6647 , 0.6381 , 0.5145 ,
↪ 0.6728 , 0.1212 , 0.8608 , 0.3301 , 0.8662 , 0.336 , 0.4992 , 0.9 & Pna2_1
↪ C_{2v}^{19} #33 (a^10) & oP40 & None & Al2O3 & $\kappa$-alumina
↪ & B. Ollivier et al., J. Mater. Chem. 7, 1049-1056 (1997)
1.000000000000000
4.843700000000000 0.000000000000000 0.000000000000000
0.000000000000000 8.330000000000000 0.000000000000000
0.000000000000000 0.000000000000000 8.954700000000000
Al O
16 24
Direct
0.678700000000000 0.841600000000000 0.000000000000000 Al (4a)
-0.678700000000000 -0.841600000000000 0.500000000000000 Al (4a)
1.178700000000000 -0.341600000000000 0.000000000000000 Al (4a)
-0.178700000000000 1.341600000000000 0.500000000000000 Al (4a)
0.184600000000000 0.343200000000000 0.786800000000000 Al (4a)
-0.184600000000000 -0.343200000000000 1.286800000000000 Al (4a)
0.684600000000000 0.156800000000000 0.786800000000000 Al (4a)
0.315400000000000 0.843200000000000 1.286800000000000 Al (4a)
0.811500000000000 0.648900000000000 0.697200000000000 Al (4a)
-0.811500000000000 -0.648900000000000 1.197200000000000 Al (4a)
1.311500000000000 -0.148900000000000 0.697200000000000 Al (4a)
-0.311500000000000 1.148900000000000 1.197200000000000 Al (4a)
0.667700000000000 0.469600000000000 0.999300000000000 Al (4a)
-0.667700000000000 -0.469600000000000 1.499300000000000 Al (4a)
1.167700000000000 0.030400000000000 0.999300000000000 Al (4a)
-0.167700000000000 0.969600000000000 1.499300000000000 Al (4a)
0.329000000000000 0.831300000000000 0.892700000000000 O (4a)
-0.329000000000000 -0.831300000000000 1.392700000000000 O (4a)
0.829000000000000 -0.331300000000000 0.892700000000000 O (4a)
0.171000000000000 1.331300000000000 1.392700000000000 O (4a)
0.024800000000000 0.490800000000000 0.629200000000000 O (4a)
-0.024800000000000 -0.490800000000000 1.129200000000000 O (4a)
0.524800000000000 0.009200000000000 0.629200000000000 O (4a)
0.475200000000000 0.990800000000000 1.129200000000000 O (4a)
0.471700000000000 0.664700000000000 0.638100000000000 O (4a)
-0.471700000000000 -0.664700000000000 1.138100000000000 O (4a)
0.971700000000000 -0.164700000000000 0.638100000000000 O (4a)
0.028300000000000 1.164700000000000 1.138100000000000 O (4a)
0.514500000000000 0.672800000000000 0.121200000000000 O (4a)
-0.514500000000000 -0.672800000000000 0.621200000000000 O (4a)
1.014500000000000 -0.172800000000000 0.121200000000000 O (4a)
-0.014500000000000 1.172800000000000 0.621200000000000 O (4a)
0.860800000000000 0.330100000000000 0.866200000000000 O (4a)
-0.860800000000000 -0.330100000000000 1.366200000000000 O (4a)
1.360800000000000 0.169900000000000 0.866200000000000 O (4a)
-0.360800000000000 0.830100000000000 1.366200000000000 O (4a)
0.336000000000000 0.499200000000000 0.900000000000000 O (4a)
-0.336000000000000 -0.499200000000000 1.400000000000000 O (4a)
0.836000000000000 0.000800000000000 0.900000000000000 O (4a)
0.164000000000000 0.999200000000000 1.400000000000000 O (4a)

```

**TiAl<sub>2</sub>Br<sub>3</sub>: A2B8C\_oP22\_34\_c\_4c\_a - CIF**

```

# CIF file
data_findsym-output

```

```

_audit_creation_method FINDSYM
_chemical_name_mineral 'TiAl2Br8'
_chemical_formula_sum 'Al2 Br8 Ti'

loop_
_publ_author_name
'S. I. Troyanov'
'V. B. Rybakov'
'V. M. Ionov'
_journal_name_full_name
:
Russian Journal of Inorganic Chemistry
:
_journal_volume 35
_journal_year 1990
_journal_page_first 882
_journal_page_last 887
_publ_section_title
:
Synthesis and Crystal Structure of TiBr_{4}$, TiBr_{3}$ and Ti(AlBr_{
↪ {4}$)_{2}$
:
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'TiAlS_{2}SBrS_{8}$ Structure'
_aflow_proto 'A2B8C_oP22_34_c_4c_a'
_aflow_params 'a,b/a,c/a,z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6}'
↪ {4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6}'
_aflow_params_values '6.2740008991,2.04032515143,1.38284985656,0.5,0.605
↪ ,0.8135,0.499,0.7349,0.6796,0.009,0.743,-0.0925,0.3064,0.2388,
↪ 0.5935,0.2196,0.7131,0.6459,0.513'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP22'

_cell_length_a 6.2740008991
_cell_length_b 12.8010018345
_cell_length_c 8.6760012434
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P n n 2"
_symmetry_Int_Tables_number 34

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x+1/2,y+1/2,z+1/2
4 x+1/2,-y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ti1 Ti 2 a 0.00000 0.00000 0.50000 1.00000
Al1 Al 4 c 0.60500 0.81350 0.49900 1.00000
Br1 Br 4 c 0.73490 0.67960 0.00900 1.00000
Br2 Br 4 c 0.74300 -0.09250 0.30640 1.00000
Br3 Br 4 c 0.23880 0.59350 0.21960 1.00000
Br4 Br 4 c 0.71310 0.64590 0.51300 1.00000

```

**TiAl<sub>2</sub>Br<sub>3</sub>: A2B8C\_oP22\_34\_c\_4c\_a - POSCAR**

```

A2B8C_oP22_34_c_4c_a & a,b/a,c/a,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,
↪ x6,y6,z6 --params=6.2740008991,2.04032515143,1.38284985656,0.5,
↪ 0.605,0.8135,0.499,0.7349,0.6796,0.009,0.743,-0.0925,0.3064,
↪ 0.2388,0.5935,0.2196,0.7131,0.6459,0.513 & Pnn2_C_{2v}^{10} #34
↪ (ac^5) & oP22 & None & TiAl2Br8 & S. I. Troyanov and V. B.
↪ Rybakov and V. M. Ionov, Russ. J. Inorg. Chem. 35, 882-887 (
↪ 1990)
1.000000000000000
6.27400089910000 0.0000000000000 0.000000000000000
0.000000000000000 12.80100183450000 0.000000000000000
0.000000000000000 0.000000000000000 8.676001243400000
Al Br Ti
4 16 2
Direct
0.605000000000000 0.813500000000000 0.499000000000000 Al (4c)
-0.605000000000000 -0.813500000000000 0.499000000000000 Al (4c)
1.105000000000000 -0.313500000000000 0.999000000000000 Al (4c)
-0.105000000000000 1.313500000000000 0.999000000000000 Al (4c)
0.734900000000000 0.679600000000000 0.009000000000000 Br (4c)
-0.734900000000000 -0.679600000000000 0.009000000000000 Br (4c)
1.234900000000000 -0.179600000000000 0.509000000000000 Br (4c)
-0.234900000000000 1.179600000000000 0.509000000000000 Br (4c)
0.743000000000000 -0.092500000000000 0.306400000000000 Br (4c)
-0.743000000000000 0.092500000000000 0.306400000000000 Br (4c)
1.243000000000000 0.592500000000000 0.219600000000000 Br (4c)
-0.243000000000000 -0.592500000000000 0.219600000000000 Br (4c)
0.238800000000000 0.593500000000000 0.219600000000000 Br (4c)
-0.238800000000000 -0.593500000000000 0.219600000000000 Br (4c)
0.738800000000000 -0.093500000000000 0.719600000000000 Br (4c)
0.261200000000000 1.093500000000000 0.719600000000000 Br (4c)
0.713100000000000 0.645900000000000 0.513000000000000 Br (4c)
-0.713100000000000 -0.645900000000000 0.513000000000000 Br (4c)

```



1.21310000000000	-0.14590000000000	1.01300000000000	Br	(4c)
-0.21310000000000	1.14590000000000	1.01300000000000	Br	(4c)
0.00000000000000	0.00000000000000	0.50000000000000	Ti	(2a)
0.50000000000000	0.50000000000000	1.00000000000000	Ti	(2a)

FeSb<sub>2</sub>: AB2\_oP6\_34\_a\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'FeSb2'
_chemical_formula_sum 'Fe Sb2'

loop_
_publ_author_name
'H. Holseth'
'A. Kjekshus'
_journal_name_full_name
;
Acta Chemica Scandinavica
;
_journal_volume 23
_journal_year 1969
_journal_page_first 3043
_journal_page_last 3050
_publ_section_title
;
Compounds with the Marcasite Type Crystal Structure. IV. The Crystal
  ↳ Structure of FeSb2{2}$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title 'FeSb2{2}$ Structure'
_aflow_proto 'AB2_oP6_34_a_c'
_aflow_params 'a,b/a,c/a,z_{1},x_{2},y_{2},z_{2}'
_aflow_params_values '5.8327827022,1.12083390481,0.548158688784,0.5,
  ↳ 0.6881,0.8565,0.0097'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP6'

_cell_length_a 5.8327827022
_cell_length_b 6.5375806120
_cell_length_c 3.1972905180
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P n n 2"
_symmetry_Int_Tables_number 34

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x+1/2,y+1/2,z+1/2
4 x+1/2,-y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Fe1 Fe 2 a 0.00000 0.00000 0.50000 1.00000
Sb1 Sb 4 c 0.68810 0.85650 0.00970 1.00000
```

FeSb<sub>2</sub>: AB2\_oP6\_34\_a\_c - POSCAR

```
AB2_oP6_34_a_c & a,b/a,c/a,z1,x2,y2,z2 --params=5.8327827022,
  ↳ 1.12083390481,0.548158688784,0.5,0.6881,0.8565,0.0097 & Pnn2 C_
  ↳ {2v}^{10} #34 (ac) & oP6 & None & FeSb2 & H. Holseth and A.
  ↳ Kjekshus, Acta Chem. Scand. 23, 3043-3050 (1969)
1.00000000000000
5.83278270220000 0.00000000000000 0.00000000000000
0.00000000000000 6.53758061200000 0.00000000000000
0.00000000000000 0.00000000000000 3.19729051800000
Fe Sb
2 4
Direct
0.00000000000000 0.00000000000000 0.50000000000000 Fe (2a)
0.50000000000000 0.50000000000000 1.00000000000000 Fe (2a)
0.68810000000000 0.85650000000000 0.00970000000000 Sb (4c)
-0.68810000000000 -0.85650000000000 0.00970000000000 Sb (4c)
1.18810000000000 -0.35650000000000 0.50970000000000 Sb (4c)
-0.18810000000000 1.35650000000000 0.50970000000000 Sb (4c)
```

V<sub>2</sub>MoO<sub>8</sub>: AB8C2\_oC22\_35\_a\_ab3e\_e - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'V2MoO8'
_chemical_formula_sum 'Mo O8 V2'

loop_
_publ_author_name
'E. S\{a}ndor'
'R. F. C. Farrow'
_journal_name_full_name
;
Nature
;
_journal_volume 213
_journal_year 1967
```

```
'P. Mah{\e}-Pailleret'
_journal_year 1970
_publ_section_title
;
Contribution {\a}l\{\e)tude chimique et structurale des compos{\
  ↳ e}s ABS_{2}$O rencontr{\e}s dans les syst{\e}mes Mo-VO, UVO
  ↳ et U-Mo-O
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title 'VS_{2}$MoOs_{8}$ Structure'
_aflow_proto 'AB8C2_oC22_35_a_ab3e_e'
_aflow_params 'a,b/a,c/a,z_{1},z_{2},z_{3},y_{4},z_{4},y_{5},z_{5},y_{6}
  ↳ ,z_{6},y_{7},z_{7}'
_aflow_params_values '4.534758023,1.1408839779,2.72580110498,0.0,0.5838
  ↳ ,-0.042,0.189,0.5461,0.0961,0.122,0.2982,0.1399,0.1866,0.0038'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC22'

_cell_length_a 4.5347580230
_cell_length_b 5.1736327721
_cell_length_c 12.3608484299
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "C m m 2"
_symmetry_Int_Tables_number 35

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x,y,z
4 x,-y,z
5 x+1/2,y+1/2,z
6 -x+1/2,-y+1/2,z
7 -x+1/2,y+1/2,z
8 x+1/2,-y+1/2,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mo1 Mo 2 a 0.00000 0.00000 0.00000 1.00000
O1 O 2 a 0.00000 0.00000 0.58380 1.00000
O2 O 2 b 0.00000 0.50000 -0.04200 1.00000
O3 O 4 e 0.00000 0.18900 0.54610 1.00000
O4 O 4 e 0.00000 0.09610 0.12200 1.00000
O5 O 4 e 0.00000 0.29820 0.13990 1.00000
V1 V 4 e 0.00000 0.18660 0.00380 1.00000
```

V<sub>2</sub>MoO<sub>8</sub>: AB8C2\_oC22\_35\_a\_ab3e\_e - POSCAR

```
AB8C2_oC22_35_a_ab3e_e & a,b/a,c/a,z1,z2,z3,y4,z4,y5,z5,y6,y7,z7 --
  ↳ params=4.534758023,1.1408839779,2.72580110498,0.0,0.5838,-0.042
  ↳ ,0.189,0.5461,0.0961,0.122,0.2982,0.1399,0.1866,0.0038 & Cmm2
  ↳ C_{2v}^{11} #35 (a^2be^4) & oC22 & None & V2MoO8 & P. Mah{\
  ↳ e}-Pailleret, (1970)
1.00000000000000
2.26737901150000 -2.58681638605000 0.00000000000000
2.26737901150000 2.58681638605000 0.00000000000000
0.00000000000000 0.00000000000000 12.36084842990000
Mo O V
1 8 2
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Mo (2a)
0.00000000000000 0.00000000000000 0.58380000000000 O (2a)
0.50000000000000 0.50000000000000 -0.04200000000000 O (2b)
-0.18900000000000 0.18900000000000 0.54610000000000 O (4e)
0.18900000000000 -0.18900000000000 0.54610000000000 O (4e)
-0.09610000000000 0.09610000000000 0.12200000000000 O (4e)
-0.09610000000000 -0.09610000000000 0.12200000000000 O (4e)
-0.29820000000000 0.29820000000000 0.13990000000000 O (4e)
0.29820000000000 -0.29820000000000 0.13990000000000 O (4e)
-0.18660000000000 0.18660000000000 0.00380000000000 V (4e)
0.18660000000000 -0.18660000000000 0.00380000000000 V (4e)
```

HCl: AB\_oC8\_36\_a\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'HCl'
_chemical_formula_sum 'Cl H'

loop_
_publ_author_name
'E. S\{a}ndor'
'R. F. C. Farrow'
_journal_name_full_name
;
Nature
;
_journal_volume 213
_journal_year 1967
```

```

_journal_page_first 171
_journal_page_last 172
_publ_Section_title
;
Crystal Structure of Solid Hydrogen Chloride and Deuterium Chloride
;
_aflow_title 'HCl Structure'
_aflow_proto 'AB_oC8_36_a_a'
_aflow_params 'a,b/a,c/a,y_{1},z_{1},y_{2},z_{2}'
_aflow_params_values '5.825,0.945115879828,0.922403433476,0.25,0.0,0.081
↪ ,0.83'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC8'
_symmetry_space_group_name_H-M "C m c 21"
_symmetry_Int_Tables_number 36
_cell_length_a 5.82500
_cell_length_b 5.50530
_cell_length_c 5.37300
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z+1/2
3 -x,y,z
4 x,-y,z+1/2
5 x+1/2,y+1/2,z
6 -x+1/2,-y+1/2,z+1/2
7 -x+1/2,y+1/2,z
8 x+1/2,-y+1/2,z+1/2
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cl1 Cl 4 a 0.00000 0.25000 0.00000 1.00000
H1 H 4 a 0.00000 0.08100 0.83000 1.00000

```

HCl: AB\_oC8\_36\_a\_a - POSCAR

```

AB_oC8_36_a_a & a,b/a,c/a,y1,z1,y2,z2 --params=5.825,0.945115879828,
↪ 0.922403433476,0.25,0.0,0.081,0.83 & Cmc2_{1} C_{2v}^{12} #36 (
↪ a^2) & oC8 & None & HCl & HCl & E. S\'{a}ndor and R. F. C.
↪ Farrow, Nature 213, 171-172 (1967)
1.0000000000000000
2.9125000000000000 -2.7526500000000000 0.0000000000000000
2.9125000000000000 2.7526500000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.3730000000000000
Cl H
2 2
Direct
-0.2500000000000000 0.2500000000000000 0.0000000000000000 Cl (4a)
0.2500000000000000 -0.2500000000000000 0.5000000000000000 Cl (4a)
-0.0810000000000000 0.0810000000000000 0.8300000000000000 H (4a)
0.0810000000000000 -0.0810000000000000 1.3300000000000000 H (4a)

```

Li<sub>2</sub>Si<sub>2</sub>O<sub>5</sub>: A2B5C2\_oC36\_37\_d\_c2d\_d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Li2Si2O5'
_chemical_formula_sum 'Li2 O5 Si2'
loop_
_publ_author_name
'B. H. W. S [de Jong]'
'P. G. G. Slaats'
'H. T. J. Sup[e]r'
'N. Veldman'
'A. L. Spek'
_journal_name_full_name
;
Journal of Non-Crystalline Solids
;
_journal_volume 176
_journal_year 1994
_journal_page_first 164
_journal_page_last 171
_publ_Section_title
;
Extended structures in crystalline phyllosilicates: silica ring systems
↪ in lithium, rubidium, cesium, and cesium/lithium
↪ phyllosilicate
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013
_aflow_title 'Li_{2}Si_{2}O_{5} Structure'
_aflow_proto 'A2B5C2_oC36_37_d_c2d_d'
_aflow_params 'a,b/a,c/a,z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4}
↪ ,y_{4},z_{4},x_{5},y_{5},z_{5}'

```

```

_aflow_params_values '5.8071602545,2.51110728429,0.821939039086,0.0,
↪ 0.654,0.0584,0.0469,0.6705,0.0718,0.471,0.0932,0.1377,0.4004,
↪ 0.1552,0.14836,0.0571'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC36'
_cell_length_a 5.8071602545
_cell_length_b 14.5824024161
_cell_length_c 4.7731317194
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000
_symmetry_space_group_name_H-M "C c c 2"
_symmetry_Int_Tables_number 37
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x,y,z+1/2
4 x,-y,z+1/2
5 x+1/2,y+1/2,z
6 -x+1/2,-y+1/2,z
7 -x+1/2,y+1/2,z+1/2
8 x+1/2,-y+1/2,z+1/2
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 4 c 0.25000 0.25000 0.00000 1.00000
Li1 Li 8 d 0.65400 0.05840 0.04690 1.00000
O2 O 8 d 0.67050 0.07180 0.47100 1.00000
O3 O 8 d 0.09320 0.13770 0.40040 1.00000
Si1 Si 8 d 0.15520 0.14836 0.05710 1.00000

```

Li<sub>2</sub>Si<sub>2</sub>O<sub>5</sub>: A2B5C2\_oC36\_37\_d\_c2d\_d - POSCAR

```

A2B5C2_oC36_37_d_c2d_d & a,b/a,c/a,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,
↪ z5 --params=5.8071602545,2.51110728429,0.821939039086,0.0,0.654
↪ ,0.0584,0.0469,0.6705,0.0718,0.471,0.0932,0.1377,0.4004,0.1552,
↪ 0.14836,0.0571 & Ccc2_C_{2v}^{13} #37 (cd^4) & oC36 & None &
↪ Li2Si2O5 & B. H. W. S [de Jong] et al., J. Non Cryst. Solids
↪ 176, 164-171 (1994)
1.0000000000000000
2.90358012725000 -7.29120120805000 0.0000000000000000
2.90358012725000 7.29120120805000 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.77313171940000
Li O Si
4 10 4
Direct
0.5956000000000000 0.7124000000000000 0.0469000000000000 Li (8d)
-0.5956000000000000 -0.7124000000000000 0.0469000000000000 Li (8d)
0.7124000000000000 -0.5956000000000000 0.5469000000000000 Li (8d)
-0.7124000000000000 -0.5956000000000000 0.5469000000000000 Li (8d)
0.0000000000000000 0.5000000000000000 0.0000000000000000 O (4c)
0.5000000000000000 0.0000000000000000 0.5000000000000000 O (4c)
0.5987000000000000 0.7423000000000000 0.4710000000000000 O (8d)
-0.5987000000000000 -0.7423000000000000 0.4710000000000000 O (8d)
0.7423000000000000 0.5987000000000000 0.9710000000000000 O (8d)
-0.7423000000000000 -0.5987000000000000 0.9710000000000000 O (8d)
-0.0445000000000000 0.2309000000000000 0.4004000000000000 O (8d)
0.0445000000000000 -0.2309000000000000 0.4004000000000000 O (8d)
0.2309000000000000 -0.0445000000000000 0.9004000000000000 O (8d)
-0.2309000000000000 0.0445000000000000 0.9004000000000000 O (8d)
0.0068400000000000 0.3035600000000000 0.0571000000000000 Si (8d)
-0.0068400000000000 -0.3035600000000000 0.0571000000000000 Si (8d)
0.3035600000000000 0.0068400000000000 0.5571000000000000 Si (8d)
-0.3035600000000000 -0.0068400000000000 0.5571000000000000 Si (8d)

```

Ta<sub>3</sub>S<sub>2</sub>: A2B3\_oC40\_39\_2d\_2c2d - CIF

```

# CIF file# This file was generated by FINDSYM
# Harold T. Stokes, Branton J. Campbell, Dorian M. Hatch
# Brigham Young University, Provo, Utah, USA
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Ta3S2'
_chemical_formula_sum 'S2 Ta3'
loop_
_publ_author_name
'S. J. Kim'
'K. S. Nanjundaswamy'
'T. Hughbanks'
_journal_name_full_name
;
Inorganic Chemistry
;
_journal_volume 30
_journal_year 1991
_journal_page_first 159
_journal_page_last 164
_publ_Section_title
;

```

```

Single-crystal structure of tantalum sulfide (TaS3)  

  ↳ Structure and bonding in the Ta6Sn (Sn = 1, 3, 4, 5?)  

  ↳ pentagonal-antiprismatic chain compounds  

;
# Found in Pearson's Crystal Data - Crystal Structure Database for  

  ↳ Inorganic Compounds, 2013

_aflow_title 'TaS3 Structure'  

_aflow_proto 'A2B3_oC40_39_2d_2c2d'  

_aflow_params 'a,b/a,c/a,x1,z1,x2,z2,x3,y3,z3,x4,  

  ↳ y4,z4,x5,y5,z5,x6,y6,z6'  

_aflow_params_values '7.47831,2.30292940517,0.749515599113,0.3449,0.5,  

  ↳ 0.0058,0.7654,0.173,0.5398,0.3889,0.5843,0.6154,0.3917,0.28104,  

  ↳ 0.16619,0.0206,0.10455,0.6073,0.0144'  

_aflow_Strukturbericht 'None'  

_aflow_Pearson 'oC40'

_symmetry_space_group_name_H-M 'A b m 2'  

_symmetry_Int_Tables_number 39

_cell_length_a 7.47831  

_cell_length_b 17.22202  

_cell_length_c 5.60511  

_cell_angle_alpha 90.00000  

_cell_angle_beta 90.00000  

_cell_angle_gamma 90.00000

loop_  

_space_group_symop_id  

_space_group_symop_operation_xyz  

1 x,y,z  

2 -x,-y,z  

3 x,-y,z+1/2  

4 -x,y,z+1/2  

5 x,y+1/2,z+1/2  

6 -x,-y+1/2,z+1/2  

7 x,-y+1/2,z  

8 -x,y+1/2,z

loop_  

_atom_site_label  

_atom_site_type_symbol  

_atom_site_symmetry_multiplicity  

_atom_site_Wyckoff_label  

_atom_site_fract_x  

_atom_site_fract_y  

_atom_site_fract_z  

_atom_site_occupancy  

Ta1 Ta 4 c 0.34490 0.25000 0.50000 1.00000  

Ta2 Ta 4 c 0.00580 0.25000 0.76540 1.00000  

S1 S 8 d 0.17300 0.53980 0.38890 1.00000  

S2 S 8 d 0.58430 0.61540 0.39170 1.00000  

Ta3 Ta 8 d 0.28104 0.16619 0.02060 1.00000  

Ta4 Ta 8 d 0.10455 0.60730 0.01440 1.00000

```

Ta<sub>3</sub>S<sub>2</sub>: A2B3\_oC40\_39\_2d\_2c2d - POSCAR

```

A2B3_oC40_39_2d_2c2d & a,b/a,c/a,x1,z1,x2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,  

  ↳ x6,y6,z6 --params=7.47831,2.30292940517,0.749515599113,0.3449,  

  ↳ 0.5,0.0058,0.7654,0.173,0.5398,0.3889,0.5843,0.6154,0.3917,  

  ↳ 0.28104,0.16619,0.0206,0.10455,0.6073,0.0144 & Abm2 C2v^{15}  

  ↳ #39 (c^2d^4) & oC40 & None & Ta3S2 & S. J. Kim and K. S.  

  ↳ Nanjundaswamy and T. Hughbanks, Inorg. Chem. 30, 159-164 (1991)
1.0000000000000000
7.4783100000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.6110100000000000 -2.8025550000000000
0.0000000000000000 8.6110100000000000 2.8025550000000000
S Ta  

8 12
Direct
0.1730000000000000 0.1509000000000000 0.9287000000000000 S (8d)
-0.1730000000000000 -0.9287000000000000 -0.1509000000000000 S (8d)
0.1730000000000000 -0.4287000000000000 0.3491000000000000 S (8d)
-0.1730000000000000 0.6509000000000000 1.4287000000000000 S (8d)
0.5843000000000000 0.2237000000000000 1.0071000000000000 S (8d)
-0.5843000000000000 -1.0071000000000000 -0.2237000000000000 S (8d)
0.5843000000000000 -0.5071000000000000 0.2763000000000000 S (8d)
-0.5843000000000000 0.7237000000000000 1.5071000000000000 S (8d)
0.3449000000000000 -0.2500000000000000 0.7500000000000000 Ta (4c)
-0.3449000000000000 0.2500000000000000 1.2500000000000000 Ta (4c)
0.0058000000000000 -0.5154000000000000 1.0154000000000000 Ta (4c)
-0.0058000000000000 -0.0154000000000000 1.5154000000000000 Ta (4c)
0.2810400000000000 0.1455900000000000 0.1867900000000000 Ta (8d)
-0.2810400000000000 -0.1867900000000000 -0.1455900000000000 Ta (8d)
0.2810400000000000 0.3132100000000000 0.3544100000000000 Ta (8d)
-0.2810400000000000 0.6455900000000000 0.6867900000000000 Ta (8d)
0.1045500000000000 0.5929000000000000 0.6217000000000000 Ta (8d)
-0.1045500000000000 -0.6217000000000000 -0.5929000000000000 Ta (8d)
0.1045500000000000 -0.1217000000000000 -0.0929000000000000 Ta (8d)
-0.1045500000000000 1.0929000000000000 1.1217000000000000 Ta (8d)

```

VPCl<sub>9</sub>: A9BC\_oC44\_39\_3c3d\_a\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'VPCl9'
_chemical_formula_sum 'Cl9 P V'

loop_
_publ_author_name
'M. L. Ziegler'
'B. Nuber'

```

```

'K. Weidenhammer'
'G. Hoch'
_journal_name_full_name
;
Zeitschrift f{"u}r Naturforschung B
;
_journal_volume 32
_journal_year 1977
_journal_page_first 18
_journal_page_last 21
_publ_section_title
;
Die Molek{"u}l- und Kristallstruktur von
  ↳ Tetrachlorphosphoniumpentachlorovanadat (IV), [PCl5]{4}[
  ↳ VCl5]/ The Molecular and Crystal Structure of
  ↳ Tetrachlorphosphoniumpentachlorovanadate (IV), [PCl5]{4}[
  ↳ VCl5]{4}
;

```

# Found in Pearson's Crystal Data - Crystal Structure Database for  
 ↳ Inorganic Compounds, 2013

```

_aflow_title 'VPCl9 Structure'  

_aflow_proto 'A9BC_oC44_39_3c3d_a_c'  

_aflow_params 'a,b/a,c/a,z1,x2,z2,x3,z3,x4,z4,x5,  

  ↳ z5,x6,y6,z6,x7,y7,z7,x8,y8,z8'  

_aflow_params_values '6.2123847492,1.90215711527,2.62509658728,0.5,  

  ↳ 0.2673,0.7493,0.6176,0.8879,0.6246,0.6059,0.6191,0.7476,0.2266,  

  ↳ 0.0857,0.2459,0.1789,0.5932,0.0649,0.18,0.5948,0.4281'  

_aflow_Strukturbericht 'None'  

_aflow_Pearson 'oC44'

_cell_length_a 6.2123847492  

_cell_length_b 11.8169318535  

_cell_length_c 16.3081100040  

_cell_angle_alpha 90.0000000000  

_cell_angle_beta 90.0000000000  

_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'A b m 2'  

_symmetry_Int_Tables_number 39

loop_  

_space_group_symop_id  

_space_group_symop_operation_xyz  

1 x,y,z  

2 -x,-y,z  

3 x,-y,z+1/2  

4 -x,y,z+1/2  

5 x,y+1/2,z+1/2  

6 -x,-y+1/2,z+1/2  

7 x,-y+1/2,z  

8 -x,y+1/2,z

loop_  

_atom_site_label  

_atom_site_type_symbol  

_atom_site_symmetry_multiplicity  

_atom_site_Wyckoff_label  

_atom_site_fract_x  

_atom_site_fract_y  

_atom_site_fract_z  

_atom_site_occupancy  

P1 P 4 a 0.00000 0.00000 0.50000 1.00000  

Cl1 Cl 4 c 0.26730 0.25000 0.74930 1.00000  

Cl2 Cl 4 c 0.61760 0.25000 0.88790 1.00000  

Cl3 Cl 4 c 0.62460 0.25000 0.60590 1.00000  

V1 V 4 c 0.61910 0.25000 0.74760 1.00000  

Cl4 Cl 8 d 0.22660 0.08570 0.24590 1.00000  

Cl5 Cl 8 d 0.17890 0.59320 0.06490 1.00000  

Cl6 Cl 8 d 0.18000 0.59480 0.42810 1.00000

```

VPCl<sub>9</sub>: A9BC\_oC44\_39\_3c3d\_a\_c - POSCAR

```

A9BC_oC44_39_3c3d_a_c & a,b/a,c/a,z1,x2,z2,x3,z3,x4,z4,x5,z5,x6,y6,z6,x7,  

  ↳ y7,z7,x8,y8,z8 --params=6.2123847492,1.90215711527,  

  ↳ 2.62509658728,0.5,0.2673,0.7493,0.6176,0.8879,0.6246,0.6059,  

  ↳ 0.6191,0.7476,0.2266,0.0857,0.2459,0.1789,0.5932,0.0649,0.18,  

  ↳ 0.5948,0.4281 & Abm2 C2v^{15} #39 (ac^4d^3) & oC44 & None &  

  ↳ VPCl9 & M. L. Ziegler et al., Z. Naturforsch. B 32, 18-21 (1977)
1.0000000000000000
6.2123847492000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.9084659267500000 -8.1540550020000000
0.0000000000000000 5.9084659267500000 8.1540550020000000
Cl P V  

18 2 2
Direct
0.2673000000000000 -0.4993000000000000 0.9993000000000000 Cl (4c)
-0.2673000000000000 0.0007000000000000 1.4993000000000000 Cl (4c)
0.6176000000000000 -0.6379000000000000 1.1379000000000000 Cl (4c)
-0.6176000000000000 -0.1379000000000000 1.6379000000000000 Cl (4c)
0.6246000000000000 -0.3559000000000000 0.8559000000000000 Cl (4c)
-0.6246000000000000 0.1441000000000000 1.3559000000000000 Cl (4c)
0.2266000000000000 -0.1602000000000000 0.3316000000000000 Cl (8d)
-0.2266000000000000 -0.3316000000000000 0.1602000000000000 Cl (8d)
0.2266000000000000 0.1684000000000000 0.6602000000000000 Cl (8d)
-0.2266000000000000 0.3398000000000000 0.8316000000000000 Cl (8d)
0.1789000000000000 0.5283000000000000 0.6581000000000000 Cl (8d)
-0.1789000000000000 -0.6581000000000000 -0.5283000000000000 Cl (8d)
0.1789000000000000 -0.1581000000000000 -0.0283000000000000 Cl (8d)
-0.1789000000000000 1.0283000000000000 1.1581000000000000 Cl (8d)
0.1800000000000000 0.1667000000000000 1.0229000000000000 Cl (8d)
-0.1800000000000000 -1.0229000000000000 -0.1667000000000000 Cl (8d)
0.1800000000000000 -0.5229000000000000 0.3333000000000000 Cl (8d)

```

```

-0.18000000000000 0.66670000000000 1.52290000000000 Cl (8d)
0.00000000000000 -0.50000000000000 0.50000000000000 P (4a)
0.00000000000000 0.00000000000000 1.00000000000000 P (4a)
0.61910000000000 -0.49760000000000 0.99760000000000 V (4c)
-0.61910000000000 0.00240000000000 1.49760000000000 V (4c)

```

K<sub>2</sub>CdPb: AB2C\_oC16\_40\_a\_2b\_b - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'K2CdPb'
_chemical_formula_sum 'Cd K2 Pb'

loop_
_publ_author_name
'R. Matthes'
'H.-U. Schuster'
_journal_name_full_name
;
Zeitschrift f {\u}r Naturforschung B
;
_journal_volume 34
_journal_year 1979
_journal_page_first 541
_journal_page_last 543
_publ_section_title
;
Synthese und Struktur der Phasen KS_{2}SCdSn und KS_{2}SCdPb/ Synthesis
and Structure of the Phase KS_{2}SCdSn and KS_{2}SCdPb
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
Inorganic Compounds, 2013

_aflow_title 'KS_{2}SCdPb Structure'
_aflow_proto 'AB2C_oC16_40_a_2b_b'
_aflow_params 'a,b/a,c/a,z_{1},y_{2},z_{2},y_{3},z_{3},y_{4},z_{4}'
_aflow_params_values '6.4580033647,1.33199132859,1.69634561784,0.0,
0.3467,0.1773,0.8661,0.3301,0.7281,0.0093'
_aflow_strukturbericht 'None'
_aflow_pearson 'oC16'

_cell_length_a 6.4580033647
_cell_length_b 8.6020044818
_cell_length_c 10.9550057077
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'A m a 2'
_symmetry_Int_Tables_number 40

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 x+1/2,-y,z
4 -x+1/2,y,z
5 x,y+1/2,z+1/2
6 -x,-y+1/2,z+1/2
7 x+1/2,-y+1/2,z+1/2
8 -x+1/2,y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cd1 Cd 4 a 0.00000 0.00000 0.00000 1.00000
K1 K 4 b 0.25000 0.34670 0.17730 1.00000
K2 K 4 b 0.25000 0.86610 0.33010 1.00000
Pb1 Pb 4 b 0.25000 0.72810 0.00930 1.00000

```

K<sub>2</sub>CdPb: AB2C\_oC16\_40\_a\_2b\_b - POSCAR

```

AB2C_oC16_40_a_2b_b & a,b/a,c/a,z1,y2,z2,y3,z3,y4,z4 --params=
6.4580033647,1.33199132859,1.69634561784,0.0,0.3467,0.1773,
0.8661,0.3301,0.7281,0.0093 & Ama2 C_{2v}^{16} #40 (ab^3) &
oC16 & None & K2CdPb & R. Matthes and H.-U. Schuster, Z.
Naturforsch. B 34, 541-543 (1979)
1.00000000000000
6.45800336470000 0.00000000000000 0.00000000000000
0.00000000000000 4.30100224090000 -5.47750285385000
0.00000000000000 4.30100224090000 5.47750285385000
Cd K Pb
2 4 2
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Cd (4a)
0.50000000000000 0.00000000000000 0.00000000000000 Cd (4a)
0.25000000000000 0.16940000000000 0.52400000000000 K (4b)
0.75000000000000 -0.52400000000000 -0.16940000000000 K (4b)
0.25000000000000 0.53600000000000 1.19620000000000 K (4b)
0.75000000000000 -1.19620000000000 -0.53600000000000 K (4b)
0.25000000000000 0.71880000000000 0.73740000000000 Pb (4b)
0.75000000000000 -0.73740000000000 -0.71880000000000 Pb (4b)

```

CeTe<sub>3</sub>: AB<sub>3</sub>\_oC16\_40\_b\_3b - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'CeTe3'
_chemical_formula_sum 'Ce Te3'

loop_
_publ_author_name
'C. Malliakas'
'S. J. L. Billinge'
'H. J. Kim'
'M. G. Kanatzidis'
_journal_name_full_name
;
Journal of the American Chemical Society
;
_journal_volume 127
_journal_year 2005
_journal_page_first 6510
_journal_page_last 6511
_publ_section_title
;
Square Nets of Tellurium: Rare-Earth Dependent Variation in the
Charge-Density Wave of $RETe_{3}$ ($RES$ = Rare-Earth Element
)
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
Inorganic Compounds, 2013

_aflow_title 'CeTe_{3}$ Structure'
_aflow_proto 'AB3_oC16_40_b_3b'
_aflow_params 'a,b/a,c/a,y_{1},z_{1},y_{2},z_{2},y_{3},z_{3},y_{4},z_{4}'
_aflow_params_values '4.3850022361,5.92335058951,0.997331752147,0.83109,
0.0,0.70417,0.0021,0.56971,0.4966,-0.07002,0.4978'
_aflow_strukturbericht 'None'
_aflow_pearson 'oC16'

_cell_length_a 4.3850022361
_cell_length_b 25.9739055802
_cell_length_c 4.3733019633
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'A m a 2'
_symmetry_Int_Tables_number 40

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 x+1/2,-y,z
4 -x+1/2,y,z
5 x,y+1/2,z+1/2
6 -x,-y+1/2,z+1/2
7 x+1/2,-y+1/2,z+1/2
8 -x+1/2,y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ce1 Ce 4 b 0.25000 0.83109 0.00000 1.00000
Te1 Te 4 b 0.25000 0.70417 0.00210 1.00000
Te2 Te 4 b 0.25000 0.56971 0.49660 1.00000
Te3 Te 4 b 0.25000 -0.07002 0.49780 1.00000

```

CeTe<sub>3</sub>: AB<sub>3</sub>\_oC16\_40\_b\_3b - POSCAR

```

AB3_oC16_40_b_3b & a,b/a,c/a,y1,z1,y2,z2,y3,z3,y4,z4 --params=
4.3850022361,5.92335058951,0.997331752147,0.83109,0.0,0.70417,
0.0021,0.56971,0.4966,-0.07002,0.4978 & Ama2 C_{2v}^{16} #40 (b
^4) & oC16 & None & CeTe3 & C. Malliakas et al., J. Am.
Chem. Soc. 127, 6510-6511 (2005)
1.00000000000000
4.38500223610000 0.00000000000000 0.00000000000000
0.00000000000000 12.98695279010000 -2.18665098165000
0.00000000000000 12.98695279010000 2.18665098165000
Ce Te
2 6
Direct
0.25000000000000 0.83109000000000 0.83109000000000 Ce (4b)
0.75000000000000 -0.83109000000000 -0.83109000000000 Ce (4b)
0.25000000000000 0.70207000000000 0.70627000000000 Te (4b)
0.75000000000000 -0.70627000000000 -0.70207000000000 Te (4b)
0.25000000000000 0.07311000000000 1.06631000000000 Te (4b)
0.75000000000000 -1.06631000000000 -0.07311000000000 Te (4b)
0.25000000000000 -0.56782000000000 0.42778000000000 Te (4b)
0.75000000000000 -0.42778000000000 0.56782000000000 Te (4b)

```

W<sub>3</sub>O<sub>10</sub>: A10B<sub>3</sub>\_oF52\_42\_2abce\_ab - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

```

```

_chemical_name_mineral 'W3O10'
_chemical_formula_sum 'O10 W3'

loop_
  _publ_author_name
    'B. Gerand'
    'G. Nowogrocki'
    'M. Figlarz'
  _journal_name_full_name
    ;
  Journal of Solid State Chemistry
  ;
  _journal_volume 38
  _journal_year 1981
  _journal_page_first 312
  _journal_page_last 320
  _publ_section_title
    ;
  A new tungsten trioxide hydrate, WOS_{3}$\{\text{periodcentered}\}1/3H_{2}
    ↪ SO: Preparation, characterization, and crystallographic study
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'WS_{3}$O_{10}$ Structure'
_aflow_proto 'A10B3_oF52_42_2abce_ab'
_aflow_params 'a,b/a,c/a,z_{1},z_{2},z_{3},z_{4},z_{5},y_{6},z_{6},x_{7}
  ↪ ,y_{7},z_{7}'
_aflow_params_values '7.4494846573,1.70036689767,1.04688136975,0.76,0.27
  ↪ ,0.0,0.31,0.06,0.79,0.6,0.17,0.11,0.07'
_aflow_strukturbericht 'None'
_aflow_pearson 'oF52'

_cell_length_a 7.4494846573
_cell_length_b 12.6668571160
_cell_length_c 7.7987267020
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "F m m 2"
_symmetry_int_tables_number 42

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 -x,-y,z
  3 -x,y,z
  4 x,-y,z
  5 x,y+1/2,z+1/2
  6 -x,-y+1/2,z+1/2
  7 -x,y+1/2,z+1/2
  8 x,-y+1/2,z+1/2
  9 x+1/2,y,z+1/2
  10 -x+1/2,-y,z+1/2
  11 -x+1/2,y,z+1/2
  12 x+1/2,-y,z+1/2
  13 x+1/2,y+1/2,z
  14 -x+1/2,-y+1/2,z
  15 -x+1/2,y+1/2,z
  16 x+1/2,-y+1/2,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  O1 O 4 a 0.00000 0.00000 0.76000 1.00000
  O2 O 4 a 0.00000 0.00000 0.27000 1.00000
  W1 W 4 a 0.00000 0.00000 0.00000 1.00000
  O3 O 8 b 0.25000 0.25000 0.31000 1.00000
  W2 W 8 b 0.25000 0.25000 0.06000 1.00000
  O4 O 8 c 0.00000 0.79000 0.60000 1.00000
  O5 O 16 e 0.17000 0.11000 0.07000 1.00000

```

W<sub>3</sub>O<sub>10</sub>: A10B3\_oF52\_42\_2abce\_ab - POSCAR

```

A10B3_oF52_42_2abce_ab & a,b/a,c/a,z1,z2,z3,z4,z5,y6,z6,x7,y7,z7 --
  ↪ params=7.4494846573,1.70036689767,1.04688136975,0.76,0.27,0.0,
  ↪ 0.31,0.06,0.79,0.6,0.17,0.11,0.07 & Fmm2 C_{2v}^{18} #42 (a^3b^
  ↪ 2c) & oF52 & None & W3O10 & B. Gerand and G. Nowogrocki and
  ↪ M. Figlarz, J. Solid State Chem. 38, 312-320 (1981)
  1.0000000000000000
  0.0000000000000000 6.33342855800000 3.89936335100000
  3.72474232865000 0.00000000000000 3.89936335100000
  3.72474232865000 6.33342855800000 0.00000000000000
  O W
  10 3
Direct
  0.760000000000000 0.760000000000000 -0.760000000000000 O (4a)
  0.270000000000000 0.270000000000000 -0.270000000000000 O (4a)
  0.310000000000000 0.310000000000000 0.190000000000000 O (8b)
  0.810000000000000 0.810000000000000 -0.310000000000000 O (8b)
  1.390000000000000 -0.190000000000000 0.190000000000000 O (8c)
  -0.190000000000000 1.390000000000000 -1.390000000000000 O (8c)
  0.010000000000000 0.130000000000000 0.210000000000000 O (16e)
  0.130000000000000 0.010000000000000 -0.350000000000000 O (16e)
  -0.210000000000000 0.350000000000000 -0.010000000000000 O (16e)

```

```

0.350000000000000 -0.210000000000000 -0.130000000000000 O (16e)
0.000000000000000 0.000000000000000 0.000000000000000 W (4a)
0.060000000000000 0.060000000000000 0.440000000000000 W (8b)
0.560000000000000 0.560000000000000 -0.060000000000000 W (8b)

```

BN (High-pressure, high-temperature): AB\_oF8\_42\_a\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'BN'
_chemical_formula_sum 'B N'

loop_
  _publ_author_name
    'A. V. Kurdyumov'
    'G. S. Olejnik'
  _journal_name_full_name
    ;
  Kristallografiya, English title: Crystallography Reports
  ;
  _journal_volume 29
  _journal_year 1984
  _journal_page_first 792
  _journal_page_last 793
  _publ_section_title
    ;
  On metastable structures of graphite-like boron nitride
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'BN (High-pressure, high-temperature) Structure'
_aflow_proto 'AB_oF8_42_a_a'
_aflow_params 'a,b/a,c/a,z_{1},z_{2}'
_aflow_params_values '2.5000573158,1.33999999999,1.73599999999,0.0,0.333
  ↪ '
_aflow_strukturbericht 'None'
_aflow_pearson 'oF8'

_cell_length_a 2.5000573158
_cell_length_b 3.3500768031
_cell_length_c 4.3400995002
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "F m m 2"
_symmetry_int_tables_number 42

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 -x,-y,z
  3 -x,y,z
  4 x,-y,z
  5 x,y+1/2,z+1/2
  6 -x,-y+1/2,z+1/2
  7 -x,y+1/2,z+1/2
  8 x,-y+1/2,z+1/2
  9 x+1/2,y,z+1/2
  10 -x+1/2,-y,z+1/2
  11 -x+1/2,y,z+1/2
  12 x+1/2,-y,z+1/2
  13 x+1/2,y+1/2,z
  14 -x+1/2,-y+1/2,z
  15 -x+1/2,y+1/2,z
  16 x+1/2,-y+1/2,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  B1 B 4 a 0.00000 0.00000 0.00000 1.00000
  N1 N 4 a 0.00000 0.00000 0.33300 1.00000

```

BN (High-pressure, high-temperature): AB\_oF8\_42\_a\_a - POSCAR

```

AB_oF8_42_a_a & a,b/a,c/a,z1,z2 --params=2.5000573158,1.33999999999,
  ↪ 1.73599999999,0.0,0.333 & Fmm2 C_{2v}^{18} #42 (a^2) & oF8 &
  ↪ None & BN & A. V. Kurdyumov and G. S. Olejnik,
  ↪ Kristallografiya 29, 792-793 (1984)
  1.0000000000000000
  0.000000000000000 1.67503840155000 2.17004975010000
  1.25002865790000 0.00000000000000 2.17004975010000
  1.25002865790000 1.67503840155000 0.00000000000000
  B N
  1 1
Direct
  0.000000000000000 0.000000000000000 0.000000000000000 B (4a)
  0.333000000000000 0.333000000000000 -0.333000000000000 N (4a)

```

MnGa<sub>2</sub>Sb<sub>2</sub>: A2B2C\_oI20\_45\_c\_b\_c - CIF

```

# CIF file
data_findsym-output

```

```

_audit_creation_method FINDSYM
_chemical_name_mineral 'MnGa2Sb2'
_chemical_formula_sum 'Ga2 Mn Sb2'

loop_
  _publ_author_name
    'W. Sakakibara'
    'Y. Hayashi'
    'H. Takizawa'
  _journal_name_full_name
    'Journal of The Ceramic Society of Japan'
  _journal_volume 117
  _journal_year 2009
  _journal_page_first 72
  _journal_page_last 75
  _publ_section_title
    'MnGa2Sb2, a new ferromagnetic compound synthesized under high
    ↪ pressure'
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'MnGa2Sb2 Structure'
_aflow_proto 'A2BC2_oI20_45_c_b_c'
_aflow_params 'a,b/a,c/a,z1,x2,y2,z2,x3,y3,z3'
_aflow_params_values '5.9678340183,1.97721179624,0.981568364609,0.25,
↪ 0.2729,0.629,0.493,0.2296,0.8629,0.474'
_aflow_strukturbericht 'None'
_aflow_pearson 'oI20'

_cell_length_a 5.9678340183
_cell_length_b 11.7996718190
_cell_length_c 5.8578370776
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I b a 2"
_symmetry_Int_Tables_number 45

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x,y,z+1/2
4 x,-y,z+1/2
5 x+1/2,y+1/2,z+1/2
6 -x+1/2,-y+1/2,z+1/2
7 -x+1/2,y+1/2,z
8 x+1/2,-y+1/2,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Mn1 Mn 4 b 0.0000 0.5000 0.2500 1.0000
Ga Ga 8 c 0.2729 0.6290 0.4930 1.0000
Sb1 Sb 8 c 0.2296 0.8629 0.4740 1.0000

```

MnGa<sub>2</sub>Sb<sub>2</sub>: A2BC2\_oI20\_45\_c\_b\_c - POSCAR

```

A2BC2_oI20_45_c_b_c & a,b/a,c/a,z1,x2,y2,z2,x3,y3,z3 --params=
↪ 5.9678340183,1.97721179624,0.981568364609,0.25,0.2729,0.629,
↪ 0.493,0.2296,0.8629,0.474 & Iba2_C_{2v}^{[21]} #45 (bc^2) & oI20
↪ & None & MnGa2Sb2 & W. Sakakibara and Y. Hayashi and H.
↪ Takizawa, J. Ceram. Soc. Jpn. 117, 72-75 (2009)
1.00000000000000
-2.98391700915000 5.89983590950000 2.92891853880000
2.98391700915000 -5.89983590950000 2.92891853880000
2.98391700915000 5.89983590950000 -2.92891853880000
Ga Mn Sb
4 2 4
Direct
1.12200000000000 0.76590000000000 0.90190000000000 Ga (8c)
-0.13600000000000 0.22010000000000 -0.90190000000000 Ga (8c)
0.36400000000000 1.26590000000000 -0.35610000000000 Ga (8c)
1.62200000000000 0.72010000000000 0.35610000000000 Ga (8c)
0.75000000000000 0.25000000000000 0.50000000000000 Mn (4b)
0.25000000000000 0.75000000000000 0.50000000000000 Mn (4b)
1.33690000000000 0.70360000000000 1.09250000000000 Sb (8c)
-0.38890000000000 0.24440000000000 -1.09250000000000 Sb (8c)
0.11110000000000 1.20360000000000 -0.63330000000000 Sb (8c)
1.83690000000000 0.74440000000000 0.63330000000000 Sb (8c)

```

TiFeSi: ABC\_oI36\_46\_ac\_bc\_3b - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'TiFeSi'
_chemical_formula_sum 'Fe Si Ti'
loop_

```

```

  _publ_author_name
    'W. Jeitschko'
  _journal_name_full_name
    'Acta Crystallographica Section B: Structural Science'
  _journal_volume 26
  _journal_year 1970
  _journal_page_first 815
  _journal_page_last 822
  _publ_section_title
    'The crystal structure of TiFeSi and related compounds'
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'TiFeSi Structure'
_aflow_proto 'ABC_oI36_46_ac_bc_3b'
_aflow_params 'a,b/a,c/a,z1,y2,z2,x2,y2,z2,x3,y3,z3,y4,z4,y5,z5'
↪ ,z5,x6,y6,z6,x7,y7,z7'
_aflow_params_values '6.9969353511,1.54780620265,0.898527940538,0.25,
↪ 0.5253,0.0054,0.7207,0.7706,-0.0021,-0.0823,0.2996,0.7963,
↪ 0.5295,0.6236,0.1199,0.006,0.3325,0.4952'
_aflow_strukturbericht 'None'
_aflow_pearson 'oI36'

_cell_length_a 6.9969353511
_cell_length_b 10.8298999360
_cell_length_c 6.2869419111
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I m a 2"
_symmetry_Int_Tables_number 46

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x+1/2,y,z
4 x+1/2,-y,z
5 x+1/2,y+1/2,z+1/2
6 -x+1/2,-y+1/2,z+1/2
7 -x,y+1/2,z+1/2
8 x,-y+1/2,z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Fe1 Fe 4 a 0.0000 0.0000 0.2500 1.0000
Si1 Si 4 b 0.2500 0.5253 0.0054 1.0000
Ti1 Ti 4 b 0.2500 0.7207 0.7706 1.0000
Ti2 Ti 4 b 0.2500 -0.0021 -0.0823 1.0000
Ti3 Ti 4 b 0.2500 0.2996 0.7963 1.0000
Fe2 Fe 8 c 0.5295 0.6236 0.1199 1.0000
Si2 Si 8 c 0.0060 0.3325 0.4952 1.0000

```

TiFeSi: ABC\_oI36\_46\_ac\_bc\_3b - POSCAR

```

ABC_oI36_46_ac_bc_3b & a,b/a,c/a,z1,y2,z2,y3,z3,y4,z4,y5,z5,x6,y6,z6,x7,
↪ y7,z7 --params=6.9969353511,1.54780620265,0.898527940538,0.25,
↪ 0.5253,0.0054,0.7207,0.7706,-0.0021,-0.0823,0.2996,0.7963,
↪ 0.5295,0.6236,0.1199,0.006,0.3325,0.4952 & Ima2_C_{2v}^{[22]} #46
↪ (ab^4c^2) & oI36 & None & TiFeSi & W. Jeitschko, Acta
↪ Crystallogr. Sect. B Struct. Sci. 26, 815-822 (1970)
1.00000000000000
-3.49846767555000 5.41494996800000 3.14347095555000
3.49846767555000 -5.41494996800000 3.14347095555000
3.49846767555000 5.41494996800000 -3.14347095555000
Fe Si Ti
6 6 6
Direct
0.25000000000000 0.25000000000000 0.00000000000000 Fe (4a)
0.25000000000000 0.75000000000000 0.50000000000000 Fe (4a)
0.74350000000000 0.64940000000000 1.15310000000000 Fe (8c)
-0.50370000000000 -0.40960000000000 -1.15310000000000 Fe (8c)
-0.50370000000000 1.14940000000000 0.40590000000000 Fe (8c)
0.74350000000000 0.09040000000000 0.59410000000000 Fe (8c)
0.53070000000000 0.25540000000000 0.77530000000000 Si (4b)
-0.51990000000000 0.75540000000000 0.22470000000000 Si (4b)
0.82770000000000 0.50120000000000 0.33850000000000 Si (8c)
0.16270000000000 0.48920000000000 -0.33850000000000 Si (8c)
0.16270000000000 1.00120000000000 0.17350000000000 Si (8c)
0.82770000000000 0.98920000000000 0.82650000000000 Si (8c)
1.49130000000000 1.02060000000000 0.97070000000000 Ti (4b)
0.04990000000000 1.52060000000000 0.02930000000000 Ti (4b)
-0.08440000000000 0.16770000000000 0.24790000000000 Ti (4b)
-0.08020000000000 0.66770000000000 0.75210000000000 Ti (4b)
1.09590000000000 1.04630000000000 0.54960000000000 Ti (4b)
0.49670000000000 1.54630000000000 0.45040000000000 Ti (4b)

```

α-RbPr[MoO<sub>4</sub>]<sub>2</sub>: A2B8CD\_oP24\_48\_k\_2m\_d\_b - CIF

```

# CIF file
data_findsym-output

```

```

_audit_creation_method FINDSYM
_chemical_name_mineral 'alpha-RbPr[MoO4]2'
_chemical_formula_sum 'Mo2 O8 Pr Rb'

loop_
  _publ_author_name
  'R. F. Klevtsova'
  'P. V. Klevtsov'
  _journal_name_full_name
  ;
  Kristallografiya, English title: Crystallography Reports
  ;
  _journal_volume 15
  _journal_year 1970
  _journal_page_first 466
  _journal_page_last 470
  _publ_section_title
  ;
  Polymorphism of rubidium-praseodymium molybdate, RbPr(MoO4)2
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title '$\alpha$-RbPr[MoO4]2 Structure'
_aflow_proto 'A2B8CD_oP24_48_k_2m_d_b'
_aflow_params 'a,b/a,c/a,z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5}'
_aflow_params_values '6.3302356554,1.0,1.50710900473,0.4978,0.56,0.629,
  ↳ 0.114,0.642,0.558,0.601'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP24'

_cell_length_a 6.3302356554
_cell_length_b 6.3302356554
_cell_length_c 9.5403551583
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2/n 2/n 2/n (origin choice 2)"
_symmetry_Int_Tables_number 48

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x,-y+1/2,-z+1/2
  3 -x+1/2,y,-z+1/2
  4 -x+1/2,-y+1/2,z
  5 -x,-y,-z
  6 -x,y+1/2,z+1/2
  7 x+1/2,-y,z+1/2
  8 x+1/2,y+1/2,-z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Rb1 Rb 2 b 0.75000 0.25000 0.25000 1.00000
  Pr1 Pr 2 d 0.25000 0.75000 0.25000 1.00000
  Mo1 Mo 4 k 0.25000 0.25000 0.49780 1.00000
  O1 O 8 m 0.56000 0.62900 0.11400 1.00000
  O2 O 8 m 0.64200 0.55800 0.60100 1.00000

```

$\alpha$ -RbPr[MoO<sub>4</sub>]<sub>2</sub>: A2B8CD\_oP24\_48\_k\_2m\_d\_b - POSCAR

```

A2B8CD_oP24_48_k_2m_d_b & a,b/a,c/a,z3,x4,y4,z4,x5,y5,z5 --params=
  ↳ 6.3302356554,1.0,1.50710900473,0.4978,0.56,0.629,0.114,0.642,
  ↳ 0.558,0.601 & Pnnn D_{2h}^{2} #48 (bdkm^2) & oP24 & None & RbPr
  ↳ [MoO4]2 & alpha & R. F. Klevtsova and P. V. Klevtsov,
  ↳ Kristallografiya 15, 466-470 (1970)
  1.00000000000000
  6.33023565540000 0.00000000000000 0.00000000000000
  0.00000000000000 6.33023565540000 0.00000000000000
  0.00000000000000 0.00000000000000 9.54035515830000
  Mo O Pr Rb
  4 16 2 2
Direct
  0.25000000000000 0.25000000000000 0.49780000000000 Mo (4k)
  0.25000000000000 0.25000000000000 0.00220000000000 Mo (4k)
  0.75000000000000 0.75000000000000 -0.49780000000000 Mo (4k)
  0.75000000000000 0.75000000000000 0.99780000000000 Mo (4k)
  0.56000000000000 0.62900000000000 0.11400000000000 O (8m)
  -0.06000000000000 -0.12900000000000 0.11400000000000 O (8m)
  -0.06000000000000 0.62900000000000 0.38600000000000 O (8m)
  0.56000000000000 -0.12900000000000 0.38600000000000 O (8m)
  -0.56000000000000 -0.62900000000000 -0.11400000000000 O (8m)
  1.06000000000000 1.12900000000000 -0.11400000000000 O (8m)
  1.06000000000000 -0.62900000000000 0.61400000000000 O (8m)
  -0.56000000000000 1.12900000000000 0.61400000000000 O (8m)
  0.64200000000000 0.55800000000000 0.60100000000000 O (8m)
  -0.14200000000000 -0.05800000000000 0.60100000000000 O (8m)
  -0.14200000000000 0.55800000000000 -0.10100000000000 O (8m)
  0.64200000000000 -0.05800000000000 -0.10100000000000 O (8m)
  -0.64200000000000 -0.55800000000000 -0.60100000000000 O (8m)
  1.14200000000000 1.05800000000000 -0.60100000000000 O (8m)
  1.14200000000000 -0.55800000000000 1.10100000000000 O (8m)
  -0.64200000000000 1.05800000000000 1.10100000000000 O (8m)
  0.25000000000000 0.75000000000000 0.25000000000000 Pr (2d)

```

0.75000000000000	0.25000000000000	0.75000000000000	Pr	(2d)
0.75000000000000	0.25000000000000	0.25000000000000	Rb	(2b)
0.25000000000000	0.75000000000000	0.75000000000000	Rb	(2b)

$\beta$ -Ta<sub>2</sub>O<sub>5</sub>: ASB2\_oP14\_49\_dehq\_ab - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'beta-Ta2O5'
_chemical_formula_sum 'O5 Ta2'

loop_
  _publ_author_name
  'L. A. Aleshina'
  'S. V. Loginova'
  _journal_name_full_name
  ;
  Crystallography Reports
  ;
  _journal_volume 47
  _journal_year 2002
  _journal_page_first 415
  _journal_page_last 419
  _publ_section_title
  ;
  Rietveld analysis of X-ray diffraction pattern from $\beta$Ta2O5
  ↳ {5}$ oxide
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title '$\beta$Ta2O5 Structure'
_aflow_proto 'ASB2_oP14_49_dehq_ab'
_aflow_params 'a,b/a,c/a,x_{6},y_{6}'
_aflow_params_values '3.6705354001,1.69539132804,2.12544314151,0.002,
  ↳ 0.681'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP14'

_cell_length_a 3.6705354001
_cell_length_b 6.2229938866
_cell_length_c 7.8015142918
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2/c 2/c 2/m"
_symmetry_Int_Tables_number 49

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x,-y,-z+1/2
  3 -x,y,-z+1/2
  4 -x,-y,z
  5 -x,-y,-z
  6 -x,y,z+1/2
  7 x,-y,z+1/2
  8 x,y,-z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Ta1 Ta 2 a 0.00000 0.00000 0.00000 1.00000
  Ta2 Ta 2 b 0.50000 0.50000 0.00000 1.00000
  O1 O 2 d 0.50000 0.00000 0.00000 1.00000
  O2 O 2 e 0.00000 0.00000 0.25000 1.00000
  O3 O 2 h 0.50000 0.50000 0.25000 1.00000
  O4 O 4 q 0.00200 0.68100 0.00000 1.00000

```

$\beta$ -Ta<sub>2</sub>O<sub>5</sub>: ASB2\_oP14\_49\_dehq\_ab - POSCAR

```

ASB2_oP14_49_dehq_ab & a,b/a,c/a,x6,y6 --params=3.6705354001,
  ↳ 1.69539132804,2.12544314151,0.002,0.681 & Pcm D_{2h}^{3} #49 (
  ↳ abdehq) & oP14 & None & Ta2O5 & beta & L. A. Aleshina and S. V.
  ↳ Loginova, Crystallogr. Rep. 47, 415-419 (2002)
  1.00000000000000
  3.67053540010000 0.00000000000000 0.00000000000000
  0.00000000000000 6.22299388660000 0.00000000000000
  0.00000000000000 0.00000000000000 7.80151429180000
  O Ta
  10 4
Direct
  0.50000000000000 0.00000000000000 0.00000000000000 O (2d)
  0.50000000000000 0.00000000000000 0.50000000000000 O (2d)
  0.00000000000000 0.00000000000000 0.25000000000000 O (2e)
  0.00000000000000 0.00000000000000 0.75000000000000 O (2e)
  0.50000000000000 0.50000000000000 0.25000000000000 O (2h)
  0.50000000000000 0.50000000000000 0.75000000000000 O (2h)
  0.00200000000000 0.68100000000000 0.00000000000000 O (4q)
  -0.00200000000000 -0.68100000000000 0.00000000000000 O (4q)
  -0.00200000000000 0.68100000000000 0.50000000000000 O (4q)
  0.00200000000000 -0.68100000000000 0.50000000000000 O (4q)
  0.00000000000000 0.00000000000000 0.00000000000000 Ta (2a)
  0.00000000000000 0.00000000000000 0.50000000000000 Ta (2a)

```

0.5000000000000000	0.5000000000000000	0.0000000000000000	Ta	(2b)
0.5000000000000000	0.5000000000000000	0.5000000000000000	Ta	(2b)

CsPr[MoO<sub>4</sub>]<sub>2</sub>: AB2C8D\_oP24\_49\_g\_q\_2qr\_e - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'CsPr[MoO4]2'
_chemical_formula_sum 'Cs Mo2 O8 Pr'

loop_
_publ_author_name
'V. A. Vinokurov'
'P. V. Klevtsov'
_journal_name_full_name
;
Soviet Physics Crystallography
;
_journal_volume 17
_journal_year 1972
_journal_page_first 102
_journal_page_last 106
_publ_section_title
;
Polymorphism and crystallization of binary cesium-rare earth molybdates
↪ CsLn(MoOS_{4})_{2}
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'CsPr[MoOS_{4}]_{2} Structure'
_aflow_proto 'AB2C8D_oP24_49_g_q_2qr_e'
_aflow_params 'a,b/a,c/a,x_{3},y_{3},x_{4},y_{4},x_{5},y_{5},x_{6},y_{6}
↪ ,z_{6}'
_aflow_params_values '6.3302356554,1.0,1.50710900473,0.5184,0.7996,0.258
↪ ,-0.0697,0.3652,0.6307,0.2617,0.1943,0.8286'
_aflow_strukturbericht 'None'
_aflow_pearson 'oP24'

_cell_length_a 6.3302356554
_cell_length_b 6.3302356554
_cell_length_c 9.5403551583
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2/c 2/c 2/m"
_symmetry_Int_Tables_number 49

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z+1/2
3 -x,y,-z+1/2
4 -x,-y,z
5 -x,-y,-z
6 -x,y,z+1/2
7 x,-y,z+1/2
8 x,y,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Pr1 Pr 2 e 0.00000 0.00000 0.25000 1.00000
Cs1 Cs 2 g 0.00000 0.50000 0.25000 1.00000
Mo1 Mo 4 q 0.51840 0.79960 0.00000 1.00000
O1 O 4 q 0.25800 -0.06970 0.00000 1.00000
O2 O 4 q 0.36520 0.63070 0.00000 1.00000
O3 O 8 r 0.26170 0.19430 0.82860 1.00000
```

CsPr[MoO<sub>4</sub>]<sub>2</sub>: AB2C8D\_oP24\_49\_g\_q\_2qr\_e - POSCAR

```
AB2C8D_oP24_49_g_q_2qr_e & a,b/a,c/a,x3,y3,x4,y4,x5,y5,x6,y6,z6 --params
↪ =6.3302356554,1.0,1.50710900473,0.5184,0.7996,0.258,-0.0697,
↪ 0.3652,0.6307,0.2617,0.1943,0.8286 & Pccm D_{2h}^{3} #49 (egq^
↪ 3r) & oP24 & None & CsPr[MoO4]2 & V. A. Vinokurov and P. V.
↪ Klevtsov, Sov. Phys. Crystallogr. 17, 102-106 (1972)
1.0000000000000000
6.33023565540000 0.00000000000000 0.00000000000000
0.00000000000000 6.33023565540000 0.00000000000000
0.00000000000000 0.00000000000000 9.54035515830000
Cs Mo O Pr
2 4 16 2
Direct
0.00000000000000 0.50000000000000 0.25000000000000 Cs (2g)
0.00000000000000 0.50000000000000 0.75000000000000 Cs (2g)
0.51840000000000 0.79960000000000 0.00000000000000 Mo (4q)
-0.51840000000000 -0.79960000000000 0.00000000000000 Mo (4q)
-0.51840000000000 0.79960000000000 0.50000000000000 Mo (4q)
0.51840000000000 -0.79960000000000 0.50000000000000 Mo (4q)
0.25800000000000 -0.06970000000000 0.00000000000000 O (4q)
-0.25800000000000 0.06970000000000 0.00000000000000 O (4q)
-0.25800000000000 -0.06970000000000 0.50000000000000 O (4q)
0.25800000000000 0.06970000000000 0.50000000000000 O (4q)
0.36520000000000 0.63070000000000 0.00000000000000 O (4q)
```

-0.3652000000000000	-0.6307000000000000	0.0000000000000000	O	(4q)
-0.3652000000000000	0.6307000000000000	0.5000000000000000	O	(4q)
0.3652000000000000	-0.6307000000000000	0.5000000000000000	O	(4q)
0.2617000000000000	0.1943000000000000	0.8286000000000000	O	(8r)
-0.2617000000000000	-0.1943000000000000	0.8286000000000000	O	(8r)
-0.2617000000000000	0.1943000000000000	-0.3286000000000000	O	(8r)
0.2617000000000000	-0.1943000000000000	-0.3286000000000000	O	(8r)
0.2617000000000000	-0.1943000000000000	-0.8286000000000000	O	(8r)
0.2617000000000000	0.1943000000000000	-0.8286000000000000	O	(8r)
0.2617000000000000	-0.1943000000000000	1.3286000000000000	O	(8r)
-0.2617000000000000	0.1943000000000000	1.3286000000000000	O	(8r)
0.0000000000000000	0.0000000000000000	0.2500000000000000	Pr	(2e)
0.0000000000000000	0.0000000000000000	0.7500000000000000	Pr	(2e)

La<sub>2</sub>NiO<sub>4</sub>: A2BC4\_oP28\_50\_ij\_ac\_ijm - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'La2NiO4'
_chemical_formula_sum 'La2 Ni O4'

loop_
_publ_author_name
'P. Odier'
'M. Leblanc'
'J. Choisnet'
_journal_name_full_name
;
Materials Research Bulletin
;
_journal_volume 21
_journal_year 1986
_journal_page_first 787
_journal_page_last 796
_publ_section_title
;
Structural characterization of an orthorhombic form of La_{2}NiO_{4}
↪ $
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'La_{2}NiO_{4} Structure'
_aflow_proto 'A2BC4_oP28_50_ij_ac_ijm'
_aflow_params 'a,b/a,c/a,y_{3},y_{4},y_{5},y_{6},x_{7},y_{7},z_{7}'
_aflow_params_values '5.5348069961,2.26684733515,0.987895212291,0.8726,
↪ 0.445,0.3867,-0.076,0.5,0.743,0.226'
_aflow_strukturbericht 'None'
_aflow_pearson 'oP28'

_cell_length_a 5.5348069961
_cell_length_b 12.5465624897
_cell_length_c 5.4678093324
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2/b 2/a 2/n (origin choice 2)"
_symmetry_Int_Tables_number 50

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y+1/2,-z
3 -x+1/2,y,-z
4 -x+1/2,-y+1/2,z
5 -x,-y,-z
6 -x,y+1/2,z
7 x+1/2,-y,z
8 x+1/2,y+1/2,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ni1 Ni 2 a 0.25000 0.25000 0.00000 1.00000
Ni2 Ni 2 c 0.75000 0.25000 0.50000 1.00000
La1 La 4 i 0.25000 0.87260 0.00000 1.00000
O1 O 4 i 0.25000 0.44500 0.00000 1.00000
La2 La 4 j 0.25000 0.38670 0.50000 1.00000
O2 O 4 j 0.25000 -0.07600 0.50000 1.00000
O3 O 8 m 0.50000 0.74300 0.22600 1.00000
```

La<sub>2</sub>NiO<sub>4</sub>: A2BC4\_oP28\_50\_ij\_ac\_ijm - POSCAR

```
A2BC4_oP28_50_ij_ac_ijm & a,b/a,c/a,y3,y4,y5,y6,x7,y7,z7 --params=
↪ 5.5348069961,2.26684733515,0.987895212291,0.8726,0.445,0.3867,-
↪ 0.076,0.5,0.743,0.226 & Pban D_{2h}^{4} #50 (aci^2j^2m) & oP28
↪ & None & La2NiO4 & P. Odier and M. Leblanc and J. Choisnet,
↪ Mater. Res. Bull. 21, 787-796 (1986)
1.0000000000000000
5.53480699610000 0.00000000000000 0.00000000000000
0.00000000000000 12.54656248970000 0.00000000000000
0.00000000000000 0.00000000000000 5.46780933240000
La Ni O
8 4 16
```



```
Direct
0.25000000000000 0.87260000000000 0.00000000000000 La (4i)
0.25000000000000 -0.37260000000000 0.00000000000000 La (4i)
0.75000000000000 -0.87260000000000 0.00000000000000 La (4i)
0.75000000000000 1.37260000000000 0.00000000000000 La (4i)
0.25000000000000 0.38670000000000 0.50000000000000 La (4j)
0.25000000000000 0.11330000000000 0.50000000000000 La (4j)
0.75000000000000 -0.38670000000000 0.50000000000000 La (4j)
0.75000000000000 0.88670000000000 0.50000000000000 La (4j)
0.25000000000000 0.25000000000000 0.00000000000000 Ni (2a)
0.75000000000000 0.75000000000000 0.00000000000000 Ni (2a)
0.75000000000000 0.25000000000000 0.50000000000000 Ni (2c)
0.25000000000000 0.75000000000000 0.50000000000000 Ni (2c)
0.25000000000000 0.44500000000000 0.00000000000000 O (4i)
0.25000000000000 0.05500000000000 0.00000000000000 O (4i)
0.75000000000000 -0.44500000000000 0.00000000000000 O (4i)
0.75000000000000 0.94500000000000 0.00000000000000 O (4i)
0.25000000000000 -0.07600000000000 0.50000000000000 O (4j)
0.25000000000000 0.57600000000000 0.50000000000000 O (4j)
0.75000000000000 0.07600000000000 0.50000000000000 O (4j)
0.75000000000000 0.42400000000000 0.50000000000000 O (4j)
0.50000000000000 0.74300000000000 0.22600000000000 O (8m)
0.00000000000000 -0.24300000000000 0.22600000000000 O (8m)
0.00000000000000 0.74300000000000 -0.22600000000000 O (8m)
0.50000000000000 -0.24300000000000 -0.22600000000000 O (8m)
-0.50000000000000 -0.74300000000000 -0.22600000000000 O (8m)
1.00000000000000 1.24300000000000 -0.22600000000000 O (8m)
1.00000000000000 -0.74300000000000 0.22600000000000 O (8m)
-0.50000000000000 1.24300000000000 0.22600000000000 O (8m)
```

$\alpha$ - $\text{Ti}_2\text{TeO}_3$ : A3BC2\_oP48\_50\_3m\_m\_2m - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'alpha-Ti2TeO3'
_chemical_formula_sum 'O3 Te Ti2'

loop_
  _publ_author_name
  'F. Rieger'
  'A.-V. Mudring'
  _journal_name_full_name
  ;
  Inorganic Chemistry
  ;
  _journal_volume 46
  _journal_year 2007
  _journal_page_first 446
  _journal_page_last 452
  _publ_section_title
  ;
  Phase transition in  $\text{TiS}_2$  and  $\text{TeO}_3$ : Influence and origin of the
  ↪ thallium lone pair distortion
  ;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title '$\alpha$-TiS2-TeO3 Structure'
_aflow_proto 'A3BC2_oP48_50_3m_m_2m'
_aflow_params 'a,b/a,c/a,x{1},y{1},z{1},x{2},y{2},z{2},x{3},y{3},z{3},x{4},y{4},z{4},x{5},y{5},z{5},x{6},y{6},z{6}'
  ↪ ,z{3},x{4},y{4},z{4},x{5},y{5},z{5},x{6},y{6},z{6}'
_aflow_params_values '11.0940438033, 1.50045069408, 0.472480620154, 0.0515,
  ↪ 0.8152, 0.238, 0.602, 0.5567, 0.315, 0.604, 0.8447, 0.116, 0.61286,
  ↪ 0.66266, 0.2344, 0.11964, 0.66839, 0.2479, 0.63183, 0.00412, 0.2439'
_aflow_strukturbericht 'None'
_aflow_pearson 'oP48'

_cell_length_a 11.0940438033
_cell_length_b 16.6460657248
_cell_length_c 5.2417206962
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2/b 2/a 2/n (origin choice 2)"
_symmetry_Int_Tables_number 50

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x,-y+1/2,-z
  3 -x+1/2,y,-z
  4 -x+1/2,-y+1/2,z
  5 -x,-y,-z
  6 -x,y+1/2,z
  7 x+1/2,-y,z
  8 x+1/2,y+1/2,-z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  O1 O 8 m 0.05150 0.81520 0.23800 1.00000
  O2 O 8 m 0.60200 0.55670 0.31500 1.00000
  O3 O 8 m 0.60400 0.84470 0.11600 1.00000
  Te1 Te 8 m 0.61286 0.66266 0.23440 1.00000
```

```
T11 Ti 8 m 0.11964 0.66839 0.24790 1.00000
T12 Ti 8 m 0.63183 0.00412 0.24390 1.00000
```

$\alpha$ - $\text{Ti}_2\text{TeO}_3$ : A3BC2\_oP48\_50\_3m\_m\_2m - POSCAR

```
A3BC2_oP48_50_3m_m_2m & a,b/a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5
  ↪ ,y5,z5,x6,y6,z6 --params=11.0940438033, 1.50045069408,
  ↪ 0.472480620154, 0.0515, 0.8152, 0.238, 0.602, 0.5567, 0.315, 0.604,
  ↪ 0.8447, 0.116, 0.61286, 0.66266, 0.2344, 0.11964, 0.66839, 0.2479,
  ↪ 0.63183, 0.00412, 0.2439 & Ph.D. #50 (m6) & oP48 &
  ↪ None &  $\text{Ti}_2\text{TeO}_3$  & alpha & F. Rieger and A.-V. Mudring, Inorg.
  ↪ Chem. 46, 446-452 (2007)
```

```
1.0000000000000000
11.09404380330000 0.00000000000000 0.00000000000000
0.00000000000000 16.64606572480000 0.00000000000000
0.00000000000000 0.00000000000000 5.24172069620000
O Te Ti
24 8 16
```

```
Direct
0.05150000000000 0.81520000000000 0.23800000000000 O (8m)
0.44850000000000 -0.31520000000000 0.23800000000000 O (8m)
0.44850000000000 0.81520000000000 -0.23800000000000 O (8m)
0.05150000000000 -0.31520000000000 -0.23800000000000 O (8m)
-0.05150000000000 -0.81520000000000 -0.23800000000000 O (8m)
0.55150000000000 1.31520000000000 -0.23800000000000 O (8m)
0.55150000000000 -0.81520000000000 0.23800000000000 O (8m)
-0.05150000000000 1.31520000000000 0.23800000000000 O (8m)
0.60200000000000 0.55670000000000 0.31500000000000 O (8m)
-0.10200000000000 -0.05670000000000 0.31500000000000 O (8m)
-0.10200000000000 0.55670000000000 -0.31500000000000 O (8m)
0.60200000000000 -0.05670000000000 -0.31500000000000 O (8m)
-0.60200000000000 -0.55670000000000 -0.31500000000000 O (8m)
1.10200000000000 1.05670000000000 -0.31500000000000 O (8m)
1.10200000000000 -0.55670000000000 0.31500000000000 O (8m)
-0.60200000000000 1.05670000000000 0.31500000000000 O (8m)
0.60400000000000 0.84470000000000 0.11600000000000 O (8m)
-0.10400000000000 -0.34470000000000 0.11600000000000 O (8m)
0.10400000000000 0.84470000000000 -0.11600000000000 O (8m)
0.60400000000000 -0.34470000000000 -0.11600000000000 O (8m)
-0.60400000000000 -0.84470000000000 -0.11600000000000 O (8m)
1.10400000000000 1.34470000000000 -0.11600000000000 O (8m)
1.10400000000000 -0.84470000000000 0.11600000000000 O (8m)
-0.60400000000000 1.34470000000000 0.11600000000000 O (8m)
0.61286000000000 0.66266000000000 0.23440000000000 Te (8m)
-0.11286000000000 -0.16266000000000 0.23440000000000 Te (8m)
-0.11286000000000 0.66266000000000 -0.23440000000000 Te (8m)
0.61286000000000 -0.16266000000000 -0.23440000000000 Te (8m)
-0.61286000000000 0.66266000000000 -0.23440000000000 Te (8m)
1.11286000000000 1.16266000000000 -0.23440000000000 Te (8m)
1.11286000000000 -0.66266000000000 0.23440000000000 Te (8m)
-0.61286000000000 1.16266000000000 0.23440000000000 Te (8m)
0.11964000000000 0.66839000000000 0.24790000000000 Ti (8m)
0.38036000000000 -0.16839000000000 0.24790000000000 Ti (8m)
0.38036000000000 0.66839000000000 -0.24790000000000 Ti (8m)
0.11964000000000 -0.16839000000000 -0.24790000000000 Ti (8m)
-0.11964000000000 -0.66839000000000 -0.24790000000000 Ti (8m)
0.61964000000000 1.16839000000000 -0.24790000000000 Ti (8m)
0.61964000000000 -0.66839000000000 0.24790000000000 Ti (8m)
-0.11964000000000 1.16839000000000 0.24790000000000 Ti (8m)
0.63183000000000 0.00412000000000 0.24390000000000 Ti (8m)
-0.13183000000000 0.49588000000000 0.24390000000000 Ti (8m)
0.63183000000000 0.00412000000000 -0.24390000000000 Ti (8m)
0.63183000000000 0.49588000000000 -0.24390000000000 Ti (8m)
-0.63183000000000 -0.00412000000000 -0.24390000000000 Ti (8m)
1.13183000000000 0.50412000000000 -0.24390000000000 Ti (8m)
1.13183000000000 -0.00412000000000 0.24390000000000 Ti (8m)
-0.63183000000000 0.50412000000000 0.24390000000000 Ti (8m)
```

$\text{GaCl}_2$  (High-temperature): A2B\_oP24\_52\_2e\_cd - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'GaCl2'
_chemical_formula_sum 'Cl2 Ga'

loop_
  _publ_author_name
  'A. P. Wilkinson'
  'A. K. Cheetham'
  'D. E. Cox'
  _journal_name_full_name
  ;
  Acta Crystallographica Section B: Structural Science
  ;
  _journal_volume 47
  _journal_year 1991
  _journal_page_first 155
  _journal_page_last 161
  _publ_section_title
  ;
  Study of oxidation-state contrast in gallium dichloride by synchrotron
  ↪ X-ray anomalous scattering
  ;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'GaCl2 (High-temperature) Structure'
_aflow_proto 'A2B_oP24_52_2e_cd'
_aflow_params 'a,b/a,c/a,z{1},x{2},x{3},y{3},z{3},x{4},y{4},z{4}'
  ↪ )'
_aflow_params_values '7.2235008877, 1.34576036547, 1.32098013428, 0.3175,
  ↪ 0.6759, 0.8271, 0.1762, 0.5576, 0.5093, 0.0419, 0.8142'
```

```

_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP24'

_cell_length_a 7.2235008877
_cell_length_b 9.7211011946
_cell_length_c 9.5421011726
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2/n 21/n 2/a"
_symmetry_Int_Tables_number 52

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y+1/2, -z+1/2
3 -x+1/2, y+1/2, -z+1/2
4 -x+1/2, -y, z
5 -x, -y, -z
6 -x, y+1/2, z+1/2
7 x+1/2, -y+1/2, z+1/2
8 x+1/2, y, -z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ga1 Ga 4 c 0.25000 0.00000 0.31750 1.00000
Ga2 Ga 4 d 0.67590 0.25000 0.25000 1.00000
Cl1 Cl 8 e 0.82710 0.17620 0.55760 1.00000
Cl2 Cl 8 e 0.50930 0.04190 0.81420 1.00000

```

GaCl<sub>2</sub> (High-temperature): A2B<sub>2</sub>oP24\_52\_2e\_cd - POSCAR

```

A2B2oP24_52_2e_cd & a,b/a,c/a,z1,x2,x3,y3,z3,x4,y4,z4 --params=
↪ 7.2235008877, 1.34576036547, 1.32098013428, 0.3175, 0.6759, 0.8271,
↪ 0.1762, 0.5576, 0.5093, 0.0419, 0.8142 & Pnna D2h^{6} #52 (cde^2
↪ ) & oP24 & None & GaCl2 & A. P. Wilkinson and A. K. Cheetham
↪ and D. E. Cox, Acta Crystallogr. Sect. B Struct. Sci. 47,
↪ 155-161 (1991)
1.0000000000000000
7.22350088770000 0.00000000000000 0.00000000000000
0.00000000000000 9.72110119460000 0.00000000000000
0.00000000000000 0.00000000000000 9.54210117260000
Cl Ga
16 8
Direct
0.82710000000000 0.17620000000000 0.55760000000000 Cl (8e)
-0.32710000000000 -0.17620000000000 0.55760000000000 Cl (8e)
-0.32710000000000 0.67620000000000 -0.05760000000000 Cl (8e)
0.82710000000000 0.32380000000000 -0.05760000000000 Cl (8e)
-0.82710000000000 -0.17620000000000 -0.55760000000000 Cl (8e)
1.32710000000000 0.17620000000000 -0.55760000000000 Cl (8e)
1.32710000000000 0.32380000000000 1.05760000000000 Cl (8e)
-0.82710000000000 0.67620000000000 1.05760000000000 Cl (8e)
0.50930000000000 0.04190000000000 0.81420000000000 Cl (8e)
-0.00930000000000 -0.04190000000000 0.81420000000000 Cl (8e)
-0.00930000000000 0.54190000000000 -0.31420000000000 Cl (8e)
0.50930000000000 0.45810000000000 -0.31420000000000 Cl (8e)
-0.50930000000000 -0.04190000000000 -0.81420000000000 Cl (8e)
1.00930000000000 0.04190000000000 -0.81420000000000 Cl (8e)
1.00930000000000 0.45810000000000 1.31420000000000 Cl (8e)
-0.50930000000000 0.54190000000000 1.31420000000000 Cl (8e)
0.25000000000000 0.00000000000000 0.31750000000000 Ga (4c)
0.25000000000000 0.50000000000000 0.18250000000000 Ga (4c)
0.75000000000000 0.00000000000000 -0.31750000000000 Ga (4c)
0.75000000000000 0.50000000000000 0.81750000000000 Ga (4c)
0.67590000000000 0.25000000000000 0.25000000000000 Ga (4d)
-0.17590000000000 0.75000000000000 0.25000000000000 Ga (4d)
-0.67590000000000 0.75000000000000 0.75000000000000 Ga (4d)
1.17590000000000 0.25000000000000 0.75000000000000 Ga (4d)

```

Sr<sub>2</sub>Bi<sub>3</sub>: A3B<sub>2</sub>oP20\_52\_de\_cd - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Sr2Bi3'
_chemical_formula_sum 'Bi3 Sr2'

loop_
_publ_author_name
'F. Merlo'
'M. L. Fornasini'
_journal_name_full_name
;
Materials Research Bulletin
;
_journal_volume 29
_journal_year 1994
_journal_page_first 149
_journal_page_last 154
_publ_section_title
;
Crystal structure of some phases and alloying behaviour in alkaline
↪ earths, europium and ytterbium pnictides
;

```

```

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'SrS2Bi3 Structure'
_aflow_proto 'A3B2_oP20_52_de_cd'
_aflow_params 'a,b/a,c/a,z_{1},x_{2},x_{3},x_{4},y_{4},z_{4}'
_aflow_params_values '15.5832022616,0.434585119311,0.426069989123,0.443,
↪ 0.4294,0.0001,0.6539,0.064,0.0788'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP20'

_cell_length_a 15.5832022616
_cell_length_b 6.7722278141
_cell_length_c 6.6395348181
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2/n 21/n 2/a"
_symmetry_Int_Tables_number 52

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y+1/2, -z+1/2
3 -x+1/2, y+1/2, -z+1/2
4 -x+1/2, -y, z
5 -x, -y, -z
6 -x, y+1/2, z+1/2
7 x+1/2, -y+1/2, z+1/2
8 x+1/2, y, -z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Sr1 Sr 4 c 0.25000 0.00000 0.44300 1.00000
Bi1 Bi 4 d 0.42940 0.25000 0.25000 1.00000
Sr2 Sr 4 d 0.00010 0.25000 0.25000 1.00000
Bi2 Bi 8 e 0.65390 0.06400 0.07880 1.00000

```

Sr<sub>2</sub>Bi<sub>3</sub>: A3B<sub>2</sub>oP20\_52\_de\_cd - POSCAR

```

A3B2oP20_52_de_cd & a,b/a,c/a,z1,x2,x3,y4,z4 --params=15.5832022616,
↪ 0.434585119311, 0.426069989123, 0.443, 0.4294, 0.0001, 0.6539, 0.064,
↪ 0.0788 & Pnna D2h^{6} #52 (cd^2e) & oP20 & None & Sr2Bi3 &
↪ F. Merlo and M. L. Fornasini, Mater. Res. Bull. 29, 149-154 (
↪ 1994)
1.0000000000000000
15.58320226160000 0.00000000000000 0.00000000000000
0.00000000000000 6.77222781410000 0.00000000000000
0.00000000000000 0.00000000000000 6.63953481810000
Bi Sr
12 8
Direct
0.42940000000000 0.25000000000000 0.25000000000000 Bi (4d)
0.07060000000000 0.75000000000000 0.25000000000000 Bi (4d)
-0.42940000000000 0.75000000000000 0.75000000000000 Bi (4d)
0.92940000000000 0.25000000000000 0.75000000000000 Bi (4d)
0.65390000000000 0.06400000000000 0.07880000000000 Bi (8e)
-0.15390000000000 -0.06400000000000 0.07880000000000 Bi (8e)
-0.15390000000000 0.56400000000000 0.42120000000000 Bi (8e)
0.65390000000000 0.43600000000000 0.42120000000000 Bi (8e)
-0.65390000000000 -0.06400000000000 -0.07880000000000 Bi (8e)
1.15390000000000 0.06400000000000 -0.07880000000000 Bi (8e)
1.15390000000000 0.43600000000000 0.57880000000000 Bi (8e)
-0.65390000000000 0.56400000000000 0.57880000000000 Bi (8e)
0.25000000000000 0.00000000000000 0.44300000000000 Sr (4c)
0.25000000000000 0.50000000000000 0.05700000000000 Sr (4c)
0.75000000000000 0.00000000000000 -0.44300000000000 Sr (4c)
0.75000000000000 0.50000000000000 0.94300000000000 Sr (4c)
0.00100000000000 0.25000000000000 0.25000000000000 Sr (4d)
0.49990000000000 0.75000000000000 0.25000000000000 Sr (4d)
-0.00100000000000 0.75000000000000 0.75000000000000 Sr (4d)
0.50010000000000 0.25000000000000 0.75000000000000 Sr (4d)

```

TaNiTe<sub>2</sub>: ABC<sub>2</sub>oP16\_53\_h\_e\_gh - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'TaNiTe2'
_chemical_formula_sum 'Ni Ta Te2'

loop_
_publ_author_name
'W. Tremel'
_journal_name_full_name
;
Angewandte Chemie (International ed.)
;
_journal_volume 30
_journal_year 1991
_journal_page_first 840
_journal_page_last 843
_publ_section_title
;

```

```

Isolated and Condensed TaS2NiS2 Clusters in the Layered
↳ Tellurides TaS2NiS2Te4 and TaS2NiS3Te5
↳ ]S
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'TaNiTeS2 Structure'
_aflow_proto 'ABC2_oP16_53_h_e_g_h'
_aflow_params 'a,b/a,c/a,x1,y2,y3,z3,y4,z4'
_aflow_params_values '11.6904618594,0.282132455361,0.78890717994,0.79514
↳ ,0.3193,0.1198,0.3549,0.224,0.7493'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP16'

_cell_length_a 11.6904618594
_cell_length_b 3.2982587087
_cell_length_c 9.2226892977
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2/m 2/n 21/a"
_symmetry_Int_Tables_number 53

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x+1/2,y,-z+1/2
4 -x+1/2,-y,z+1/2
5 -x,-y,-z
6 -x,y,z
7 x+1/2,-y,z+1/2
8 x+1/2,y,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ta1 Ta 4 e 0.79514 0.00000 0.00000 1.00000
Te1 Te 4 g 0.25000 0.31930 0.25000 1.00000
Ni1 Ni 4 h 0.00000 0.11980 0.35490 1.00000
Te2 Te 4 h 0.00000 0.22400 0.74930 1.00000

```

TaNiTe<sub>2</sub>: ABC2\_oP16\_53\_h\_e\_g\_h - POSCAR

```

ABC2_oP16_53_h_e_g_h & a,b/a,c/a,x1,y2,y3,z3,y4,z4 --params=11.6904618594
↳ ,0.282132455361,0.78890717994,0.79514,0.3193,0.1198,0.3549,
↳ 0.224,0.7493 & Pmna D2h7 #53 (egh2) & oP16 & None &
↳ TaNiTe2 & W. Tremel, Angew. Chem. Int. Ed. 30, 840-843 (1991
↳ )
1.0000000000000000
11.69046185940000 0.00000000000000 0.00000000000000
0.00000000000000 3.29825870870000 0.00000000000000
0.00000000000000 0.00000000000000 9.22268929770000
Ni Ta Te
4 4 8
Direct
0.00000000000000 0.11980000000000 0.35490000000000 Ni (4h)
0.50000000000000 -0.11980000000000 0.85490000000000 Ni (4h)
0.50000000000000 0.11980000000000 0.14510000000000 Ni (4h)
0.00000000000000 -0.11980000000000 -0.35490000000000 Ni (4h)
0.79514000000000 0.00000000000000 0.00000000000000 Ta (4e)
-0.29514000000000 0.00000000000000 0.50000000000000 Ta (4e)
-0.79514000000000 0.00000000000000 0.00000000000000 Ta (4e)
1.29514000000000 0.00000000000000 0.50000000000000 Ta (4e)
0.25000000000000 0.31930000000000 0.25000000000000 Te (4g)
0.25000000000000 -0.31930000000000 0.75000000000000 Te (4g)
0.75000000000000 -0.31930000000000 0.75000000000000 Te (4g)
0.75000000000000 0.31930000000000 0.25000000000000 Te (4g)
0.00000000000000 0.22400000000000 0.74930000000000 Te (4h)
0.50000000000000 -0.22400000000000 1.24930000000000 Te (4h)
0.50000000000000 0.22400000000000 -0.24930000000000 Te (4h)
0.00000000000000 -0.22400000000000 -0.74930000000000 Te (4h)

```

CuBrSe<sub>3</sub>: ABC3\_oP20\_53\_e\_g\_hi - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'CuBrSe3'
_chemical_formula_sum 'Br Cu Se3'

loop_
_publ_author_name
'H. M. Haendler'
'P. M. Carkner'
_journal_name_full_name
;
Journal of Solid State Chemistry
;
_journal_volume 29
_journal_year 1979
_journal_page_first 35
_journal_page_last 39
_publ_section_title

```

```

;
The crystal structure of copper bromide triselenide, CuBrSe3
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'CuBrSe3 Structure'
_aflow_proto 'ABC3_oP20_53_e_g_hi'
_aflow_params 'a,b/a,c/a,x1,y2,y3,z3,x4,y4,z4'
_aflow_params_values '14.3630679002,0.312469539787,0.535821207264,0.6826
↳ ,0.2856,0.3458,0.2708,0.6247,0.6057,0.3575'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP20'

_cell_length_a 14.3630679002
_cell_length_b 4.4880212167
_cell_length_c 7.6960363823
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2/m 2/n 21/a"
_symmetry_Int_Tables_number 53

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x+1/2,y,-z+1/2
4 -x+1/2,-y,z+1/2
5 -x,-y,-z
6 -x,y,z
7 x+1/2,-y,z+1/2
8 x+1/2,y,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Br1 Br 4 e 0.68260 0.00000 0.00000 1.00000
Cu1 Cu 4 g 0.25000 0.28560 0.25000 1.00000
Se1 Se 4 h 0.00000 0.34580 0.27080 1.00000
Se2 Se 8 i 0.62470 0.60570 0.35750 1.00000

```

CuBrSe<sub>3</sub>: ABC3\_oP20\_53\_e\_g\_hi - POSCAR

```

ABC3_oP20_53_e_g_hi & a,b/a,c/a,x1,y2,y3,z3,x4,y4,z4 --params=
↳ 14.3630679002,0.312469539787,0.535821207264,0.6826,0.2856,
↳ 0.3458,0.2708,0.6247,0.6057,0.3575 & Pmna D2h7 #53 (eghi)
↳ & oP20 & None & CuBrSe3 & H. M. Haendler and P. M. Carkner,
↳ J. Solid State Chem. 29, 35-39 (1979)
1.0000000000000000
14.36306790020000 0.00000000000000 0.00000000000000
0.00000000000000 4.48802121670000 0.00000000000000
0.00000000000000 0.00000000000000 7.69603638230000
Br Cu Se
4 4 12
Direct
0.68260000000000 0.00000000000000 0.00000000000000 Br (4e)
-0.18260000000000 0.00000000000000 0.50000000000000 Br (4e)
-0.68260000000000 0.00000000000000 0.00000000000000 Br (4e)
1.18260000000000 0.00000000000000 0.50000000000000 Br (4e)
0.25000000000000 0.28560000000000 0.25000000000000 Cu (4g)
0.25000000000000 -0.28560000000000 0.75000000000000 Cu (4g)
0.75000000000000 -0.28560000000000 0.75000000000000 Cu (4g)
0.75000000000000 0.28560000000000 0.25000000000000 Cu (4g)
0.00000000000000 0.34580000000000 0.27080000000000 Se (4h)
0.50000000000000 -0.34580000000000 0.77080000000000 Se (4h)
0.50000000000000 0.34580000000000 0.22920000000000 Se (4h)
0.00000000000000 -0.34580000000000 -0.27080000000000 Se (4h)
0.62470000000000 0.60570000000000 0.35750000000000 Se (8i)
-0.12470000000000 -0.60570000000000 0.85750000000000 Se (8i)
-0.12470000000000 0.60570000000000 0.14250000000000 Se (8i)
0.62470000000000 -0.60570000000000 -0.35750000000000 Se (8i)
-0.62470000000000 -0.60570000000000 -0.35750000000000 Se (8i)
1.12470000000000 0.60570000000000 0.14250000000000 Se (8i)
1.12470000000000 -0.60570000000000 0.85750000000000 Se (8i)
-0.62470000000000 0.60570000000000 0.35750000000000 Se (8i)

```

BiGaO<sub>3</sub>: ABC3\_oP20\_54\_e\_d\_cf - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'BiGaO3'
_chemical_formula_sum 'Bi Ga O3'

loop_
_publ_author_name
'H. Yusa'
'A. A. Belik'
'E. {Takayama-Muromachi}'
'N. Hirao'
'Y. Ohishi'
_journal_name_full_name
;
Physical Review B

```

```

:
_journal_volume 80
_journal_year 2009
_journal_page_first 214103
_journal_page_last 214103
_publ_Section_title
:
High-pressure phase transitions in Bi2MSO5 (MS = Al, Ga, and In):
  ↳ (vit In situ) x-ray diffraction and Raman scattering
  ↳ experiments
:
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title 'BiGaO5 Structure'
_aflow_proto 'ABC3oP20_54_e_d_cf'
_aflow_params 'a,b/a,c/a,y1,z2,z3,x4,y4,z4'
_aflow_params_values '5.3467489374,0.956627452436,1.81710213776,0.8667,
  ↳ 0.6417,0.8902,0.4055,0.2686,0.5503'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP20'

_cell_length_a 5.3467489374
_cell_length_b 5.1148468148
_cell_length_c 9.7155889242
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 21/c 2/c 2/a"
_symmetry_Int_Tables_number 54

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x+1/2, -y, -z+1/2
3 -x, -y, z+1/2
4 -x+1/2, -y, z
5 -x, -y, -z
6 -x+1/2, y, z+1/2
7 x, -y, z+1/2
8 x+1/2, y, -z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 4 c 0.00000 0.86670 0.25000 1.00000
Ga1 Ga 4 d 0.25000 0.00000 0.64170 1.00000
Bi1 Bi 4 e 0.25000 0.50000 0.89020 1.00000
O2 O 8 f 0.40550 0.26860 0.55030 1.00000

```

BiGaO<sub>5</sub>: ABC<sub>3</sub>oP20\_54\_e\_d\_cf - POSCAR

```

ABC3oP20_54_e_d_cf & a,b/a,c/a,y1,z2,z3,x4,y4,z4 --params=5.3467489374,
  ↳ 0.956627452436,1.81710213776,0.8667,0.6417,0.8902,0.4055,0.2686
  ↳ ,0.5503 & Pecca D2h^8 #54 (cdef) & oP20 & None & BiGaO5 &
  ↳ & H. Yusa et al., Phys. Rev. B 80, 214103 (2009)

1.0000000000000000
5.34674893740000 0.00000000000000 0.00000000000000
0.00000000000000 5.11484681480000 0.00000000000000
0.00000000000000 0.00000000000000 9.71558892420000
Bi Ga O
4 4 12
Direct
0.25000000000000 0.50000000000000 0.89020000000000 Bi (4e)
0.75000000000000 0.50000000000000 -0.39020000000000 Bi (4e)
0.75000000000000 0.50000000000000 -0.89020000000000 Bi (4e)
0.25000000000000 0.50000000000000 1.39020000000000 Bi (4e)
0.25000000000000 0.00000000000000 0.64170000000000 Ga (4d)
0.75000000000000 0.00000000000000 -0.14170000000000 Ga (4d)
0.75000000000000 0.00000000000000 -0.64170000000000 Ga (4d)
0.25000000000000 0.00000000000000 1.14170000000000 Ga (4d)
0.00000000000000 0.86670000000000 0.25000000000000 O (4c)
0.50000000000000 -0.86670000000000 0.25000000000000 O (4c)
0.00000000000000 -0.86670000000000 0.75000000000000 O (4c)
0.50000000000000 0.86670000000000 0.75000000000000 O (4c)
0.40550000000000 0.26860000000000 0.55030000000000 O (8f)
0.09450000000000 -0.26860000000000 0.55030000000000 O (8f)
-0.40550000000000 0.26860000000000 -0.05030000000000 O (8f)
0.90550000000000 -0.26860000000000 -0.05030000000000 O (8f)
-0.40550000000000 -0.26860000000000 -0.55030000000000 O (8f)
0.90550000000000 0.26860000000000 -0.55030000000000 O (8f)
0.40550000000000 -0.26860000000000 1.05030000000000 O (8f)
0.09450000000000 0.26860000000000 1.05030000000000 O (8f)

```

GeAs<sub>2</sub>: A2B\_oP24\_55\_2g2h\_gh - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'GeAs2'
_chemical_formula_sum 'As2 Ge'

loop_
_publ_author_name
'T. Wadsten'

```

```

_journal_name_full_name
:
Acta Chemica Scandinavica
:
_journal_volume 21
_journal_year 1967
_journal_page_first 593
_journal_page_last 594
_publ_Section_title
:
Crystal structures of SiP2S, SiAs2S, and GeP
:
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title 'GeAs2 Structure'
_aflow_proto 'A2B_oP24_55_2g2h_gh'
_aflow_params 'a,b/a,c/a,x1,y1,x2,y2,x3,y3,x4,y4,
  ↳ x5,y5,x6,y6'
_aflow_params_values '10.1600191136,1.45275590551,0.366929133855,0.0628,
  ↳ 0.4022,0.1014,0.1118,0.2024,0.2667,0.226,0.0384,0.3532,0.2953,
  ↳ 0.4192,0.1378'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP24'

_cell_length_a 10.1600191136
_cell_length_b 14.7600277674
_cell_length_c 3.7280070133
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 21/b 21/a 2/m"
_symmetry_Int_Tables_number 55

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x+1/2, -y+1/2, -z
3 -x+1/2, y+1/2, -z
4 -x, -y, z
5 -x, -y, -z
6 -x+1/2, y+1/2, z
7 x+1/2, -y+1/2, z
8 x, y, -z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
As1 As 4 g 0.06280 0.40220 0.00000 1.00000
As2 As 4 g 0.10140 0.11180 0.00000 1.00000
Ge1 Ge 4 g 0.20240 0.26670 0.00000 1.00000
As3 As 4 h 0.22600 0.03840 0.50000 1.00000
As4 As 4 h 0.35320 0.29530 0.50000 1.00000
Ge2 Ge 4 h 0.41920 0.13780 0.50000 1.00000

```

GeAs<sub>2</sub>: A2B\_oP24\_55\_2g2h\_gh - POSCAR

```

A2B_oP24_55_2g2h_gh & a,b/a,c/a,x1,y1,x2,y2,x3,y3,x4,y4,x5,y5,x6,y6 --
  ↳ params=10.1600191136,1.45275590551,0.366929133855,0.0628,0.4022
  ↳ ,0.1014,0.1118,0.2024,0.2667,0.226,0.0384,0.3532,0.2953,0.4192,
  ↳ 0.1378 & Pbam D2h^9 #55 (g3h3) & oP24 & None & GeAs2 &
  ↳ & T. Wadsten, Acta Chem. Scand. 21, 593-594 (1967)

1.0000000000000000
10.16001911360000 0.00000000000000 0.00000000000000
0.00000000000000 14.76002776740000 0.00000000000000
0.00000000000000 0.00000000000000 3.72800701330000
As Ge
16 8
Direct
0.06280000000000 0.40220000000000 0.00000000000000 As (4g)
-0.06280000000000 -0.40220000000000 0.00000000000000 As (4g)
0.43720000000000 0.90220000000000 0.00000000000000 As (4g)
0.56280000000000 0.09780000000000 0.00000000000000 As (4g)
0.10140000000000 0.11180000000000 0.00000000000000 As (4g)
-0.10140000000000 -0.11180000000000 0.00000000000000 As (4g)
0.39860000000000 0.61180000000000 0.00000000000000 As (4g)
0.60140000000000 0.38820000000000 0.00000000000000 As (4g)
0.22600000000000 0.03840000000000 0.50000000000000 As (4h)
-0.22600000000000 -0.03840000000000 0.50000000000000 As (4h)
0.27400000000000 0.53840000000000 0.50000000000000 As (4h)
0.72600000000000 0.46160000000000 0.50000000000000 As (4h)
0.35320000000000 0.29530000000000 0.50000000000000 As (4h)
-0.35320000000000 -0.29530000000000 0.50000000000000 As (4h)
0.14680000000000 0.79530000000000 0.50000000000000 As (4h)
0.85320000000000 0.20470000000000 0.50000000000000 As (4h)
0.20240000000000 0.26670000000000 0.00000000000000 Ge (4g)
-0.20240000000000 -0.26670000000000 0.00000000000000 Ge (4g)
0.29760000000000 0.76670000000000 0.00000000000000 Ge (4g)
0.70240000000000 0.23330000000000 0.00000000000000 Ge (4g)
0.41920000000000 0.13780000000000 0.50000000000000 Ge (4h)
-0.41920000000000 -0.13780000000000 0.50000000000000 Ge (4h)
0.08080000000000 0.63780000000000 0.50000000000000 Ge (4h)
0.91920000000000 0.36220000000000 0.50000000000000 Ge (4h)

```

Rh<sub>5</sub>Ge<sub>3</sub>: A3B<sub>5</sub>oP16\_55\_ch\_agh - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Rh5Ge3'
_chemical_formula_sum 'Ge3 Rh5'

loop_
  _publ_author_name
  'S. Geller'
  _journal_name_full_name
  :
  Acta Crystallographica
  :
  _journal_volume 8
  _journal_year 1955
  _journal_page_first 15
  _journal_page_last 21
  _publ_section_title
  :
  The rhodium--germanium system. I. The crystal structures of Rh5Ge3
  ↪ Rh5Ge3 and RhGe
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'Rh5Ge3 Structure'
_aflow_proto 'A3B5_oP16_55_ch_agh'
_aflow_params 'a,b/a,c/a,x_{3},y_{3},x_{4},y_{4},x_{5},y_{5}'
_aflow_params_values '5.4199981729,1.90405904061,0.730627306278,0.348,
↪ 0.22,0.112,0.152,0.17,0.393'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP16'

_cell_length_a 5.4199981729
_cell_length_b 10.3199965212
_cell_length_c 3.9599986651
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 21/b 21/a 2/m"
_symmetry_Int_Tables_number 55

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x+1/2,-y+1/2,-z
  3 -x+1/2,y+1/2,-z
  4 -x,-y,z
  5 -x,-y,-z
  6 -x+1/2,y+1/2,z
  7 x+1/2,-y+1/2,z
  8 x,y,-z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Rh1 Rh 2 a 0.0000 0.0000 0.0000 1.0000
  Ge1 Ge 2 c 0.0000 0.5000 0.0000 1.0000
  Rh2 Rh 4 g 0.3480 0.2200 0.0000 1.0000
  Ge2 Ge 4 h 0.1120 0.1520 0.5000 1.0000
  Rh3 Rh 4 h 0.1700 0.3930 0.5000 1.0000
```

Rh<sub>5</sub>Ge<sub>3</sub>: A3B5\_oP16\_55\_ch\_agh - POSCAR

```
A3B5_oP16_55_ch_agh & a,b/a,c/a,x3,y3,x4,y4,x5,y5 --params=5.4199981729,
↪ 1.90405904061,0.730627306278,0.348,0.22,0.112,0.152,0.17,0.393
↪ & Pbam D_{2h}^{9} #55 (acgh^2) & oP16 & None & Rh5Ge3 & S.
↪ Geller, Acta Cryst. 8, 15-21 (1955)
1.0000000000000000
5.41999817290000 0.00000000000000 0.00000000000000
0.00000000000000 10.31999652120000 0.00000000000000
0.00000000000000 0.00000000000000 3.95999866510000
Ge Rh
6 10
Direct
0.00000000000000 0.50000000000000 0.00000000000000 Ge (2c)
0.50000000000000 0.00000000000000 0.00000000000000 Ge (2c)
0.11200000000000 0.15200000000000 0.50000000000000 Ge (4h)
-0.11200000000000 -0.15200000000000 0.50000000000000 Ge (4h)
0.38800000000000 0.65200000000000 0.50000000000000 Ge (4h)
0.61200000000000 0.34800000000000 0.50000000000000 Ge (4h)
0.00000000000000 0.00000000000000 0.00000000000000 Rh (2a)
0.50000000000000 0.50000000000000 0.00000000000000 Rh (2a)
0.34800000000000 0.22000000000000 0.00000000000000 Rh (4g)
-0.34800000000000 -0.22000000000000 0.00000000000000 Rh (4g)
0.15200000000000 0.72000000000000 0.00000000000000 Rh (4g)
0.84800000000000 0.28000000000000 0.00000000000000 Rh (4g)
0.17000000000000 0.39300000000000 0.50000000000000 Rh (4h)
-0.17000000000000 -0.39300000000000 0.50000000000000 Rh (4h)
0.33000000000000 0.89300000000000 0.50000000000000 Rh (4h)
0.67000000000000 0.10700000000000 0.50000000000000 Rh (4h)
```

R-carbon: A\_oP16\_55\_2g2h - CIF

```
# CIF file
```

```
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'R-carbon'
_chemical_formula_sum 'C'

loop_
  _publ_author_name
  'H. Niu'
  'X.-Q. Chen'
  'S. Wang'
  'D. Li'
  'W. L. Mao'
  'Y. Li'
  _journal_name_full_name
  :
  Physical Review Letters
  :
  _journal_volume 108
  _journal_year 2012
  _journal_page_first 135501
  _journal_page_last 135501
  _publ_section_title
  :
  Families of Superhard Crystalline Carbon Allotropes Constructed via
  ↪ Cold Compression of Graphite and Nanotubes
  ;

_aflow_title 'R-carbon Structure'
_aflow_proto 'A_oP16_55_2g2h'
_aflow_params 'a,b/a,c/a,x_{1},y_{1},x_{2},y_{2},x_{3},y_{3},x_{4},y_{4}
↪ '
_aflow_params_values '7.7886,0.613101199189,0.320442698303,0.6731,-0.037
↪ ,0.8435,0.8087,-0.0454,0.8613,0.5704,0.8926'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP16'

_symmetry_space_group_name_H-M "P 21/b 21/a 2/m"
_symmetry_Int_Tables_number 55

_cell_length_a 7.78860
_cell_length_b 4.77520
_cell_length_c 2.49580
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x+1/2,-y+1/2,-z
  3 -x+1/2,y+1/2,-z
  4 -x,-y,z
  5 -x,-y,-z
  6 -x+1/2,y+1/2,z
  7 x+1/2,-y+1/2,z
  8 x,y,-z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  C1 C 4 g 0.67310 -0.03700 0.00000 1.00000
  C2 C 4 g 0.84350 0.80870 0.00000 1.00000
  C3 C 4 h -0.04540 0.86130 0.50000 1.00000
  C4 C 4 h 0.57040 0.89260 0.50000 1.00000
```

R-carbon: A\_oP16\_55\_2g2h - POSCAR

```
A_oP16_55_2g2h & a,b/a,c/a,x1,y1,x2,y2,x3,y3,x4,y4 --params=7.7886,
↪ 0.613101199189,0.320442698303,0.6731,-0.037,0.8435,0.8087,-
↪ 0.0454,0.8613,0.5704,0.8926 & Pbam D_{2h}^{9} #55 (g^2h^2) &
↪ oP16 & None & C & R-carbon & H. Niu et al., Phys. Rev. Lett.
↪ 108, 135501 (2012)
1.00000000000000
7.78860000000000 0.00000000000000 0.00000000000000
0.00000000000000 4.77520000000000 0.00000000000000
0.00000000000000 0.00000000000000 2.49580000000000
C
16
Direct
0.67310000000000 -0.03700000000000 0.00000000000000 C (4g)
-0.67310000000000 0.03700000000000 0.00000000000000 C (4g)
-0.17310000000000 0.46300000000000 0.00000000000000 C (4g)
1.17310000000000 0.53700000000000 0.00000000000000 C (4g)
0.84350000000000 0.80870000000000 0.00000000000000 C (4g)
-0.84350000000000 -0.80870000000000 0.00000000000000 C (4g)
-0.34350000000000 1.30870000000000 0.00000000000000 C (4g)
1.34350000000000 -0.30870000000000 0.00000000000000 C (4g)
-0.04540000000000 0.86130000000000 0.50000000000000 C (4h)
0.04540000000000 -0.86130000000000 0.50000000000000 C (4h)
0.54540000000000 1.36130000000000 0.50000000000000 C (4h)
0.45460000000000 -0.36130000000000 0.50000000000000 C (4h)
0.57040000000000 0.89260000000000 0.50000000000000 C (4h)
-0.57040000000000 -0.89260000000000 0.50000000000000 C (4h)
-0.07040000000000 1.39260000000000 0.50000000000000 C (4h)
1.07040000000000 -0.39260000000000 0.50000000000000 C (4h)
```

α-PdCl<sub>2</sub> (C50): A2B\_oP6\_58\_g\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '$\alpha$-PdCl2'
_chemical_formula_sum 'Cl2 Pd'

loop_
_publ_author_name
'J. Evers'
'W. Beck'
'M. G\{o}bel'
'S. Jakob'
'P. Mayer'
'G. Oehlinger'
'M. Rotter'
'T. M. Klap\{o}tke'
_journal_name_full_name
;
Angewandte Chemie (International ed.)
;
_journal_volume 49
_journal_year 2010
_journal_page_first 5677
_journal_page_last 5682
_publ_section_title
;
The Structures of $\delta$-PdClS_{2}$ and $\gamma$-PdClS_{2}$: Phases
↪ with Negative Thermal Expansion in One Direction
;
_aflow_title '$\alpha$-PdClS_{2}$ (SC50S) Structure'
_aflow_proto 'A2B_oP6_58_g_a'
_aflow_params 'a,b/a,c/a,x_{2},y_{2}'
_aflow_params_values '3.7572,2.89952624295,0.89063664431,0.3326,0.63309'
_aflow_Strukturbericht 'SC50S'
_aflow_Pearson 'oP6'

_symmetry_space_group_name_H-M "P 21/n 21/n 2/m"
_symmetry_Int_Tables_number 58

_cell_length_a 3.75720
_cell_length_b 10.89410
_cell_length_c 3.34630
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x+1/2,y+1/2,-z+1/2
4 -x,-y,-z
5 -x,-y,-z
6 -x+1/2,y+1/2,z+1/2
7 x+1/2,-y+1/2,z+1/2
8 x,y,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Pd1 Pd 2 a 0.00000 0.00000 0.00000 1.00000
Cl1 Cl 4 g 0.33260 0.63309 0.00000 1.00000
```

$\alpha$ -PdCl<sub>2</sub> (C50): A2B\_oP6\_58\_g\_a - POSCAR

```
A2B_oP6_58_g_a & a,b/a,c/a,x2,y2 --params=3.7572,2.89952624295,
↪ 0.89063664431,0.3326,0.63309 & Pmm D_{2h}^{12} #58 (ag) & oP6
↪ & SC50S & PdCl2 & $\alpha$-PdCl2 & J. Evers et al., Angew.
↪ Chem. Int. Ed. 49, 5677-5682 (2010)
1.0000000000000000
3.7572000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.8941000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 3.3463000000000000
Cl Pd
4 2
Direct
0.3326000000000000 0.6330900000000000 0.0000000000000000 Cl (4g)
-0.3326000000000000 -0.6330900000000000 0.0000000000000000 Cl (4g)
0.1674000000000000 -1.1330900000000000 0.5000000000000000 Cl (4g)
0.8326000000000000 -0.1330900000000000 0.5000000000000000 Cl (4g)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Pd (2a)
0.5000000000000000 0.5000000000000000 0.5000000000000000 Pd (2a)
```

FeOCl: ABC\_oP6\_59\_a\_b\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'FeOCl'
_chemical_formula_sum 'Cl Fe O'

loop_
_publ_author_name
'S. M. Kauzlarich'
```

```
'J. L. Stanton'
'J. Faber'
'B. A. Averill'
_journal_name_full_name
;
Journal of the American Chemical Society
;
_journal_volume 108
_journal_year 1986
_journal_page_first 7946
_journal_page_last 7951
_publ_section_title
;
Neutron profile refinement of the structure of FeOCl and FeOCl(TTF)$_{1}
↪ /8.5)$
;
_aflow_title 'FeOCl Structure'
_aflow_proto 'ABC_oP6_59_a_b_a'
_aflow_params 'a,b/a,c/a,z_{1},z_{2},z_{3}'
_aflow_params_values '3.301,1.14298697364,2.39612238716,0.32961,-0.04795'
↪ ,0.89243'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP6'

_symmetry_space_group_name_H-M "P m m n :2"
_symmetry_Int_Tables_number 59

_cell_length_a 3.30100
_cell_length_b 3.77300
_cell_length_c 7.90960
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y,-z
3 -x,y+1/2,-z
4 -x+1/2,-y+1/2,z
5 -x,-y,-z
6 -x+1/2,y,z
7 x,-y+1/2,z
8 x+1/2,y+1/2,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cl1 Cl 2 a 0.25000 0.25000 1.00000
O1 O 2 a 0.25000 0.25000 -0.04795 1.00000
Fe1 Fe 2 b 0.25000 0.75000 0.89243 1.00000
```

FeOCl: ABC\_oP6\_59\_a\_b\_a - POSCAR

```
ABC_oP6_59_a_b_a & a,b/a,c/a,z1,z2,z3 --params=3.301,1.14298697364,
↪ 2.39612238716,0.32961,-0.04795,0.89243 & Pmm D_{2h}^{13} #59 (
↪ a^2b) & oP6 & None & FeOCl & FeOCl & S. M. Kauzlarich et al.,
↪ J. Am. Chem. Soc. 108, 7946-7951 (1986)
1.0000000000000000
3.3010000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 3.7730000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.9096000000000000
Cl Fe O
2 2 2
Direct
0.2500000000000000 0.2500000000000000 0.3296100000000000 Cl (2a)
0.7500000000000000 0.7500000000000000 -0.3296100000000000 Cl (2a)
0.2500000000000000 0.7500000000000000 0.8924300000000000 Fe (2b)
0.7500000000000000 0.2500000000000000 -0.8924300000000000 Fe (2b)
0.2500000000000000 0.2500000000000000 -0.0479500000000000 O (2a)
0.7500000000000000 0.7500000000000000 0.0479500000000000 O (2a)
```

Rh<sub>2</sub>S<sub>3</sub>: A2B3\_oP20\_60\_d\_cd - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Rh2S3'
_chemical_formula_sum 'Rh2 S3'

loop_
_publ_author_name
'E. Parth\{e} F.'
'Hulliger'
_journal_year 1966
_publ_section_title
;
The crystal structure of RhS_{2}SS_{3}$
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'RhS_{2}SS_{3}$ Structure'
_aflow_proto 'A2B3_oP20_60_d_cd'
_aflow_params 'a,b/a,c/a,y_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3}'
```

```

_aflow_params_values '8.4598035458 , 0.706855791961 , 0.724586288418 , 0.547 ,
↪ 0.394 , 0.75 , 0.033 , 0.348 , 0.611 , 0.396 '
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP20'

_cell_length_a 8.4598035458
_cell_length_b 5.9798611352
_cell_length_c 6.1298576520
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 21/b 2/c 21/n"
_symmetry_Int_Tables_number 60

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x+1/2, -y+1/2, -z
3 -x, y, -z+1/2
4 -x+1/2, -y+1/2, z+1/2
5 -x, -y, -z
6 -x+1/2, y+1/2, z
7 x, -y, z+1/2
8 x+1/2, y+1/2, -z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
S1 S 4 c 0.00000 0.54700 0.25000 1.00000
Rh1 Rh 8 d 0.39400 0.75000 0.03300 1.00000
S2 S 8 d 0.34800 0.61100 0.39600 1.00000

```

Rh<sub>2</sub>S<sub>3</sub>: A2B<sub>3</sub>\_oP20\_60\_d\_cd - POSCAR

```

A2B3_oP20_60_d_cd & a, b/a, c/a, x1, y1, x2, y2, z2, x3, y3, z3 --params=8.4598035458
↪ 0.706855791961, 0.724586288418, 0.547, 0.394, 0.75, 0.033, 0.348,
↪ 0.611, 0.396 & Pbcn D_{2h}^{14} #60 (cd^2) & oP20 & None & Rh2S3
↪ & E. Parth{\^e} F. and Hulliger, (1966)
1.0000000000000000
8.45980354580000 0.00000000000000 0.00000000000000
0.00000000000000 5.97986113520000 0.00000000000000
0.00000000000000 0.00000000000000 6.12985765200000
Rh S
8 12
Direct
0.39400000000000 0.75000000000000 0.03300000000000 Rh (8d)
0.10600000000000 -0.25000000000000 0.53300000000000 Rh (8d)
-0.39400000000000 0.75000000000000 0.46700000000000 Rh (8d)
0.89400000000000 -0.25000000000000 -0.03300000000000 Rh (8d)
-0.39400000000000 -0.75000000000000 -0.03300000000000 Rh (8d)
0.89400000000000 1.25000000000000 0.46700000000000 Rh (8d)
0.39400000000000 -0.75000000000000 0.53300000000000 Rh (8d)
0.10600000000000 1.25000000000000 0.03300000000000 Rh (8d)
0.00000000000000 0.54700000000000 0.25000000000000 S (4c)
0.50000000000000 -0.04700000000000 0.75000000000000 S (4c)
0.00000000000000 -0.54700000000000 0.75000000000000 S (4c)
0.50000000000000 1.04700000000000 0.25000000000000 S (4c)
0.34800000000000 0.61100000000000 0.39600000000000 S (8d)
0.15200000000000 -0.11100000000000 0.89600000000000 S (8d)
-0.34800000000000 0.61100000000000 0.10400000000000 S (8d)
0.84800000000000 -0.11100000000000 -0.39600000000000 S (8d)
-0.34800000000000 -0.61100000000000 -0.39600000000000 S (8d)
0.84800000000000 1.11100000000000 0.10400000000000 S (8d)
0.34800000000000 -0.61100000000000 0.89600000000000 S (8d)
0.15200000000000 1.11100000000000 0.39600000000000 S (8d)

```

WO<sub>3</sub>: A3B\_oP32\_60\_3d\_d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'WO3'
_chemical_formula_sum 'O3 W'

loop_
_publ_author_name
'T. Vogt'
'P. M. Woodward'
'B. A. Hunter'
_journal_name_full_name
'Journal of Solid State Chemistry'
;
_journal_volume 144
_journal_year 1999
_journal_page_first 209
_journal_page_last 215
_publ_section_title
;
The high-temperature phases of WO3{3}$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'WO3{3}$ Structure'

```

```

_aflow_proto 'A3B_oP32_60_3d_d'
_aflow_params 'a, b/a, c/a, x_{1}, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}'
↪ , z_{3}, x_{4}, y_{4}, z_{4}'
_aflow_params_values '7.3397836195 , 1.05524748967 , 1.03197678378 , 0.5016 ,
↪ 0.7205 , 0.0322 , 0.2167 , 0.7591 , 0.2582 , 0.2197 , 0.5016 , 0.013 , 0.248 ,
↪ 0.783 , 0.0291 '
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP32'

_cell_length_a 7.3397836195
_cell_length_b 7.7452882392
_cell_length_c 7.5744862933
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 21/b 2/c 21/n"
_symmetry_Int_Tables_number 60

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x+1/2, -y+1/2, -z
3 -x, y, -z+1/2
4 -x+1/2, -y+1/2, z+1/2
5 -x, -y, -z
6 -x+1/2, y+1/2, z
7 x, -y, z+1/2
8 x+1/2, y+1/2, -z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 8 d 0.50160 0.72050 0.03220 1.00000
O2 O 8 d 0.21670 0.75910 0.25820 1.00000
O3 O 8 d 0.21970 0.50160 0.01300 1.00000
W1 W 8 d 0.24800 0.78300 0.02910 1.00000

```

WO<sub>3</sub>: A3B\_oP32\_60\_3d\_d - POSCAR

```

A3B_oP32_60_3d_d & a, b/a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4 --
↪ params=7.3397836195 , 1.05524748967 , 1.03197678378 , 0.5016 , 0.7205 ,
↪ 0.0322 , 0.2167 , 0.7591 , 0.2582 , 0.2197 , 0.5016 , 0.013 , 0.248 , 0.783 ,
↪ 0.0291 & Pbcn D_{2h}^{14} #60 (d^4) & oP32 & None & WO3 & T.
↪ Vogt and P. M. Woodward and B. A. Hunter, J. Solid State Chem.
↪ 144, 209-215 (1999)
1.0000000000000000
7.33978361950000 0.00000000000000 0.00000000000000
0.00000000000000 7.74528823920000 0.00000000000000
0.00000000000000 0.00000000000000 7.57448629330000
O W
24 8
Direct
0.50160000000000 0.72050000000000 0.03220000000000 O (8d)
-0.00160000000000 -0.22050000000000 0.53220000000000 O (8d)
-0.50160000000000 0.72050000000000 0.46780000000000 O (8d)
1.00160000000000 -0.22050000000000 -0.03220000000000 O (8d)
-0.50160000000000 -0.72050000000000 -0.03220000000000 O (8d)
1.00160000000000 1.22050000000000 0.46780000000000 O (8d)
0.50160000000000 -0.72050000000000 0.53220000000000 O (8d)
-0.00160000000000 1.22050000000000 0.03220000000000 O (8d)
0.21670000000000 0.75910000000000 0.25820000000000 O (8d)
0.28330000000000 -0.25910000000000 0.75820000000000 O (8d)
-0.21670000000000 0.75910000000000 0.24180000000000 O (8d)
0.71670000000000 -0.25910000000000 -0.25820000000000 O (8d)
-0.21670000000000 -0.75910000000000 -0.25820000000000 O (8d)
0.71670000000000 1.25910000000000 0.24180000000000 O (8d)
0.21670000000000 -0.75910000000000 0.75820000000000 O (8d)
0.28330000000000 1.25910000000000 0.25820000000000 O (8d)
0.21970000000000 0.50160000000000 0.01300000000000 O (8d)
0.28030000000000 -0.00160000000000 0.51300000000000 O (8d)
-0.21970000000000 0.50160000000000 0.48700000000000 O (8d)
0.71970000000000 -0.00160000000000 -0.01300000000000 O (8d)
-0.21970000000000 -0.50160000000000 -0.01300000000000 O (8d)
0.71970000000000 1.00160000000000 0.48700000000000 O (8d)
0.21970000000000 -0.50160000000000 0.51300000000000 O (8d)
0.28030000000000 1.00160000000000 0.01300000000000 O (8d)
0.24800000000000 0.78300000000000 0.02910000000000 W (8d)
0.25200000000000 -0.28300000000000 0.52910000000000 W (8d)
-0.24800000000000 0.78300000000000 0.47090000000000 W (8d)
0.74800000000000 -0.28300000000000 -0.02910000000000 W (8d)
-0.24800000000000 -0.78300000000000 -0.02910000000000 W (8d)
0.74800000000000 1.28300000000000 0.47090000000000 W (8d)
0.24800000000000 -0.78300000000000 0.52910000000000 W (8d)
0.25200000000000 1.28300000000000 0.02910000000000 W (8d)

```

β-Toluene: A7B8\_oP120\_60\_7d\_8d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'beta-Toluene'
_chemical_formula_sum 'C7 H8'

loop_
_publ_author_name
'D. Andre'

```

```

'R. Fourme'
'J. {Bruneaux-Pouille}'
'L. Bosio'
_journal_name_full_name
:
Journal of Molecular Structure
:
_journal_volume 81
_journal_year 1982
_journal_page_first 253
_journal_page_last 259
_publ_section_title
:
Crystal structure of the metastable $\beta$-phase of toluene
:
_aflow_title '$\beta$-Toluene Structure'
_aflow_proto 'A7B8_oP120_60_7d_8d'
_aflow_params 'a,b/a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},y_{7},z_{7},x_{8},y_{8},z_{8},x_{9},y_{9},z_{9},x_{10},y_{10},z_{10},x_{11},y_{11},z_{11},x_{12},y_{12},z_{12},x_{13},y_{13},z_{13},x_{14},y_{14},z_{14},x_{15},y_{15},z_{15}'
_aflow_params_values '13.85,0.824548736462,0.53357400722,0.382,0.3932,0.5783,0.2764,0.38,0.5411,0.2264,0.4631,0.4411,0.1289,0.4507,0.4069,0.0794,0.3554,0.4717,0.1276,0.2723,0.571,0.2251,0.2844,0.6054,0.2616,0.5329,0.393,0.094,0.5116,0.3344,0.0088,0.3466,0.4468,0.0917,0.2026,0.6185,0.2593,0.2232,0.6779,0.3972,0.4784,0.595,0.4192,0.3624,0.4724,0.4002,0.3492,0.6895'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oP120'

_symmetry_space_group_name_H-M "P 21/b 2/c 21/n"
_symmetry_Int_Tables_number 60

_cell_length_a 13.85000
_cell_length_b 11.42000
_cell_length_c 7.39000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z
3 -x,-y,z+1/2
4 -x+1/2,-y+1/2,z+1/2
5 -x,-y,-z
6 -x+1/2,y+1/2,z
7 x,-y,z+1/2
8 x+1/2,y+1/2,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
C1 C 8 d 0.38200 0.39320 0.57830 1.00000
C2 C 8 d 0.27640 0.38000 0.54110 1.00000
C3 C 8 d 0.22640 0.46310 0.44110 1.00000
C4 C 8 d 0.12890 0.45070 0.40690 1.00000
C5 C 8 d 0.07940 0.35540 0.47170 1.00000
C6 C 8 d 0.12760 0.27230 0.57100 1.00000
C7 C 8 d 0.22510 0.28440 0.60540 1.00000
H1 H 8 d 0.26160 0.53290 0.39300 1.00000
H2 H 8 d 0.09400 0.51160 0.33440 1.00000
H3 H 8 d 0.00880 0.34660 0.44680 1.00000
H4 H 8 d 0.09170 0.20260 0.61850 1.00000
H5 H 8 d 0.25930 0.22320 0.67790 1.00000
H6 H 8 d 0.39720 0.47840 0.59500 1.00000
H7 H 8 d 0.41920 0.36240 0.47240 1.00000
H8 H 8 d 0.40020 0.34920 0.68950 1.00000

```

**\$\beta\$-Toluene: A7B8\_oP120\_60\_7d\_8d - POSCAR**

```

A7B8_oP120_60_7d_8d & a,b/a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,
y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11,y11,
z11,x12,y12,z12,x13,y13,z13,x14,y14,z14,x15,y15,z15 --params=
13.85,0.824548736462,0.53357400722,0.382,0.3932,0.5783,0.2764,
0.38,0.5411,0.2264,0.4631,0.4411,0.1289,0.4507,0.4069,0.0794,
0.3554,0.4717,0.1276,0.2723,0.571,0.2251,0.2844,0.6054,0.2616,
0.5329,0.393,0.094,0.5116,0.3344,0.0088,0.3466,0.4468,0.0917,
0.2026,0.6185,0.2593,0.2232,0.6779,0.3972,0.4784,0.595,0.4192,
0.3624,0.4724,0.4002,0.3492,0.6895 & Pbcn D_{2h}^{14} #60 (d^{15})
) & oP120 & None & C7H8 & beta-Toluene & D. Andre et al., J.
Mol. Struct. 81, 253-259 (1982)
1.0000000000000000
13.850000000000000 0.000000000000000 0.000000000000000
0.000000000000000 11.420000000000000 0.000000000000000
0.000000000000000 0.000000000000000 7.390000000000000
C H
56 64
Direct
0.382000000000000 0.393200000000000 0.578300000000000 C (8d)
0.118000000000000 0.106800000000000 1.078300000000000 C (8d)
-0.382000000000000 0.393200000000000 -0.078300000000000 C (8d)
0.882000000000000 0.106800000000000 -0.578300000000000 C (8d)
-0.382000000000000 -0.393200000000000 -0.578300000000000 C (8d)
0.882000000000000 0.893200000000000 -0.078300000000000 C (8d)

```

```

0.382000000000000 -0.393200000000000 1.078300000000000 C (8d)
0.118000000000000 0.893200000000000 0.578300000000000 C (8d)
0.276400000000000 0.380000000000000 0.541100000000000 C (8d)
0.223600000000000 0.120000000000000 1.041100000000000 C (8d)
-0.276400000000000 0.380000000000000 -0.041100000000000 C (8d)
0.776400000000000 0.120000000000000 -0.541100000000000 C (8d)
-0.276400000000000 -0.380000000000000 -0.541100000000000 C (8d)
0.776400000000000 0.880000000000000 -0.041100000000000 C (8d)
0.276400000000000 -0.380000000000000 1.041100000000000 C (8d)
0.223600000000000 0.880000000000000 0.541100000000000 C (8d)
0.226400000000000 0.463100000000000 0.441100000000000 C (8d)
0.273600000000000 0.036900000000000 0.941100000000000 C (8d)
-0.226400000000000 0.463100000000000 0.058900000000000 C (8d)
0.726400000000000 0.036900000000000 -0.441100000000000 C (8d)
-0.226400000000000 -0.463100000000000 -0.441100000000000 C (8d)
0.726400000000000 0.963100000000000 0.058900000000000 C (8d)
0.226400000000000 -0.463100000000000 0.941100000000000 C (8d)
0.273600000000000 0.963100000000000 0.441100000000000 C (8d)
0.128900000000000 0.450700000000000 0.406900000000000 C (8d)
0.371100000000000 0.049300000000000 0.906900000000000 C (8d)
-0.128900000000000 0.450700000000000 0.093100000000000 C (8d)
0.628900000000000 0.049300000000000 -0.406900000000000 C (8d)
-0.128900000000000 -0.450700000000000 -0.406900000000000 C (8d)
0.628900000000000 0.950700000000000 0.950700000000000 C (8d)
0.128900000000000 -0.450700000000000 0.906900000000000 C (8d)
0.371100000000000 0.950700000000000 0.406900000000000 C (8d)
0.079400000000000 0.355400000000000 0.471700000000000 C (8d)
0.420600000000000 0.144600000000000 0.971700000000000 C (8d)
-0.079400000000000 0.355400000000000 0.028300000000000 C (8d)
0.579400000000000 0.144600000000000 -0.471700000000000 C (8d)
-0.079400000000000 -0.355400000000000 -0.471700000000000 C (8d)
0.579400000000000 0.855400000000000 0.028300000000000 C (8d)
0.079400000000000 -0.355400000000000 0.971700000000000 C (8d)
0.420600000000000 0.855400000000000 0.471700000000000 C (8d)
0.127600000000000 0.272300000000000 0.571000000000000 C (8d)
0.372400000000000 0.227700000000000 1.071000000000000 C (8d)
-0.127600000000000 0.272300000000000 -0.071000000000000 C (8d)
0.627600000000000 0.227700000000000 -0.571000000000000 C (8d)
-0.127600000000000 -0.272300000000000 -0.571000000000000 C (8d)
0.627600000000000 0.772300000000000 -0.071000000000000 C (8d)
0.127600000000000 -0.272300000000000 1.071000000000000 C (8d)
0.372400000000000 0.772300000000000 0.571000000000000 C (8d)
0.225100000000000 0.284400000000000 0.605400000000000 C (8d)
0.274900000000000 0.215600000000000 1.105400000000000 C (8d)
-0.225100000000000 0.284400000000000 -0.105400000000000 C (8d)
0.725100000000000 0.215600000000000 -0.605400000000000 C (8d)
-0.225100000000000 -0.284400000000000 -0.605400000000000 C (8d)
0.725100000000000 0.784400000000000 -0.105400000000000 C (8d)
0.225100000000000 -0.284400000000000 1.105400000000000 C (8d)
0.274900000000000 0.784400000000000 0.605400000000000 C (8d)
0.261600000000000 0.532900000000000 0.393000000000000 H (8d)
0.238400000000000 -0.032900000000000 0.893000000000000 H (8d)
-0.261600000000000 0.532900000000000 0.107000000000000 H (8d)
0.761600000000000 -0.032900000000000 -0.393000000000000 H (8d)
-0.261600000000000 -0.532900000000000 -0.393000000000000 H (8d)
0.761600000000000 1.032900000000000 0.107000000000000 H (8d)
0.261600000000000 -0.532900000000000 0.893000000000000 H (8d)
0.238400000000000 1.032900000000000 0.393000000000000 H (8d)
0.094000000000000 0.511600000000000 0.334400000000000 H (8d)
0.406000000000000 -0.011600000000000 0.834400000000000 H (8d)
-0.094000000000000 0.511600000000000 0.165600000000000 H (8d)
0.594000000000000 -0.011600000000000 -0.334400000000000 H (8d)
-0.094000000000000 -0.511600000000000 -0.334400000000000 H (8d)
0.594000000000000 1.011600000000000 0.165600000000000 H (8d)
0.094000000000000 -0.511600000000000 0.834400000000000 H (8d)
0.406000000000000 1.011600000000000 0.334400000000000 H (8d)
0.008800000000000 0.346600000000000 0.446800000000000 H (8d)
0.491200000000000 0.153400000000000 0.946800000000000 H (8d)
-0.008800000000000 0.346600000000000 0.053200000000000 H (8d)
0.508800000000000 0.153400000000000 -0.446800000000000 H (8d)
-0.008800000000000 -0.346600000000000 -0.446800000000000 H (8d)
0.508800000000000 0.846600000000000 0.053200000000000 H (8d)
0.008800000000000 -0.346600000000000 0.946800000000000 H (8d)
0.491200000000000 0.846600000000000 0.446800000000000 H (8d)
0.091700000000000 0.202600000000000 0.618500000000000 H (8d)
0.408300000000000 0.297400000000000 1.118500000000000 H (8d)
-0.091700000000000 0.202600000000000 -0.118500000000000 H (8d)
0.591700000000000 0.297400000000000 -0.618500000000000 H (8d)
-0.091700000000000 -0.202600000000000 -0.618500000000000 H (8d)
0.591700000000000 0.702600000000000 -0.118500000000000 H (8d)
0.091700000000000 -0.202600000000000 1.118500000000000 H (8d)
0.408300000000000 0.702600000000000 0.618500000000000 H (8d)
0.259300000000000 0.223200000000000 0.677900000000000 H (8d)
0.240700000000000 0.276800000000000 1.177900000000000 H (8d)
-0.259300000000000 0.223200000000000 -0.177900000000000 H (8d)
0.759300000000000 0.276800000000000 -0.677900000000000 H (8d)
-0.259300000000000 -0.223200000000000 -0.677900000000000 H (8d)
0.759300000000000 0.723200000000000 -0.177900000000000 H (8d)
0.259300000000000 -0.223200000000000 1.177900000000000 H (8d)
0.240700000000000 0.723200000000000 0.677900000000000 H (8d)
0.397200000000000 0.478400000000000 0.595000000000000 H (8d)
0.102800000000000 0.021600000000000 1.095000000000000 H (8d)
-0.397200000000000 0.478400000000000 -0.095000000000000 H (8d)
0.897200000000000 0.021600000000000 -0.595000000000000 H (8d)
-0.397200000000000 -0.478400000000000 -0.595000000000000 H (8d)
0.897200000000000 0.978400000000000 -0.095000000000000 H (8d)
0.397200000000000 -0.478400000000000 1.095000000000000 H (8d)
0.102800000000000 0.978400000000000 0.595000000000000 H (8d)
0.419200000000000 0.362400000000000 0.472400000000000 H (8d)
0.080800000000000 0.137600000000000 0.972400000000000 H (8d)
-0.419200000000000 0.362400000000000 0.027600000000000 H (8d)
0.919200000000000 0.137600000000000 -0.472400000000000 H (8d)
-0.419200000000000 -0.362400000000000 -0.472400000000000 H (8d)
0.919200000000000 0.862400000000000 0.027600000000000 H (8d)
0.419200000000000 -0.362400000000000 0.972400000000000 H (8d)

```



0.08080000000000	0.86240000000000	0.47240000000000	H	(8d)
0.40020000000000	0.34920000000000	0.68950000000000	H	(8d)
0.09980000000000	0.15080000000000	1.18950000000000	H	(8d)
-0.40020000000000	0.34920000000000	-0.18950000000000	H	(8d)
0.90020000000000	0.15080000000000	-0.68950000000000	H	(8d)
-0.40020000000000	-0.34920000000000	-0.68950000000000	H	(8d)
0.90020000000000	0.84920000000000	-0.18950000000000	H	(8d)
0.40020000000000	-0.34920000000000	1.18950000000000	H	(8d)
0.09980000000000	0.84920000000000	0.68950000000000	H	(8d)

Benzene: AB\_oP48\_61\_3c\_3c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Benzene'
_chemical_formula_sum 'C H'

loop_
_publ_author_name
'S. K Nayak'
'R. Sathishkumar'
'T. N. {Guru Row}'
_journal_name_full_name
;
CrystEngComm
;
_journal_volume 12
_journal_year 2010
_journal_page_first 3112
_journal_page_last 3118
_publ_Section_title
;
Directing role of functional groups in selective generation of C-H-S
  -> pi$ interactions: In situ cryo-crystallographic studies on
  -> benzyl derivatives
;

_aware_title 'Benzene Structure'
_aware_proto 'AB_oP48_61_3c_3c'
_aware_params 'a,b/a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6}'
_aware_params_values '6.914,1.08128435059,1.38313566676,0.1297,0.5762,
  -> 0.40803,0.1235,0.6328,0.54518,0.0057,0.4432,0.36289,0.2172,
  -> 0.6275,0.346,0.2068,0.7225,0.5756,0.0095,0.4051,0.2704'
_aware_Strukturbericht 'None'
_aware_Pearson 'oP48'

_symmetry_space_group_name_H-M "P 21/b 21/c 21/a"
_symmetry_Int_Tables_number 61

_cell_length_a 6.91400
_cell_length_b 7.47600
_cell_length_c 9.56300
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z
3 -x,y+1/2,-z+1/2
4 -x+1/2,-y,z+1/2
5 -x,-y,-z
6 -x+1/2,y+1/2,z
7 x,-y+1/2,z+1/2
8 x+1/2,y,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
C1 C 8 c 0.12970 0.57620 0.40803 1.00000
C2 C 8 c 0.12350 0.63280 0.54518 1.00000
C3 C 8 c 0.00570 0.44320 0.36289 1.00000
H1 H 8 c 0.21720 0.62750 0.34600 1.00000
H2 H 8 c 0.20680 0.72250 0.57560 1.00000
H3 H 8 c 0.00950 0.40510 0.27040 1.00000
```

Benzene: AB\_oP48\_61\_3c\_3c - POSCAR

```
AB_oP48_61_3c_3c & a,b/a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,
  -> z5,x6,y6,z6 --params=6.914,1.08128435059,1.38313566676,0.1297,
  -> 0.5762,0.40803,0.1235,0.6328,0.54518,0.0057,0.4432,0.36289,
  -> 0.2172,0.6275,0.346,0.2068,0.7225,0.5756,0.0095,0.4051,0.2704 &
  -> PbcA D_{2h}^{15} #61 (c^6) & oP48 & None & Benzene & Benzene &
  -> S. K Nayak and R. Sathishkumar and T. N. {Guru Row},
  -> CrystEngComm 12, 3112-3118 (2010)
1.00000000000000
6.91400000000000 0.00000000000000 0.00000000000000
0.00000000000000 7.47600000000000 0.00000000000000
0.00000000000000 0.00000000000000 9.56300000000000
C H
24 24
Direct
0.12970000000000 0.57620000000000 0.40803000000000 C (8c)
0.37030000000000 -0.57620000000000 0.90803000000000 C (8c)
```

-0.12970000000000	1.07620000000000	0.09197000000000	C	(8c)
0.62970000000000	-0.07620000000000	-0.40803000000000	C	(8c)
-0.12970000000000	-0.57620000000000	-0.40803000000000	C	(8c)
0.62970000000000	0.57620000000000	0.09197000000000	C	(8c)
0.12970000000000	-0.07620000000000	0.90803000000000	C	(8c)
0.37030000000000	1.07620000000000	0.40803000000000	C	(8c)
0.12350000000000	0.63280000000000	0.54518000000000	C	(8c)
0.37650000000000	-0.63280000000000	1.04518000000000	C	(8c)
-0.12350000000000	1.13280000000000	-0.04518000000000	C	(8c)
0.62350000000000	-0.13280000000000	-0.54518000000000	C	(8c)
-0.12350000000000	-0.63280000000000	-0.54518000000000	C	(8c)
0.62350000000000	0.63280000000000	-0.04518000000000	C	(8c)
0.12350000000000	-0.13280000000000	1.04518000000000	C	(8c)
0.37650000000000	1.13280000000000	0.54518000000000	C	(8c)
0.00570000000000	0.44320000000000	0.36289000000000	C	(8c)
0.49430000000000	-0.44320000000000	0.86289000000000	C	(8c)
-0.00570000000000	0.94320000000000	-0.13711000000000	C	(8c)
0.50570000000000	0.05680000000000	-0.36289000000000	C	(8c)
-0.00570000000000	-0.44320000000000	-0.36289000000000	C	(8c)
0.50570000000000	0.44320000000000	0.13711000000000	C	(8c)
0.00570000000000	0.05680000000000	0.86289000000000	C	(8c)
0.49430000000000	0.94320000000000	0.36289000000000	C	(8c)
0.21720000000000	0.62750000000000	0.34600000000000	H	(8c)
0.28280000000000	-0.62750000000000	0.84600000000000	H	(8c)
-0.21720000000000	1.12750000000000	0.15400000000000	H	(8c)
0.71720000000000	-0.12750000000000	-0.34600000000000	H	(8c)
-0.21720000000000	-0.62750000000000	-0.34600000000000	H	(8c)
0.71720000000000	0.62750000000000	0.15400000000000	H	(8c)
0.21720000000000	-0.12750000000000	0.84600000000000	H	(8c)
0.28280000000000	1.12750000000000	0.34600000000000	H	(8c)
0.20680000000000	0.72250000000000	0.57560000000000	H	(8c)
0.29320000000000	-0.72250000000000	1.07560000000000	H	(8c)
-0.20680000000000	1.22250000000000	-0.07560000000000	H	(8c)
0.70680000000000	-0.22250000000000	-0.57560000000000	H	(8c)
-0.20680000000000	-0.72250000000000	-0.57560000000000	H	(8c)
0.70680000000000	0.72250000000000	-0.07560000000000	H	(8c)
0.20680000000000	-0.22250000000000	1.07560000000000	H	(8c)
0.29320000000000	1.22250000000000	0.57560000000000	H	(8c)
0.00950000000000	0.40510000000000	0.27040000000000	H	(8c)
0.49050000000000	-0.40510000000000	0.77040000000000	H	(8c)
-0.00950000000000	0.90510000000000	0.22960000000000	H	(8c)
0.50950000000000	0.09490000000000	-0.27040000000000	H	(8c)
-0.00950000000000	-0.40510000000000	-0.27040000000000	H	(8c)
0.50950000000000	0.40510000000000	0.22960000000000	H	(8c)
0.00950000000000	0.09490000000000	0.77040000000000	H	(8c)
0.49050000000000	0.90510000000000	0.27040000000000	H	(8c)

Tongbaite (Cr<sub>3</sub>C<sub>2</sub>, D<sub>5h</sub>): A2B<sub>3</sub>oP20\_62\_2c\_3c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Tongbaite'
_chemical_formula_sum 'C2 Cr3'

loop_
_publ_author_name
'S. Rundqvist'
'G. Runnsj {\\"o'}'
_journal_name_full_name
;
Acta Chemica Scandinavica
;
_journal_volume 23
_journal_year 1969
_journal_page_first 1191
_journal_page_last 1199
_publ_Section_title
;
Crystal Structure Refinement of Cr$_{3}$C$_{2}$
;

_aware_title 'Tongbaite (Cr$_{3}$C$_{2}$), $D_{5h}(10)$ Structure'
_aware_proto 'A2B3_oP20_62_2c_3c'
_aware_params 'a,b/a,c/a,x_{1},z_{1},x_{2},z_{2},x_{3},z_{3},x_{4},z_{4},x_{5},z_{5}'
_aware_params_values '5.5329,0.511305102207,2.07339731425,0.1008,0.2055,
  -> 0.2432,-0.0464,0.0157,0.4015,0.1808,0.7737,0.8691,-0.0688'
_aware_Strukturbericht '$D_{5h}(10)$'
_aware_Pearson 'oP20'

_symmetry_space_group_name_H-M "P 21/n 21/m 21/a"
_symmetry_Int_Tables_number 62

_cell_length_a 5.53290
_cell_length_b 2.82900
_cell_length_c 11.47190
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x,y+1/2,-z
4 -x+1/2,-y,z+1/2
5 -x,-y,-z
6 -x+1/2,y+1/2,z+1/2
7 x,-y+1/2,z
8 x+1/2,y,-z+1/2

loop_
```

```

_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
C1 C 4 c 0.10080 0.25000 0.20550 1.00000
C2 C 4 c 0.24320 0.25000 -0.04640 1.00000
Cr1 Cr 4 c 0.01570 0.25000 0.40150 1.00000
Cr2 Cr 4 c 0.18080 0.25000 0.77370 1.00000
Cr3 Cr 4 c 0.86910 0.25000 -0.06880 1.00000

```

Tongbaite (Cr<sub>3</sub>C<sub>2</sub>, D<sub>5</sub><sub>10</sub>): A2B<sub>3</sub>oP20\_62\_2c\_3c - POSCAR

```

A2B3_oP20_62_2c_3c & a,b/a,c/a,x1,z1,x2,z2,x3,z3,x4,z4,x5,z5 --params=
↪ 5.5329, 0.511305102207, 2.07339731425, 0.1008, 0.2055, 0.2432, -
↪ 0.0464, 0.0157, 0.4015, 0.1808, 0.7737, 0.8691, -0.0688 & Pnma D_2h
↪ ]^[16] #62 (c^5) & oP20 & SD5_{10}$ & Cr3C2 & Tongbaite & S.
↪ Rundqvist and G. Runnsj[\o], Acta Chem. Scand. 23, 1191-1199 (
↪ 1969)
1.0000000000000000
5.5329000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 2.8290000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 11.4719000000000000
C Cr
8 12
Direct
0.1008000000000000 0.2500000000000000 0.2055000000000000 C (4c)
0.3992000000000000 0.0000000000000000 0.7055000000000000 C (4c)
-0.1008000000000000 0.7500000000000000 -0.2055000000000000 C (4c)
0.6008000000000000 0.2500000000000000 0.2945000000000000 C (4c)
0.2432000000000000 0.2500000000000000 -0.0464000000000000 C (4c)
0.2568000000000000 0.7500000000000000 0.4536000000000000 C (4c)
-0.2432000000000000 0.7500000000000000 0.0464000000000000 C (4c)
0.7432000000000000 0.2500000000000000 0.5464000000000000 C (4c)
0.0157000000000000 0.2500000000000000 0.4015000000000000 Cr (4c)
0.4843000000000000 0.7500000000000000 0.9015000000000000 Cr (4c)
-0.0157000000000000 0.7500000000000000 -0.4015000000000000 Cr (4c)
0.5157000000000000 0.2500000000000000 0.0985000000000000 Cr (4c)
0.1808000000000000 0.2500000000000000 0.7737000000000000 Cr (4c)
0.3192000000000000 0.7500000000000000 1.2737000000000000 Cr (4c)
-0.1808000000000000 0.7500000000000000 -0.7737000000000000 Cr (4c)
0.6808000000000000 0.2500000000000000 -0.2737000000000000 Cr (4c)
0.8691000000000000 0.2500000000000000 -0.0688000000000000 Cr (4c)
-0.3691000000000000 0.7500000000000000 0.4312000000000000 Cr (4c)
-0.8691000000000000 0.7500000000000000 0.0688000000000000 Cr (4c)
1.3691000000000000 0.2500000000000000 0.5688000000000000 Cr (4c)

```

Forsterite (Mg<sub>2</sub>SiO<sub>4</sub>, S<sub>12</sub>): A2B4C\_oP28\_62\_ac\_2cd\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Forsterite'
_chemical_formula_sum 'Mg2 O4 Si'
loop_
_publ_author_name
'R. M. Hazen'
_journal_name_full_name
:
American Mineralogist
:
_journal_volume 61
_journal_year 1976
_journal_page_first 1280
_journal_page_last 1293
_publ_Section_title
:
Effects of temperature and pressure on the crystal structure of
↪ forsterite
:
_aflow_title 'Forsterite (Mg_{2})SiO_{4}$, SS1_{2})$ Structure'
_aflow_proto 'A2B4C_oP28_62_ac_2cd_c'
_aflow_params 'a,b/a,c/a,x_{2},z_{2},x_{3},z_{3},x_{4},z_{4},x_{5},z_{5}
↪ ],x_{6},y_{6},z_{6}'
_aflow_params_values '10.193, 0.586382811734, 0.466202295693, 0.2774, -
↪ 0.0085, 0.0913, 0.7657, 0.4474, 0.2215, 0.094, 0.4262, 0.1628, 0.0331,
↪ 0.2777'
_aflow_Strukturbericht 'SS1_{2})$'
_aflow_Pearson 'oP28'
_symmetry_space_group_name_H-M "P 21/n 21/m 21/a"
_symmetry_Int_Tables_number 62
_cell_length_a 10.19300
_cell_length_b 5.97700
_cell_length_c 4.75200
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x,y+1/2,-z
4 -x+1/2,-y,z+1/2
5 -x,-y,-z
6 -x+1/2,y+1/2,z+1/2

```

```

7 x,-y+1/2,z
8 x+1/2,y,-z+1/2
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mg1 Mg 4 a 0.00000 0.00000 0.00000 1.00000
Mg2 Mg 4 c 0.27740 0.25000 -0.00850 1.00000
O1 O 4 c 0.09130 0.25000 0.76570 1.00000
O2 O 4 c 0.44740 0.25000 0.22150 1.00000
Si1 Si 4 c 0.09400 0.25000 0.42620 1.00000
O3 O 8 d 0.16280 0.03310 0.27770 1.00000

```

Forsterite (Mg<sub>2</sub>SiO<sub>4</sub>, S<sub>12</sub>): A2B4C\_oP28\_62\_ac\_2cd\_c - POSCAR

```

A2B4C_oP28_62_ac_2cd_c & a,b/a,c/a,x2,z2,x3,z3,x4,z4,x5,z5,x6,y6,z6 --
↪ params=10.193, 0.586382811734, 0.466202295693, 0.2774, -0.0085,
↪ 0.0913, 0.7657, 0.4474, 0.2215, 0.094, 0.4262, 0.1628, 0.0331, 0.2777 &
↪ Pnma D_{2h}^[16] #62 (ac^4d) & oP28 & SS1_{2})$ & Mg2SiO4 &
↪ Forsterite & R. M. Hazen, Am. Mineral. 61, 1280-1293 (1976)
1.0000000000000000
10.1930000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.9770000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.7520000000000000
Mg O Si
8 16 4
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 Mg (4a)
0.5000000000000000 0.0000000000000000 0.5000000000000000 Mg (4a)
0.0000000000000000 0.5000000000000000 0.0000000000000000 Mg (4a)
0.5000000000000000 0.5000000000000000 0.5000000000000000 Mg (4a)
0.2774000000000000 0.2500000000000000 -0.0085000000000000 Mg (4c)
0.2226000000000000 0.7500000000000000 0.4915000000000000 Mg (4c)
-0.2774000000000000 0.7500000000000000 0.0085000000000000 Mg (4c)
0.7774000000000000 0.2500000000000000 0.5085000000000000 Mg (4c)
0.0913000000000000 0.2500000000000000 0.7657000000000000 O (4c)
0.4087000000000000 0.7500000000000000 1.2657000000000000 O (4c)
-0.0913000000000000 0.7500000000000000 -0.7657000000000000 O (4c)
0.5913000000000000 0.2500000000000000 -0.2657000000000000 O (4c)
0.4474000000000000 0.2500000000000000 0.2215000000000000 O (4c)
0.0526000000000000 0.7500000000000000 0.7215000000000000 O (4c)
-0.4474000000000000 0.7500000000000000 -0.2215000000000000 O (4c)
0.9474000000000000 0.2500000000000000 0.2785000000000000 O (4c)
0.1628000000000000 0.0331000000000000 0.2777000000000000 O (8d)
0.3372000000000000 -0.0331000000000000 0.7777000000000000 O (8d)
-0.1628000000000000 0.5331000000000000 -0.2777000000000000 O (8d)
0.6628000000000000 0.4669000000000000 0.2223000000000000 O (8d)
-0.1628000000000000 -0.0331000000000000 -0.2777000000000000 O (8d)
0.6628000000000000 0.0331000000000000 0.2223000000000000 O (8d)
0.1628000000000000 0.4669000000000000 0.2777000000000000 O (8d)
0.3372000000000000 0.5331000000000000 0.7777000000000000 O (8d)
0.0940000000000000 0.2500000000000000 0.4262000000000000 Si (4c)
0.4060000000000000 0.7500000000000000 0.9262000000000000 Si (4c)
-0.0940000000000000 0.7500000000000000 -0.4262000000000000 Si (4c)
0.5940000000000000 0.2500000000000000 0.0738000000000000 Si (4c)

```

SrH<sub>2</sub> (C29): A2B\_oP12\_62\_2c\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'SrH2'
_chemical_formula_sum 'H2 Sr'
loop_
_publ_author_name
'R. C. Ropp'
_journal_year 2013
_publ_Section_title
:
Encyclopedia of the Alkaline Earth Compounds
:
_aflow_title 'SrHS_{2})$ (SC29)$ Structure'
_aflow_proto 'A2B_oP12_62_2c_c'
_aflow_params 'a,b/a,c/a,x_{1},z_{1},x_{2},z_{2},x_{3},z_{3}'
_aflow_params_values '3.875, 1.64232258065, 1.89496774194, 0.004, 0.758, 0.24
↪ , 0.07, 0.24, 0.39'
_aflow_Strukturbericht 'SC29$'
_aflow_Pearson 'oP12'
_symmetry_space_group_name_H-M "P 21/n 21/m 21/a"
_symmetry_Int_Tables_number 62
_cell_length_a 3.87500
_cell_length_b 6.36400
_cell_length_c 7.34300
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x,y+1/2,-z
4 -x+1/2,-y,z+1/2

```

```
5 -x,-y,-z
6 -x+1/2,y+1/2,z+1/2
7 x,-y+1/2,z
8 x+1/2,y,-z+1/2
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 c 0.00400 0.25000 0.75800 1.00000
H2 H 4 c 0.24000 0.25000 0.07000 1.00000
Sr1 Sr 4 c 0.24000 0.25000 0.39000 1.00000
```

#### SrH<sub>2</sub> (C29): A2B\_oP12\_62\_2c\_c - POSCAR

```
A2B_oP12_62_2c_c & a,b/a,c/a,x1,z1,x2,z2,x3,z3 --params=3.875,
↳ 1.64232258065,1.89496774194,0.004,0.758,0.24,0.07,0.24,0.39 &
↳ Pnma D_{2h}^{16} #62 (c^3) & oP12 & $C29$ & SrH2 & SrH2 & R. C.
↳ Ropp., (2013)
1.0000000000000000
3.8750000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 6.3640000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.3430000000000000
H Sr
8 4
Direct
0.0040000000000000 0.2500000000000000 0.7580000000000000 H (4c)
0.4960000000000000 0.7500000000000000 1.2580000000000000 H (4c)
-0.0040000000000000 0.7500000000000000 -0.7580000000000000 H (4c)
0.5040000000000000 0.2500000000000000 -0.2580000000000000 H (4c)
0.2400000000000000 0.2500000000000000 0.0700000000000000 H (4c)
0.2600000000000000 0.7500000000000000 0.5700000000000000 H (4c)
-0.2400000000000000 0.7500000000000000 -0.0700000000000000 H (4c)
0.7400000000000000 0.2500000000000000 0.4300000000000000 H (4c)
0.2400000000000000 0.2500000000000000 0.3900000000000000 Sr (4c)
0.2600000000000000 0.7500000000000000 0.8900000000000000 Sr (4c)
-0.2400000000000000 0.7500000000000000 -0.3900000000000000 Sr (4c)
0.7400000000000000 0.2500000000000000 0.1100000000000000 Sr (4c)
```

#### e-NiAl<sub>3</sub> (D0<sub>20</sub>): A3B\_oP16\_62\_cd\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '$\epsilon$-NiAl_{3}$'
_chemical_formula_sum 'Al3 Ni'

loop_
_publ_author_name
'A. J. Bradley'
'A. Taylor'
_journal_name_full_name
;
Philosophical Magazine
;
_journal_volume 23
_journal_year 1937
_journal_page_first 1049
_journal_page_last 1067
_publ_section_title
;
The crystal structures of Ni_{2}Al_{3}$ and NiAl_{3}$
;

# Found in A Handbook of Lattice Spacings and Structures of Metals and
Alloys, 1958

_aware_title '$\epsilon$-NiAl_{3}$ (SD0_{20}$) Structure'
_aware_proto 'A3B_oP16_62_cd_c'
_aware_params 'a,b/a,c/a,x_{1},z_{1},x_{2},z_{2},x_{3},y_{3},z_{3}'
_aware_params_values '6.5982,1.11416750023,0.727789397108,0.011,0.415,
↳ 0.369,0.555,0.174,0.053,0.856'
_aware_strukturbericht 'SD0_{20}$'
_aware_pearson 'oP16'

_symmetry_space_group_name_H-M "P 21/n 21/m 21/a"
_symmetry_Int_Tables_number 62

_cell_length_a 6.59820
_cell_length_b 7.35150
_cell_length_c 4.80210
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x,y+1/2,-z
4 -x+1/2,-y,z+1/2
5 -x,-y,-z
6 -x+1/2,y+1/2,z+1/2
7 x,-y+1/2,z
8 x+1/2,y,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
```

```
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 4 c 0.01100 0.25000 0.41500 1.00000
Ni1 Ni 4 c 0.36900 0.25000 0.55500 1.00000
Al2 Al 8 d 0.17400 0.05300 0.85600 1.00000
```

#### e-NiAl<sub>3</sub> (D0<sub>20</sub>): A3B\_oP16\_62\_cd\_c - POSCAR

```
A3B_oP16_62_cd_c & a,b/a,c/a,x1,z1,x2,z2,x3,y3,z3 --params=6.5982,
↳ 1.11416750023,0.727789397108,0.011,0.415,0.369,0.555,0.174,
↳ 0.053,0.856 & Pnma D_{2h}^{16} #62 (c^2d) & oP16 & $SD0_{20}$ &
↳ NiAl3 & $\epsilon$-NiAl_{3}$ & A. J. Bradley and A. Taylor,
↳ Philos. Mag. 23, 1049-1067 (1937)
1.0000000000000000
6.5982000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.3515000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.8021000000000000
Al Ni
12 4
Direct
0.0110000000000000 0.2500000000000000 0.4150000000000000 Al (4c)
0.4890000000000000 0.7500000000000000 0.9150000000000000 Al (4c)
-0.0110000000000000 0.7500000000000000 -0.4150000000000000 Al (4c)
0.5110000000000000 0.2500000000000000 0.0850000000000000 Al (4c)
0.1740000000000000 0.0530000000000000 0.8560000000000000 Al (8d)
0.3260000000000000 -0.0530000000000000 1.3560000000000000 Al (8d)
-0.1740000000000000 0.5530000000000000 -0.8560000000000000 Al (8d)
0.6740000000000000 0.4470000000000000 -0.3560000000000000 Al (8d)
-0.1740000000000000 -0.0530000000000000 -0.8560000000000000 Al (8d)
0.6740000000000000 0.0530000000000000 -0.3560000000000000 Al (8d)
0.1740000000000000 0.4470000000000000 0.8560000000000000 Al (8d)
0.3260000000000000 0.5530000000000000 1.3560000000000000 Al (8d)
0.3690000000000000 0.2500000000000000 0.5550000000000000 Ni (4c)
0.1310000000000000 0.7500000000000000 1.0550000000000000 Ni (4c)
-0.3690000000000000 0.7500000000000000 -0.5550000000000000 Ni (4c)
0.8690000000000000 0.2500000000000000 -0.0550000000000000 Ni (4c)
```

#### Cubanite (CuFe<sub>2</sub>S<sub>3</sub>, E<sub>9</sub>): AB2C3\_oP24\_62\_c\_d\_cd - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Cubanite'
_chemical_formula_sum 'Cu Fe2 S3'

loop_
_publ_author_name
'T. Szyma{\n}ski'
_journal_name_full_name
;
Zeitschrift f{"u}r Kristallographie - Crystalline Materials
;
_journal_volume 140
_journal_year 1974
_journal_page_first 218
_journal_page_last 239
_publ_section_title
;
A refinement of the structure of cubanite, CuFe_{2}S_{3}$
;

_aware_title 'Cubanite (CuFe_{2}S_{3}$, SE9_{e}$) Structure'
_aware_proto 'AB2C3_oP24_62_c_d_cd'
_aware_params 'a,b/a,c/a,x_{1},z_{1},x_{2},z_{2},x_{3},y_{3},z_{3},x_{4}
↳ ,y_{4},z_{4}'
_aware_params_values '6.231,1.78414379714,1.03787514043,0.123,0.0823,
↳ 0.2579,0.4127,0.1366,0.087,0.5853,0.267,0.0846,-0.088'
_aware_strukturbericht 'SE9_{e}$'
_aware_pearson 'oP24'

_symmetry_space_group_name_H-M "P 21/n 21/m 21/a"
_symmetry_Int_Tables_number 62

_cell_length_a 6.23100
_cell_length_b 11.11700
_cell_length_c 6.46700
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x,y+1/2,-z
4 -x+1/2,-y,z+1/2
5 -x,-y,-z
6 -x+1/2,y+1/2,z+1/2
7 x,-y+1/2,z
8 x+1/2,y,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
```

```

_atom_site_fract_z
_atom_site_occupancy
Cu1 Cu 4 c 0.12300 0.25000 0.08230 1.00000
S1 S 4 c 0.25790 0.25000 0.41270 1.00000
Fe1 Fe 8 d 0.13660 0.08700 0.58530 1.00000
S2 S 8 d 0.26700 0.08460 -0.08800 1.00000

```

Cubanite (CuFe<sub>2</sub>S<sub>3</sub>, E<sub>9</sub>): AB2C3\_op24\_62\_c\_d\_cd - POSCAR

```

AB2C3_op24_62_c_d_cd & a,b/a,c/a,x1,z1,x2,z2,x3,y3,z3,x4,y4,z4 --params=
↳ 6.231,1.78414379714,1.03787514043,0.123,0.0823,0.2579,0.4127,
↳ 0.1366,0.087,0.5853,0.267,0.0846,-0.088 & Pnma D_{2h}^{16} #62
↳ (c^2d^2) & oP24 & SE9_{e}S & CuFe2S3 & Cubanite & T. Szyma{\n}
↳ ski, Zeitschrift f{u}r Kristallographie - Crystalline
↳ Materials 140, 218-239 (1974)
1.0000000000000000
6.231000000000000 0.000000000000000 0.000000000000000
0.000000000000000 11.117000000000000 0.000000000000000
0.000000000000000 0.000000000000000 6.467000000000000
Cu Fe S
4 8 12
Direct
0.123000000000000 0.250000000000000 0.082300000000000 Cu (4c)
0.377000000000000 0.750000000000000 0.582300000000000 Cu (4c)
-0.123000000000000 0.750000000000000 -0.082300000000000 Cu (4c)
0.623000000000000 0.250000000000000 0.417700000000000 Cu (4c)
0.136600000000000 0.087000000000000 0.585300000000000 Fe (8d)
0.363400000000000 -0.087000000000000 1.085300000000000 Fe (8d)
-0.136600000000000 0.087000000000000 -0.585300000000000 Fe (8d)
0.636600000000000 0.413000000000000 -0.085300000000000 Fe (8d)
-0.136600000000000 -0.087000000000000 -0.585300000000000 Fe (8d)
0.636600000000000 0.087000000000000 -0.085300000000000 Fe (8d)
0.136600000000000 0.413000000000000 0.585300000000000 Fe (8d)
0.363400000000000 0.087000000000000 1.085300000000000 Fe (8d)
0.257900000000000 0.250000000000000 0.412700000000000 S (4c)
0.242100000000000 0.750000000000000 0.912700000000000 S (4c)
-0.257900000000000 0.750000000000000 -0.412700000000000 S (4c)
0.757900000000000 0.250000000000000 0.087300000000000 S (4c)
0.267000000000000 0.084600000000000 -0.088000000000000 S (8d)
0.233000000000000 -0.084600000000000 0.412000000000000 S (8d)
-0.267000000000000 0.584600000000000 0.088000000000000 S (8d)
0.767000000000000 0.415400000000000 0.588000000000000 S (8d)
-0.267000000000000 -0.084600000000000 0.088000000000000 S (8d)
0.767000000000000 0.084600000000000 0.588000000000000 S (8d)
0.267000000000000 0.415400000000000 -0.088000000000000 S (8d)
0.233000000000000 0.584600000000000 0.412000000000000 S (8d)

```

Molybdate (MoO<sub>3</sub>, D<sub>0g</sub>): AB3\_op16\_62\_c\_3c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Molybdate'
_chemical_formula_sum 'Mo O3'

loop_
_publ_author_name
'H. Sitepu'
'B. H. {O}Connor'
'D. Li'
_journal_name_full_name
;
Journal of Applied Crystallography
;
_journal_volume 38
_journal_year 2005
_journal_page_first 158
_journal_page_last 167
_publ_section_title
;
Comparative evaluation of the March and generalized spherical harmonic
↳ preferred orientation models using X-ray diffraction data for
↳ molybdate and calcite powders
;

_aflow_title 'Molybdate (MoO3_{3}$, $D0_{8}$) Structure'
_aflow_proto 'AB3_op16_62_c_3c'
_aflow_params 'a,b/a,c/a,x_{1},z_{1},x_{2},z_{2},x_{3},z_{3},x_{4},z_{4}'
↳ '
_aflow_params_values '13.855,0.266791771923,0.28601948755,0.398,0.425,
↳ 0.074,-0.026,0.414,-0.066,0.276,0.49'
_aflow_Strukturbericht '$D0_{8}$'
_aflow_Pearson 'oP16'

_symmetry_space_group_name_H-M 'P n m a'
_symmetry_Int_Tables_number 62

_cell_length_a 13.85500
_cell_length_b 3.69640
_cell_length_c 3.96280
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x,y+1/2,-z
4 -x+1/2,-y,z+1/2
5 -x,-y,-z
6 -x+1/2,y+1/2,z+1/2
7 x,-y+1/2,z

```

```

8 x+1/2,y,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mo1 Mo 4 c 0.39800 0.25000 0.42500 1.00000
O1 O 4 c 0.07400 0.25000 -0.02600 1.00000
O2 O 4 c 0.41400 0.25000 -0.06600 1.00000
O3 O 4 c 0.27600 0.25000 0.49000 1.00000

```

Molybdate (MoO<sub>3</sub>, D<sub>0g</sub>): AB3\_op16\_62\_c\_3c - POSCAR

```

AB3_op16_62_c_3c & a,b/a,c/a,x1,z1,x2,z2,x3,z3,x4,z4 --params=13.855,
↳ 0.266791771923,0.28601948755,0.398,0.425,0.074,-0.026,0.414,-
↳ 0.066,0.276,0.49 & Pnma D_{2h}^{16} #62 (c^4) & oP16 & SD0_{8}$
↳ & MoO3 & Molybdate & H. Sitepu and B. H. {O}Connor and D. Li,
↳ J. Appl. Crystallogr. 38, 158-167 (2005)
1.0000000000000000
13.855000000000000 0.000000000000000 0.000000000000000
0.000000000000000 3.696400000000000 0.000000000000000
0.000000000000000 0.000000000000000 3.962800000000000
Mo O
4 12
Direct
0.398000000000000 0.250000000000000 0.425000000000000 Mo (4c)
0.102000000000000 0.750000000000000 0.925000000000000 Mo (4c)
-0.398000000000000 0.750000000000000 -0.425000000000000 Mo (4c)
0.898000000000000 0.250000000000000 0.075000000000000 Mo (4c)
0.074000000000000 0.250000000000000 -0.026000000000000 O (4c)
0.426000000000000 0.750000000000000 0.474000000000000 O (4c)
-0.074000000000000 0.750000000000000 0.026000000000000 O (4c)
0.574000000000000 0.250000000000000 0.526000000000000 O (4c)
0.414000000000000 0.250000000000000 -0.066000000000000 O (4c)
0.086000000000000 0.750000000000000 0.434000000000000 O (4c)
-0.414000000000000 0.750000000000000 0.066000000000000 O (4c)
0.914000000000000 0.250000000000000 0.566000000000000 O (4c)
0.276000000000000 0.250000000000000 0.490000000000000 O (4c)
0.224000000000000 0.750000000000000 0.990000000000000 O (4c)
-0.276000000000000 0.750000000000000 -0.490000000000000 O (4c)
0.776000000000000 0.250000000000000 0.010000000000000 O (4c)

```

Barite (BaSO<sub>4</sub>, H<sub>02</sub>): AB4C\_op24\_62\_c\_2cd\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Barite'
_chemical_formula_sum 'Ba O4 S'

loop_
_publ_author_name
'A. A. Colville'
'K. Staudhammer'
_journal_name_full_name
;
American Mineralogist
;
_journal_volume 52
_journal_year 1967
_journal_page_first 1877
_journal_page_last 1880
_publ_section_title
;
A refinement of the structure of barite
;

# Found in Mineralogy Database, 2012 Found in Mineralogy Database, {
↳ Barite},

_aflow_title 'Barite (BaSO4_{4}$, $H0_{2}$) Structure'
_aflow_proto 'AB4C_op24_62_c_2cd_c'
_aflow_params 'a,b/a,c/a,x_{1},z_{1},x_{2},z_{2},x_{3},z_{3},x_{4},z_{4}'
↳ ',x_{5},y_{5},z_{5}'
_aflow_params_values '8.884,0.614362899595,0.805155335434,0.8154,0.3419,
↳ 0.5878,0.6062,0.3192,0.5515,0.437,0.6914,0.4186,0.4702,0.819'
_aflow_Strukturbericht '$H0_{2}$'
_aflow_Pearson 'oP24'

_symmetry_space_group_name_H-M 'P 21/n 21/m 21/a'
_symmetry_Int_Tables_number 62

_cell_length_a 8.88400
_cell_length_b 5.45800
_cell_length_c 7.15300
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x,y+1/2,-z
4 -x+1/2,-y,z+1/2
5 -x,-y,-z
6 -x+1/2,y+1/2,z+1/2
7 x,-y+1/2,z

```

```

8 x+1/2,y,-z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Ba1 Ba 4 c 0.81540 0.25000 0.34190 1.00000
O1 O 4 c 0.58780 0.25000 0.60620 1.00000
O2 O 4 c 0.31920 0.25000 0.55150 1.00000
S1 S 4 c 0.43700 0.25000 0.69140 1.00000
O3 O 8 d 0.41860 0.47020 0.81900 1.00000

```

Barite (BaSO<sub>4</sub>, H<sub>0</sub>): AB4C\_oP24\_62\_c\_2cd\_c - POSCAR

```

AB4C_oP24_62_c_2cd_c & a,b/a,c/a,x1,z1,x2,z2,x3,z3,x4,z4,x5,y5,z5 --
↳ params=8.884,0.614362899595,0.805155335434,0.8154,0.3419,0.5878
↳ 0.6062,0.3192,0.5515,0.437,0.6914,0.4186,0.4702,0.819 & Pnma
↳ D_{2h}^{16} #62 (c^4d) & oP24 & $H0_{2}$ & BaSO4 & Barite & A.
↳ A. Colville and K. Staudhammer, Am. Mineral. 52, 1877-1880 (
↳ 1967)
1.0000000000000000
8.8840000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.4580000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.1530000000000000
Ba O S
4 16 4
Direct
0.8154000000000000 0.2500000000000000 0.3419000000000000 Ba (4c)
-0.3154000000000000 0.7500000000000000 0.8419000000000000 Ba (4c)
-0.8154000000000000 0.7500000000000000 -0.3419000000000000 Ba (4c)
1.3154000000000000 0.2500000000000000 0.1581000000000000 Ba (4c)
0.5878000000000000 0.2500000000000000 0.6062000000000000 O (4c)
-0.0878000000000000 0.7500000000000000 1.1062000000000000 O (4c)
-0.5878000000000000 0.7500000000000000 -0.6062000000000000 O (4c)
1.0878000000000000 0.2500000000000000 -0.1062000000000000 O (4c)
0.3192000000000000 0.2500000000000000 0.5515000000000000 O (4c)
0.1808000000000000 0.7500000000000000 1.0515000000000000 O (4c)
-0.3192000000000000 0.7500000000000000 -0.5515000000000000 O (4c)
0.8192000000000000 0.2500000000000000 -0.0515000000000000 O (4c)
0.4186000000000000 0.4702000000000000 0.8190000000000000 O (8d)
0.0814000000000000 -0.4702000000000000 1.3190000000000000 O (8d)
-0.4186000000000000 0.9702000000000000 -0.8190000000000000 O (8d)
0.9186000000000000 0.0298000000000000 -0.3190000000000000 O (8d)
-0.4186000000000000 -0.4702000000000000 -0.8190000000000000 O (8d)
0.9186000000000000 0.4702000000000000 -0.3190000000000000 O (8d)
0.4186000000000000 0.0298000000000000 0.8190000000000000 O (8d)
0.0814000000000000 0.9702000000000000 1.3190000000000000 O (8d)
0.4370000000000000 0.2500000000000000 0.6914000000000000 S (4c)
0.0630000000000000 0.7500000000000000 1.1914000000000000 S (4c)
-0.4370000000000000 0.7500000000000000 -0.6914000000000000 S (4c)
0.9370000000000000 0.2500000000000000 -0.1914000000000000 S (4c)

```

Westerveldite (FeAs, B14): AB\_oP8\_62\_c\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Westerveldite'
_chemical_formula_sum 'As Fe'

loop_
  _publ_author_name
  'K. Selte'
  'A. Kjekshus'
  'A. F. Andresen'
  _journal_name_full_name
  ;
Acta Chemica Scandinavica
;
_journal_volume 26
_journal_year 1972
_journal_page_first 3101
_journal_page_last 3113
_publ_section_title
;
Magnetic Structure and Properties of FeAs
;

# Found in Interplay between magnetism, structure, and strong
↳ electron-phonon coupling in binary FeAs under pressure, 2011

_aflow_title 'Westerveldite (FeAs, $B14$) Structure'
_aflow_proto 'AB_oP8_62_c_c'
_aflow_params 'a,b/a,c/a,x_{1},z_{1},x_{2},z_{2}'
_aflow_params_values '5.454,0.609644297763,1.10542720939,0.2005,0.5741,
↳ 0.0058,0.1993'
_aflow_Strukturbericht '$B14$'
_aflow_Pearson 'oP8'

_symmetry_space_group_name_H-M 'P 21/n 21/m 21/a'
_symmetry_Int_Tables_number 62

_cell_length_a 5.45400
_cell_length_b 3.32500
_cell_length_c 6.02900
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

```

```

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x,y+1/2,-z
4 -x+1/2,-y,z+1/2
5 -x,-y,-z
6 -x+1/2,y+1/2,z+1/2
7 x,-y+1/2,z
8 x+1/2,y,-z+1/2

```

```

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
As1 As 4 c 0.20050 0.25000 0.57410 1.00000
Fe1 Fe 4 c 0.00580 0.25000 0.19930 1.00000

```

Westerveldite (FeAs, B14): AB\_oP8\_62\_c\_c - POSCAR

```

AB_oP8_62_c_c & a,b/a,c/a,x1,z1,x2,z2 --params=5.454,0.609644297763,
↳ 1.10542720939,0.2005,0.5741,0.0058,0.1993 & Pnma D_{2h}^{16} #
↳ 62 (c^2) & oP8 & $B14$ & FeAs & Westerveldite & K. Selte and A.
↳ Kjekshus and A. F. Andresen, Acta Chem. Scand. 26, 3101-3113 (
↳ 1972)
1.0000000000000000
5.4540000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 3.3250000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.0290000000000000
As Fe
4 4
Direct
0.2005000000000000 0.2500000000000000 0.5741000000000000 As (4c)
0.2995000000000000 0.7500000000000000 1.0741000000000000 As (4c)
-0.2005000000000000 0.7500000000000000 -0.5741000000000000 As (4c)
0.7005000000000000 0.2500000000000000 -0.0741000000000000 As (4c)
0.0058000000000000 0.2500000000000000 0.1993000000000000 Fe (4c)
0.4942000000000000 0.7500000000000000 0.6993000000000000 Fe (4c)
-0.0058000000000000 0.7500000000000000 -0.1993000000000000 Fe (4c)
0.5058000000000000 0.2500000000000000 0.3007000000000000 Fe (4c)

```

Rasvumite (KFe<sub>2</sub>S<sub>3</sub>): A2BC3\_oC24\_63\_e\_c\_cg - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Rasvumite'
_chemical_formula_sum 'Fe2 K S3'

loop_
  _publ_author_name
  'J. R. Clark'
  'G. E. {Brown, Jr.}'
  _journal_name_full_name
  ;
American Mineralogist
;
_journal_volume 65
_journal_year 1980
_journal_page_first 477
_journal_page_last 482
_publ_section_title
;
Crystal structure of rasvumite, KFe$_{2}$S$_{3}$
;

# Found in The American Mineralogist Crystal Structure Database, 2003

_aflow_title 'Rasvumite (KFe$_{2}$S$_{3}$) Structure'
_aflow_proto 'A2BC3_oC24_63_e_c_cg'
_aflow_params 'a,b/a,c/a,y_{1},y_{2},x_{3},x_{4},y_{4}'
_aflow_params_values '9.049,1.21770361366,0.600176815118,0.6699,0.1191,
↳ 0.8502,0.2174,0.3859'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC24'

_symmetry_space_group_name_H-M 'C 2/m 2/c 21/m'
_symmetry_Int_Tables_number 63

_cell_length_a 9.04900
_cell_length_b 11.01900
_cell_length_c 5.43100
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z+1/2
4 -x,-y,z+1/2
5 -x,-y,-z
6 -x,y,z
7 x,-y,z+1/2
8 x,y,-z+1/2
9 x+1/2,y+1/2,z

```

```

10 x+1/2,-y+1/2,-z
11 -x+1/2,y+1/2,-z+1/2
12 -x+1/2,-y+1/2,z+1/2
13 -x+1/2,-y+1/2,-z
14 -x+1/2,y+1/2,z
15 x+1/2,-y+1/2,z+1/2
16 x+1/2,y+1/2,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
K1 K 4 c 0.00000 0.66990 0.25000 1.00000
S1 S 4 c 0.00000 0.11910 0.25000 1.00000
Fe1 Fe 8 e 0.85020 0.00000 0.00000 1.00000
S2 S 8 g 0.21740 0.38590 0.25000 1.00000

```

Rasvumite (KFe<sub>2</sub>S<sub>3</sub>): A2BC3\_oC24\_63\_e\_c\_cg - POSCAR

```

A2BC3_oC24_63_e_c_cg & a,b/a,c/a,y1,y2,x3,x4,y4 --params=9.049,
↳ 1.21770361366,0.600176815118,0.6699,0.1191,0.8502,0.2174,0.3859
↳ & Cmc D_{2h}^{17} #63 (c^2eg) & oC24 & None & KFe2S3 &
↳ Rasvumite & J. R. Clark and G. E. {Brown, Jr.}, Am. Mineral. 65
↳ , 477-482 (1980)
1.000000000000000
4.524500000000000 -5.509500000000000 0.000000000000000
4.524500000000000 5.509500000000000 0.000000000000000
0.000000000000000 0.000000000000000 5.431000000000000
Fe K S
4 2 6
Direct
0.850200000000000 0.850200000000000 0.000000000000000 Fe (8e)
-0.850200000000000 -0.850200000000000 0.500000000000000 Fe (8e)
-0.850200000000000 -0.850200000000000 0.000000000000000 Fe (8e)
0.850200000000000 0.850200000000000 0.500000000000000 Fe (8e)
-0.669900000000000 0.669900000000000 0.250000000000000 K (4c)
0.669900000000000 -0.669900000000000 0.750000000000000 K (4c)
-0.119100000000000 0.119100000000000 0.250000000000000 S (4c)
0.119100000000000 -0.119100000000000 0.750000000000000 S (4c)
-0.168500000000000 0.603300000000000 0.250000000000000 S (8g)
0.168500000000000 -0.603300000000000 0.750000000000000 S (8g)
-0.603300000000000 0.168500000000000 0.250000000000000 S (8g)
0.603300000000000 -0.168500000000000 0.750000000000000 S (8g)

```

La<sub>3</sub>Ni<sub>17</sub>Mg<sub>5</sub>: A43B5C17\_oC260\_63\_c8fg6h\_cfg\_ce3f2h - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'La43Ni17Mg5'
_chemical_formula_sum 'La43 Mg5 Ni17'

loop_
_publ_author_name
'P. Solokha'
'S. {De Negri}'
'V. Pavlyuk'
'A. Saccone'
_journal_name_full_name
;
Inorganic Chemistry
;
_journal_volume 48
_journal_year 2009
_journal_page_first 11586
_journal_page_last 11593
_publ_section_title
;
Anti-Mackay Polyicosahedral Clusters in {La-Ni-Mg} Ternary Compounds:
↳ Synthesis and Crystal Structure of the LaS_{43}NiS_{17}MgS_{5}
↳ }S} New Intermetallic Phase
;
_aflow_title 'LaS_{43}NiS_{17}MgS_{5} Structure'
_aflow_proto 'A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h'
_aflow_params 'a,b/a,c/a,y_{1},y_{2},y_{3},x_{4},y_{5},z_{5},y_{6},z_{6}
↳ ),y_{7},z_{7},y_{8},z_{8},y_{9},z_{9},y_{10},z_{10},y_{11},z_{11},z_{12},z_{13},z_{14},z_{15},y_{16},z_{16},x_{17},y_{17},x_{18},y_{18},x_{19},y_{19},z_{20},y_{20},z_{20},x_{21},y_{21},z_{21},x_{22},y_{22},z_{22},x_{23},y_{23},z_{23},x_{24},y_{24},z_{24},x_{25},y_{25},z_{25},x_{26},y_{26},z_{26} --
↳ )
_aflow_params_values '10.11895,1.73974572461,4.16742843872,0.38998,
↳ 0.0432,0.5987,0.1275,0.13992,0.17412,0.7278,0.20648,0.19723,
↳ 0.62632,0.1388,0.02884,0.39065,0.0988,0.06788,0.55569,0.59876,
↳ 0.1328,0.28079,0.54761,0.0678,0.6912,0.07797,0.09224,0.45337,
↳ 0.1675,0.43146,0.0091,0.18607,0.20422,0.3338,0.3774,0.18828,
↳ 0.32898,0.174,0.19344,0.2014,0.10123,0.30731,0.03499,0.20655,
↳ 0.30495,0.49596,0.12681,0.19578,0.33018,0.026,0.31697,0.03483,
↳ 0.04522,0.2812,0.17213,0.16828,0.2807,0.35936,0.09067'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC260'

_symmetry_space_group_name_H-M 'C 2/m 2/c 21/m'
_symmetry_Int_Tables_number 63

_cell_length_a 10.11895
_cell_length_b 17.60440
_cell_length_c 42.17000

```

```

_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z+1/2
4 -x,-y,z+1/2
5 -x,-y,-z
6 -x,y,z
7 x,-y,z+1/2
8 x,y,-z+1/2
9 x+1/2,y+1/2,z
10 x+1/2,-y+1/2,-z
11 -x+1/2,y+1/2,-z+1/2
12 -x+1/2,-y+1/2,z+1/2
13 -x+1/2,-y+1/2,-z
14 -x+1/2,y+1/2,z
15 x+1/2,-y+1/2,z+1/2
16 x+1/2,y+1/2,-z+1/2

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
La1 La 4 c 0.00000 0.38998 0.25000 1.00000
Mg1 Mg 4 c 0.00000 0.04320 0.25000 1.00000
Ni1 Ni 4 c 0.00000 0.59870 0.25000 1.00000
Ni2 Ni 8 e 0.12750 0.00000 0.00000 1.00000
La2 La 8 f 0.00000 0.13992 0.17412 1.00000
La3 La 8 f 0.00000 0.72780 0.20648 1.00000
La4 La 8 f 0.00000 0.19723 0.62632 1.00000
La5 La 8 f 0.00000 0.13880 0.02884 1.00000
La6 La 8 f 0.00000 0.39065 0.09880 1.00000
La7 La 8 f 0.00000 0.06788 0.55569 1.00000
La8 La 8 f 0.00000 0.59876 0.13280 1.00000
La9 La 8 f 0.00000 0.28079 0.54761 1.00000
Mg2 Mg 8 f 0.00000 0.06780 0.69120 1.00000
Ni3 Ni 8 f 0.00000 0.07797 0.09224 1.00000
Ni4 Ni 8 f 0.00000 0.45337 0.16750 1.00000
Ni5 Ni 8 f 0.00000 0.43146 0.00910 1.00000
La10 La 8 g 0.18607 0.20422 0.25000 1.00000
Mg3 Mg 8 g 0.33380 0.37740 0.25000 1.00000
La11 La 16 h 0.18828 0.32898 0.17400 1.00000
La12 La 16 h 0.19344 0.20140 0.10123 1.00000
La13 La 16 h 0.30731 0.03499 0.20655 1.00000
La14 La 16 h 0.30495 0.49596 0.12681 1.00000
La15 La 16 h 0.19578 0.33018 0.02600 1.00000
La16 La 16 h 0.31697 0.03483 0.04522 1.00000
Ni6 Ni 16 h 0.28120 0.17213 0.16828 1.00000
Ni7 Ni 16 h 0.28070 0.35936 0.09067 1.00000

```

La<sub>3</sub>Ni<sub>17</sub>Mg<sub>5</sub>: A43B5C17\_oC260\_63\_c8fg6h\_cfg\_ce3f2h - POSCAR

```

A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h & a,b/a,c/a,y1,y2,y3,x4,y5,z5,y6,z6,
↳ y7,z7,y8,z8,y9,z9,y10,z10,y11,z11,y12,z12,y13,z13,y14,z14,y15,
↳ z15,y16,z16,x17,y17,x18,y18,x19,y19,z19,x20,y20,z20,x21,y21,z21
↳ ,x22,y22,z22,x23,y23,z23,x24,y24,z24,x25,y25,z25,x26,y26,z26 --
↳ )
params=10.11895,1.73974572461,4.16742843872,0.38998,0.0432,
↳ 0.5987,0.1275,0.13992,0.17412,0.7278,0.20648,0.19723,0.62632,
↳ 0.1388,0.02884,0.39065,0.0988,0.06788,0.55569,0.59876,0.1328,
↳ 0.28079,0.54761,0.0678,0.6912,0.07797,0.09224,0.45337,0.1675,
↳ 0.43146,0.0091,0.18607,0.20422,0.3338,0.3774,0.18828,0.32898,
↳ 0.174,0.19344,0.2014,0.10123,0.30731,0.03499,0.20655,0.30495,
↳ 0.49596,0.12681,0.19578,0.33018,0.026,0.31697,0.03483,0.04522,
↳ 0.2812,0.17213,0.16828,0.2807,0.35936,0.09067 & Cmc D_{2h}^{17}
↳ ) #63 (c^3ef^12g^2h^8) & oC260 & None & La43Ni17Mg5 &
↳ La43Ni17Mg5 & P. Solokha et al., Inorg. Chem. 48, 11586-11593 (
↳ 2009)
1.000000000000000
5.059475000000000 -8.802200000000000 0.000000000000000
5.059475000000000 8.802200000000000 0.000000000000000
0.000000000000000 0.000000000000000 42.170000000000000
La Mg Ni
86 10 34
Direct
-0.389980000000000 0.389980000000000 0.250000000000000 La (4c)
0.389980000000000 -0.389980000000000 0.750000000000000 La (4c)
-0.139920000000000 0.139920000000000 0.174120000000000 La (8f)
0.139920000000000 -0.139920000000000 0.674120000000000 La (8f)
-0.139920000000000 0.139920000000000 0.325880000000000 La (8f)
0.139920000000000 -0.139920000000000 -0.174120000000000 La (8f)
-0.727800000000000 0.727800000000000 0.206480000000000 La (8f)
0.727800000000000 -0.727800000000000 0.706480000000000 La (8f)
-0.727800000000000 0.727800000000000 0.293520000000000 La (8f)
0.727800000000000 -0.727800000000000 -0.206480000000000 La (8f)
-0.197230000000000 0.197230000000000 0.626320000000000 La (8f)
0.197230000000000 -0.197230000000000 1.263200000000000 La (8f)
-0.197230000000000 0.197230000000000 -0.126320000000000 La (8f)
0.197230000000000 -0.197230000000000 -0.626320000000000 La (8f)
-0.138800000000000 0.138800000000000 0.028840000000000 La (8f)
0.138800000000000 -0.138800000000000 0.528840000000000 La (8f)
-0.138800000000000 0.138800000000000 0.471160000000000 La (8f)
0.138800000000000 -0.138800000000000 -0.028840000000000 La (8f)
-0.390650000000000 0.390650000000000 0.098800000000000 La (8f)
0.390650000000000 -0.390650000000000 0.598800000000000 La (8f)
-0.390650000000000 0.390650000000000 0.401200000000000 La (8f)

```

```

0.39065000000000 -0.39065000000000 -0.09880000000000 La (8f)
-0.06788000000000 -0.06788000000000 0.55569000000000 La (8f)
0.06788000000000 -0.06788000000000 1.05569000000000 La (8f)
-0.06788000000000 -0.06788000000000 -0.05569000000000 La (8f)
0.06788000000000 -0.06788000000000 -0.55569000000000 La (8f)
-0.59876000000000 0.59876000000000 0.13280000000000 La (8f)
0.59876000000000 -0.59876000000000 0.63280000000000 La (8f)
-0.59876000000000 0.59876000000000 0.36720000000000 La (8f)
0.59876000000000 -0.59876000000000 -0.13280000000000 La (8f)
-0.28079000000000 0.28079000000000 0.54761000000000 La (8f)
0.28079000000000 -0.28079000000000 1.04761000000000 La (8f)
-0.28079000000000 0.28079000000000 -0.04761000000000 La (8f)
0.28079000000000 -0.28079000000000 -0.54761000000000 La (8f)
-0.01815000000000 0.39029000000000 0.25000000000000 La (8g)
0.01815000000000 -0.39029000000000 0.75000000000000 La (8g)
-0.39029000000000 0.01815000000000 0.25000000000000 La (8g)
0.39029000000000 -0.01815000000000 0.75000000000000 La (8g)
-0.14070000000000 0.51726000000000 0.17400000000000 La (16h)
0.14070000000000 -0.51726000000000 0.67400000000000 La (16h)
-0.51726000000000 0.14070000000000 0.32600000000000 La (16h)
0.51726000000000 -0.14070000000000 -0.17400000000000 La (16h)
0.14070000000000 -0.51726000000000 -0.17400000000000 La (16h)
-0.14070000000000 0.51726000000000 0.32600000000000 La (16h)
0.51726000000000 -0.14070000000000 0.67400000000000 La (16h)
-0.51726000000000 0.14070000000000 0.17400000000000 La (16h)
-0.00796000000000 0.39484000000000 0.10123000000000 La (16h)
0.00796000000000 -0.39484000000000 0.60123000000000 La (16h)
-0.39484000000000 0.00796000000000 0.39877000000000 La (16h)
0.39484000000000 -0.00796000000000 -0.10123000000000 La (16h)
0.00796000000000 -0.39484000000000 -0.10123000000000 La (16h)
-0.00796000000000 0.39484000000000 0.39877000000000 La (16h)
0.39484000000000 -0.00796000000000 0.60123000000000 La (16h)
-0.39484000000000 0.00796000000000 0.10123000000000 La (16h)
0.27232000000000 0.34230000000000 0.20655000000000 La (16h)
-0.27232000000000 -0.34230000000000 0.70655000000000 La (16h)
0.34230000000000 -0.27232000000000 0.29345000000000 La (16h)
-0.34230000000000 0.27232000000000 -0.20655000000000 La (16h)
0.27232000000000 0.34230000000000 0.29345000000000 La (16h)
-0.34230000000000 -0.27232000000000 0.70655000000000 La (16h)
0.34230000000000 -0.27232000000000 0.20655000000000 La (16h)
-0.19101000000000 0.80091000000000 0.12681000000000 La (16h)
0.19101000000000 -0.80091000000000 0.62681000000000 La (16h)
-0.80091000000000 0.19101000000000 0.37319000000000 La (16h)
0.80091000000000 -0.19101000000000 -0.12681000000000 La (16h)
0.19101000000000 -0.80091000000000 -0.12681000000000 La (16h)
-0.19101000000000 0.80091000000000 0.37319000000000 La (16h)
0.80091000000000 -0.19101000000000 0.62681000000000 La (16h)
-0.80091000000000 0.19101000000000 0.12681000000000 La (16h)
-0.13440000000000 0.52596000000000 0.02600000000000 La (16h)
0.13440000000000 -0.52596000000000 0.52600000000000 La (16h)
-0.52596000000000 0.13440000000000 0.47400000000000 La (16h)
0.52596000000000 -0.13440000000000 -0.02600000000000 La (16h)
0.13440000000000 -0.52596000000000 -0.02600000000000 La (16h)
-0.13440000000000 0.52596000000000 0.47400000000000 La (16h)
0.52596000000000 -0.13440000000000 0.52600000000000 La (16h)
-0.28214000000000 0.35180000000000 0.04522000000000 La (16h)
0.28214000000000 -0.35180000000000 0.54522000000000 La (16h)
-0.35180000000000 0.28214000000000 0.45478000000000 La (16h)
0.35180000000000 -0.28214000000000 -0.04522000000000 La (16h)
-0.28214000000000 0.35180000000000 -0.04522000000000 La (16h)
0.28214000000000 -0.35180000000000 0.45478000000000 La (16h)
0.35180000000000 0.28214000000000 0.54522000000000 La (16h)
-0.35180000000000 -0.28214000000000 0.04522000000000 La (16h)
-0.04320000000000 0.04320000000000 0.25000000000000 Mg (4c)
0.04320000000000 -0.04320000000000 0.75000000000000 Mg (4c)
-0.06780000000000 0.06780000000000 0.69120000000000 Mg (8f)
0.06780000000000 -0.06780000000000 1.19120000000000 Mg (8f)
-0.06780000000000 0.06780000000000 -0.19120000000000 Mg (8f)
0.06780000000000 -0.06780000000000 -0.69120000000000 Mg (8f)
-0.04360000000000 0.71120000000000 0.25000000000000 Mg (8g)
0.04360000000000 -0.71120000000000 0.75000000000000 Mg (8g)
0.71120000000000 0.04360000000000 0.25000000000000 Mg (8g)
-0.71120000000000 -0.04360000000000 0.75000000000000 Mg (8g)
0.59870000000000 0.59870000000000 0.25000000000000 Ni (4c)
-0.59870000000000 -0.59870000000000 0.75000000000000 Ni (4c)
0.12750000000000 0.12750000000000 0.00000000000000 Ni (8e)
-0.12750000000000 -0.12750000000000 0.50000000000000 Ni (8e)
0.12750000000000 -0.12750000000000 0.00000000000000 Ni (8e)
-0.12750000000000 0.12750000000000 0.50000000000000 Ni (8e)
-0.07797000000000 0.07797000000000 0.09224000000000 Ni (8f)
0.07797000000000 -0.07797000000000 0.59224000000000 Ni (8f)
-0.07797000000000 0.07797000000000 0.40776000000000 Ni (8f)
0.07797000000000 -0.07797000000000 -0.09224000000000 Ni (8f)
-0.45337000000000 0.45337000000000 0.16750000000000 Ni (8f)
0.45337000000000 -0.45337000000000 0.66750000000000 Ni (8f)
-0.45337000000000 0.45337000000000 0.33250000000000 Ni (8f)
0.45337000000000 -0.45337000000000 -0.16750000000000 Ni (8f)
-0.43146000000000 0.43146000000000 0.00910000000000 Ni (8f)
0.43146000000000 -0.43146000000000 0.50910000000000 Ni (8f)
-0.43146000000000 0.43146000000000 0.49090000000000 Ni (8f)
0.43146000000000 -0.43146000000000 -0.00910000000000 Ni (8f)
0.10907000000000 0.45333000000000 0.16828000000000 Ni (16h)
-0.10907000000000 -0.45333000000000 0.66828000000000 Ni (16h)
-0.45333000000000 0.10907000000000 0.33172000000000 Ni (16h)
0.45333000000000 -0.10907000000000 -0.16828000000000 Ni (16h)
-0.10907000000000 0.45333000000000 0.33172000000000 Ni (16h)
-0.45333000000000 -0.10907000000000 -0.16828000000000 Ni (16h)
0.10907000000000 0.45333000000000 0.33172000000000 Ni (16h)
-0.45333000000000 -0.10907000000000 0.66828000000000 Ni (16h)
-0.45333000000000 0.10907000000000 0.16828000000000 Ni (16h)
-0.07866000000000 0.64006000000000 0.09067000000000 Ni (16h)
0.07866000000000 -0.64006000000000 0.59067000000000 Ni (16h)
-0.64006000000000 0.07866000000000 0.40933000000000 Ni (16h)
0.64006000000000 -0.07866000000000 -0.09067000000000 Ni (16h)

```

```

0.07866000000000 -0.64006000000000 -0.09067000000000 Ni (16h)
-0.07866000000000 0.64006000000000 0.40933000000000 Ni (16h)
0.64006000000000 -0.07866000000000 0.59067000000000 Ni (16h)
-0.64006000000000 0.07866000000000 0.09067000000000 Ni (16h)

```

MnAl<sub>6</sub> (D<sub>2h</sub>): A6B<sub>6</sub>Oc28\_63\_efg\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'MnAl6'
_chemical_formula_sum 'Al6 Mn'

loop_
  _publ_author_name
  'A. Kontio'
  'P. Coppens'
  _journal_name_full_name
  ;
  Acta Crystallographica Section B: Structural Science
  ;
  _journal_volume 37
  _journal_year 1981
  _journal_page_first 433
  _journal_page_last 435
  _publ_section_title
  ;
  New study of the structure of MnAl6{6}$
  ;

_flow_title 'MnAl6{6}$ (SD2_{h}$) Structure'
_flow_proto 'A6B6Oc28_63_efg_c'
_flow_params 'a,b/a,c/a,y_{1},x_{2},y_{3},z_{3},x_{4},y_{4}'
_flow_params_values '7.5551,0.860266574896,1.17435904224,0.45686,
  ↪ 0.32602,0.13917,0.10039,0.31768,0.28622'
_flow_strukturbericht 'SD2_{h}$'
_flow_pearson 'oC28'

_symmetry_space_group_name_H-M 'C 2/m 2/c 21/m'
_symmetry_Int_Tables_number 63

_cell_length_a 7.55510
_cell_length_b 6.49940
_cell_length_c 8.87240
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x,-y,-z
  3 -x,-y,-z+1/2
  4 -x,-y,z+1/2
  5 -x,-y,-z
  6 -x,y,z
  7 x,-y,z+1/2
  8 x,y,-z+1/2
  9 x+1/2,y+1/2,z
  10 x+1/2,-y+1/2,-z
  11 -x+1/2,y+1/2,-z+1/2
  12 -x+1/2,-y+1/2,z+1/2
  13 -x+1/2,-y+1/2,-z
  14 -x+1/2,y+1/2,z
  15 x+1/2,-y+1/2,z+1/2
  16 x+1/2,y+1/2,-z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Mn1 Mn 4 c 0.00000 0.45686 0.25000 1.00000
  Al1 Al 8 e 0.32602 0.00000 0.00000 1.00000
  Al2 Al 8 f 0.00000 0.13917 0.10039 1.00000
  Al3 Al 8 g 0.31768 0.28622 0.25000 1.00000

```

MnAl<sub>6</sub> (D<sub>2h</sub>): A6B<sub>6</sub>Oc28\_63\_efg\_c - POSCAR

```

A6B6Oc28_63_efg_c & a,b/a,c/a,y1,x2,y3,z3,x4,y4 --params=7.5551,
  ↪ 0.860266574896,1.17435904224,0.45686,0.32602,0.13917,0.10039,
  ↪ 0.31768,0.28622 & CnmD_2{2h}^{17} #63 (cefg) & oC28 & SD2_{h}$
  ↪ & MnAl6 & MnAl6 & A. Kontio & P. Coppens, Acta Crystallogr.
  ↪ Sect. B Struct. Sci. 37, 433-435 (1981)
1.00000000000000
3.77755000000000 -3.24970000000000 0.00000000000000
3.77755000000000 3.24970000000000 0.00000000000000
0.00000000000000 0.00000000000000 8.87240000000000
Al Mn
12 2
Direct
0.32602000000000 0.32602000000000 0.00000000000000 Al (8e)
-0.32602000000000 -0.32602000000000 0.50000000000000 Al (8e)
-0.32602000000000 -0.32602000000000 0.00000000000000 Al (8e)
0.32602000000000 0.32602000000000 0.50000000000000 Al (8e)
-0.13917000000000 0.13917000000000 0.10039000000000 Al (8f)
0.13917000000000 -0.13917000000000 0.60039000000000 Al (8f)
-0.13917000000000 0.13917000000000 0.39961000000000 Al (8f)
0.13917000000000 -0.13917000000000 -0.10039000000000 Al (8f)

```

0.03146000000000	0.60390000000000	0.25000000000000	Al	(8g)
-0.03146000000000	-0.60390000000000	0.75000000000000	Al	(8g)
-0.60390000000000	-0.03146000000000	0.25000000000000	Al	(8g)
0.60390000000000	0.03146000000000	0.75000000000000	Al	(8g)
-0.45686000000000	0.45686000000000	0.25000000000000	Mn	(4c)
0.45686000000000	-0.45686000000000	0.75000000000000	Mn	(4c)

Post-perovskite (MgSiO<sub>3</sub>): AB3C\_oC20\_63\_a\_cf\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Post-perovskite MgSiO3_{3}$'
_chemical_formula_sum 'Mg O3 Si'

loop_
_publ_author_name
'M. Murakami'
'K. Hirose'
'K. Kawamura'
'N. Sata'
'Y. Ohishi'
_journal_name_full_name
;
Science
;
_journal_volume 304
_journal_year 2004
_journal_page_first 855
_journal_page_last 858
_publ_section_title
;
Post-Perovskite Phase Transition in MgSiO3_{3}$
;

_aflow_title 'Post-perovskite (MgSiO3_{3}$) Structure'
_aflow_proto 'AB3C_oC20_63_a_cf_c'
_aflow_params 'a,b/a,c/a,y_{2},y_{3},y_{4},z_{4}'
_aflow_params_values '2.456, 3.27442996743, 2.48086319218, 0.077, 0.747,
↪ 0.631,-0.064'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC20'

_symmetry_space_group_name_H-M 'C m c m'
_symmetry_Int_Tables_number 63

_cell_length_a 2.45600
_cell_length_b 8.04200
_cell_length_c 6.09300
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z+1/2
4 -x,-y,z+1/2
5 -x,-y,-z
6 -x,y,z
7 x,-y,z+1/2
8 x,y,-z+1/2
9 x+1/2,y+1/2,z
10 x+1/2,-y+1/2,-z
11 -x+1/2,y+1/2,-z+1/2
12 -x+1/2,-y+1/2,z+1/2
13 -x+1/2,-y+1/2,-z
14 -x+1/2,y+1/2,z
15 x+1/2,-y+1/2,z+1/2
16 x+1/2,y+1/2,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mg1 Mg 4 a 0.00000 0.00000 0.00000 1.00000
O1 O 4 c 0.00000 0.07700 0.25000 1.00000
Si1 Si 4 c 0.00000 0.74700 0.25000 1.00000
O2 O 8 f 0.00000 0.63100 -0.06400 1.00000
```

Post-perovskite (MgSiO<sub>3</sub>): AB3C\_oC20\_63\_a\_cf\_c - POSCAR

```
AB3C_oC20_63_a_cf_c & a,b/a,c/a,y2,y3,y4,z4 --params=2.456,3.27442996743
↪ ,2.48086319218,0.077,0.747,0.631,-0.064 & Cmcn D_{2h}^{17} #63
↪ (ac^2f) & oC20 & None & MgSiO3 & Post-perovskite MgSiO3_{3}$ &
↪ M. Murakami et al., Science 304, 855-858 (2004)

1.00000000000000
1.22800000000000 -4.02100000000000 0.00000000000000
1.22800000000000 4.02100000000000 0.00000000000000
0.00000000000000 0.00000000000000 6.09300000000000
Mg O Si
2 6 2
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Mg (4a)
0.00000000000000 0.00000000000000 0.50000000000000 Mg (4a)
-0.07700000000000 0.07700000000000 0.25000000000000 O (4c)
0.07700000000000 -0.07700000000000 0.75000000000000 O (4c)
```

-0.63100000000000	0.63100000000000	-0.06400000000000	O	(8f)
0.63100000000000	-0.63100000000000	0.43600000000000	O	(8f)
-0.63100000000000	0.63100000000000	0.56400000000000	O	(8f)
0.63100000000000	-0.63100000000000	0.06400000000000	O	(8f)
-0.74700000000000	0.74700000000000	0.25000000000000	Si	(4c)
0.74700000000000	-0.74700000000000	0.75000000000000	Si	(4c)

MgSO<sub>4</sub>: AB4C\_oC24\_63\_a\_fg\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Mg O4 S'

loop_
_publ_author_name
'P. J. Rentzeperis'
'C. T. Soldatos'
_journal_name_full_name
;
Acta Crystallographica
;
_journal_volume 11
_journal_year 1958
_journal_page_first 686
_journal_page_last 688
_publ_section_title
;
The crystal structure of the anhydrous magnesium sulphate
;

# Found in The American Mineralogist Crystal Structure Database, 2003

_aflow_title 'MgSO4_{4}$ Structure'
_aflow_proto 'AB4C_oC24_63_a_fg_c'
_aflow_params 'a,b/a,c/a,y_{2},y_{3},z_{3},x_{4},y_{4}'
_aflow_params_values '5.182, 1.52315708221, 1.25549980702, 0.37, 0.25, 0.06,
↪ 0.25, 0.47'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC24'

_symmetry_space_group_name_H-M 'C 2/m 2/c 21/m'
_symmetry_Int_Tables_number 63

_cell_length_a 5.18200
_cell_length_b 7.89300
_cell_length_c 6.50600
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z+1/2
4 -x,-y,z+1/2
5 -x,-y,-z
6 -x,y,z
7 x,-y,z+1/2
8 x,y,-z+1/2
9 x+1/2,y+1/2,z
10 x+1/2,-y+1/2,-z
11 -x+1/2,y+1/2,-z+1/2
12 -x+1/2,-y+1/2,z+1/2
13 -x+1/2,-y+1/2,-z
14 -x+1/2,y+1/2,z
15 x+1/2,-y+1/2,z+1/2
16 x+1/2,y+1/2,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mg1 Mg 4 a 0.00000 0.00000 0.00000 1.00000
S1 S 4 c 0.00000 0.37000 0.25000 1.00000
O1 O 8 f 0.00000 0.25000 0.06000 1.00000
O2 O 8 g 0.25000 0.47000 0.25000 1.00000
```

MgSO<sub>4</sub>: AB4C\_oC24\_63\_a\_fg\_c - POSCAR

```
AB4C_oC24_63_a_fg_c & a,b/a,c/a,y2,y3,z3,x4,y4 --params=5.182,
↪ 1.52315708221, 1.25549980702, 0.37, 0.25, 0.06, 0.25, 0.47 & Cmcn D_{
↪ 2h}^{17} #63 (acfg) & oC24 & None & MgO4S & & P. J.
↪ Rentzeperis and C. T. Soldatos, Acta Cryst. 11, 686-688 (1958)

1.00000000000000
2.59100000000000 -3.94650000000000 0.00000000000000
2.59100000000000 3.94650000000000 0.00000000000000
0.00000000000000 0.00000000000000 6.50600000000000
Mg O S
2 8 2
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Mg (4a)
0.00000000000000 0.00000000000000 0.50000000000000 Mg (4a)
-0.25000000000000 0.25000000000000 0.06000000000000 O (8f)
0.25000000000000 -0.25000000000000 0.56000000000000 O (8f)
-0.25000000000000 0.25000000000000 0.44000000000000 O (8f)
```



0.2500000000000000	-0.2500000000000000	-0.0600000000000000	O	(8f)
-0.2200000000000000	0.7200000000000000	0.2500000000000000	O	(8g)
0.2200000000000000	-0.7200000000000000	0.7500000000000000	O	(8g)
-0.7200000000000000	0.2200000000000000	0.2500000000000000	O	(8g)
0.7200000000000000	-0.2200000000000000	0.7500000000000000	O	(8g)
-0.3700000000000000	0.3700000000000000	0.2500000000000000	S	(4c)
0.3700000000000000	-0.3700000000000000	0.7500000000000000	S	(4c)

Anhydrite (CaSO<sub>4</sub>, H<sub>0</sub>): AB4C\_oC24\_63\_c\_fg\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Anhydrite'
_chemical_formula_sum 'Ca O4 S'

loop_
  _publ_author_name
    'F. C. Hawthorne'
    'R. B. Ferguson'
  _journal_name_full_name
    ;
  Canadian Mineralogist
  ;
  _journal_volume 13
  _journal_year 1975
  _journal_page_first 289
  _journal_page_last 292
  _publ_section_title
    ;
  Anhydrous sulphates. II. Refinement of the crystal structure of
    ↪ anhydrite
  ;

_aflow_title 'Anhydrite (CaSO4{4}$, $H0_{1}$) Structure'
_aflow_proto 'AB4C_oC24_63_c_fg_c'
_aflow_params 'a,b/a,c/a,y_{1},y_{2},y_{3},z_{3},x_{4},y_{4}'
_aflow_params_values '6.995,0.892780557541,0.999714081487,0.6524,0.15556
    ↪ 0.7025,-0.0819,0.1699,0.0162'
_aflow_Strukturbericht '$H0_{1}$'
_aflow_Pearson 'oC24'

_symmetry_space_group_name_H-M 'C 2/m 2/c 21/m'
_symmetry_Int_Tables_number 63

_cell_length_a 6.99500
_cell_length_b 6.24500
_cell_length_c 6.99300
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x,-y,-z
  3 -x,y,-z+1/2
  4 -x,-y,z+1/2
  5 -x,-y,-z
  6 -x,y,z
  7 x,-y,z+1/2
  8 x,y,-z+1/2
  9 x+1/2,y+1/2,z
  10 x+1/2,-y+1/2,-z
  11 -x+1/2,y+1/2,-z+1/2
  12 -x+1/2,-y+1/2,z+1/2
  13 -x+1/2,-y+1/2,-z
  14 -x+1/2,y+1/2,z
  15 x+1/2,-y+1/2,z+1/2
  16 x+1/2,y+1/2,-z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Ca1 Ca 4 c 0.00000 0.65240 0.25000 1.00000
  S1 S 4 c 0.00000 0.15556 0.25000 1.00000
  O1 O 8 f 0.00000 0.70250 -0.08190 1.00000
  O2 O 8 g 0.16990 0.01620 0.25000 1.00000
```

Anhydrite (CaSO<sub>4</sub>, H<sub>0</sub>): AB4C\_oC24\_63\_c\_fg\_c - POSCAR

```
AB4C_oC24_63_c_fg_c & a,b/a,c/a,y1,y2,y3,z3,x4,y4 --params=6.995,
    ↪ 0.892780557541,0.999714081487,0.6524,0.15556,0.7025,-0.0819,
    ↪ 0.1699,0.0162 & Cmc2 D_{2h}^{17} #63 (c^2fg) & oC24 & $H0_{1}$
    ↪ CaSO4 & Anhydrite & F. C. Hawthorne and R. B. Ferguson, Can.
    ↪ Mineral. 13, 289-292 (1975)
1.0000000000000000
3.4975000000000000 -3.1225000000000000 0.0000000000000000
3.4975000000000000 3.1225000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.9930000000000000
Ca O S
2 8 2
Direct
-0.6524000000000000 0.6524000000000000 0.2500000000000000 Ca (4c)
0.6524000000000000 -0.6524000000000000 0.7500000000000000 Ca (4c)
-0.7025000000000000 0.7025000000000000 -0.0819000000000000 O (8f)
0.7025000000000000 -0.7025000000000000 0.4181000000000000 O (8f)
```

-0.7025000000000000	0.7025000000000000	0.5819000000000000	O	(8f)
0.7025000000000000	-0.7025000000000000	0.0819000000000000	O	(8f)
0.1537000000000000	0.1861000000000000	0.2500000000000000	O	(8g)
-0.1537000000000000	-0.1861000000000000	0.7500000000000000	O	(8g)
-0.1861000000000000	0.1537000000000000	0.2500000000000000	O	(8g)
0.1861000000000000	0.1537000000000000	0.7500000000000000	O	(8g)
-0.1555600000000000	0.1555600000000000	0.2500000000000000	S	(4c)
0.1555600000000000	-0.1555600000000000	0.7500000000000000	S	(4c)

H<sub>2</sub>S (170 GPa): A2B\_oC24\_64\_2f\_f - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'H2S'
_chemical_formula_sum 'H2 S'

loop_
  _publ_author_name
    'Y. Li'
    'J. Hao'
    'H. Liu'
    'Y. Li'
    'Y. Ma'
  _journal_name_full_name
    ;
  Journal of Chemical Physics
  ;
  _journal_volume 140
  _journal_year 2014
  _journal_page_first 174712
  _journal_page_last 174712
  _publ_section_title
    ;
  The metallization and superconductivity of dense hydrogen sulfide
  ;

_aflow_title 'H2S (170-GPa) Structure'
_aflow_proto 'A2B_oC24_64_2f_f'
_aflow_params 'a,b/a,c/a,y_{1},y_{2},y_{3},z_{3}'
_aflow_params_values '2.9986,1.44314013206,2.534682852,0.372,0.27,0.6,
    ↪ 0.092,0.371,0.615'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC24'

_symmetry_space_group_name_H-M 'C 2/m 2/c 21/a'
_symmetry_Int_Tables_number 64

_cell_length_a 2.99860
_cell_length_b 4.32740
_cell_length_c 7.60050
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x,-y,-z
  3 -x+1/2,y,-z+1/2
  4 -x+1/2,-y,z+1/2
  5 -x,-y,-z
  6 -x,y,z
  7 x+1/2,-y,z+1/2
  8 x+1/2,y,-z+1/2
  9 x+1/2,y+1/2,z
  10 x+1/2,-y+1/2,-z
  11 -x,y+1/2,-z+1/2
  12 -x,-y+1/2,z+1/2
  13 -x+1/2,-y+1/2,-z
  14 -x+1/2,y+1/2,z
  15 x,-y+1/2,z+1/2
  16 x,y+1/2,-z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  H1 H 8 f 0.00000 0.37200 0.27000 1.00000
  H2 H 8 f 0.00000 0.60000 0.09200 1.00000
  S1 S 8 f 0.00000 0.37100 0.61500 1.00000
```

H<sub>2</sub>S (170 GPa): A2B\_oC24\_64\_2f\_f - POSCAR

```
A2B_oC24_64_2f_f & a,b/a,c/a,y1,z1,y2,z2,y3,z3 --params=2.9986,
    ↪ 1.44314013206,2.534682852,0.372,0.27,0.6,0.092,0.371,0.615 &
    ↪ Cmc2 D_{2h}^{18} #64 (f^3) & oC24 & None & H2S & H2S & Y. Li et
    ↪ al., J. Chem. Phys. 140, 174712(2014)
1.0000000000000000
1.4993000000000000 -2.1637000000000000 0.0000000000000000
1.4993000000000000 2.1637000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.6005000000000000
H S
8 4
Direct
-0.3720000000000000 0.3720000000000000 0.2700000000000000 H (8f)
0.8720000000000000 0.1280000000000000 0.7700000000000000 H (8f)
0.1280000000000000 0.8720000000000000 0.2300000000000000 H (8f)
```

0.37200000000000	-0.37200000000000	-0.27000000000000	H	(8f)
-0.60000000000000	0.60000000000000	0.09200000000000	H	(8f)
1.10000000000000	-0.10000000000000	0.59200000000000	H	(8f)
-0.10000000000000	1.10000000000000	0.40800000000000	H	(8f)
0.60000000000000	-0.60000000000000	-0.09200000000000	H	(8f)
-0.37100000000000	0.37100000000000	0.61500000000000	S	(8f)
0.87100000000000	0.12900000000000	1.11500000000000	S	(8f)
0.12900000000000	0.87100000000000	-0.11500000000000	S	(8f)
0.37100000000000	-0.37100000000000	-0.61500000000000	S	(8f)

SrAl<sub>2</sub>Se<sub>4</sub>: A2B4C\_oC28\_66\_1\_kl\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'SrAl2Se4'
_chemical_formula_sum 'Al2 Se4 Sr'

loop_
_publ_author_name
'W. Klee'
'H. Sch{"a}fer'
_journal_name_full_name
';
Zeitschrift f{"u}r Naturforschung B
;
_journal_volume 33
_journal_year 1978
_journal_page_first 829
_journal_page_last 833
_publ_section_title
;
CaAlS_{2}$SeS_{4}$ und SrAlS_{2}$SeS_{4}$-Strukturvarianten des
↪ TiSe-Typs / CaAlS_{2}$SeS_{4}$ and SrAlS_{2}$SeS_{4}$-Variants
↪ of the TiSe-Structure
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'SrAlS_{2}$SeS_{4}$ Structure'
_aflow_proto 'A2B4C_oC28_66_1_kl_a'
_aflow_params 'a,b/a,c/a,z_{2},x_{3},y_{3},x_{4},y_{4}'
_aflow_params_values '6.2700590867,1.72567783094,1.73046251993,0.833,
↪ 0.005,0.268,0.737,0.42'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC28'

_cell_length_a 6.2700590867
_cell_length_b 10.8201019646
_cell_length_c 10.8501022473
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'C 2/c 2/c 2/m'
_symmetry_Int_Tables_number 66

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z+1/2
3 -x,y,-z+1/2
4 -x,-y,z
5 -x,-y,-z
6 -x,y,z+1/2
7 x,-y,z+1/2
8 x,y,-z
9 x+1/2,y+1/2,z
10 x+1/2,-y+1/2,-z+1/2
11 -x+1/2,y+1/2,-z+1/2
12 -x+1/2,-y+1/2,z
13 -x+1/2,-y+1/2,-z
14 -x+1/2,y+1/2,z+1/2
15 x+1/2,-y+1/2,z+1/2
16 x+1/2,y+1/2,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Sr1 Sr 4 a 0.00000 0.00000 0.25000 1.00000
Se1 Se 8 k 0.25000 0.25000 0.83300 1.00000
Al1 Al 8 l 0.00500 0.26800 0.00000 1.00000
Se2 Se 8 l 0.73700 0.42000 0.00000 1.00000
```

SrAl<sub>2</sub>Se<sub>4</sub>: A2B4C\_oC28\_66\_1\_kl\_a - POSCAR

```
A2B4C_oC28_66_1_kl_a & a,b/a,c/a,z2,x3,y3,x4,y4 --params=6.2700590867,
↪ 1.72567783094,1.73046251993,0.833,0.005,0.268,0.737,0.42 & Cccm
↪ D_{2h}^{12} #66 (ak1'2) & oC28 & None & SrAl2Se4 & W. Klee
↪ & H. Sch{"a}fer, Z. Naturforsch. B 33, 829-833 (1978)

1.00000000000000
3.13502954335000 -5.41005098230000 0.00000000000000
3.13502954335000 5.41005098230000 0.00000000000000
0.00000000000000 0.00000000000000 10.85010224730000

Al Se Sr
4 8 2
```

Direct				
-0.26300000000000	0.27300000000000	0.00000000000000	Al	(8i)
0.26300000000000	-0.27300000000000	0.00000000000000	Al	(8i)
-0.27300000000000	0.26300000000000	0.50000000000000	Al	(8i)
0.27300000000000	-0.26300000000000	0.50000000000000	Al	(8i)
0.00000000000000	0.50000000000000	0.83300000000000	Se	(8k)
0.50000000000000	0.00000000000000	-0.33300000000000	Se	(8k)
0.00000000000000	0.50000000000000	-0.83300000000000	Se	(8k)
0.50000000000000	0.00000000000000	1.33300000000000	Se	(8k)
0.31700000000000	1.15700000000000	0.00000000000000	Se	(8l)
-0.31700000000000	-1.15700000000000	0.00000000000000	Se	(8l)
-1.15700000000000	-0.31700000000000	0.50000000000000	Se	(8l)
1.15700000000000	0.31700000000000	0.50000000000000	Se	(8l)
0.00000000000000	0.00000000000000	0.25000000000000	Sr	(4a)
0.00000000000000	0.00000000000000	0.75000000000000	Sr	(4a)

H<sub>3</sub>S (60 GPa): A3B\_oC64\_66\_gi2lm\_21 - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'H3S'
_chemical_formula_sum 'H3 S'

_aflow_title 'HS_{3}$S (60-GPa) Structure'
_aflow_proto 'A3B_oC64_66_gi2lm_21'
_aflow_params 'a,b/a,c/a,x_{1},z_{2},x_{3},y_{3},x_{4},y_{4},x_{5},y_{5}
↪ ,x_{6},y_{6},x_{7},y_{7},z_{7}'
_aflow_params_values '8.157,1.00294225818,0.59212945936,0.54552,0.3287,
↪ 0.39296,0.16145,0.33837,0.89039,0.24136,0.07877,0.42337,0.74171
↪ ,0.33285,0.66798,0.24948'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC64'

_symmetry_space_group_name_H-M 'C 2/c 2/c 2/m'
_symmetry_Int_Tables_number 66

_cell_length_a 8.15700
_cell_length_b 8.18100
_cell_length_c 4.83000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z+1/2
3 -x,y,-z+1/2
4 -x,-y,z
5 -x,-y,-z
6 -x,y,z+1/2
7 x,-y,z+1/2
8 x,y,-z
9 x+1/2,y+1/2,z
10 x+1/2,-y+1/2,-z+1/2
11 -x+1/2,y+1/2,-z+1/2
12 -x+1/2,-y+1/2,z
13 -x+1/2,-y+1/2,-z
14 -x+1/2,y+1/2,z+1/2
15 x+1/2,-y+1/2,z+1/2
16 x+1/2,y+1/2,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 8 g 0.54552 0.00000 0.25000 1.00000
H2 H 8 i 0.00000 0.00000 0.32870 1.00000
H3 H 8 l 0.39296 0.16145 0.00000 1.00000
H4 H 8 l 0.33837 0.89039 0.00000 1.00000
S1 S 8 l 0.24136 0.07877 0.00000 1.00000
S2 S 8 l 0.42337 0.74171 0.00000 1.00000
H5 H 16 m 0.33285 0.66798 0.24948 1.00000
```

H<sub>3</sub>S (60 GPa): A3B\_oC64\_66\_gi2lm\_21 - POSCAR

```
A3B_oC64_66_gi2lm_21 & a,b/a,c/a,x1,z2,x3,y3,x4,y4,x5,y5,x6,y6,x7,y7,z7
↪ --params=8.157,1.00294225818,0.59212945936,0.54552,0.3287,
↪ 0.39296,0.16145,0.33837,0.89039,0.24136,0.07877,0.42337,0.74171
↪ ,0.33285,0.66798,0.24948 & Cccm D_{2h}^{12} #66 (gil^4m) & oC64
↪ & None & H3S & H3S &

1.00000000000000
4.07850000000000 -4.09050000000000 0.00000000000000
4.07850000000000 4.09050000000000 0.00000000000000
0.00000000000000 0.00000000000000 4.83000000000000

H S
24 8

Direct
0.54552000000000 0.54552000000000 0.25000000000000 H (8g)
-0.54552000000000 -0.54552000000000 0.25000000000000 H (8g)
-0.54552000000000 -0.54552000000000 0.75000000000000 H (8g)
0.54552000000000 0.54552000000000 0.75000000000000 H (8i)
0.00000000000000 0.00000000000000 0.32870000000000 H (8i)
0.00000000000000 0.00000000000000 0.17130000000000 H (8i)
0.00000000000000 0.00000000000000 -0.32870000000000 H (8i)
0.00000000000000 0.00000000000000 0.82870000000000 H (8i)
0.23151000000000 0.55441000000000 0.00000000000000 H (8l)
```

-0.23151000000000	-0.55441000000000	0.00000000000000	H	(81)
-0.55441000000000	-0.23151000000000	0.50000000000000	H	(81)
0.55441000000000	0.23151000000000	0.50000000000000	H	(81)
-0.55202000000000	1.22876000000000	0.00000000000000	H	(81)
0.55202000000000	-1.22876000000000	0.00000000000000	H	(81)
-1.22876000000000	0.55202000000000	0.50000000000000	H	(81)
1.22876000000000	-0.55202000000000	0.50000000000000	H	(81)
-0.33513000000000	1.00083000000000	0.24948000000000	H	(16m)
0.33513000000000	-1.00083000000000	0.24948000000000	H	(16m)
-1.00083000000000	0.33513000000000	0.25052000000000	H	(16m)
1.00083000000000	-0.33513000000000	0.25052000000000	H	(16m)
0.33513000000000	-1.00083000000000	-0.24948000000000	H	(16m)
-0.33513000000000	1.00083000000000	-0.24948000000000	H	(16m)
1.00083000000000	-0.33513000000000	0.74948000000000	H	(16m)
-1.00083000000000	0.33513000000000	0.74948000000000	H	(16m)
0.16259000000000	0.32013000000000	0.00000000000000	S	(81)
-0.16259000000000	-0.32013000000000	0.00000000000000	S	(81)
-0.32013000000000	-0.16259000000000	0.50000000000000	S	(81)
0.32013000000000	0.16259000000000	0.50000000000000	S	(81)
-0.31834000000000	1.16508000000000	0.00000000000000	S	(81)
0.31834000000000	-1.16508000000000	0.00000000000000	S	(81)
-1.16508000000000	0.31834000000000	0.50000000000000	S	(81)
1.16508000000000	-0.31834000000000	0.50000000000000	S	(81)

$\beta$ -Th<sub>3</sub>: A3B\_oC64\_66\_kl2m\_bdl - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral '\beta$-ThI3_{3}$'
_chemical_formula_sum 'I3 Th'

loop_
  _publ_author_name
    'H. P. Beck'
    'C. Strobel'
  _journal_name_full_name
  ;
  Angewandte Chemie
  ;
  _journal_volume 94
  _journal_year 1982
  _journal_page_first 558
  _journal_page_last 559
  _publ_section_title
  ;
  ThI3_{3}$, ein Janus unter den Verbindungen mit
    ↪ Metall-Metall-Wechselwirkungen
  ;

# Found in The American Mineralogist Crystal Structure Database, 2003

_aflow_title '\beta$-ThI3_{3}$ Structure'
_aflow_proto 'A3B_oC64_66_kl2m_bdl'
_aflow_params 'a,b/a,c/a,z_{3},x_{4},y_{4},x_{5},y_{5},x_{6},y_{6},z_{6}
  ↪ ,x_{7},y_{7},z_{7}'
_aflow_params_values '8.735,2.32364052662,1.67842014883,0.1826,-0.0318,
  ↪ 0.1994,0.327,0.1716,0.2894,0.451,0.1302,0.1133,0.3773,0.3708'
_aflow_strukturbericht 'None'
_aflow_pearson 'oC64'

_symmetry_space_group_name_H-M "C 2/c 2/c 2/m"
_symmetry_Int_Tables_number 66

_cell_length_a 8.73500
_cell_length_b 20.29700
_cell_length_c 14.66100
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x,-y,-z+1/2
  3 -x,y,-z+1/2
  4 -x,-y,z
  5 -x,-y,-z
  6 -x,y,z+1/2
  7 x,-y,z+1/2
  8 x,y,-z
  9 x+1/2,y+1/2,z
  10 x+1/2,-y+1/2,-z+1/2
  11 -x+1/2,y+1/2,-z+1/2
  12 -x+1/2,-y+1/2,z
  13 -x+1/2,-y+1/2,-z
  14 -x+1/2,y+1/2,z+1/2
  15 x+1/2,-y+1/2,z+1/2
  16 x+1/2,y+1/2,-z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Th1 Th 4 b 0.00000 0.50000 0.25000 1.00000
  Th2 Th 4 d 0.00000 0.50000 0.00000 1.00000
  I1 I 8 k 0.25000 0.25000 0.18260 1.00000
  I2 I 8 l -0.03180 0.19940 0.00000 1.00000
```

Th3	Th	8	l	0.32700	0.17160	0.00000	1.00000
I3	I	16	m	0.28940	0.45100	0.13020	1.00000
I4	I	16	m	0.11330	0.37730	0.37080	1.00000

$\beta$ -Th<sub>3</sub>: A3B\_oC64\_66\_kl2m\_bdl - POSCAR

```
A3B_oC64_66_kl2m_bdl & a,b/a,c/a,z3,x4,y4,x5,y5,x6,y6,x7,y7,z7 --
  ↪ params=8.735,2.32364052662,1.67842014883,0.1826,-0.0318,0.1994,
  ↪ 0.327,0.1716,0.2894,0.451,0.1302,0.1133,0.3773,0.3708 & Ccm D_
  ↪ [2h]^20 #66 (bdkl^2m^2) & oC64 & None & ThI3 & \beta$-ThI3_{
  ↪ 3}$ & H. P. Beck and C. Strobel, Angew. Chem. 94, 558-559 (1982)
  ↪

1.0000000000000000
4.3675000000000000 -10.1485000000000000 0.0000000000000000
4.3675000000000000 10.1485000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 14.6610000000000000

I Th
24 8

Direct
0.0000000000000000 0.5000000000000000 0.1826000000000000 I (8k)
0.5000000000000000 0.0000000000000000 0.3174000000000000 I (8k)
0.0000000000000000 0.5000000000000000 -0.1826000000000000 I (8k)
0.5000000000000000 0.0000000000000000 0.6826000000000000 I (8k)
-0.2312000000000000 0.1676000000000000 0.0000000000000000 I (81)
0.2312000000000000 -0.1676000000000000 0.0000000000000000 I (81)
-0.1676000000000000 0.2312000000000000 0.5000000000000000 I (81)
0.1676000000000000 -0.2312000000000000 0.5000000000000000 I (81)
-0.1616000000000000 0.7404000000000000 0.1302000000000000 I (16m)
0.1616000000000000 -0.7404000000000000 0.1302000000000000 I (16m)
-0.7404000000000000 0.1616000000000000 0.3698000000000000 I (16m)
0.7404000000000000 -0.1616000000000000 0.3698000000000000 I (16m)
0.1616000000000000 -0.7404000000000000 -0.1302000000000000 I (16m)
-0.1616000000000000 0.7404000000000000 -0.1302000000000000 I (16m)
0.7404000000000000 -0.1616000000000000 0.6302000000000000 I (16m)
-0.7404000000000000 0.1616000000000000 0.6302000000000000 I (16m)
-0.2640000000000000 0.4906000000000000 0.3708000000000000 I (16m)
0.2640000000000000 -0.4906000000000000 0.3708000000000000 I (16m)
-0.4906000000000000 0.2640000000000000 0.1292000000000000 I (16m)
0.4906000000000000 -0.2640000000000000 0.1292000000000000 I (16m)
0.2640000000000000 -0.4906000000000000 -0.3708000000000000 I (16m)
-0.2640000000000000 0.4906000000000000 -0.3708000000000000 I (16m)
0.4906000000000000 -0.2640000000000000 0.8708000000000000 I (16m)
-0.4906000000000000 0.2640000000000000 0.8708000000000000 I (16m)
0.5000000000000000 0.5000000000000000 0.2500000000000000 Th (4b)
0.5000000000000000 0.5000000000000000 0.7500000000000000 Th (4b)
0.5000000000000000 0.5000000000000000 0.0000000000000000 Th (4d)
0.5000000000000000 0.5000000000000000 0.5000000000000000 Th (4d)
0.1554000000000000 0.4986000000000000 0.0000000000000000 Th (81)
-0.1554000000000000 -0.4986000000000000 0.0000000000000000 Th (81)
-0.4986000000000000 0.1554000000000000 0.5000000000000000 Th (81)
0.4986000000000000 -0.1554000000000000 0.5000000000000000 Th (81)
```

Al<sub>2</sub>CuIr: A2BC\_oC16\_67\_ag\_b\_g - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Al2CuIr'
_chemical_formula_sum 'Al2 Cu Ir'

loop_
  _publ_author_name
    'L. Meshi'
    'V. Ezersky'
    'D. Kapush'
    'B. Grushko'
  _journal_name_full_name
  ;
  Journal of Alloys and Compounds
  ;
  _journal_volume 496
  _journal_year 2010
  _journal_page_first 208
  _journal_page_last 211
  _publ_section_title
  ;
  Crystal structure of the Al_{2}$CuIr phase
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'Al_{2}$CuIr Structure'
_aflow_proto 'A2BC_oC16_67_ag_b_g'
_aflow_params 'a,b/a,c/a,z_{3},z_{4}'
_aflow_params_values '5.0644067238,1.60320657112,1.02379259962,0.3305,
  ↪ 0.8198'
_aflow_strukturbericht 'None'
_aflow_pearson 'oC16'

_cell_length_a 5.0644067238
_cell_length_b 8.1192901384
_cell_length_c 5.1849021253
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "C 2/m 2/m 2/a"
_symmetry_Int_Tables_number 67

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
```

```

2 x,-y,-z
3 -x+1/2,y,-z
4 -x+1/2,-y,z
5 -x,-y,-z
6 -x,y,z
7 x+1/2,-y,z
8 x+1/2,y,-z
9 x+1/2,y+1/2,z
10 x+1/2,-y+1/2,-z
11 -x,y+1/2,-z
12 -x,-y+1/2,z
13 -x+1/2,-y+1/2,-z
14 -x+1/2,y+1/2,z
15 x,-y+1/2,z
16 x,y+1/2,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 4 a 0.25000 0.00000 0.00000 1.00000
Cu1 Cu 4 b 0.25000 0.00000 0.50000 1.00000
Al2 Al 4 g 0.00000 0.25000 0.33050 1.00000
Ir1 Ir 4 g 0.00000 0.25000 0.81980 1.00000

```

Al<sub>2</sub>CuIr: A2BC<sub>o</sub>C16<sub>b</sub>67<sub>g</sub> - POSCAR

```

A2BCoC16b67g & a,b/a,c/a,z3,z4 --params=5.0644067238,
↪ 1.60320657112,1.02379259962,0.3305,0.8198 & Cmma D2h^121 #
↪ 67 (abg^2) & oC16 & None & Al2CuIr & L. Meshi et al., J.
↪ Alloys Compd. 496, 208-211 (2010)
1.0000000000000000
2.53220336190000 -4.05964506920000 0.0000000000000000
2.53220336190000 4.05964506920000 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.18490212530000
Al Cu Ir
4 2 2
Direct
0.2500000000000000 0.2500000000000000 0.0000000000000000 Al (4a)
0.7500000000000000 0.7500000000000000 0.0000000000000000 Al (4a)
0.7500000000000000 0.2500000000000000 0.3305000000000000 Al (4g)
0.2500000000000000 0.7500000000000000 -0.3305000000000000 Al (4g)
0.2500000000000000 0.2500000000000000 0.5000000000000000 Cu (4b)
0.7500000000000000 0.7500000000000000 0.5000000000000000 Cu (4b)
0.7500000000000000 0.2500000000000000 0.8198000000000000 Ir (4g)
0.2500000000000000 0.7500000000000000 -0.8198000000000000 Ir (4g)

```

HoCuP<sub>2</sub>: ABC<sub>2</sub>oC16<sub>b</sub>67<sub>g</sub> - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'HoCuP2'
_chemical_formula_sum 'Cu Ho P2'

loop_
_publ_author_name
'Y. Mozharivsky'
'D. Kaczorowski'
'H. F. Franzen'
_journal_name_full_name
;
Zeitschrift fur Anorganische und Allgemeine Chemie
;
_journal_volume 627
_journal_year 2001
_journal_page_first 2163
_journal_page_last 2172
_publ_section_title
;
Symmetry-Breaking Transitions in HoCuAs2-xPSx and ErCuAs2-xPSx
↪ )PSx( $x=0-2$): Crystal Structure, Application of Landau
↪ Theory, Magnetic and Electrical Properties
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'HoCuP2 Structure'
_aflow_proto 'ABC2oC16b67g ag'
_aflow_params 'a,b/a,c/a,z_{3},z_{4}'
_aflow_params_values '5.2729860526,1.00606865161,1.82912952778,0.765,
↪ 0.3403'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC16'

_cell_length_a 5.2729860526
_cell_length_b 5.3049859679
_cell_length_c 9.6449744884
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "C 2/m 2/m 2/a"
_symmetry_Int_Tables_number 67

loop_
_space_group_symop_id
_space_group_symop_operation_xyz

```

```

1 x,y,z
2 x,-y,-z
3 -x+1/2,y,-z
4 -x+1/2,-y,z
5 -x,-y,-z
6 -x,y,z
7 x+1/2,-y,z
8 x+1/2,y,-z
9 x+1/2,y+1/2,z
10 x+1/2,-y+1/2,-z
11 -x,y+1/2,-z
12 -x,-y+1/2,z
13 -x+1/2,-y+1/2,-z
14 -x+1/2,y+1/2,z
15 x,-y+1/2,z
16 x,y+1/2,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
P1 P 4 a 0.25000 0.00000 0.00000 1.00000
Cu1 Cu 4 b 0.25000 0.00000 0.50000 1.00000
Ho1 Ho 4 g 0.00000 0.25000 0.76500 1.00000
P2 P 4 g 0.00000 0.25000 0.34030 1.00000

```

HoCuP<sub>2</sub>: ABC<sub>2</sub>oC16<sub>b</sub>67<sub>g</sub> - POSCAR

```

ABC2oC16b67g & a,b/a,c/a,z3,z4 --params=5.2729860526,
↪ 1.00606865161,1.82912952778,0.765,0.3403 & Cmma D2h^121 #67
↪ (abg^2) & oC16 & None & HoCuP2 & Y. Mozharivsky and D.
↪ Kaczorowski and H. F. Franzen, Z. Anorg. Allg. Chem. 627,
↪ 2163-2172 (2001)
1.0000000000000000
2.63649302630000 -2.65249298395000 0.0000000000000000
2.63649302630000 2.65249298395000 0.0000000000000000
0.0000000000000000 0.0000000000000000 9.64497448840000
Cu Ho P
2 2 4
Direct
0.2500000000000000 0.2500000000000000 0.5000000000000000 Cu (4b)
0.7500000000000000 0.7500000000000000 0.5000000000000000 Cu (4b)
0.7500000000000000 0.2500000000000000 0.7650000000000000 Ho (4g)
0.2500000000000000 0.7500000000000000 -0.7650000000000000 Ho (4g)
0.2500000000000000 0.2500000000000000 0.0000000000000000 P (4a)
0.7500000000000000 0.7500000000000000 0.0000000000000000 P (4a)
0.7500000000000000 0.2500000000000000 0.3403000000000000 P (4g)
0.2500000000000000 0.7500000000000000 -0.3403000000000000 P (4g)

```

α-FeSe: AB<sub>o</sub>C8<sub>b</sub>67<sub>g</sub> - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '$\alpha$-FeSe'
_chemical_formula_sum 'Fe Se'

loop_
_publ_author_name
'D. Louca'
'K. Horigane'
'A. Llobet'
'R. Arita'
'S. Ji'
'N. Katayama'
'S. Konbu'
'K. Nakamura'
'T.-Y. Koo'
'P. Tong'
'K. Yamada'
_journal_name_full_name
;
Physical Review B
;
_journal_volume 81
_journal_year 2010
_journal_page_first 134524
_journal_page_last 134524
_publ_section_title
;
Local atomic structure of superconducting FeSe1-xTex
;

_aflow_title '$\alpha$-FeSe Structure'
_aflow_proto 'ABoC8b67g a_g'
_aflow_params 'a,b/a,c/a,z_{2}'
_aflow_params_values '5.32495,0.997010300566,1.02896740814,0.26686'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC8'

_symmetry_space_group_name_H-M "C 2/m 2/m 2/a"
_symmetry_Int_Tables_number 67

_cell_length_a 5.32495
_cell_length_b 5.30903
_cell_length_c 5.47920
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

```

```

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x+1/2,y,-z
4 -x+1/2,-y,z
5 -x,-y,-z
6 -x,y,z
7 x+1/2,-y,z
8 x+1/2,y,-z
9 x+1/2,y+1/2,z
10 x+1/2,-y+1/2,-z
11 -x,y+1/2,-z
12 -x,-y+1/2,z
13 -x+1/2,-y+1/2,-z
14 -x+1/2,y+1/2,z
15 x,-y+1/2,z
16 x,y+1/2,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Fe1 Fe 4 a 0.25000 0.00000 0.00000 1.00000
Se1 Se 4 g 0.00000 0.25000 0.26686 1.00000

```

$\alpha$ -FeSe: AB\_oC8\_67\_a\_g - POSCAR

```

AB_oC8_67_a_g & a,b/a,c/a,z2 --params=5.32495,0.997010300566,
↪ 1.02896740814,0.26686 & Cmma D_{2h}^{[21]} #67 (ag) & oC8 & None
↪ & FeSe & $\alpha$-FeSe & D. Louca et al., Phys. Rev. B 81,
↪ 134524(2010)
1.0000000000000000
2.6624750000000000 -2.654515000000000 0.000000000000000
2.6624750000000000 2.6545150000000000 0.000000000000000
0.0000000000000000 0.0000000000000000 5.479200000000000
Fe Se
2 2
Direct
0.2500000000000000 0.2500000000000000 0.000000000000000 Fe (4a)
0.7500000000000000 0.7500000000000000 0.000000000000000 Fe (4a)
0.7500000000000000 0.2500000000000000 0.266860000000000 Se (4g)
0.2500000000000000 0.7500000000000000 -0.266860000000000 Se (4g)

```

$\alpha$ -PbO: AB\_oC8\_67\_a\_g - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'alpha-PbO'
_chemical_formula_sum 'O Pb'

loop_
_publ_author_name
'P. Boher'
'P. Garnier'
'J. R. Gavarri'
'A. W. Hewat'
_journal_name_full_name
;
Journal of Solid State Chemistry
;
_journal_volume 57
_journal_year 1985
_journal_page_first 343
_journal_page_last 350
_publ_section_title
;
Monoxyde quadratique PbO$\alpha$ (I): Description de la transition
↪ structurale ferro($\alpha$)lastique
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title '$\alpha$-PbO Structure'
_aflow_proto 'AB_oC8_67_a_g'
_aflow_params 'a,b/a,c/a,z_{2}'
_aflow_params_values '5.6124272786,0.999376380873,0.8895303257,0.7642'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC8'

_cell_length_a 5.6124272786
_cell_length_b 5.6089272616
_cell_length_c 4.9924242651
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "C 2/m 2/m 2/a"
_symmetry_Int_Tables_number 67

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z

```

```

3 -x+1/2,y,-z
4 -x+1/2,-y,z
5 -x,-y,-z
6 -x,y,z
7 x+1/2,-y,z
8 x+1/2,y,-z
9 x+1/2,y+1/2,z
10 x+1/2,-y+1/2,-z
11 -x,y+1/2,-z
12 -x,-y+1/2,z
13 -x+1/2,-y+1/2,-z
14 -x+1/2,y+1/2,z
15 x,-y+1/2,z
16 x,y+1/2,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 4 a 0.25000 0.00000 0.00000 1.00000
Pb1 Pb 4 g 0.00000 0.25000 0.76420 1.00000

```

$\alpha$ -PbO: AB\_oC8\_67\_a\_g - POSCAR

```

AB_oC8_67_a_g & a,b/a,c/a,z2 --params=5.6124272786,0.999376380873,
↪ 0.8895303257,0.7642 & Cmma D_{2h}^{[21]} #67 (ag) & oC8 & None &
↪ PbO & alpha & P. Boher et al., J. Solid State Chem. 57, 343-350
↪ (1985)
1.0000000000000000
2.8062136393000000 -2.804463630800000 0.000000000000000
2.8062136393000000 2.804463630800000 0.000000000000000
0.0000000000000000 0.0000000000000000 4.99242426510000
O Pb
2 2
Direct
0.2500000000000000 0.2500000000000000 0.000000000000000 O (4a)
0.7500000000000000 0.7500000000000000 0.000000000000000 O (4a)
0.7500000000000000 0.2500000000000000 0.764200000000000 Pb (4g)
0.2500000000000000 0.7500000000000000 -0.764200000000000 Pb (4g)

```

PdSn<sub>4</sub>: AB<sub>4</sub>oC20\_68\_a\_i - CIF

```

# CIF file# This file was generated by FINDSYM
# Harold T. Stokes, Branton J. Campbell, Dorian M. Hatch
# Brigham Young University, Provo, Utah, USA

data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'PdSn4'
_chemical_formula_sum 'Pd Sn4'

loop_
_publ_author_name
'J. Nyl {\e}n'
'F. J. {Garc {\i}a Garc {\i}a}'
'B. D. Mosel'
'R. P {\o}ttgen'
'U. H {\a}ussermann'
_journal_name_full_name
;
Solid State Sciences
;
_journal_volume 6
_journal_year 2004
_journal_page_first 147
_journal_page_last 155
_publ_section_title
;
Structural relationships, phase stability and bonding of compounds
↪ PdSn_{n}$ (Sn = 2, 3, 4)
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'PdSn_{4}$ Structure'
_aflow_proto 'AB4_oC20_68_a_i'
_aflow_params 'a,b/a,c/a,x_{2},y_{2},z_{2}'
_aflow_params_values '6.44222,1.77662048176,0.991771470083,0.3313,0.1233
↪ ,0.0801'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'oC20'

_symmetry_space_group_name_H-M "C 2/c 2/c 2/a (origin choice 2)"
_symmetry_Int_Tables_number 68

_cell_length_a 6.44222
_cell_length_b 11.44538
_cell_length_c 6.38921
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y+1/2,-z+1/2
3 -x,y,-z+1/2

```

```
4 -x,-y+1/2,z
5 -x+1/2,-y+1/2,-z
6 -x+1/2,y,z+1/2
7 x+1/2,-y+1/2,z+1/2
8 x+1/2,y,-z
9 x+1/2,y+1/2,z
10 x+1/2,-y,-z+1/2
11 -x+1/2,y+1/2,-z+1/2
12 -x+1/2,-y,z
13 -x,-y,-z
14 -x,y+1/2,z+1/2
15 x,-y,z+1/2
16 x,y+1/2,-z
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Pd1 Pd 4 a 0.00000 0.25000 0.25000 1.00000
Sn1 Sn 16 i 0.33130 0.12330 0.08010 1.00000
```

PdSn<sub>4</sub>: AB<sub>4</sub>oC20\_68\_a\_i - POSCAR

```
AB4_oC20_68_a_i & a,b/a,c/a,x2,y2,z2 --params=6.44222,1.77662048176,
↪ 0.991771470083,0.3313,0.1233,0.0801 & Ccca_D_{2h}^{22} #68 (ai)
↪ & oC20 & None & PdSn4 & J. Nyl{\e}n et al., Solid State
↪ Sci. 6, 147-155 (2004)
1.0000000000000000
3.2211100000000000 -5.7226900000000000 0.0000000000000000
3.2211100000000000 5.7226900000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.3892100000000000
Pd Sn
2 8
Direct
0.7500000000000000 0.2500000000000000 0.2500000000000000 Pd (4a)
0.2500000000000000 0.7500000000000000 0.7500000000000000 Pd (4a)
0.2080000000000000 0.4546000000000000 0.0801000000000000 Sn (16i)
0.2920000000000000 0.0454000000000000 0.0801000000000000 Sn (16i)
-0.4546000000000000 -0.2080000000000000 0.4199000000000000 Sn (16i)
0.9546000000000000 0.7080000000000000 0.4199000000000000 Sn (16i)
-0.2080000000000000 -0.4546000000000000 -0.0801000000000000 Sn (16i)
0.7080000000000000 0.9546000000000000 -0.0801000000000000 Sn (16i)
0.4546000000000000 0.2080000000000000 0.5801000000000000 Sn (16i)
0.0454000000000000 0.2920000000000000 0.5801000000000000 Sn (16i)
```

Mn<sub>2</sub>B (D<sub>1f</sub>): AB<sub>2</sub>oF48\_70\_fg - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Mn2B'
_chemical_formula_sum 'B Mn2'
loop_
_publ_author_name
'L.-E. Tergenius'
_journal_name_full_name
;
Journal of the Less-Common Metals
;
_journal_volume 82
_journal_year 1981
_journal_page_first 335
_journal_page_last 340
_publ_Section_title
;
Refinement of the crystal structure of orthorhombic MnS_{2}SB (formerly
↪ denoted MnS_{4}SB)
;
_aflow_title 'MnS_{2}SB (SD1_{f}) Structure'
_aflow_proto 'AB2_oF48_70_fg'
_aflow_params 'a,b/a,c/a,y_{1},y_{2},z_{3}'
_aflow_params_values '4.2082,3.45504015969,1.7326647973,0.2495,0.54337,
↪ 0.29445'
_aflow_Strukturbericht 'SD1_{f}'
_aflow_Pearson 'oF48'
;
_symmetry_space_group_name_H-M "F 2/d 2/d 2/d (origin choice 2)"
_symmetry_Int_Tables_number 70
;
_cell_length_a 4.20820
_cell_length_b 14.53950
_cell_length_c 7.29140
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y+3/4,-z+3/4
3 -x+3/4,y,-z+3/4
4 -x+3/4,-y+3/4,z
5 -x,-y,-z
6 -x,y+1/4,z+1/4
7 x+1/4,-y,z+1/4
8 x+1/4,y+1/4,-z
```

```
9 x,y+1/2,z+1/2
10 x,-y+1/4,-z+1/4
11 -x+3/4,y+1/2,-z+1/4
12 -x+3/4,-y+1/4,z+1/2
13 -x,-y+1/2,-z+1/2
14 -x,y+3/4,z+3/4
15 x+1/4,-y+1/2,z+3/4
16 x+1/4,y+3/4,-z+1/2
17 x+1/2,y,z+1/2
18 x+1/2,-y+3/4,-z+1/4
19 -x+1/4,y,-z+1/4
20 -x+1/4,-y+3/4,z+1/2
21 -x+1/2,-y,-z+1/2
22 -x+1/2,y+1/4,z+3/4
23 x+3/4,-y,z+3/4
24 x+3/4,y+1/4,-z+1/2
25 x+1/2,y+1/2,z
26 x+1/2,-y+1/4,-z+3/4
27 -x+1/4,y+1/2,-z+3/4
28 -x+1/4,-y+1/4,z
29 -x+1/2,-y+1/2,-z
30 -x+1/2,y+3/4,z+1/4
31 x+3/4,-y+1/2,z+1/4
32 x+3/4,y+3/4,-z
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
B1 B 16 f 0.12500 0.24950 0.12500 1.00000
Mn1 Mn 16 f 0.12500 0.54337 0.12500 1.00000
Mn2 Mn 16 g 0.12500 0.12500 0.29445 1.00000
```

Mn<sub>2</sub>B (D<sub>1f</sub>): AB<sub>2</sub>oF48\_70\_fg - POSCAR

```
AB2_oF48_70_fg & a,b/a,c/a,y1,y2,z3 --params=4.2082,3.45504015969,
↪ 1.7326647973,0.2495,0.54337,0.29445 & Fddd_D_{2h}^{24} #70 (f^
↪ 2g) & oF48 & SD1_{f} & Mn2B & Mn2B & L.-E. Tergenius, J.
↪ Less-Common Met. 82, 335-340 (1981)
1.0000000000000000
0.0000000000000000 7.2697500000000000 3.6457000000000000
2.1041000000000000 0.0000000000000000 3.6457000000000000
2.1041000000000000 7.2697500000000000 0.0000000000000000
B Mn
4 8
Direct
0.2495000000000000 0.0005000000000000 0.2495000000000000 B (16f)
0.0005000000000000 0.2495000000000000 0.0005000000000000 B (16f)
-0.2495000000000000 0.9995000000000000 -0.2495000000000000 B (16f)
0.9995000000000000 -0.2495000000000000 0.9995000000000000 B (16f)
0.5433700000000000 -0.2933700000000000 0.5433700000000000 Mn (16f)
-0.2933700000000000 0.5433700000000000 -0.2933700000000000 Mn (16f)
-0.5433700000000000 1.2933700000000000 -0.5433700000000000 Mn (16f)
1.2933700000000000 -0.5433700000000000 1.2933700000000000 Mn (16f)
0.2944500000000000 0.2944500000000000 -0.0444500000000000 Mn (16g)
-0.0444500000000000 -0.0444500000000000 0.2944500000000000 Mn (16g)
-0.2944500000000000 -0.2944500000000000 1.0444500000000000 Mn (16g)
1.0444500000000000 1.0444500000000000 -0.2944500000000000 Mn (16g)
```

Ta<sub>3</sub>B<sub>4</sub> (D<sub>7b</sub>): A4B3\_oI14\_71\_gh\_cg - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Ta3B4'
_chemical_formula_sum 'B4 Ta3'
loop_
_publ_author_name
'R. Kiessling'
_journal_name_full_name
;
Acta Chemica Scandinavica
;
_journal_volume 3
_journal_year 1949
_journal_page_first 603
_journal_page_last 615
_publ_Section_title
;
The Borides of Tantalum
;
# Found in Transition-metal borides with the tantalum boride (TaS_{3})
↪ SBS_{4}) crystal structure: their electronic and bonding
↪ properties, 1991
;
_aflow_title 'TaS_{3}SBS_{4} (SD7_{b}) Structure'
_aflow_proto 'A4B3_oI14_71_gh_cg'
_aflow_params 'a,b/a,c/a,y_{2},y_{3},y_{4}'
_aflow_params_values '3.29,4.25531914894,0.951367781155,0.375,0.18,0.444
↪ '
_aflow_Strukturbericht 'SD7_{b}'
_aflow_Pearson 'oI14'
;
_symmetry_space_group_name_H-M "I 2/m 2/m 2/m"
_symmetry_Int_Tables_number 71
;
_cell_length_a 3.29000
```

```

_cell_length_b 14.00000
_cell_length_c 3.13000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y, -z
4 -x, -y, z
5 -x, -y, -z
6 -x, y, z
7 x, -y, z
8 x, y, -z
9 x+1/2, y+1/2, z+1/2
10 x+1/2, -y+1/2, -z+1/2
11 -x+1/2, y+1/2, -z+1/2
12 -x+1/2, -y+1/2, z+1/2
13 -x+1/2, -y+1/2, -z+1/2
14 -x+1/2, y+1/2, z+1/2
15 x+1/2, -y+1/2, z+1/2
16 x+1/2, y+1/2, -z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ta1 Ta 2 c 0.50000 0.50000 0.00000 1.00000
B1 B 4 g 0.00000 0.37500 0.00000 1.00000
Ta2 Ta 4 g 0.00000 0.18000 0.00000 1.00000
B2 B 4 h 0.00000 0.44400 0.50000 1.00000

```

Ta<sub>3</sub>B<sub>4</sub> (D7<sub>h</sub>): A4B3\_oI14\_71\_gh\_cg - POSCAR

```

A4B3_oI14_71_gh_cg & a, b/a, c/a, y2, y3, y4 --params=3.29, 4.25531914894,
↪ 0.951367781155, 0.375, 0.18, 0.444 & Immm D_{2h}^{25} #71 (cg^2h)
↪ oI14 & SD7_{b}S & Ta3B4 & Ta3B4 & R. Kiessling, Acta Chem.
↪ Scand. 3, 603-615 (1949)
1.0000000000000000
-1.6450000000000000 7.0000000000000000 1.5650000000000000
1.6450000000000000 -7.0000000000000000 1.5650000000000000
1.6450000000000000 7.0000000000000000 -1.5650000000000000
B Ta
4 3
Direct
0.3750000000000000 0.0000000000000000 0.3750000000000000 B (4g)
-0.3750000000000000 0.0000000000000000 -0.3750000000000000 B (4g)
0.9440000000000000 0.5000000000000000 0.4440000000000000 B (4h)
0.0560000000000000 0.5000000000000000 -0.4440000000000000 B (4h)
0.5000000000000000 0.5000000000000000 0.0000000000000000 Ta (2c)
0.1800000000000000 0.0000000000000000 0.1800000000000000 Ta (4g)
-0.1800000000000000 0.0000000000000000 -0.1800000000000000 Ta (4g)

```

NbPS: ABC\_oI12\_71\_h\_j\_g - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Nb P S'

loop_
_publ_author_name
'P. C. Donohue'
'P. E. Bierstedt'
_journal_name_full_name
;
Inorganic Chemistry
;
_journal_volume 8
_journal_year 1969
_journal_page_first 2690
_journal_page_last 2694
_publ_section_title
;
Synthesis, crystal structure, and superconducting properties of niobium
↪ phosphorus sulfide, niobium phosphorus selenide and tantalum
↪ phosphorus sulfide
;
_aflow_title 'NbPS Structure'
_aflow_proto 'ABC_oI12_71_h_j_g'
_aflow_params 'a, b/a, c/a, y_{1}, y_{2}, z_{3}'
_aflow_params_values '3.438, 3.4554973822, 1.37434554974, 0.212, 0.1232,
↪ 0.235'
_aflow_strukturbericht 'None'
_aflow_pearson 'oI12'

_symmetry_space_group_name_H-M "I 2/m 2/m 2/m"
_symmetry_Int_tables_number 71

_cell_length_a 3.43800
_cell_length_b 11.88000
_cell_length_c 4.72500
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000

```

```

_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y, -z
4 -x, -y, z
5 -x, -y, -z
6 -x, y, z
7 x, -y, z
8 x, y, -z
9 x+1/2, y+1/2, z+1/2
10 x+1/2, -y+1/2, -z+1/2
11 -x+1/2, y+1/2, -z+1/2
12 -x+1/2, -y+1/2, z+1/2
13 -x+1/2, -y+1/2, -z+1/2
14 -x+1/2, y+1/2, z+1/2
15 x+1/2, -y+1/2, z+1/2
16 x+1/2, y+1/2, -z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
S1 S 4 g 0.00000 0.21200 0.00000 1.00000
Nb1 Nb 4 h 0.00000 0.12320 0.50000 1.00000
P1 P 4 j 0.50000 0.00000 0.23500 1.00000

```

NbPS: ABC\_oI12\_71\_h\_j\_g - POSCAR

```

ABC_oI12_71_h_j_g & a, b/a, c/a, y1, y2, z3 --params=3.438, 3.4554973822,
↪ 1.37434554974, 0.212, 0.1232, 0.235 & Immm D_{2h}^{25} #71 (ghj) &
↪ oI12 & None & NbPS & P. C. Donohue and P. E. Bierstedt,
↪ Inorg. Chem. 8, 2690-2694 (1969)
1.0000000000000000
-1.7190000000000000 5.9400000000000000 2.3625000000000000
1.7190000000000000 -5.9400000000000000 2.3625000000000000
1.7190000000000000 5.9400000000000000 -2.3625000000000000
Nb P S
2 2 2
Direct
0.6232000000000000 0.5000000000000000 0.1232000000000000 Nb (4h)
0.3768000000000000 0.5000000000000000 -0.1232000000000000 Nb (4h)
0.2350000000000000 0.7350000000000000 0.5000000000000000 P (4j)
-0.2350000000000000 0.2650000000000000 0.5000000000000000 P (4j)
0.2120000000000000 0.0000000000000000 0.2120000000000000 S (4g)
-0.2120000000000000 0.0000000000000000 -0.2120000000000000 S (4g)

```

KAg[CO<sub>3</sub>]: ABCD3\_oI48\_73\_d\_e\_ef - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'KAg[CO3]'
_chemical_formula_sum 'Ag C K O3'

loop_
_publ_author_name
'Y.-Q. Zheng'
'L.-X. Zhou'
'J.-L. Lin'
'S.-W. Zhang'
_journal_name_full_name
;
Zeitschrift f{"u}r Kristallographie - New Crystal Structures
;
_journal_volume 215
_journal_year 2000
_journal_page_first 467
_journal_page_last 468
_publ_section_title
;
Refinement of the crystal structure of potassium {\it catena}--
↪ carbonato--argentate(I), K[Ag(CO3_{3}S)]
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'KAg[CO3_{3}S] Structure'
_aflow_proto 'ABCD3_oI48_73_d_e_ef'
_aflow_params 'a, b/a, c/a, y_{1}, z_{2}, z_{3}, z_{4}, x_{5}, y_{5}, z_{5}'
_aflow_params_values '5.7750411261, 1.02926406926, 3.53056277057, 0.63427,
↪ 0.3734, 0.18032, 0.311, 0.1349, 0.6124, 0.0967'
_aflow_strukturbericht 'None'
_aflow_pearson 'oI48'

_cell_length_a 5.7750411261
_cell_length_b 5.9440423296
_cell_length_c 20.3891451983
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 21/b 21/c 21/a"
_symmetry_Int_tables_number 73

```

```

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z+1/2
3 -x+1/2, y, -z
4 -x, -y+1/2, z
5 -x, -y, -z
6 -x, y, z+1/2
7 x+1/2, -y, z
8 x, y+1/2, -z
9 x+1/2, y+1/2, z+1/2
10 x+1/2, -y+1/2, -z
11 -x, y+1/2, -z+1/2
12 -x+1/2, -y, z+1/2
13 -x+1/2, -y+1/2, -z+1/2
14 -x+1/2, y+1/2, z
15 x, -y+1/2, z+1/2
16 x+1/2, y, -z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1 Ag 8 d 0.25000 0.63427 0.00000 1.00000
Cl C 8 e 0.00000 0.25000 0.37340 1.00000
K1 K 8 e 0.00000 0.25000 0.18032 1.00000
O1 O 8 e 0.00000 0.25000 0.31100 1.00000
O2 O 16 f 0.13490 0.61240 0.09670 1.00000

```

KAg[CO<sub>3</sub>]: ABCD3\_ol48\_73\_d\_e\_e\_f - POSCAR

```

ABCD3_ol48_73_d_e_e_f & a,b/a,c/a,y1,z2,z3,z4,x5,y5,z5 --params=
↪ 5.7750411261, 1.02926406926, 3.53056277057, 0.63427, 0.3734, 0.18032
↪ 0.311, 0.1349, 0.6124, 0.0967 & lbca D_{2h}^{[27]} #73 (de^3f) &
↪ ol48 & None & KAg[CO3] & Y.-Q. Zheng et al., Zeitschrift f"
↪ ur Kristallographie - New Crystal Structures 215, 467-468 (
↪ 2000)
1.0000000000000000
-2.88752056305000 2.97202116480000 10.19457259915000
2.88752056305000 -2.97202116480000 10.19457259915000
2.88752056305000 2.97202116480000 -10.19457259915000
Ag C K O
4 4 4 12
Direct
0.634270000000000 0.250000000000000 0.884270000000000 Ag (8d)
-0.134270000000000 0.750000000000000 -0.384270000000000 Ag (8d)
-0.634270000000000 0.750000000000000 0.115730000000000 Ag (8d)
1.134270000000000 0.250000000000000 1.384270000000000 Ag (8d)
0.623400000000000 0.373400000000000 0.250000000000000 C (8e)
-0.123400000000000 0.126600000000000 0.750000000000000 C (8e)
0.376600000000000 -0.373400000000000 0.750000000000000 C (8e)
1.123400000000000 0.873400000000000 0.250000000000000 C (8e)
0.430320000000000 0.180320000000000 0.250000000000000 K (8e)
0.069680000000000 0.319680000000000 0.750000000000000 K (8e)
0.569680000000000 -0.180320000000000 0.750000000000000 K (8e)
0.930320000000000 0.680320000000000 0.250000000000000 K (8e)
0.561000000000000 0.311000000000000 0.250000000000000 O (8e)
-0.061000000000000 0.189000000000000 0.750000000000000 O (8e)
0.439000000000000 -0.311000000000000 0.750000000000000 O (8e)
1.061000000000000 0.811000000000000 0.250000000000000 O (8e)
0.709100000000000 0.231600000000000 0.747300000000000 O (16f)
-0.015700000000000 -0.038200000000000 -0.247300000000000 O (16f)
0.515700000000000 0.268400000000000 0.977500000000000 O (16f)
-0.209100000000000 0.538200000000000 -0.477500000000000 O (16f)
-0.709100000000000 -0.231600000000000 -0.747300000000000 O (16f)
1.015700000000000 0.038200000000000 1.247300000000000 O (16f)
-0.515700000000000 0.731600000000000 0.022500000000000 O (16f)
1.209100000000000 0.461800000000000 0.477500000000000 O (16f)

```

KHg<sub>2</sub>: A2B\_ol12\_74\_h\_e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'KHg2'
_chemical_formula_sum 'Hg2 K'

loop_
_publ_author_name
'E. J. Duwell'
'N. C. Baenziger'
_journal_name_full_name
;
Acta Crystallographica
;
_journal_volume 8
_journal_year 1955
_journal_page_first 705
_journal_page_last 710
_publ_section_title
;
The crystal structures of KHg and KHg_{2}$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013
_aflow_title 'KHg_{2}$ Structure'

```

```

_aflow_proto 'A2B_ol12_74_h_e'
_aflow_params 'a,b/a,c/a,z_{1},y_{2},z_{2}'
_aflow_params_values '5.158858099,1.56976744188,1.70096899227,-0.047,
↪ 0.56,0.663'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'ol12'

_cell_length_a 5.1588580990
_cell_length_b 8.0982074811
_cell_length_c 8.7750576619
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 21/m 21/m 21/a"
_symmetry_Int_Tables_number 74

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y+1/2, -z
4 -x, -y+1/2, z
5 -x, -y, -z
6 -x, y, z
7 x, -y+1/2, z
8 x, y+1/2, -z
9 x+1/2, y+1/2, z+1/2
10 x+1/2, -y+1/2, -z+1/2
11 -x+1/2, y, -z+1/2
12 -x+1/2, -y, z+1/2
13 -x+1/2, -y+1/2, -z+1/2
14 -x+1/2, y+1/2, z+1/2
15 x+1/2, -y, z+1/2
16 x+1/2, y, -z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
K1 K 4 e 0.00000 0.25000 -0.04700 1.00000
Hg1 Hg 8 h 0.00000 0.56000 0.66300 1.00000

```

KHg<sub>2</sub>: A2B\_ol12\_74\_h\_e - POSCAR

```

A2B_ol12_74_h_e & a,b/a,c/a,z1,y2,z2 --params=5.158858099,1.56976744188,
↪ 1.70096899227,-0.047,0.56,0.663 & Imma D_{2h}^{[28]} #74 (eh) &
↪ ol12 & None & KHg2 & E. J. Duwell and N. C. Baenziger, Acta
↪ Cryst. 8, 705-710 (1955)
1.0000000000000000
-2.57942904950000 4.04910374055000 4.38752883095000
2.57942904950000 -4.04910374055000 4.38752883095000
2.57942904950000 4.04910374055000 -4.38752883095000
Hg K
4 2
Direct
1.223000000000000 0.663000000000000 0.560000000000000 Hg (8h)
0.603000000000000 0.663000000000000 -0.060000000000000 Hg (8h)
0.397000000000000 -0.663000000000000 1.060000000000000 Hg (8h)
-1.223000000000000 -0.663000000000000 -0.560000000000000 Hg (8h)
0.203000000000000 -0.047000000000000 0.250000000000000 K (4e)
0.797000000000000 0.047000000000000 0.750000000000000 K (4e)

```

Al<sub>4</sub>U (D1<sub>6</sub>): A4B\_ol20\_74\_beh\_e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Al4 U'

loop_
_publ_author_name
'H. U. Borgstedt'
'H. Wedemeyer'
_journal_year 1989
_publ_section_title
;
Gmelin Handbook of Inorganic Chemistry
;

_aflow_title 'Al_{4}$U ($D1_{b}$) Structure'
_aflow_proto 'A4B_ol20_74_beh_e'
_aflow_params 'a,b/a,c/a,z_{2},z_{3},y_{4},z_{4}'
_aflow_params_values '4.39,1.4236902501,3.12528473804,-0.111,0.111,-
↪ 0.033,0.314'
_aflow_Strukturbericht '$D1_{b}$'
_aflow_Pearson 'ol20'

_symmetry_space_group_name_H-M "I 21/m 21/m 21/a"
_symmetry_Int_Tables_number 74

_cell_length_a 4.39000
_cell_length_b 6.25000
_cell_length_c 13.72000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

```



```

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y+1/2, -z
4 -x, -y+1/2, z
5 -x, -y, -z
6 -x, y, z
7 x, -y+1/2, z
8 x, y+1/2, -z
9 x+1/2, y+1/2, z+1/2
10 x+1/2, -y+1/2, -z+1/2
11 -x+1/2, y, -z+1/2
12 -x+1/2, -y, z+1/2
13 -x+1/2, -y+1/2, -z+1/2
14 -x+1/2, y+1/2, z+1/2
15 x+1/2, -y, z+1/2
16 x+1/2, y, -z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 4 b 0.00000 0.00000 0.50000 1.00000
Al2 Al 4 e 0.00000 0.25000 -0.11100 1.00000
U1 U 4 e 0.00000 0.25000 0.11100 1.00000
Al3 Al 8 h 0.00000 -0.03300 0.31400 1.00000

```

Al<sub>4</sub>U (D<sub>16</sub>): A4B\_oI20\_74\_beh\_e - POSCAR

```

A4B_oI20_74_beh_e & a, b/a, c/a, z2, z3, y4, z4 --params=4.39, 1.42369020501,
↳ 3.12528473804, -0.111, 0.111, -0.033, 0.314 & Imma D_{2h}^{28} #74
↳ (be^2h) & oI20 & $D1_{b}$ & Al4U & & H. U. Borgstedt and H.
↳ Wedemeyer, (1989)
1.0000000000000000
-2.1950000000000000 3.1250000000000000 6.8600000000000000
2.1950000000000000 -3.1250000000000000 6.8600000000000000
2.1950000000000000 3.1250000000000000 -6.8600000000000000
Al U
8 2
Direct
0.5000000000000000 0.5000000000000000 0.0000000000000000 Al (4b)
0.0000000000000000 0.5000000000000000 0.0000000000000000 Al (4b)
0.1390000000000000 -0.1110000000000000 0.2500000000000000 Al (4e)
0.8610000000000000 0.1110000000000000 0.7500000000000000 Al (4e)
0.2810000000000000 0.3140000000000000 -0.0330000000000000 Al (8h)
0.8470000000000000 0.3140000000000000 0.5330000000000000 Al (8h)
0.1530000000000000 -0.3140000000000000 0.4670000000000000 Al (8h)
-0.2810000000000000 -0.3140000000000000 0.0330000000000000 Al (8h)
0.3610000000000000 0.1110000000000000 0.2500000000000000 U (4e)
0.6390000000000000 -0.1110000000000000 0.7500000000000000 U (4e)

```

BaCr<sub>2</sub>Ru<sub>4</sub>O<sub>12</sub>: AB2C12D4\_tP76\_75\_2a2b\_2d\_12d\_4d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'BaCr2Ru4O12'
_chemical_formula_sum 'Ba Cr2 O12 Ru4'

loop_
_publ_author_name
'M. C. Cad{\e}'
'A. Prodan'
_journal_name_full_name
;
Materials Research Bulletin
;
_journal_volume 14
_journal_year 1979
_journal_page_first 613
_journal_page_last 618
_publ_section_title
;
Tripling of the short axis in the hollandite structure
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'BaCr_{2}Ru_{4}O_{12} Structure'
_aflow_proto 'AB2C12D4_tP76_75_2a2b_2d_12d_4d'
_aflow_params 'a, c/a, z_{1}, z_{2}, z_{3}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}, x_{7}, y_{7}, z_{7}, x_{8}, y_{8}, z_{8}, x_{9}, y_{9}, z_{9}, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22}, y_{22}, z_{22}'
_aflow_params_values '9.8880614494, 0.922431229769, 0.3333, 0.0, 0.5003,
↳ 0.1666, 0.167, 0.348, 0.1666, 0.333, 0.152, 0.0, 0.208, 0.152, 0.8333,
↳ 0.458, 0.152, 0.8333, 0.292, 0.348, 0.6666, 0.042, 0.348, 0.6666, 0.208,
↳ 0.152, 0.5, 0.458, 0.152, 0.5, 0.292, 0.348, 0.3333, 0.042, 0.348, 0.3333
↳ 0.208, 0.152, 0.1666, 0.458, 0.152, 0.1666, 0.292, 0.348, 0.0, 0.042,
↳ 0.348, 0.0, 0.167, 0.348, 0.8333, 0.333, 0.152, 0.6666, 0.167, 0.348, 0.5,
↳ 0.333, 0.152, 0.3333'
_aflow_strukturbericht 'None'

```

```

_aflow_Pearson 'tP76'

_cell_length_a 9.8880614494
_cell_length_b 9.8880614494
_cell_length_c 9.1210566828
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'P 4'
_symmetry_Int_Tables_number 75

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -x, -y, z
3 -y, x, z
4 y, -x, z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ba1 Ba 1 a 0.00000 0.00000 0.33330 1.00000
Ba2 Ba 1 a 0.00000 0.00000 0.00000 1.00000
Ba3 Ba 1 b 0.50000 0.50000 0.50030 1.00000
Ba4 Ba 1 b 0.50000 0.50000 0.16660 1.00000
Cr1 Cr 4 d 0.16700 0.34800 0.16660 1.00000
Cr2 Cr 4 d 0.33300 0.15200 0.00000 1.00000
O1 O 4 d 0.20800 0.15200 0.83330 1.00000
O2 O 4 d 0.45800 0.15200 0.83330 1.00000
O3 O 4 d 0.29200 0.34800 0.66660 1.00000
O4 O 4 d 0.04200 0.34800 0.66660 1.00000
O5 O 4 d 0.20800 0.15200 0.50000 1.00000
O6 O 4 d 0.45800 0.15200 0.50000 1.00000
O7 O 4 d 0.29200 0.34800 0.33330 1.00000
O8 O 4 d 0.04200 0.34800 0.33330 1.00000
O9 O 4 d 0.20800 0.15200 0.16660 1.00000
O10 O 4 d 0.45800 0.15200 0.16660 1.00000
O11 O 4 d 0.29200 0.34800 0.00000 1.00000
O12 O 4 d 0.04200 0.34800 0.00000 1.00000
Ru1 Ru 4 d 0.16700 0.34800 0.83330 1.00000
Ru2 Ru 4 d 0.33300 0.15200 0.66660 1.00000
Ru3 Ru 4 d 0.16700 0.34800 0.50000 1.00000
Ru4 Ru 4 d 0.33300 0.15200 0.33330 1.00000

```

BaCr<sub>2</sub>Ru<sub>4</sub>O<sub>12</sub>: AB2C12D4\_tP76\_75\_2a2b\_2d\_12d\_4d - POSCAR

```

AB2C12D4_tP76_75_2a2b_2d_12d_4d & a, c/a, z1, z2, z3, z4, x5, y5, z5, x6, y6, z6, x7,
↳ y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12,
↳ x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18,
↳ y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22 --
↳ params=9.8880614494, 0.922431229769, 0.3333, 0.0, 0.5003, 0.1666,
↳ 0.167, 0.348, 0.1666, 0.333, 0.152, 0.0, 0.208, 0.152, 0.8333, 0.458,
↳ 0.152, 0.8333, 0.292, 0.348, 0.6666, 0.042, 0.348, 0.6666, 0.208, 0.152,
↳ 0.5, 0.458, 0.152, 0.5, 0.292, 0.348, 0.3333, 0.042, 0.348, 0.3333, 0.208
↳ 0.152, 0.1666, 0.458, 0.152, 0.1666, 0.292, 0.348, 0.0, 0.042, 0.348,
↳ 0.0, 0.167, 0.348, 0.8333, 0.333, 0.152, 0.6666, 0.167, 0.348, 0.5, 0.333
↳ 0.152, 0.3333 & P4 C_{4}^{1} #75 (a^2b^2d^18) & P76 & None &
↳ BaCr2Ru4O12 & M. C. Cad{\e} and A. Prodan, Mater. Res.
↳ Bull. 14, 613-618 (1979)
1.0000000000000000
9.88806144940000 0.00000000000000 0.00000000000000
0.00000000000000 9.88806144940000 0.00000000000000
0.00000000000000 0.00000000000000 9.12105668280000
Ba Cr O Ru
4 8 48 16
Direct
0.00000000000000 0.00000000000000 0.33330000000000 Ba (1a)
0.00000000000000 0.00000000000000 0.00000000000000 Ba (1a)
0.50000000000000 0.50000000000000 0.50030000000000 Ba (1b)
0.50000000000000 0.50000000000000 0.16660000000000 Ba (1b)
0.16700000000000 0.34800000000000 0.16660000000000 Cr (4d)
-0.16700000000000 -0.34800000000000 0.16660000000000 Cr (4d)
-0.34800000000000 0.16700000000000 0.16660000000000 Cr (4d)
0.33300000000000 0.15200000000000 0.00000000000000 Cr (4d)
-0.33300000000000 -0.15200000000000 0.00000000000000 Cr (4d)
-0.15200000000000 0.33300000000000 0.00000000000000 Cr (4d)
0.15200000000000 -0.33300000000000 0.00000000000000 Cr (4d)
0.20800000000000 0.15200000000000 0.83330000000000 O (4d)
-0.20800000000000 -0.15200000000000 0.83330000000000 O (4d)
-0.15200000000000 0.20800000000000 0.83330000000000 O (4d)
0.15200000000000 -0.20800000000000 0.83330000000000 O (4d)
0.45800000000000 0.15200000000000 0.83330000000000 O (4d)
-0.45800000000000 -0.15200000000000 0.83330000000000 O (4d)
-0.15200000000000 0.45800000000000 0.83330000000000 O (4d)
0.15200000000000 -0.45800000000000 0.83330000000000 O (4d)
0.29200000000000 0.34800000000000 0.66660000000000 O (4d)
-0.29200000000000 -0.34800000000000 0.66660000000000 O (4d)
-0.34800000000000 0.29200000000000 0.66660000000000 O (4d)
0.34800000000000 -0.29200000000000 0.66660000000000 O (4d)
0.04200000000000 0.34800000000000 0.66660000000000 O (4d)
-0.04200000000000 -0.34800000000000 0.66660000000000 O (4d)
-0.34800000000000 0.04200000000000 0.66660000000000 O (4d)
0.34800000000000 -0.04200000000000 0.66660000000000 O (4d)
0.20800000000000 0.15200000000000 0.50000000000000 O (4d)
-0.20800000000000 -0.15200000000000 0.50000000000000 O (4d)
-0.15200000000000 0.20800000000000 0.50000000000000 O (4d)

```

```
0.1520000000000000 -0.2080000000000000 0.5000000000000000 O (4d)
0.4580000000000000 0.1520000000000000 0.5000000000000000 O (4d)
-0.4580000000000000 -0.1520000000000000 0.5000000000000000 O (4d)
-0.1520000000000000 0.4580000000000000 0.5000000000000000 O (4d)
0.1520000000000000 -0.4580000000000000 0.5000000000000000 O (4d)
0.2920000000000000 0.3480000000000000 0.3333000000000000 O (4d)
-0.2920000000000000 -0.3480000000000000 0.3333000000000000 O (4d)
-0.3480000000000000 0.2920000000000000 0.3333000000000000 O (4d)
0.3480000000000000 -0.2920000000000000 0.3333000000000000 O (4d)
0.0420000000000000 0.3480000000000000 0.3333000000000000 O (4d)
-0.0420000000000000 -0.3480000000000000 0.3333000000000000 O (4d)
-0.3480000000000000 0.0420000000000000 0.3333000000000000 O (4d)
0.3480000000000000 -0.0420000000000000 0.3333000000000000 O (4d)
0.2080000000000000 0.1520000000000000 0.1666000000000000 O (4d)
-0.2080000000000000 -0.1520000000000000 0.1666000000000000 O (4d)
-0.1520000000000000 0.2080000000000000 0.1666000000000000 O (4d)
0.1520000000000000 -0.2080000000000000 0.1666000000000000 O (4d)
0.4580000000000000 0.1520000000000000 0.1666000000000000 O (4d)
-0.4580000000000000 -0.1520000000000000 0.1666000000000000 O (4d)
-0.1520000000000000 0.4580000000000000 0.1666000000000000 O (4d)
0.1520000000000000 -0.4580000000000000 0.1666000000000000 O (4d)
0.2920000000000000 0.3480000000000000 0.0000000000000000 O (4d)
-0.2920000000000000 -0.3480000000000000 0.0000000000000000 O (4d)
-0.3480000000000000 0.2920000000000000 0.0000000000000000 O (4d)
0.3480000000000000 -0.2920000000000000 0.0000000000000000 O (4d)
0.0420000000000000 0.3480000000000000 0.0000000000000000 O (4d)
-0.0420000000000000 -0.3480000000000000 0.0000000000000000 O (4d)
-0.3480000000000000 0.0420000000000000 0.0000000000000000 O (4d)
0.3480000000000000 -0.0420000000000000 0.0000000000000000 O (4d)
0.1670000000000000 0.3480000000000000 0.8333000000000000 Ru (4d)
-0.1670000000000000 -0.3480000000000000 0.8333000000000000 Ru (4d)
-0.3480000000000000 0.1670000000000000 0.8333000000000000 Ru (4d)
0.3480000000000000 -0.1670000000000000 0.8333000000000000 Ru (4d)
0.3330000000000000 0.1520000000000000 0.6666000000000000 Ru (4d)
-0.3330000000000000 -0.1520000000000000 0.6666000000000000 Ru (4d)
-0.1520000000000000 0.3330000000000000 0.6666000000000000 Ru (4d)
0.1520000000000000 -0.3330000000000000 0.6666000000000000 Ru (4d)
0.1670000000000000 0.3480000000000000 0.5000000000000000 Ru (4d)
-0.1670000000000000 -0.3480000000000000 0.5000000000000000 Ru (4d)
-0.3480000000000000 0.1670000000000000 0.5000000000000000 Ru (4d)
0.3480000000000000 -0.1670000000000000 0.5000000000000000 Ru (4d)
0.3330000000000000 0.1520000000000000 0.3333000000000000 Ru (4d)
-0.3330000000000000 -0.1520000000000000 0.3333000000000000 Ru (4d)
-0.1520000000000000 0.3330000000000000 0.3333000000000000 Ru (4d)
0.1520000000000000 -0.3330000000000000 0.3333000000000000 Ru (4d)
```

LaRhC<sub>2</sub>: A2BC\_tP16\_76\_2a\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'LaRhC2'
_chemical_formula_sum 'C2 La Rh'

loop_
_publ_author_name
'A. O. Tsokol'
'O. I. Bodak'
'E. P. Marusin'
'V. E. Zavodnik'
_journal_name_full_name
;
Kristallografiya, English title: Crystallography Reports
;
_journal_volume 33
_journal_year 1988
_journal_page_first 345
_journal_page_last 348
_publ_section_title
;
X-ray diffraction studies of ternary SRSRhC2 (SRS = La, Ce, Pr, Nd
↪ , Sm) compounds
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'LaRhC2{2} Structure'
_aflow_proto 'A2BC_tP16_76_2a_a'
_aflow_params 'a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},z_{4}'
↪ '3},x_{4},y_{4},z_{4}'
_aflow_params_values '3.9810644174,3.85606631503,0.143,0.173,0.1347,
↪ 0.353,0.141,0.2027,0.3461,0.3475,0.5937,0.1519,0.1578,0.0'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP16'

_cell_length_a 3.9810644174
_cell_length_b 3.9810644174
_cell_length_c 15.3512483979
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'P 41'
_symmetry_Int_Tables_number 76

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z+1/2
3 -y,x,z+1/4
4 y,-x,z+3/4
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
C1 C 4 a 0.14300 0.17300 0.13470 1.00000
C2 C 4 a 0.35300 0.14100 0.20270 1.00000
La1 La 4 a 0.34610 0.34750 0.59370 1.00000
Rh1 Rh 4 a 0.15190 0.15780 0.00000 1.00000
```

LaRhC<sub>2</sub>: A2BC\_tP16\_76\_2a\_a - POSCAR

```
A2BC_tP16_76_2a_a & a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4 --params
↪ =3.9810644174,3.85606631503,0.143,0.173,0.1347,0.353,0.141,
↪ 0.2027,0.3461,0.3475,0.5937,0.1519,0.1578,0.0 & P4_1 C_{4}^{2}
↪ } #76 (a^4) & tP16 & None & LaRhC2 & A. O. Tsokol' et al.,
↪ Kristallografiya 33, 345-348 (1988)
1.0000000000000000
3.98106441740000 0.00000000000000 0.0000000000000000
0.00000000000000 3.98106441740000 0.0000000000000000
0.00000000000000 0.00000000000000 15.35124839790000
C La Rh
8 4 4
Direct
0.143000000000000 0.173000000000000 0.134700000000000 C (4a)
-0.143000000000000 -0.173000000000000 0.634700000000000 C (4a)
-0.173000000000000 -0.143000000000000 0.384700000000000 C (4a)
0.173000000000000 -0.143000000000000 0.884700000000000 C (4a)
0.353000000000000 0.141000000000000 0.202700000000000 C (4a)
-0.353000000000000 -0.141000000000000 0.702700000000000 C (4a)
-0.141000000000000 0.353000000000000 0.452700000000000 C (4a)
0.141000000000000 -0.353000000000000 0.952700000000000 C (4a)
0.346100000000000 0.347500000000000 0.593700000000000 La (4a)
-0.346100000000000 -0.347500000000000 1.093700000000000 La (4a)
-0.347500000000000 0.346100000000000 0.843700000000000 La (4a)
0.347500000000000 -0.346100000000000 1.343700000000000 La (4a)
0.151900000000000 0.157800000000000 0.000000000000000 Rh (4a)
-0.151900000000000 -0.157800000000000 0.500000000000000 Rh (4a)
-0.157800000000000 0.151900000000000 0.250000000000000 Rh (4a)
0.157800000000000 -0.151900000000000 0.750000000000000 Rh (4a)
```

Cs<sub>3</sub>P<sub>7</sub>: A3B7\_tP40\_76\_3a\_7a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Cs3 P7'

loop_
_publ_author_name
'T. Meyer'
'W. H. {o}nle'
'H. G. {von Schnering}'
_journal_name_full_name
;
Zeitschrift fur Anorganische und Allgemeine Chemie
;
_journal_volume 552
_journal_year 1987
_journal_page_first 69
_journal_page_last 80
_publ_section_title
;
Zur Chemie und Strukturchemie von Phosphiden und Polyphosphiden. 44.
↪ Tric{a}siumheptaphosphid Cs3PS7: Darstellung,
↪ Struktur und Eigenschaften
;
# Found in Crystals and Crystal Structures, 2006

_aflow_title 'Cs3PS7 Structure'
_aflow_proto 'A3B7_tP40_76_3a_7a'
_aflow_params 'a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},z_{4}'
↪ '3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},y_{7},z_{7},x_{8},y_{8},z_{8},x_{9},y_{9},z_{9},x_{10},y_{10},z_{10}'
_aflow_params_values '9.046,1.84766747734,0.7435,0.3852,0.0,0.4169,0.733
↪ 0.8359,0.026,0.8404,-0.0086,0.79,0.6,0.8105,0.443,0.095,-0.053
↪ 0.106,0.473,0.8928,0.357,0.024,0.061,0.629,0.794,0.017,-0.002,
↪ 0.341,0.7049,0.011,0.29,0.84'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP40'

_symmetry_space_group_name_H-M 'P 41'
_symmetry_Int_Tables_number 76

_cell_length_a 9.04600
_cell_length_b 9.04600
_cell_length_c 16.71400
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z+1/2
3 -y,x,z+1/4
```

```

4 y,-x,z+3/4

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Cs1 Cs 4 a 0.74350 0.38520 0.00000 1.00000
Cs2 Cs 4 a 0.41690 0.73300 0.83590 1.00000
Cs3 Cs 4 a 0.02600 0.84040 -0.00860 1.00000
P1 P 4 a 0.79000 0.60000 0.81050 1.00000
P2 P 4 a 0.44300 0.09500 -0.05300 1.00000
P3 P 4 a 0.10600 0.47300 0.89280 1.00000
P4 P 4 a 0.35700 0.02400 0.06100 1.00000
P5 P 4 a 0.62900 0.79400 0.01700 1.00000
P6 P 4 a -0.00200 0.34100 0.70490 1.00000
P7 P 4 a 0.01100 0.29000 0.84000 1.00000

```

Cs<sub>3</sub>P<sub>7</sub>: A3B7\_tP40\_76\_3a\_7a - POSCAR

```

A3B7_tP40_76_3a_7a & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5,
  x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10 --params=9.046,
  1.84766747734, 0.7435, 0.3852, 0.0, 0.4169, 0.733, 0.8359, 0.026,
  0.8404, -0.0086, 0.79, 0.6, 0.8105, 0.443, 0.095, -0.053, 0.106, 0.473,
  0.8928, 0.357, 0.024, 0.061, 0.629, 0.794, 0.017, -0.002, 0.341, 0.7049,
  0.011, 0.29, 0.84 & P4_{1} C_{4}^{[2]} #76 (a^10) & tP40 & None &
  Cs3P7 & & T. Meyer and W. H\''{o}nle and H. G. {von Schnering},
  Z. Anorg. Allg. Chem. 552, 69-80 (1987)

1.0000000000000000
9.0460000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 9.0460000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 16.7140000000000000

Cs P
12 28

Direct
0.7435000000000000 0.3852000000000000 0.0000000000000000 Cs (4a)
-0.7435000000000000 -0.3852000000000000 0.5000000000000000 Cs (4a)
-0.3852000000000000 0.7435000000000000 0.2500000000000000 Cs (4a)
0.3852000000000000 -0.7435000000000000 0.7500000000000000 Cs (4a)
0.4169000000000000 0.7330000000000000 0.8359000000000000 Cs (4a)
-0.4169000000000000 -0.7330000000000000 1.3359000000000000 Cs (4a)
-0.7330000000000000 0.4169000000000000 1.0859000000000000 Cs (4a)
0.7330000000000000 -0.4169000000000000 1.5859000000000000 Cs (4a)
0.0260000000000000 0.8404000000000000 -0.0086000000000000 Cs (4a)
-0.0260000000000000 -0.8404000000000000 0.4914000000000000 Cs (4a)
-0.8404000000000000 0.0260000000000000 0.2414000000000000 Cs (4a)
0.8404000000000000 -0.0260000000000000 0.7414000000000000 Cs (4a)
0.7900000000000000 0.6000000000000000 0.8105000000000000 P (4a)
-0.7900000000000000 -0.6000000000000000 1.3105000000000000 P (4a)
-0.6000000000000000 0.7900000000000000 1.0605000000000000 P (4a)
0.6000000000000000 -0.7900000000000000 1.5605000000000000 P (4a)
0.4430000000000000 0.0950000000000000 -0.0530000000000000 P (4a)
-0.4430000000000000 -0.0950000000000000 0.4470000000000000 P (4a)
-0.0950000000000000 0.4430000000000000 0.1970000000000000 P (4a)
0.0950000000000000 -0.4430000000000000 0.6970000000000000 P (4a)
0.1060000000000000 0.4730000000000000 0.8928000000000000 P (4a)
-0.1060000000000000 -0.4730000000000000 1.3928000000000000 P (4a)
-0.4730000000000000 0.1060000000000000 1.1428000000000000 P (4a)
0.4730000000000000 -0.1060000000000000 1.6428000000000000 P (4a)
0.3570000000000000 0.0240000000000000 0.0610000000000000 P (4a)
-0.3570000000000000 -0.0240000000000000 0.5610000000000000 P (4a)
-0.0240000000000000 0.3570000000000000 0.3110000000000000 P (4a)
0.0240000000000000 -0.3570000000000000 0.8110000000000000 P (4a)
0.6290000000000000 0.7940000000000000 0.0170000000000000 P (4a)
-0.6290000000000000 -0.7940000000000000 0.5170000000000000 P (4a)
-0.7940000000000000 0.6290000000000000 0.2670000000000000 P (4a)
0.7940000000000000 -0.6290000000000000 0.7670000000000000 P (4a)
-0.0020000000000000 0.3410000000000000 0.7049000000000000 P (4a)
0.0020000000000000 -0.3410000000000000 1.2049000000000000 P (4a)
-0.3410000000000000 0.0020000000000000 0.9549000000000000 P (4a)
0.3410000000000000 0.0020000000000000 1.4549000000000000 P (4a)
0.0110000000000000 0.2900000000000000 0.8400000000000000 P (4a)
-0.0110000000000000 -0.2900000000000000 1.3400000000000000 P (4a)
-0.2900000000000000 0.0110000000000000 1.0900000000000000 P (4a)
0.2900000000000000 -0.0110000000000000 1.5900000000000000 P (4a)

```

Pinnoite (Mg<sub>2</sub>O(OH)<sub>6</sub>): A2B6CD7\_tP64\_77\_2d\_6d\_d\_ab6d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'MgB2O(OH)6'
_chemical_formula_sum 'B2 H6 Mg O7'

loop_
  _publ_author_name
  'E. A. Genkina'
  'Y. A. Malinovskii'
  _journal_name_full_name
  'Soviet Physics Crystallography'
  _journal_volume 28
  _journal_year 1983
  _journal_page_first 475
  _journal_page_last 477
  _publ_Section_title
  'Refinement of the structure of pinnoite: Location of hydrogen atoms'

```

```

# Found in Pearson's Crystal Data - Crystal Structure Database for
  Inorganic Compounds, 2013

_abbrev_title 'Pinnoite (MgB2(OH)6) Structure'
_abbrev_proto 'A2B6CD7_tP64_77_2d_6d_d_ab6d'
_abbrev_params 'a, c/a, z_{1}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}, x_{7}, y_{7}, z_{7}, x_{8}, y_{8}, z_{8}, x_{9}, y_{9}, z_{9}, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}'
_abbrev_params_values '7.6159522234, 1.07480314961, 0.0, 0.035, 0.1167, 0.1203, 0.418, 0.392, 0.3817, 0.132, 0.362, 0.099, 0.309, 0.136, 0.393, 0.161, 0.192, 0.355, 0.442, 0.312, 0.133, 0.03, 0.028, 0.14, 0.14, 0.47, 0.35, 0.32, 0.2491, 0.7483, 0.273, 0.2602, 0.0188, 0.013, 0.2316, 0.4834, 0.184, 0.1644, 0.2577, 0.529, 0.3406, 0.2365, 0.012, 0.0182, 0.2119, 0.275, 0.4808, 0.3008, 0.268'
_abbrev_Structurbericht 'None'
_abbrev_Pearson 'tP64'

_cell_length_a 7.6159522234
_cell_length_b 7.6159522234
_cell_length_c 8.1856494370
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'P 42'
_symmetry_Int_Tables_number 77

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x, y, z
2 -x, -y, z
3 -y, x, z+1/2
4 y, -x, z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
O1 O 2 a 0.00000 0.00000 0.00000 1.00000
O2 O 2 b 0.50000 0.50000 0.03500 1.00000
B1 B 4 d 0.11670 0.12030 0.41800 1.00000
B2 B 4 d 0.39200 0.38170 0.13200 1.00000
H1 H 4 d 0.36200 0.09900 0.30900 1.00000
H2 H 4 d 0.13600 0.39300 0.16100 1.00000
H3 H 4 d 0.19200 0.35500 0.44200 1.00000
H4 H 4 d 0.31200 0.13300 0.03000 1.00000
H5 H 4 d 0.02800 0.14000 0.14000 1.00000
H6 H 4 d 0.47000 0.35000 0.32000 1.00000
Mg1 Mg 4 d 0.24910 0.74830 0.27300 1.00000
O3 O 4 d 0.26020 0.01880 0.01300 1.00000
O4 O 4 d 0.23160 0.48340 0.18400 1.00000
O5 O 4 d 0.16440 0.25770 0.52900 1.00000
O6 O 4 d 0.34060 0.23650 0.01200 1.00000
O7 O 4 d 0.01820 0.21190 0.27500 1.00000
O8 O 4 d 0.48080 0.30080 0.26800 1.00000

```

Pinnoite (Mg<sub>2</sub>O(OH)<sub>6</sub>): A2B6CD7\_tP64\_77\_2d\_6d\_d\_ab6d - POSCAR

```

A2B6CD7_tP64_77_2d_6d_d_ab6d & a, c/a, z1, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6,
  y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12,
  y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17,
  z17 --params=7.6159522234, 1.07480314961, 0.0, 0.035, 0.1167,
  0.1203, 0.418, 0.392, 0.3817, 0.132, 0.362, 0.099, 0.309, 0.136, 0.393,
  0.161, 0.192, 0.355, 0.442, 0.312, 0.133, 0.03, 0.028, 0.14, 0.14, 0.47,
  0.35, 0.32, 0.2491, 0.7483, 0.273, 0.2602, 0.0188, 0.013, 0.2316, 0.4834,
  0.184, 0.1644, 0.2577, 0.529, 0.3406, 0.2365, 0.012, 0.0182, 0.2119,
  0.275, 0.4808, 0.3008, 0.268 & P4_{2} C_{4}^{[3]} #77 (abd^15) &
  tP64 & None & MgB2O(OH)6 & E. A. Genkina and Y. A.
  Malinovskii, Sov. Phys. Crystallogr. 28, 475-477 (1983)

1.0000000000000000
7.6159522234000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6159522234000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 8.1856494370000000

B H Mg O
8 24 4 28

Direct
0.1167000000000000 0.1203000000000000 0.4180000000000000 B (4d)
-0.1167000000000000 -0.1203000000000000 0.4180000000000000 B (4d)
-0.1203000000000000 0.1167000000000000 0.9180000000000000 B (4d)
0.1203000000000000 -0.1167000000000000 0.9180000000000000 B (4d)
0.3920000000000000 0.3817000000000000 0.1320000000000000 B (4d)
-0.3920000000000000 -0.3817000000000000 0.1320000000000000 B (4d)
-0.3817000000000000 0.3920000000000000 0.6320000000000000 B (4d)
0.3817000000000000 -0.3920000000000000 0.6320000000000000 B (4d)
0.3620000000000000 0.0990000000000000 0.3090000000000000 H (4d)
-0.3620000000000000 -0.0990000000000000 0.3090000000000000 H (4d)
-0.0990000000000000 0.3620000000000000 0.8090000000000000 H (4d)
0.0990000000000000 -0.3620000000000000 0.8090000000000000 H (4d)
0.1360000000000000 0.3930000000000000 0.1610000000000000 H (4d)
-0.1360000000000000 -0.3930000000000000 0.1610000000000000 H (4d)
-0.3930000000000000 0.1360000000000000 0.6610000000000000 H (4d)
0.3930000000000000 -0.1360000000000000 0.6610000000000000 H (4d)
0.1920000000000000 0.3550000000000000 0.4420000000000000 H (4d)
-0.1920000000000000 -0.3550000000000000 0.4420000000000000 H (4d)
-0.3550000000000000 0.1920000000000000 0.9420000000000000 H (4d)

```

```

0.35500000000000 -0.19200000000000 0.94200000000000 H (4d)
0.31200000000000 -0.13300000000000 0.03000000000000 H (4d)
-0.31200000000000 -0.13300000000000 0.03000000000000 H (4d)
-0.13300000000000 0.31200000000000 0.53000000000000 H (4d)
0.13300000000000 -0.31200000000000 0.53000000000000 H (4d)
0.02800000000000 0.14000000000000 0.14000000000000 H (4d)
-0.02800000000000 -0.14000000000000 0.14000000000000 H (4d)
-0.14000000000000 0.02800000000000 0.64000000000000 H (4d)
0.14000000000000 -0.02800000000000 0.64000000000000 H (4d)
0.47000000000000 0.35000000000000 0.32000000000000 H (4d)
-0.47000000000000 -0.35000000000000 0.32000000000000 H (4d)
-0.35000000000000 0.47000000000000 0.82000000000000 H (4d)
0.35000000000000 -0.47000000000000 0.82000000000000 H (4d)
0.24910000000000 0.74830000000000 0.27300000000000 Mg (4d)
-0.24910000000000 -0.74830000000000 0.27300000000000 Mg (4d)
-0.74830000000000 0.24910000000000 0.77300000000000 Mg (4d)
0.74830000000000 -0.24910000000000 0.77300000000000 Mg (4d)
0.00000000000000 0.00000000000000 0.00000000000000 O (2a)
0.00000000000000 0.00000000000000 0.00000000000000 O (2a)
0.50000000000000 0.50000000000000 0.03500000000000 O (2b)
0.50000000000000 0.50000000000000 0.53500000000000 O (2b)
0.26020000000000 0.01880000000000 0.01300000000000 O (4d)
-0.26020000000000 -0.01880000000000 0.01300000000000 O (4d)
-0.01880000000000 0.26020000000000 0.51300000000000 O (4d)
0.01880000000000 -0.26020000000000 0.51300000000000 O (4d)
0.23160000000000 0.48340000000000 0.18400000000000 O (4d)
-0.23160000000000 -0.48340000000000 0.18400000000000 O (4d)
-0.48340000000000 0.23160000000000 0.68400000000000 O (4d)
0.48340000000000 -0.23160000000000 0.68400000000000 O (4d)
0.16440000000000 0.25770000000000 0.52900000000000 O (4d)
-0.16440000000000 -0.25770000000000 0.52900000000000 O (4d)
-0.25770000000000 0.16440000000000 1.02900000000000 O (4d)
0.25770000000000 -0.16440000000000 1.02900000000000 O (4d)
0.34060000000000 0.23650000000000 0.01200000000000 O (4d)
-0.34060000000000 -0.23650000000000 0.01200000000000 O (4d)
-0.23650000000000 0.34060000000000 0.51200000000000 O (4d)
0.23650000000000 -0.34060000000000 0.51200000000000 O (4d)
0.01820000000000 0.21190000000000 0.27500000000000 O (4d)
-0.01820000000000 -0.21190000000000 0.27500000000000 O (4d)
-0.21190000000000 0.01820000000000 0.77500000000000 O (4d)
0.21190000000000 -0.01820000000000 0.77500000000000 O (4d)
0.48080000000000 0.30080000000000 0.26800000000000 O (4d)
-0.48080000000000 -0.30080000000000 0.26800000000000 O (4d)
-0.30080000000000 0.48080000000000 0.76800000000000 O (4d)
0.30080000000000 -0.48080000000000 0.76800000000000 O (4d)

```

H<sub>2</sub>S III: A2B\_tP48\_77\_8d\_4d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'H2S III'
_chemical_formula_sum 'H2 S'

loop_
  _publ_author_name
    'E. S\{andor'
    'S. O. Ogunade'
  _journal_name_full_name
    'Nature'
  _journal_volume 224
  _journal_year 1969
  _journal_page_first 905
  _journal_page_last 907
  _publ_section_title
    'Structure and Phase Transition in Solid Hydrogen and Deuterium
    ↳ Sulphides'

# Found in Pressure-temperature phase diagram of solid hydrogen sulfide
↳ determined by Raman spectroscopy, 1995

_aflow_title 'HS_{2}S III Structure'
_aflow_proto 'A2B_tP48_77_8d_4d'
_aflow_params 'a, c/a, x_{1}, y_{1}, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3},
↳ x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}, x_{7},
↳ y_{7}, z_{7}, x_{8}, y_{8}, z_{8}, x_{9}, y_{9}, z_{9}, x_{10}, y_{10},
↳ z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}'
_aflow_params_values '13.47, 0.304380103935, 0.193, 0.14, 0.163, 0.091, 0.059,
↳ 0.837, 0.693, 0.14, 0.163, 0.591, 0.059, 0.837, 0.193, 0.64, 0.163, 0.193
↳ 0.64, 0.837, 0.693, 0.64, 0.837, 0.591, 0.559, 0.163, 0.11, 0.14, 0.0,
↳ 0.61, 0.14, 0.0, 0.11, 0.64, 0.0, 0.61, 0.64, 0.0'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP48'

_symmetry_space_group_name_H-M 'P 42'
_symmetry_Int_Tables_number 77

_cell_length_a 13.47000
_cell_length_b 13.47000
_cell_length_c 4.10000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x, y, z
  2 -x, -y, z
  3 -y, x, z+1/2

```

```

4 y, -x, z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
H1 H 4 d 0.19300 0.14000 0.16300 1.00000
H2 H 4 d 0.09100 0.05900 0.83700 1.00000
H3 H 4 d 0.69300 0.14000 0.16300 1.00000
H4 H 4 d 0.59100 0.05900 0.83700 1.00000
H5 H 4 d 0.19300 0.64000 0.16300 1.00000
H6 H 4 d 0.19300 0.64000 0.83700 1.00000
H7 H 4 d 0.69300 0.64000 0.83700 1.00000
H8 H 4 d 0.59100 0.55900 0.16300 1.00000
S1 S 4 d 0.11000 0.14000 0.00000 1.00000
S2 S 4 d 0.61000 0.14000 0.00000 1.00000
S3 S 4 d 0.11000 0.64000 0.00000 1.00000
S4 S 4 d 0.61000 0.64000 0.00000 1.00000

```

H<sub>2</sub>S III: A2B\_tP48\_77\_8d\_4d - POSCAR

```

A2B_tP48_77_8d_4d & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5,
↳ x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12
↳ y12, z12 --params=13.47, 0.304380103935, 0.193, 0.14, 0.163, 0.091,
↳ 0.059, 0.837, 0.693, 0.14, 0.163, 0.591, 0.059, 0.837, 0.193, 0.64, 0.163
↳ 0.193, 0.64, 0.837, 0.693, 0.64, 0.837, 0.591, 0.559, 0.163, 0.11, 0.14,
↳ 0.0, 0.61, 0.14, 0.0, 0.11, 0.64, 0.0, 0.61, 0.64, 0.0 & P4_{2} C_{4}^{3}
↳ } #77 (d^{12}) & tP48 & None & H2S & H2S III & E. S\{andor and
↳ S. O. Ogunade, Nature 224, 905-907 (1969)
1.00000000000000
13.47000000000000 0.00000000000000 0.00000000000000
0.00000000000000 13.47000000000000 0.00000000000000
0.00000000000000 0.00000000000000 4.10000000000000
H S
32 16
Direct
0.19300000000000 0.14000000000000 0.16300000000000 H (4d)
-0.19300000000000 -0.14000000000000 0.16300000000000 H (4d)
-0.14000000000000 0.19300000000000 0.66300000000000 H (4d)
0.14000000000000 -0.19300000000000 0.66300000000000 H (4d)
0.09100000000000 0.05900000000000 0.83700000000000 H (4d)
-0.09100000000000 -0.05900000000000 0.83700000000000 H (4d)
-0.05900000000000 0.09100000000000 1.33700000000000 H (4d)
0.05900000000000 -0.09100000000000 1.33700000000000 H (4d)
0.69300000000000 0.14000000000000 0.16300000000000 H (4d)
-0.69300000000000 -0.14000000000000 0.16300000000000 H (4d)
-0.14000000000000 0.69300000000000 0.66300000000000 H (4d)
0.14000000000000 -0.69300000000000 0.66300000000000 H (4d)
0.59100000000000 0.05900000000000 0.83700000000000 H (4d)
-0.59100000000000 -0.05900000000000 0.83700000000000 H (4d)
-0.05900000000000 0.59100000000000 1.33700000000000 H (4d)
0.05900000000000 -0.59100000000000 1.33700000000000 H (4d)
0.19300000000000 0.64000000000000 0.16300000000000 H (4d)
-0.19300000000000 -0.64000000000000 0.16300000000000 H (4d)
-0.64000000000000 0.19300000000000 0.66300000000000 H (4d)
0.64000000000000 -0.19300000000000 0.66300000000000 H (4d)
0.19300000000000 0.64000000000000 0.83700000000000 H (4d)
-0.19300000000000 -0.64000000000000 0.83700000000000 H (4d)
-0.64000000000000 0.19300000000000 1.33700000000000 H (4d)
0.64000000000000 -0.19300000000000 1.33700000000000 H (4d)
0.59100000000000 0.55900000000000 0.16300000000000 H (4d)
-0.59100000000000 -0.55900000000000 0.16300000000000 H (4d)
-0.55900000000000 0.59100000000000 0.66300000000000 H (4d)
0.55900000000000 -0.59100000000000 0.66300000000000 H (4d)
0.11000000000000 0.14000000000000 0.00000000000000 S (4d)
-0.11000000000000 -0.14000000000000 0.00000000000000 S (4d)
-0.14000000000000 0.11000000000000 0.50000000000000 S (4d)
0.14000000000000 -0.11000000000000 0.50000000000000 S (4d)
0.61000000000000 0.14000000000000 0.00000000000000 S (4d)
-0.61000000000000 -0.14000000000000 0.00000000000000 S (4d)
-0.14000000000000 0.61000000000000 0.50000000000000 S (4d)
0.14000000000000 -0.61000000000000 0.50000000000000 S (4d)
0.11000000000000 0.64000000000000 0.00000000000000 S (4d)
-0.11000000000000 -0.64000000000000 0.00000000000000 S (4d)
-0.64000000000000 0.11000000000000 0.50000000000000 S (4d)
0.64000000000000 -0.11000000000000 0.50000000000000 S (4d)
0.61000000000000 0.64000000000000 0.00000000000000 S (4d)
-0.61000000000000 -0.64000000000000 0.00000000000000 S (4d)
-0.64000000000000 0.61000000000000 0.50000000000000 S (4d)
0.64000000000000 -0.61000000000000 0.50000000000000 S (4d)

```

Sr<sub>2</sub>As<sub>2</sub>O<sub>7</sub>: A2B7C2\_tP88\_78\_4a\_14a\_4a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Sr2As2O7'
_chemical_formula_sum 'As2 O7 Sr2'

loop_
  _publ_author_name
    'A. Mbarek'
    'F. Edhokkar'
  _journal_name_full_name

```

Acta Crystallographica Section E: Crystallographic Communications

```

_journal_volume 69
_journal_year 2013
_journal_page_first i84
_journal_page_last i84
_publ_section_title
;
The P43(3) enantiomorph of Sr2(As2)2S2O7
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'Sr2(As2)2S2O7 Structure'
_aflow_proto 'A2B7C2_tP88_78_4a_14a_4a'
_aflow_params 'a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},y_{7},z_{7},x_{8},y_{8},z_{8},x_{9},y_{9},z_{9},x_{10},y_{10},z_{10},x_{11},y_{11},z_{11},x_{12},y_{12},z_{12},x_{13},y_{13},z_{13},x_{14},y_{14},z_{14},x_{15},y_{15},z_{15},x_{16},y_{16},z_{16},x_{17},y_{17},z_{17},x_{18},y_{18},z_{18},x_{19},y_{19},z_{19},x_{20},y_{20},z_{20},x_{21},y_{21},z_{21},x_{22},y_{22},z_{22}'
_aflow_params_values '7.1088964505,3.60337042297,0.14561,0.23414,0.69696
↳ 0.22057,0.48276,0.79885,0.18673,0.10525,0.29124,0.24906,
↳ 0.35443,0.19001,0.4586,0.3299,0.02876,0.0936,0.3899,0.1424,
↳ 0.4187,0.2147,0.16739,0.1085,0.2261,0.23449,0.2999,0.2626,
↳ 0.32782,0.0777,0.3681,0.7514,0.2725,0.3751,0.65898,0.0556,
↳ 0.3427,0.02051,0.3251,0.3037,0.52047,0.4811,0.0546,0.59334,
↳ 0.0026,0.0009,0.31632,0.3813,0.3334,0.82115,0.2817,0.0576,
↳ 0.71776,0.168,0.0503,-0.08181,0.26434,0.22687,0.42638,0.02701,
↳ 0.34822,0.57318,0.15408,0.39584,-0.07135,0.37469,0.25769,
↳ 0.06464'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP88'

_cell_length_a 7.1088964505
_cell_length_b 7.1088964505
_cell_length_c 25.6159872097
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 43"
_symmetry_Int_Tables_number 78

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z+1/2
3 -y,x,z+3/4
4 y,-x,z+1/4

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
As1 As 4 a 0.14561 0.23414 0.69696 1.00000
As2 As 4 a 0.22057 0.48276 0.79885 1.00000
As3 As 4 a 0.18673 0.10525 0.29124 1.00000
As4 As 4 a 0.24906 0.35443 0.19001 1.00000
O1 O 4 a 0.45860 0.32990 0.02876 1.00000
O2 O 4 a 0.09360 0.38990 0.14240 1.00000
O3 O 4 a 0.41870 0.21470 0.16739 1.00000
O4 O 4 a 0.10850 0.22610 0.23449 1.00000
O5 O 4 a 0.29990 0.26260 0.32782 1.00000
O6 O 4 a 0.07770 0.36810 0.75140 1.00000
O7 O 4 a 0.27250 0.37510 0.65898 1.00000
O8 O 4 a 0.05560 0.34270 0.02051 1.00000
O9 O 4 a 0.32510 0.30370 0.52047 1.00000
O10 O 4 a 0.48110 0.05460 0.59334 1.00000
O11 O 4 a 0.00260 0.00090 0.31632 1.00000
O12 O 4 a 0.38130 0.33340 0.82115 1.00000
O13 O 4 a 0.28170 0.05760 0.71776 1.00000
O14 O 4 a 0.16800 0.05030 -0.08181 1.00000
Sr1 Sr 4 a 0.26434 0.22687 0.42638 1.00000
Sr2 Sr 4 a 0.02701 0.34822 0.57318 1.00000
Sr3 Sr 4 a 0.15408 0.39584 -0.07135 1.00000
Sr4 Sr 4 a 0.37469 0.25769 0.06464 1.00000

```

Sr<sub>2</sub>As<sub>2</sub>O<sub>7</sub>: A2B7C2\_tP88\_78\_4a\_14a\_4a - POSCAR

```

A2B7C2_tP88_78_4a_14a_4a & a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,
y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11,y11,
z11,x12,y12,z12,x13,y13,z13,x14,y14,z14,x15,y15,z15,x16,y16,z16
↳ x17,y17,z17,x18,y18,z18,x19,y19,z19,x20,y20,z20,x21,y21,z21,
↳ x22,y22,z22 --params=7.1088964505,3.60337042297,0.14561,0.23414
↳ 0.69696,0.22057,0.48276,0.79885,0.18673,0.10525,0.29124,
↳ 0.24906,0.35443,0.19001,0.4586,0.3299,0.02876,0.0936,0.3899,
↳ 0.1424,0.4187,0.2147,0.16739,0.1085,0.2261,0.23449,0.2999,
↳ 0.2626,0.32782,0.0777,0.3681,0.7514,0.2725,0.3751,0.65898,
↳ 0.0556,0.3427,0.02051,0.3251,0.3037,0.52047,0.4811,0.0546,
↳ 0.59334,0.0026,0.0009,0.31632,0.3813,0.3334,0.82115,0.2817,
↳ 0.0576,0.71776,0.168,0.0503,-0.08181,0.26434,0.22687,0.42638,
↳ 0.02701,0.34822,0.57318,0.15408,0.39584,-0.07135,0.37469,
↳ 0.25769,0.06464 & P43(3) C4[4] #78 (a^22) & tP88 & None &
↳ Sr2As2O7 & A. Mbarek and F. Edhokkar, Acta Crystallogr. E 69
↳ , i84-i84 (2013)

```

```

1.000000000000000
7.10889645050000 0.00000000000000 0.00000000000000
0.00000000000000 7.10889645050000 0.00000000000000
0.00000000000000 0.00000000000000 25.6159872097000
As O Sr
16 56 16
Direct
0.14561000000000 0.23414000000000 0.69696000000000 As (4a)
-0.14561000000000 -0.23414000000000 1.19696000000000 As (4a)
-0.23414000000000 0.14561000000000 1.44696000000000 As (4a)
0.23414000000000 -0.14561000000000 0.94696000000000 As (4a)
0.10525000000000 0.48276000000000 0.79885000000000 As (4a)
-0.22057000000000 -0.48276000000000 1.29885000000000 As (4a)
-0.48276000000000 0.22057000000000 1.54885000000000 As (4a)
0.48276000000000 -0.22057000000000 1.04885000000000 As (4a)
0.18673000000000 0.10525000000000 0.29124000000000 As (4a)
-0.18673000000000 -0.10525000000000 0.79124000000000 As (4a)
-0.10525000000000 0.18673000000000 1.04124000000000 As (4a)
0.10525000000000 -0.18673000000000 0.54124000000000 As (4a)
0.24906000000000 0.35443000000000 0.19001000000000 As (4a)
-0.24906000000000 -0.35443000000000 0.69001000000000 As (4a)
-0.35443000000000 0.24906000000000 0.94001000000000 As (4a)
0.35443000000000 -0.24906000000000 0.44001000000000 As (4a)
0.45860000000000 0.32990000000000 0.02876000000000 O (4a)
-0.45860000000000 -0.32990000000000 0.52876000000000 O (4a)
-0.32990000000000 0.45860000000000 0.77876000000000 O (4a)
0.32990000000000 -0.45860000000000 0.27876000000000 O (4a)
0.09360000000000 0.38990000000000 0.14240000000000 O (4a)
-0.09360000000000 -0.38990000000000 0.64240000000000 O (4a)
-0.38990000000000 0.09360000000000 0.89240000000000 O (4a)
0.38990000000000 -0.09360000000000 0.39240000000000 O (4a)
0.41870000000000 0.21470000000000 0.16739000000000 O (4a)
-0.41870000000000 -0.21470000000000 0.66739000000000 O (4a)
-0.21470000000000 0.41870000000000 0.91739000000000 O (4a)
0.21470000000000 -0.41870000000000 0.41739000000000 O (4a)
0.10850000000000 0.22610000000000 0.23449000000000 O (4a)
-0.10850000000000 -0.22610000000000 0.73449000000000 O (4a)
-0.22610000000000 0.10850000000000 0.98449000000000 O (4a)
0.22610000000000 -0.10850000000000 0.48449000000000 O (4a)
0.29990000000000 0.26260000000000 0.32782000000000 O (4a)
-0.29990000000000 -0.26260000000000 0.82782000000000 O (4a)
-0.26260000000000 0.29990000000000 1.07782000000000 O (4a)
0.26260000000000 -0.29990000000000 0.57782000000000 O (4a)
0.07770000000000 0.36810000000000 0.75140000000000 O (4a)
-0.07770000000000 -0.36810000000000 1.25140000000000 O (4a)
-0.36810000000000 0.07770000000000 1.50140000000000 O (4a)
0.36810000000000 -0.07770000000000 1.00140000000000 O (4a)
0.27250000000000 0.37510000000000 0.65898000000000 O (4a)
-0.27250000000000 -0.37510000000000 1.15898000000000 O (4a)
-0.37510000000000 0.27250000000000 1.40898000000000 O (4a)
0.37510000000000 -0.27250000000000 0.90898000000000 O (4a)
0.05560000000000 0.34270000000000 0.02051000000000 O (4a)
-0.05560000000000 -0.34270000000000 0.52051000000000 O (4a)
0.34270000000000 0.05560000000000 0.77051000000000 O (4a)
-0.34270000000000 -0.05560000000000 0.27051000000000 O (4a)
0.32510000000000 0.30370000000000 0.52047000000000 O (4a)
-0.32510000000000 -0.30370000000000 1.02047000000000 O (4a)
-0.30370000000000 0.32510000000000 1.27047000000000 O (4a)
0.30370000000000 -0.32510000000000 0.77047000000000 O (4a)
0.48110000000000 0.05460000000000 0.59334000000000 O (4a)
-0.48110000000000 -0.05460000000000 1.09334000000000 O (4a)
-0.05460000000000 0.48110000000000 1.34334000000000 O (4a)
0.05460000000000 -0.48110000000000 0.84334000000000 O (4a)
0.00260000000000 0.00090000000000 0.31632000000000 O (4a)
-0.00260000000000 -0.00090000000000 0.81632000000000 O (4a)
-0.00090000000000 0.00260000000000 1.06632000000000 O (4a)
0.00090000000000 -0.00260000000000 0.56632000000000 O (4a)
0.38130000000000 0.33340000000000 0.82115000000000 O (4a)
-0.38130000000000 -0.33340000000000 1.32115000000000 O (4a)
-0.33340000000000 0.38130000000000 1.57115000000000 O (4a)
0.33340000000000 -0.38130000000000 1.07115000000000 O (4a)
0.28170000000000 0.05760000000000 0.71776000000000 O (4a)
-0.28170000000000 -0.05760000000000 1.21776000000000 O (4a)
-0.05760000000000 0.28170000000000 1.46776000000000 O (4a)
0.05760000000000 -0.28170000000000 0.96776000000000 O (4a)
0.16800000000000 0.05030000000000 -0.08181000000000 O (4a)
-0.16800000000000 -0.05030000000000 0.41819000000000 O (4a)
-0.05030000000000 0.16800000000000 0.66819000000000 O (4a)
0.05030000000000 -0.16800000000000 0.16819000000000 O (4a)
0.26434000000000 0.22687000000000 0.42638000000000 Sr (4a)
-0.26434000000000 -0.22687000000000 0.92638000000000 Sr (4a)
-0.22687000000000 0.26434000000000 1.17638000000000 Sr (4a)
0.22687000000000 -0.26434000000000 0.67638000000000 Sr (4a)
0.02701000000000 0.34822000000000 0.57318000000000 Sr (4a)
-0.02701000000000 -0.34822000000000 1.07318000000000 Sr (4a)
-0.34822000000000 0.02701000000000 1.32318000000000 Sr (4a)
0.34822000000000 -0.02701000000000 0.82318000000000 Sr (4a)
0.15408000000000 0.39584000000000 -0.07135000000000 Sr (4a)
-0.15408000000000 -0.39584000000000 0.42865000000000 Sr (4a)
-0.39584000000000 0.15408000000000 0.67865000000000 Sr (4a)
0.39584000000000 -0.15408000000000 0.17865000000000 Sr (4a)
0.37469000000000 0.25769000000000 0.06464000000000 Sr (4a)
-0.37469000000000 -0.25769000000000 0.56464000000000 Sr (4a)
-0.25769000000000 0.37469000000000 0.81464000000000 Sr (4a)
0.25769000000000 -0.37469000000000 0.31464000000000 Sr (4a)

```

TiZn<sub>2</sub>Sb<sub>2</sub>: A2B2C\_tI20\_79\_c\_2a\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'TiZn2Sb2'
_chemical_formula_sum 'Sb2 Ti Zn2'

```

```

loop_
  _publ_author_name
  'A. Czybulka'
  'B. Krenkel'
  'H.-U. Schuster'
  _journal_name_full_name
  ;
  Journal of the Less-Common Metals
  ;
  _journal_volume 137
  _journal_year 1988
  _journal_page_first 311
  _journal_page_last 322
  _publ_section_title
  ;
  Tern{\a}re zintl-Verbindungen mit thallium als elektronendonator
  ;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'TiZnS_{2}SSbS_{2} Structure'
_aflow_proto 'A2BC2_tI20_79_c_2a_c'
_aflow_params 'a,c/a,z_{1},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4}'
_aflow_params_values '8.6489709127,0.842525147414,0.0,0.4896,0.337,0.164
  ↪ ,0.2196,0.1519,0.1578,0.0'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tI20'

_cell_length_a 8.6489709127
_cell_length_b 8.6489709127
_cell_length_c 7.2869754932
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 4"
_symmetry_Int_Tables_number 79

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 -x,-y,z
  3 -y,x,z
  4 y,-x,z
  5 x+1/2,y+1/2,z+1/2
  6 -x+1/2,-y+1/2,z+1/2
  7 -y+1/2,x+1/2,z+1/2
  8 y+1/2,-x+1/2,z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Tl1 Tl 2 a 0.00000 0.00000 0.00000 1.00000
  Tl2 Tl 2 a 0.00000 0.00000 0.48960 1.00000
  Sb1 Sb 8 c 0.33700 0.16400 0.21960 1.00000
  Zn1 Zn 8 c 0.15190 0.15780 0.00000 1.00000

```

TlZn<sub>2</sub>Sb<sub>2</sub>: A2BC2\_tI20\_79\_c\_2a\_c - POSCAR

```

A2BC2_tI20_79_c_2a_c & a,c/a,z1,z2,x3,y3,z3,x4,y4,z4 --params=
  ↪ 8.6489709127,0.842525147414,0.0,0.4896,0.337,0.164,0.2196,
  ↪ 0.1519,0.1578,0.0 & I4 C_{4}^{[5]} #79 (a^2c^2) & tI20 & None &
  ↪ TlZn2Sb2 & A. Czybulka and B. Krenkel and H.-U. Schuster, J.
  ↪ Less-Common Met. 137, 311-322 (1988)
  1.0000000000000000
-4.32448545635000 4.32448545635000 3.64348774660000
4.32448545635000 -4.32448545635000 3.64348774660000
4.32448545635000 4.32448545635000 -3.64348774660000
Sb Tl Zn
4 2 4
Direct
0.383600000000000 0.556600000000000 0.501000000000000 Sb (8c)
0.055600000000000 -0.117400000000000 -0.501000000000000 Sb (8c)
0.556600000000000 0.055600000000000 0.173000000000000 Sb (8c)
-0.117400000000000 0.383600000000000 -0.173000000000000 Sb (8c)
0.000000000000000 0.000000000000000 0.000000000000000 Tl (2a)
0.489600000000000 0.489600000000000 0.000000000000000 Tl (2a)
0.157800000000000 0.151900000000000 0.309700000000000 Zn (8c)
-0.157800000000000 -0.151900000000000 -0.309700000000000 Zn (8c)
0.151900000000000 -0.157800000000000 -0.005900000000000 Zn (8c)
-0.151900000000000 0.157800000000000 0.005900000000000 Zn (8c)

```

β-NbO<sub>2</sub>: AB2\_tI48\_80\_2b\_4b - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '$\beta$-NbO_{2}$'
_chemical_formula_sum 'Nb O2'

loop_
  _publ_author_name
  'H.-J. Schweizer'
  'R. Gruehn'
  _journal_name_full_name
  ;

```

```

Zeitschrift f{\u}r Naturforschung B
;
_journal_volume 37
_journal_year 1982
_journal_page_first 1361
_journal_page_last 1368
_publ_section_title
;
  Zur Darstellung und Kristallstruktur von $\beta$-NbO_{2}$ / Synthesis
  ↪ and Crystal Structure of $\beta$-NbO_{2}$
;
# Found in Pearson's Handbook of Crystallographic Data, 1991

_aflow_title '$\beta$-NbO_{2}$ Structure'
_aflow_proto 'AB2_tI48_80_2b_4b'
_aflow_params 'a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6}'
_aflow_params_values '9.693,0.617455896007,0.2621,0.5076,0.0299,0.2455,
  ↪ 0.4909,0.4804,0.3974,0.1497,0.0077,0.1102,0.3642,-0.0098,0.6086
  ↪ ,0.3609,0.5064,0.65,0.1038,0.2484'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tI48'

_symmetry_space_group_name_H-M "I 41"
_symmetry_Int_Tables_number 80

_cell_length_a 9.69300
_cell_length_b 9.69300
_cell_length_c 5.98500
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 -x,-y,z
  3 -y,x+1/2,z+1/4
  4 y,-x+1/2,z+1/4
  5 x+1/2,y+1/2,z+1/2
  6 -x+1/2,-y+1/2,z+1/2
  7 -y+1/2,x,z+3/4
  8 y+1/2,-x,z+3/4

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Nb1 Nb 8 b 0.26210 0.50760 0.02990 1.00000
  Nb2 Nb 8 b 0.24550 0.49090 0.48040 1.00000
  O1 O 8 b 0.39740 0.14970 0.00770 1.00000
  O2 O 8 b 0.11020 0.36420 -0.00980 1.00000
  O3 O 8 b 0.60860 0.36090 0.50640 1.00000
  O4 O 8 b 0.65000 0.10380 0.24840 1.00000

```

β-NbO<sub>2</sub>: AB2\_tI48\_80\_2b\_4b - POSCAR

```

AB2_tI48_80_2b_4b & a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,
  ↪ x6,y6,z6 --params=9.693,0.617455896007,0.2621,0.5076,0.0299,
  ↪ 0.2455,0.4909,0.4804,0.3974,0.1497,0.0077,0.1102,0.3642,-0.0098
  ↪ ,0.6086,0.3609,0.5064,0.65,0.1038,0.2484 & I4_{1} C_{4}^{[6]} #80
  ↪ (b^6) & tI48 & None & NbO2 & $\beta$-NbO_{2}$ & H.-J.
  ↪ Schweizer and R. Gruehn, Z. Naturforsch. B 37, 1361-1368 (1982)
  1.0000000000000000
-4.846500000000000 4.846500000000000 2.992500000000000
4.846500000000000 -4.846500000000000 2.992500000000000
4.846500000000000 4.846500000000000 -2.992500000000000
Nb O
8 16
Direct
0.537500000000000 0.292000000000000 0.769700000000000 Nb (8b)
-0.477700000000000 -0.232200000000000 -0.769700000000000 Nb (8b)
1.042000000000000 -0.227700000000000 0.254500000000000 Nb (8b)
0.517800000000000 0.787500000000000 0.745500000000000 Nb (8b)
0.971300000000000 0.725900000000000 0.736400000000000 Nb (8b)
-0.010500000000000 0.234900000000000 -0.736400000000000 Nb (8b)
1.475900000000000 0.239500000000000 0.254600000000000 Nb (8b)
0.984900000000000 1.221300000000000 0.745400000000000 Nb (8b)
0.157400000000000 0.405100000000000 0.547100000000000 O (8b)
-0.142000000000000 -0.389700000000000 -0.547100000000000 O (8b)
1.155100000000000 0.108000000000000 0.747700000000000 O (8b)
0.360300000000000 0.407400000000000 0.252300000000000 O (8b)
0.354400000000000 0.100400000000000 0.474400000000000 O (8b)
-0.374000000000000 -0.120000000000000 -0.474400000000000 O (8b)
0.850400000000000 -0.124000000000000 0.246000000000000 O (8b)
0.630000000000000 0.604400000000000 0.754000000000000 O (8b)
0.867300000000000 1.115000000000000 0.969500000000000 O (8b)
0.145500000000000 -0.102200000000000 -0.969500000000000 O (8b)
1.865000000000000 0.395500000000000 0.747700000000000 O (8b)
0.647800000000000 1.117300000000000 0.252300000000000 O (8b)
0.352200000000000 0.898400000000000 0.753800000000000 O (8b)
0.144600000000000 -0.401600000000000 -0.753800000000000 O (8b)
1.648400000000000 0.394600000000000 1.046200000000000 O (8b)
0.348400000000000 0.602200000000000 -0.046200000000000 O (8b)

```

GeSe<sub>2</sub> (High-pressure): AB2\_tP12\_81\_adg\_2h - CIF

```

# CIF file

```

```

data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'GeSe2'
_chemical_formula_sum 'Ge Se2'

loop_
_publ_author_name
'A. Grzechnik'
'S. St{\o}len'
'E. Bakken'
'T. Grande'
'M. Mezouar'
_journal_name_full_name
;
Journal of Solid State Chemistry
;
_journal_volume 150
_journal_year 2000
_journal_page_first 121
_journal_page_last 127
_publ_section_title
;
Structural transformations in three-dimensional crystalline GeSe2
↪ at high pressures and high temperatures
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'GeSe2 (High-pressure) Structure'
_aflow_proto 'AB2_tP12_81_adg_2h'
_aflow_params 'a,c/a,z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5}'
_aflow_params_values '5.3391020438,1.87980670176,0.25,0.2739,0.234,0.128
↪ ,0.2289,0.23,0.6373'
_aflow_Structurbericht 'None'
_aflow_Pearson 'tP12'

_cell_length_a 5.3391020438
_cell_length_b 5.3391020438
_cell_length_c 10.0364798033
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P -4"
_symmetry_Int_Tables_number 81

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 y,-x,-z
4 -y,x,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ge1 Ge 1 a 0.00000 0.00000 0.00000 1.00000
Ge2 Ge 1 d 0.50000 0.50000 0.50000 1.00000
Ge3 Ge 2 g 0.00000 0.50000 0.25000 1.00000
Se1 Se 4 h 0.27390 0.23400 0.12800 1.00000
Se2 Se 4 h 0.22890 0.23000 0.63730 1.00000

```

GeSe<sub>2</sub> (High-pressure): AB2\_tP12\_81\_adg\_2h - POSCAR

```

AB2_tP12_81_adg_2h & a,c/a,z3,x4,y4,z4,x5,y5,z5 --params=5.3391020438,
↪ 1.87980670176,0.25,0.2739,0.234,0.128,0.2289,0.23,0.6373 & P-4
↪ S_{4}^{1} #81 (adg^2) & tP12 & None & GeSe2 & A. Grzechnik
↪ et al., J. Solid State Chem. 150, 121-127 (2000)

1.0000000000000000
5.33910204380000 0.00000000000000 0.00000000000000
0.00000000000000 5.33910204380000 0.00000000000000
0.00000000000000 0.00000000000000 10.03647980330000
Ge Se
4 8
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Ge (1a)
0.50000000000000 0.50000000000000 0.50000000000000 Ge (1d)
0.00000000000000 0.50000000000000 0.25000000000000 Ge (2g)
0.23400000000000 0.00000000000000 0.00000000000000 Ge (2g)
0.27390000000000 0.23400000000000 0.12800000000000 Se (4h)
-0.27390000000000 -0.23400000000000 0.12800000000000 Se (4h)
-0.27390000000000 -0.27390000000000 -0.12800000000000 Se (4h)
-0.23400000000000 0.27390000000000 -0.12800000000000 Se (4h)
0.22890000000000 0.23000000000000 0.63730000000000 Se (4h)
-0.22890000000000 -0.23000000000000 -0.63730000000000 Se (4h)
-0.23000000000000 0.22890000000000 -0.63730000000000 Se (4h)
-0.23000000000000 0.22890000000000 -0.63730000000000 Se (4h)

```

Ni<sub>3</sub>P (D0<sub>e</sub>): A3B\_tI32\_82\_3g\_g - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Ni3 P'

```

```

loop_
_publ_author_name
'S. Rundqvist'
'E. Hassler'
'L. Lundvik'
_journal_name_full_name
;
Acta Chemica Scandinavica
;
_journal_volume 16
_journal_year 1962
_journal_page_first 242
_journal_page_last 243
_publ_section_title
;
Refinement of the NiS3SP Structure
;

_aflow_title 'NiS3SP (SD0_{e})S Structure'
_aflow_proto 'A3B_tI32_82_3g_g'
_aflow_params 'a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},
↪ x_{4},y_{4},z_{4}'
_aflow_params_values '8.954,0.495711413893,0.0775,0.1117,0.2391,0.3649,
↪ 0.0321,0.9765,0.1689,0.22,0.7524,0.2862,0.0487,0.4807'
_aflow_Structurbericht 'SD0_{e}S'
_aflow_Pearson 'tI32'

_symmetry_space_group_name_H-M "I-4"
_symmetry_Int_Tables_number 82

_cell_length_a 8.95400
_cell_length_b 8.95400
_cell_length_c 4.43860
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 y,-x,-z
4 -y,x,-z
5 x+1/2,y+1/2,z+1/2
6 -x+1/2,-y+1/2,z+1/2
7 y+1/2,-x+1/2,-z+1/2
8 -y+1/2,x+1/2,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ni1 Ni 8 g 0.07750 0.11170 0.23910 1.00000
Ni2 Ni 8 g 0.36490 0.03210 0.97650 1.00000
Ni3 Ni 8 g 0.16890 0.22000 0.75240 1.00000
P1 P 8 g 0.28620 0.04870 0.48070 1.00000

```

Ni<sub>3</sub>P (D0<sub>e</sub>): A3B\_tI32\_82\_3g\_g - POSCAR

```

A3B_tI32_82_3g_g & a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4 --params=
↪ 8.954,0.495711413893,0.0775,0.1117,0.2391,0.3649,0.0321,0.9765,
↪ 0.1689,0.22,0.7524,0.2862,0.0487,0.4807 & I-4 S_{4}^{1} #82 (g^4)
↪ 4) & tI32 & SD0_{e}S & Ni3P & S. Rundqvist and E. Hassler
↪ and L. Lundvik, Acta Chem. Scand. 16, 242-243 (1962)

1.0000000000000000
-4.477000000000000 4.477000000000000 2.219300000000000
4.477000000000000 -4.477000000000000 2.219300000000000
4.477000000000000 4.477000000000000 -2.219300000000000
Ni P
12 4
Direct
0.350800000000000 0.316600000000000 0.189200000000000 Ni (8g)
0.127400000000000 0.161600000000000 -0.189200000000000 Ni (8g)
-0.316600000000000 -0.127400000000000 0.034200000000000 Ni (8g)
-0.161600000000000 -0.350800000000000 -0.034200000000000 Ni (8g)
1.008600000000000 1.341400000000000 0.397000000000000 Ni (8g)
0.944400000000000 0.611600000000000 -0.397000000000000 Ni (8g)
-1.341400000000000 -0.944400000000000 -0.332800000000000 Ni (8g)
-0.611600000000000 -1.008600000000000 0.332800000000000 Ni (8g)
0.972400000000000 0.921300000000000 0.388900000000000 Ni (8g)
0.532400000000000 0.583500000000000 -0.388900000000000 Ni (8g)
-0.921300000000000 -0.532400000000000 0.051100000000000 Ni (8g)
-0.583500000000000 -0.972400000000000 -0.051100000000000 Ni (8g)
0.529400000000000 0.766900000000000 0.334900000000000 P (8g)
0.432000000000000 0.194500000000000 -0.334900000000000 P (8g)
-0.766900000000000 -0.432000000000000 -0.237500000000000 P (8g)
-0.194500000000000 -0.529400000000000 0.237500000000000 P (8g)

```

Ti<sub>2</sub>Ge<sub>3</sub>: A3B2\_tP10\_83\_adk\_j - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ti2Ge3'
_chemical_formula_sum 'Ge3 Ti2'

loop_

```

```

_publ_author_name
'K. Schubert'
'H. G. Meissner'
'M. P{\o}tzschke'
'W. Rossteutscher'
'E. Stolz'
_journal_name_full_name
;
Naturwissenschaften
;
_journal_volume 49
_journal_year 1962
_journal_page_first 57
_journal_page_last 57
_publ_Section_title
;
Einige Strukturdaten metallischer Phasen (7)
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'TiS_{2}SGeS_{3} Structure'
_aflow_proto 'A3B2_tP10_83_adk_j'
_aflow_params 'a,c/a,x_{3},y_{3},x_{4},y_{4}'
_aflow_params_values '6.2840064744,0.638128580522,0.375,0.191,0.109,
↳ 0.314'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP10'

_cell_length_a 6.2840064744
_cell_length_b 6.2840064744
_cell_length_c 4.0100041315
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4/m"
_symmetry_Int_Tables_number 83

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,-y,-z
6 x,y,-z
7 y,-x,-z
8 -y,x,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ge1 Ge 1 a 0.00000 0.00000 0.00000 1.00000
Ge2 Ge 1 d 0.50000 0.50000 0.50000 1.00000
Ti1 Ti 4 j 0.37500 0.19100 0.00000 1.00000
Ge3 Ge 4 k 0.10900 0.31400 0.50000 1.00000

```

Ti2Ge3: A3B2\_tP10\_83\_adk\_j - POSCAR

```

A3B2_tP10_83_adk_j & a,c/a,x3,y3,x4,y4 --params=6.2840064744,
↳ 0.638128580522,0.375,0.191,0.109,0.314 & P4/m C_{4h}^{1} #83 (
↳ adjk) & tP10 & None & Ti2Ge3 & K. Schubert et al., {
↳ Naturwissenschaften 49, 57-57 (1962)
1.0000000000000000
6.28400647440000 0.00000000000000 0.00000000000000
0.00000000000000 6.28400647440000 0.00000000000000
0.00000000000000 0.00000000000000 4.01000413150000
Ge Ti
6 4
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Ge (1a)
0.50000000000000 0.50000000000000 0.50000000000000 Ge (1d)
0.10900000000000 0.31400000000000 0.50000000000000 Ge (4k)
-0.10900000000000 -0.31400000000000 0.50000000000000 Ge (4k)
-0.31400000000000 0.10900000000000 0.50000000000000 Ge (4k)
0.31400000000000 -0.10900000000000 0.50000000000000 Ge (4k)
0.37500000000000 0.19100000000000 0.00000000000000 Ti (4j)
-0.37500000000000 -0.19100000000000 0.00000000000000 Ti (4j)
-0.19100000000000 0.37500000000000 0.00000000000000 Ti (4j)
0.19100000000000 -0.37500000000000 0.00000000000000 Ti (4j)

```

SrBr2: A2B\_tP30\_85\_ab2g\_cg - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'SrBr2'
_chemical_formula_sum 'Br2 Sr'

loop_
_publ_author_name
'B. Frit'
'M. M. Chbany'
_journal_name_full_name
;

```

```

Journal of Inorganic and Nuclear Chemistry
;
_journal_volume 31
_journal_year 1969
_journal_page_first 2685
_journal_page_last 2693
_publ_Section_title
;
Les halogeno-carbonates de strontium
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'SrBrS_{2} Structure'
_aflow_proto 'A2B_tP30_85_ab2g_cg'
_aflow_params 'a,c/a,z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6}'
_aflow_params_values '11.6179902668,0.614391461525,0.6517,0.5428,0.6612,
↳ 0.5963,0.6531,0.541,0.1258,0.5856,0.1045,0.2524'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP30'

_cell_length_a 11.6179902668
_cell_length_b 11.6179902668
_cell_length_c 7.1379940200
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4/n (origin choice 2)"
_symmetry_Int_Tables_number 85

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x+1/2,-y+1/2,z
3 -y+1/2,x,z
4 y,-x+1/2,z
5 -x,-y,-z
6 x+1/2,y+1/2,-z
7 y+1/2,-x,-z
8 -y,x+1/2,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Br1 Br 2 a 0.25000 0.75000 0.00000 1.00000
Br2 Br 2 b 0.25000 0.75000 0.50000 1.00000
Sr1 Sr 2 c 0.25000 0.25000 0.65170 1.00000
Br3 Br 8 g 0.54280 0.66120 0.59630 1.00000
Br4 Br 8 g 0.65310 0.54100 0.12580 1.00000
Sr2 Sr 8 g 0.58560 0.10450 0.25240 1.00000

```

SrBr2: A2B\_tP30\_85\_ab2g\_cg - POSCAR

```

A2B_tP30_85_ab2g_cg & a,c/a,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6 --params=
↳ 11.6179902668,0.614391461525,0.6517,0.5428,0.6612,0.5963,0.6531
↳ ,0.541,0.1258,0.5856,0.1045,0.2524 & P4/n C_{4h}^{3} #85 (abcg^a
↳ ) & tP30 & None & SrBr2 & B. Frit and M. M. Chbany, J.
↳ Inorg. Nucl. Chem. 31, 2685-2693 (1969)
1.0000000000000000
11.61799026680000 0.00000000000000 0.00000000000000
0.00000000000000 11.61799026680000 0.00000000000000
0.00000000000000 0.00000000000000 7.13799402000000
Br Sr
20 10
Direct
0.25000000000000 0.75000000000000 0.00000000000000 Br (2a)
0.75000000000000 0.25000000000000 0.00000000000000 Br (2a)
0.25000000000000 0.75000000000000 0.50000000000000 Br (2b)
0.75000000000000 0.25000000000000 0.50000000000000 Br (2b)
0.54280000000000 0.66120000000000 0.59630000000000 Br (8g)
-0.04280000000000 -0.16120000000000 0.59630000000000 Br (8g)
0.16120000000000 0.54280000000000 0.59630000000000 Br (8g)
0.66120000000000 -0.04280000000000 0.59630000000000 Br (8g)
-0.54280000000000 -0.66120000000000 -0.59630000000000 Br (8g)
1.04280000000000 1.16120000000000 -0.59630000000000 Br (8g)
1.16120000000000 -0.54280000000000 -0.59630000000000 Br (8g)
-0.66120000000000 1.04280000000000 -0.59630000000000 Br (8g)
0.65310000000000 0.54100000000000 0.12580000000000 Br (8g)
-0.15310000000000 -0.04100000000000 0.12580000000000 Br (8g)
-0.04100000000000 0.65310000000000 0.12580000000000 Br (8g)
0.54100000000000 -0.15310000000000 0.12580000000000 Br (8g)
-0.65310000000000 -0.54100000000000 -0.12580000000000 Br (8g)
1.15310000000000 1.04100000000000 -0.12580000000000 Br (8g)
1.04100000000000 -0.65310000000000 -0.12580000000000 Br (8g)
-0.54100000000000 1.15310000000000 -0.12580000000000 Br (8g)
0.25000000000000 0.25000000000000 0.65170000000000 Sr (2c)
0.75000000000000 0.75000000000000 -0.65170000000000 Sr (2c)
0.58560000000000 0.10450000000000 0.25240000000000 Sr (8g)
-0.08560000000000 0.39550000000000 0.25240000000000 Sr (8g)
0.39550000000000 0.58560000000000 0.25240000000000 Sr (8g)
0.10450000000000 -0.08560000000000 0.25240000000000 Sr (8g)
-0.58560000000000 -0.10450000000000 -0.25240000000000 Sr (8g)
1.08560000000000 0.60450000000000 -0.25240000000000 Sr (8g)
0.60450000000000 -0.58560000000000 -0.25240000000000 Sr (8g)
-0.10450000000000 1.08560000000000 -0.25240000000000 Sr (8g)

```



Ti3P: AB3\_tP32\_86\_g\_3g - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ti3P'
_chemical_formula_sum 'P Ti3'

loop_
_publ_author_name
'V. N. Eremenko'
'V. E. Listvovichii'
_journal_year 1965
_publ_section_title
;
State diagram of the Ti-P system
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'TiS_{3}SP Structure'
_aflow_proto 'AB3_tP32_86_g_3g'
_aflow_params 'a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4}'
↳ 3),x_{4},y_{4},z_{4}'
_aflow_params_values '9.997999333,0.499899979999,0.0439,0.20812,0.5354,
↳ 0.11009,0.22151,0.0295,0.14275,0.66613,0.7153,0.53342,0.06957,
↳ 0.7593'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP32'

_cell_length_a 9.9979993330
_cell_length_b 9.9979993330
_cell_length_c 4.9979996666
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 42/n (origin choice 2)"
_symmetry_Int_Tables_number 86

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x+1/2,-y+1/2,z
3 -y,x+1/2,z+1/2
4 y+1/2,-x,z+1/2
5 -x,-y,-z
6 x+1/2,y+1/2,-z
7 y,-x+1/2,-z+1/2
8 -y+1/2,x,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
P1 P 8 g 0.04390 0.20812 0.53540 1.00000
Ti1 Ti 8 g 0.11009 0.22151 0.02950 1.00000
Ti2 Ti 8 g 0.14275 0.66613 0.71530 1.00000
Ti3 Ti 8 g 0.53342 0.06957 0.75930 1.00000
```

Ti3P: AB3\_tP32\_86\_g\_3g - POSCAR

```
AB3_tP32_86_g_3g & a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4 --params=
↳ 9.997999333,0.499899979999,0.0439,0.20812,0.5354,0.11009,
↳ 0.22151,0.0295,0.14275,0.66613,0.7153,0.53342,0.06957,0.7593 &
↳ P4_{2}]/n C_{4h}^{4} #86 (g^{4}) & tP32 & None & Ti3P & V. N.
↳ Eremenko and V. E. Listvovichii, (1965)
1.00000000000000
9.99799933300000 0.00000000000000 0.00000000000000
0.00000000000000 9.99799933300000 0.00000000000000
0.00000000000000 0.00000000000000 4.99799966660000
P Ti
8 24
Direct
0.04390000000000 0.20812000000000 0.53540000000000 P (8g)
0.45610000000000 0.29188000000000 0.53540000000000 P (8g)
-0.20812000000000 0.54390000000000 1.03540000000000 P (8g)
0.70812000000000 -0.04390000000000 1.03540000000000 P (8g)
-0.04390000000000 -0.20812000000000 -0.53540000000000 P (8g)
0.54390000000000 0.70812000000000 -0.53540000000000 P (8g)
0.20812000000000 0.45610000000000 -0.03540000000000 P (8g)
0.29188000000000 0.04390000000000 -0.03540000000000 P (8g)
0.11009000000000 0.22151000000000 0.02950000000000 Ti (8g)
0.38991000000000 0.27849000000000 0.02950000000000 Ti (8g)
-0.22151000000000 0.61009000000000 0.52950000000000 Ti (8g)
0.72151000000000 -0.11009000000000 0.52950000000000 Ti (8g)
-0.11009000000000 -0.22151000000000 -0.02950000000000 Ti (8g)
0.61009000000000 0.22151000000000 -0.02950000000000 Ti (8g)
0.22151000000000 0.38991000000000 0.47050000000000 Ti (8g)
0.27849000000000 0.11009000000000 0.47050000000000 Ti (8g)
0.14275000000000 0.66613000000000 0.71530000000000 Ti (8g)
0.35725000000000 -0.16613000000000 0.71530000000000 Ti (8g)
-0.66613000000000 0.64275000000000 1.21530000000000 Ti (8g)
1.16613000000000 -0.14275000000000 1.21530000000000 Ti (8g)
-0.14275000000000 -0.66613000000000 -0.71530000000000 Ti (8g)
0.64275000000000 1.16613000000000 -0.71530000000000 Ti (8g)
0.66613000000000 0.35725000000000 -0.21530000000000 Ti (8g)
```

```
-0.16613000000000 0.14275000000000 -0.21530000000000 Ti (8g)
0.53342000000000 0.06957000000000 0.75930000000000 Ti (8g)
-0.03342000000000 0.43043000000000 0.75930000000000 Ti (8g)
-0.06957000000000 1.03342000000000 1.25930000000000 Ti (8g)
0.56957000000000 -0.53342000000000 1.25930000000000 Ti (8g)
-0.53342000000000 -0.06957000000000 -0.75930000000000 Ti (8g)
1.03342000000000 0.56957000000000 -0.75930000000000 Ti (8g)
0.06957000000000 -0.03342000000000 -0.25930000000000 Ti (8g)
0.43043000000000 0.53342000000000 -0.25930000000000 Ti (8g)
```

ThCl4: A4B\_tI20\_88\_f\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'ThCl4'
_chemical_formula_sum 'Cl4 Th'

loop_
_publ_author_name
'J. T. Mason'
'M. C. Jha'
'P. Chiotti'
_journal_name_full_name
;
Journal of the Less-Common Metals
;
_journal_volume 34
_journal_year 1974
_journal_page_first 143
_journal_page_last 151
_publ_section_title
;
Crystal structures of ThCl_{4} polymorphs
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'ThClS_{4} Structure'
_aflow_proto 'A4B_tI20_88_f_a'
_aflow_params 'a,c/a,x_{2},y_{2},z_{2}'
_aflow_params_values '6.407994829,2.01685393259,0.147,0.017,0.298'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tI20'

_cell_length_a 6.4079948290
_cell_length_b 6.4079948290
_cell_length_c 12.9239895709
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 41/a (origin choice 2)"
_symmetry_Int_Tables_number 88

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y+1/2,z
3 -y+3/4,x+1/4,z+1/4
4 y+1/4,-x+1/4,z+1/4
5 -x,-y,-z
6 x,y+1/2,-z
7 y+1/4,-x+3/4,-z+3/4
8 -y+3/4,x+3/4,-z+3/4
9 x+1/2,y+1/2,z+1/2
10 -x+1/2,-y,z+1/2
11 -y+1/4,x+3/4,z+3/4
12 y+3/4,-x+3/4,z+3/4
13 -x+1/2,-y+1/2,-z+1/2
14 x+1/2,y,-z+1/2
15 y+3/4,-x+1/4,-z+1/4
16 -y+1/4,x+1/4,-z+1/4

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Th1 Th 4 a 0.00000 0.25000 0.12500 1.00000
Cl1 Cl 16 f 0.14700 0.01700 0.29800 1.00000
```

```
A4B_tI20_88_f_a & a,c/a,x2,y2,z2 --params=6.407994829,2.01685393259,
↳ 0.147,0.017,0.298 & I4_{1}/a C_{4h}^{6} #88 (af) & tI20 & None
↳ & ThCl4 & J. T. Mason and M. C. Jha and P. Chiotti, J.
↳ Less-Common Met. 34, 143-151 (1974)
1.00000000000000
-3.20399741450000 3.20399741450000 6.46199478545000
3.20399741450000 -3.20399741450000 6.46199478545000
3.20399741450000 3.20399741450000 -6.46199478545000
Cl Th
8 2
Direct
0.31500000000000 0.44500000000000 0.16400000000000 Cl (16f)
0.78100000000000 0.15100000000000 0.33600000000000 Cl (16f)
0.94500000000000 0.28100000000000 0.13000000000000 Cl (16f)
```

ThCl4: A4B\_tI20\_88\_f\_a - POSCAR

```
A4B_tI20_88_f_a & a,c/a,x2,y2,z2 --params=6.407994829,2.01685393259,
↳ 0.147,0.017,0.298 & I4_{1}/a C_{4h}^{6} #88 (af) & tI20 & None
↳ & ThCl4 & J. T. Mason and M. C. Jha and P. Chiotti, J.
↳ Less-Common Met. 34, 143-151 (1974)
1.00000000000000
-3.20399741450000 3.20399741450000 6.46199478545000
3.20399741450000 -3.20399741450000 6.46199478545000
3.20399741450000 3.20399741450000 -6.46199478545000
Cl Th
8 2
Direct
0.31500000000000 0.44500000000000 0.16400000000000 Cl (16f)
0.78100000000000 0.15100000000000 0.33600000000000 Cl (16f)
0.94500000000000 0.28100000000000 0.13000000000000 Cl (16f)
```

0.65100000000000	0.81500000000000	0.37000000000000	Cl (16f)
-0.31500000000000	-0.44500000000000	-0.16400000000000	Cl (16f)
0.21900000000000	-0.15100000000000	0.66400000000000	Cl (16f)
0.05500000000000	-0.28100000000000	-0.13000000000000	Cl (16f)
0.34900000000000	0.18500000000000	0.63000000000000	Cl (16f)
0.37500000000000	0.12500000000000	0.25000000000000	Th (4a)
0.62500000000000	0.87500000000000	0.75000000000000	Th (4a)

$\alpha$ -NbO<sub>2</sub>: AB2\_tI96\_88\_2f\_4f- CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '$\alpha$-NbOS_{2}$'
_chemical_formula_sum 'Nb O2'

loop_
  _publ_author_name
    'R. Pynn'
    'J. D. Axe'
    'R. Thomas'
  _journal_name_full_name
    'Physical Review B'
  _journal_volume 13
  _journal_year 1976
  _journal_page_first 2965
  _journal_page_last 2975
  _publ_section_title
    'Structural distortions in the low-temperature phase of NbOS_{2}$'
# Found in A Powder Neutron Diffraction Study of Semiconducting and
  ↪ Metallic Niobium Dioxide, 1994

_aflow_title '$\alpha$-NbOS_{2}$ Structure'
_aflow_proto 'AB2_tI96_88_2f_4f'
_aflow_params 'a, c/a, x_{1}, y_{1}, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}'
  ↪ 3, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}'
_aflow_params_values '13.66, 0.436603221083, 0.1155, 0.1249, 0.4746, 0.1356,
  ↪ 0.125, 0.0267, -0.0134, 0.1262, -0.0046, -0.0251, 0.1252, 0.5, 0.2739,
  ↪ 0.1245, -0.0002, 0.2631, 0.1241, 0.5043'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tI96'

_symmetry_space_group_name_H-M "I 41/a:2"
_symmetry_Int_Tables_number 88

_cell_length_a 13.66000
_cell_length_b 13.66000
_cell_length_c 5.96400
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x, y, z
2 -x, -y+1/2, z
3 -y+3/4, x+1/4, z+1/4
4 y+1/4, -x+1/4, z+1/4
5 -x, -y, -z
6 x, y+1/2, -z
7 y+1/4, -x+3/4, -z+3/4
8 -y+3/4, x+3/4, -z+3/4
9 x+1/2, y+1/2, z+1/2
10 -x+1/2, -y, z+1/2
11 -y+1/4, x+3/4, z+3/4
12 y+3/4, -x+3/4, z+3/4
13 -x+1/2, -y+1/2, -z+1/2
14 x+1/2, y, -z+1/2
15 y+3/4, -x+1/4, -z+1/4
16 -y+1/4, x+1/4, -z+1/4

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Nb1 Nb 16 f 0.11550 0.12490 0.47460 1.00000
Nb2 Nb 16 f 0.13560 0.12500 0.02670 1.00000
O1 O 16 f -0.01340 0.12620 -0.00460 1.00000
O2 O 16 f -0.02510 0.12520 0.50000 1.00000
O3 O 16 f 0.27390 0.12450 -0.00020 1.00000
O4 O 16 f 0.26310 0.12410 0.50430 1.00000
```

$\alpha$ -NbO<sub>2</sub>: AB2\_tI96\_88\_2f\_4f- POSCAR

```
AB2_tI96_88_2f_4f & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5,
  ↪ x6, y6, z6 --params=13.66, 0.436603221083, 0.1155, 0.1249, 0.4746,
  ↪ 0.1356, 0.125, 0.0267, -0.0134, 0.1262, -0.0046, -0.0251, 0.1252, 0.5,
  ↪ 0.2739, 0.1245, -0.0002, 0.2631, 0.1241, 0.5043 & I4_1/a C_{4h}^6
  ↪ #88 (f^6) & tI96 & None & NbO2 & $\alpha$-NbOS_{2}$ & R. Pynn
  ↪ and J. D. Axe and R. Thomas, Phys. Rev. B 13, 2965-2975 (1976)
1.00000000000000
-6.83000000000000 6.83000000000000 2.98200000000000
6.83000000000000 -6.83000000000000 2.98200000000000
```

6.83000000000000	6.83000000000000	-2.98200000000000	
Nb	O		
16	32		
Direct			
0.59950000000000	0.59010000000000	0.24040000000000	Nb (16f)
0.84970000000000	0.35910000000000	0.25960000000000	Nb (16f)
1.09010000000000	0.34970000000000	-0.00940000000000	Nb (16f)
0.85910000000000	1.09950000000000	0.50940000000000	Nb (16f)
-0.59950000000000	-0.59010000000000	-0.24040000000000	Nb (16f)
0.15030000000000	-0.35910000000000	0.74040000000000	Nb (16f)
-0.09010000000000	-0.34970000000000	0.00940000000000	Nb (16f)
0.14090000000000	-0.09950000000000	0.49060000000000	Nb (16f)
0.15170000000000	0.16230000000000	0.26060000000000	Nb (16f)
0.40170000000000	-0.10890000000000	0.23940000000000	Nb (16f)
0.66230000000000	-0.09830000000000	0.01060000000000	Nb (16f)
0.39110000000000	0.65170000000000	0.48940000000000	Nb (16f)
-0.15170000000000	-0.16230000000000	-0.26060000000000	Nb (16f)
0.59830000000000	0.10890000000000	0.76060000000000	Nb (16f)
0.33770000000000	0.09830000000000	-0.01060000000000	Nb (16f)
0.60890000000000	0.34830000000000	0.51060000000000	Nb (16f)
0.12160000000000	-0.01800000000000	0.11280000000000	O (16f)
0.36920000000000	0.00880000000000	0.38720000000000	O (16f)
0.48200000000000	-0.13080000000000	-0.13960000000000	O (16f)
0.50880000000000	0.62160000000000	0.63960000000000	O (16f)
-0.12160000000000	0.01800000000000	-0.11280000000000	O (16f)
0.63080000000000	-0.00880000000000	0.61280000000000	O (16f)
0.51800000000000	0.13080000000000	0.13960000000000	O (16f)
0.49120000000000	0.37840000000000	0.36040000000000	O (16f)
0.62520000000000	0.47490000000000	0.10010000000000	O (16f)
0.87480000000000	0.52510000000000	0.39990000000000	O (16f)
0.97490000000000	0.37480000000000	-0.15030000000000	O (16f)
1.02510000000000	1.12520000000000	0.65030000000000	O (16f)
-0.62520000000000	-0.47490000000000	-0.10010000000000	O (16f)
0.12520000000000	-0.52510000000000	0.60010000000000	O (16f)
0.02510000000000	-0.37480000000000	0.15030000000000	O (16f)
-0.02510000000000	-0.12520000000000	0.34970000000000	O (16f)
0.12430000000000	0.27370000000000	0.39840000000000	O (16f)
0.37530000000000	-0.27410000000000	0.10160000000000	O (16f)
0.77370000000000	-0.12470000000000	0.14940000000000	O (16f)
0.22590000000000	0.62430000000000	0.35060000000000	O (16f)
-0.12430000000000	-0.27370000000000	-0.39840000000000	O (16f)
0.62470000000000	0.27410000000000	0.89840000000000	O (16f)
0.22630000000000	0.12470000000000	-0.14940000000000	O (16f)
0.77410000000000	0.37570000000000	0.64940000000000	O (16f)
0.62840000000000	0.76740000000000	0.35060000000000	O (16f)
0.88020000000000	0.24120000000000	0.11280000000000	O (16f)
1.26740000000000	0.38020000000000	0.13900000000000	O (16f)
0.74120000000000	1.12840000000000	0.36100000000000	O (16f)
-0.62840000000000	-0.76740000000000	-0.38720000000000	O (16f)
0.11980000000000	-0.24120000000000	0.88720000000000	O (16f)
-0.26740000000000	-0.38020000000000	-0.13900000000000	O (16f)
0.25880000000000	-0.12840000000000	0.63900000000000	O (16f)

C17FeO4Pt: A17BC4D\_tP184\_89\_17p\_p\_4p\_io- CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'C17FeO4Pt'
_chemical_formula_sum 'C17 Fe O4 Pt'

_aflow_title 'CS_{17}$FeOS_{4}$Pt Structure'
_aflow_proto 'A17BC4D_tP184_89_17p_p_4p_io'
_aflow_params 'a, c/a, z_{1}, x_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}, x_{7}, y_{7}, z_{7}, x_{8}, y_{8}, z_{8}, x_{9}, y_{9}, z_{9}, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22}, y_{22}, z_{22}, x_{23}, y_{23}, z_{23}, x_{24}, y_{24}, z_{24}'
_aflow_params_values '16.2503, 0.81957871547, 0.86772, 0.10962, 0.1709, 0.485
  ↪ 0.7893, 0.2334, 0.4627, 0.7103, 0.2146, 0.4383, 0.6125, 0.2885, 0.416,
  ↪ 0.5631, 0.354, 0.4242, 0.6323, 0.3206, 0.4579, 0.7209, 0.234, 0.226,
  ↪ 0.661, 0.3111, 0.2275, 0.696, 0.3148, 0.2616, 0.794, 0.236, 0.287, 0.818
  ↪ 0.179, 0.265, 0.733, -0.0696, 0.3435, -0.084, -0.078, 0.2512, -0.097, -
  ↪ 0.004, 0.378, 0.549, -0.01, 0.309, 0.593, -0.003, 0.238, 0.558, -0.006,
  ↪ 0.165, 0.6, 0.2676, 0.3463, 0.6943, 0.1965, 0.4869, 0.8803, 0.096,
  ↪ 0.4889, 0.7614, 0.1143, 0.375, 0.0177, -0.0146, 0.3768, 0.8623'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP184'

_cell_length_a 16.2503000000
_cell_length_b 16.2503000000
_cell_length_c 13.3184000000
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4 2 2"
_symmetry_Int_Tables_number 89

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y, -z
4 -x, -y, z
5 -y, -x, -z
6 -y, x, z
7 y, -x, z
8 y, x, -z
```

loop_					
_atom_site_label					
_atom_site_type_symbol					
_atom_site_symmetry_multiplicity					
_atom_site_Wyckoff_label					
_atom_site_fract_x					
_atom_site_fract_y					
_atom_site_fract_z					
_atom_site_occupancy					
Pt1 Pt	4 i	0.00000	0.50000	0.86772	1.00000
Pt2 Pt	4 o	0.10962	0.50000	0.00000	1.00000
C1 C	8 p	0.17090	0.48500	0.78930	1.00000
C2 C	8 p	0.23340	0.46270	0.71030	1.00000
C3 C	8 p	0.21460	0.43830	0.61250	1.00000
C4 C	8 p	0.28850	0.41600	0.56310	1.00000
C5 C	8 p	0.35400	0.42420	0.63230	1.00000
C6 C	8 p	0.32060	0.45790	0.72090	1.00000
C7 C	8 p	0.23400	0.22600	0.66100	1.00000
C8 C	8 p	0.31110	0.22750	0.69600	1.00000
C9 C	8 p	0.31480	0.26160	0.79400	1.00000
C10 C	8 p	0.23600	0.28700	0.81800	1.00000
C11 C	8 p	0.17900	0.26500	0.73300	1.00000
C12 C	8 p	-0.06960	0.34350	-0.08400	1.00000
C13 C	8 p	-0.07800	0.25120	-0.09700	1.00000
C14 C	8 p	-0.00400	0.37800	0.54900	1.00000
C15 C	8 p	-0.01000	0.30900	0.59300	1.00000
C16 C	8 p	-0.00300	0.23800	0.55800	1.00000
C17 C	8 p	-0.00600	0.16500	0.60000	1.00000
Fe1 Fe	8 p	0.26760	0.34630	0.69430	1.00000
O1 O	8 p	0.19650	0.48690	0.88030	1.00000
O2 O	8 p	0.09600	0.48890	0.76140	1.00000
O3 O	8 p	0.11430	0.37500	0.01770	1.00000
O4 O	8 p	-0.01460	0.37680	0.86230	1.00000

C<sub>17</sub>FeO<sub>4</sub>Pt: A17BC4D\_tP184\_89\_17p\_p\_4p\_io - POSCAR

A17BC4D_tP184_89_17p_p_4p_io & a.c/a,z1,x2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6					
↪	y6,z6,x7,y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11,y11,z11,x12,				
↪	y12,z12,x13,y13,z13,x14,y14,z14,x15,y15,z15,x16,y16,z16,x17,y17				
↪	z17,x18,y18,z18,x19,y19,z19,x20,y20,z20,x21,y21,z21,x22,y22,				
↪	z22,x23,y23,z23,x24,y24,z24 --params=16.2503,0.81957871547,				
↪	0.86772,0.10962,0.1709,0.485,0.7893,0.2334,0.4627,0.7103,0.2146				
↪	,0.4383,0.6125,0.2885,0.416,0.5631,0.354,0.4242,0.6323,0.3206,				
↪	0.4579,0.7209,0.234,0.226,0.661,0.3111,0.2275,0.696,0.3148,				
↪	0.2616,0.794,0.236,0.287,0.818,0.179,0.265,0.733,-0.0696,0.3435				
↪	,-0.084,-0.078,0.2512,-0.097,-0.004,0.378,0.549,-0.01,0.309,				
↪	0.593,-0.003,0.238,0.558,-0.006,0.165,0.6,0.2676,0.3463,0.6943,				
↪	0.1965,0.4869,0.8803,0.096,0.4889,0.7614,0.1143,0.375,0.0177,-				
↪	0.0146,0.3768,0.8623 & P422 D_{4}^{1} #89 (iop^22) & tP184 &				
↪	None & C17FeO4Pt &				
	1.0000000000000000				
	16.2503000000000000	0.0000000000000000	0.0000000000000000		
	0.0000000000000000	16.2503000000000000	0.0000000000000000		
	0.0000000000000000	0.0000000000000000	13.3184000000000000		
	C	Fe	O	Pt	
	136	8	32	8	
Direct					
-0.1709000000000000	0.4850000000000000	0.7893000000000000	C	(8p)	
-0.1709000000000000	-0.4850000000000000	0.7893000000000000	C	(8p)	
-0.4850000000000000	0.1709000000000000	0.7893000000000000	C	(8p)	
0.4850000000000000	-0.1709000000000000	0.7893000000000000	C	(8p)	
-0.1709000000000000	0.4850000000000000	-0.7893000000000000	C	(8p)	
0.1709000000000000	-0.4850000000000000	-0.7893000000000000	C	(8p)	
0.4850000000000000	0.1709000000000000	-0.7893000000000000	C	(8p)	
-0.4850000000000000	-0.1709000000000000	-0.7893000000000000	C	(8p)	
0.2334000000000000	0.4627000000000000	0.7103000000000000	C	(8p)	
-0.2334000000000000	-0.4627000000000000	0.7103000000000000	C	(8p)	
-0.4627000000000000	0.2334000000000000	0.7103000000000000	C	(8p)	
0.4627000000000000	-0.2334000000000000	0.7103000000000000	C	(8p)	
-0.2334000000000000	0.4627000000000000	-0.7103000000000000	C	(8p)	
0.2334000000000000	-0.4627000000000000	-0.7103000000000000	C	(8p)	
0.4627000000000000	0.2334000000000000	-0.7103000000000000	C	(8p)	
-0.4627000000000000	-0.2334000000000000	-0.7103000000000000	C	(8p)	
0.2146000000000000	0.4383000000000000	0.6125000000000000	C	(8p)	
-0.2146000000000000	-0.4383000000000000	0.6125000000000000	C	(8p)	
-0.4383000000000000	0.2146000000000000	0.6125000000000000	C	(8p)	
0.4383000000000000	-0.2146000000000000	0.6125000000000000	C	(8p)	
-0.2146000000000000	0.4383000000000000	-0.6125000000000000	C	(8p)	
0.2146000000000000	-0.4383000000000000	-0.6125000000000000	C	(8p)	
-0.4383000000000000	0.2146000000000000	-0.6125000000000000	C	(8p)	
0.4383000000000000	-0.2146000000000000	-0.6125000000000000	C	(8p)	
-0.2885000000000000	0.4160000000000000	0.5631000000000000	C	(8p)	
-0.2885000000000000	-0.4160000000000000	0.5631000000000000	C	(8p)	
-0.4160000000000000	0.2885000000000000	0.5631000000000000	C	(8p)	
0.4160000000000000	-0.2885000000000000	0.5631000000000000	C	(8p)	
-0.2885000000000000	0.4160000000000000	-0.5631000000000000	C	(8p)	
0.2885000000000000	-0.4160000000000000	-0.5631000000000000	C	(8p)	
-0.4160000000000000	0.2885000000000000	-0.5631000000000000	C	(8p)	
0.4160000000000000	-0.2885000000000000	-0.5631000000000000	C	(8p)	
-0.3540000000000000	0.4242000000000000	0.6323000000000000	C	(8p)	
-0.3540000000000000	-0.4242000000000000	0.6323000000000000	C	(8p)	
-0.4242000000000000	0.3540000000000000	0.6323000000000000	C	(8p)	
0.4242000000000000	-0.3540000000000000	0.6323000000000000	C	(8p)	
-0.3540000000000000	0.4242000000000000	-0.6323000000000000	C	(8p)	
0.3540000000000000	-0.4242000000000000	-0.6323000000000000	C	(8p)	
-0.4242000000000000	0.3540000000000000	-0.6323000000000000	C	(8p)	
0.4242000000000000	-0.3540000000000000	-0.6323000000000000	C	(8p)	
-0.3206000000000000	0.4579000000000000	0.7209000000000000	C	(8p)	
-0.3206000000000000	-0.4579000000000000	0.7209000000000000	C	(8p)	
-0.4579000000000000	0.3206000000000000	0.7209000000000000	C	(8p)	
0.4579000000000000	-0.3206000000000000	0.7209000000000000	C	(8p)	
-0.3206000000000000	0.4579000000000000	-0.7209000000000000	C	(8p)	
0.3206000000000000	-0.4579000000000000	-0.7209000000000000	C	(8p)	
-0.4579000000000000	0.3206000000000000	-0.7209000000000000	C	(8p)	
0.4579000000000000	-0.3206000000000000	-0.7209000000000000	C	(8p)	

0.2340000000000000	0.2260000000000000	0.6610000000000000	C	(8p)	
-0.2340000000000000	-0.2260000000000000	0.6610000000000000	C	(8p)	
-0.2260000000000000	0.2340000000000000	0.6610000000000000	C	(8p)	
0.2260000000000000	-0.2340000000000000	0.6610000000000000	C	(8p)	
-0.2340000000000000	0.2260000000000000	-0.6610000000000000	C	(8p)	
0.2340000000000000	-0.2260000000000000	-0.6610000000000000	C	(8p)	
0.2260000000000000	0.2340000000000000	-0.6610000000000000	C	(8p)	
-0.2260000000000000	-0.2340000000000000	-0.6610000000000000	C	(8p)	
0.3111000000000000	0.2275000000000000	0.6960000000000000	C	(8p)	
-0.3111000000000000	-0.2275000000000000	0.6960000000000000	C	(8p)	
-0.2275000000000000	0.3111000000000000	0.6960000000000000	C	(8p)	
0.2275000000000000	-0.3111000000000000	0.6960000000000000	C	(8p)	
-0.3111000000000000	0.2275000000000000	-0.6960000000000000	C	(8p)	
0.3111000000000000	-0.2275000000000000	-0.6960000000000000	C	(8p)	
0.2275000000000000	0.3111000000000000	-0.6960000000000000	C	(8p)	
-0.2275000000000000	-0.3111000000000000	-0.6960000000000000	C	(8p)	
0.3148000000000000	0.2616000000000000	0.7940000000000000	C	(8p)	
-0.3148000000000000	-0.2616000000000000	0.7940000000000000	C	(8p)	
-0.2616000000000000	0.3148000000000000	0.7940000000000000	C	(8p)	
0.2616000000000000	-0.3148000000000000	0.7940000000000000	C	(8p)	
-0.3148000000000000	0.2616000000000000	-0.7940000000000000	C	(8p)	
0.3148000000000000	-0.2616000000000000	-0.7940000000000000	C	(8p)	
0.2616000000000000	0.3148000000000000	-0.7940000000000000	C	(8p)	
-0.2616000000000000	-0.3148000000000000	-0.7940000000000000	C	(8p)	
0.2360000000000000	0.2870000000000000	0.8180000000000000	C	(8p)	
-0.2360000000000000	-0.2870000000000000	0.8180000000000000	C	(8p)	
-0.2870000000000000	0.2360000000000000	0.8180000000000000	C	(8p)	
0.2870000000000000	-0.2360000000000000	0.8180000000000000	C	(8p)	
-0.2360000000000000	0.2870000000000000	-0.8180000000000000	C	(8p)	
0.2360000000000000	-0.2870000000000000	-0.8180000000000000	C	(8p)	
-0.2870000000000000	0.2360000000000000	-0.8180000000000000	C	(8p)	
0.2870000000000000	-0.2360000000000000	-0.8180000000000000	C	(8p)	
0.1790000000000000	0.2650000000000000	0.7330000000000000	C	(8p)	
-0.1790000000000000	-0.2650000000000000	0.7330000000000000	C	(8p)	
-0.2650000000000000	0.1790000000000000	0.7330000000000000	C	(8p)	
0.2650000000000000	-0.1790000000000000	0.7330000000000000	C	(8p)	
-0.1790000000000000	0.2650000000000000	-0.7330000000000000	C	(8p)	
0.1790000000000000	-0.2650000000000000	-0.7330000000000000	C	(8p)	
-0.2650000000000000	0.1790000000000000	-0.7330000000000000	C	(8p)	
0.2650000000000000	-0.1790000000000000	-0.7330000000000000	C	(8p)	
-0.0696000000000000	0.3435000000000000	-0.0840000000000000	C	(8p)	
0.0696000000000000	-0.3435000000000000	-0.0840000000000000	C	(8p)	
-0.3435000000000000	0.0696000000000000	-0.0840000000000000	C	(8p)	
0.3435000000000000	-0.0696000000000000	-0.0840000000000000	C	(8p)	
-0.0696000000000000	0.3435000000000000	0.0840000000000000	C	(8p)	
0.0696000000000000	-0.3435000000000000	0.0840000000000000	C	(8p)	
-0.3435000000000000	0.0696000000000000	0.0840000000000000	C	(8p)	
0.3435000000000000	-0.0696000000000000	0.0840000000000000	C	(8p)	
-0.0780000					

-0.09600000000000	-0.48890000000000	0.76140000000000	O	(8p)
-0.48890000000000	0.09600000000000	0.76140000000000	O	(8p)
0.48890000000000	-0.09600000000000	0.76140000000000	O	(8p)
-0.09600000000000	0.48890000000000	-0.76140000000000	O	(8p)
0.09600000000000	-0.48890000000000	-0.76140000000000	O	(8p)
0.48890000000000	0.09600000000000	-0.76140000000000	O	(8p)
-0.48890000000000	-0.09600000000000	-0.76140000000000	O	(8p)
0.11430000000000	0.37500000000000	0.01770000000000	O	(8p)
-0.11430000000000	-0.37500000000000	0.01770000000000	O	(8p)
-0.37500000000000	0.11430000000000	0.01770000000000	O	(8p)
0.37500000000000	-0.11430000000000	0.01770000000000	O	(8p)
-0.11430000000000	0.37500000000000	-0.01770000000000	O	(8p)
0.11430000000000	-0.37500000000000	-0.01770000000000	O	(8p)
0.37500000000000	0.11430000000000	-0.01770000000000	O	(8p)
-0.37500000000000	-0.11430000000000	-0.01770000000000	O	(8p)
-0.01460000000000	0.37680000000000	0.86230000000000	O	(8p)
0.01460000000000	-0.37680000000000	0.86230000000000	O	(8p)
-0.37680000000000	-0.01460000000000	0.86230000000000	O	(8p)
0.37680000000000	0.01460000000000	0.86230000000000	O	(8p)
0.01460000000000	0.37680000000000	-0.86230000000000	O	(8p)
-0.01460000000000	-0.37680000000000	-0.86230000000000	O	(8p)
0.37680000000000	-0.01460000000000	-0.86230000000000	O	(8p)
-0.37680000000000	0.01460000000000	-0.86230000000000	O	(8p)
0.00000000000000	0.50000000000000	0.86772000000000	Pt	(4i)
0.50000000000000	0.00000000000000	0.86772000000000	Pt	(4i)
0.00000000000000	0.50000000000000	-0.86772000000000	Pt	(4i)
0.50000000000000	0.00000000000000	-0.86772000000000	Pt	(4i)
0.10962000000000	0.50000000000000	0.00000000000000	Pt	(4o)
-0.10962000000000	0.50000000000000	0.00000000000000	Pt	(4o)
0.50000000000000	-0.10962000000000	0.00000000000000	Pt	(4o)
-0.50000000000000	0.10962000000000	0.00000000000000	Pt	(4o)

Na<sub>4</sub>Ti<sub>2</sub>Si<sub>8</sub>O<sub>22</sub>[H<sub>2</sub>O]<sub>4</sub>: A4B2C13D\_tP40\_90\_g\_d\_cef2g\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Na4Ti2Si8O22[H2O]4'
_chemical_formula_sum 'H4 Na2 O13 Ti'

loop_
  _publ_author_name
  'S. Ferdov'
  'U. Kolitsch'
  'C. Lengauer'
  'E. Tillmanns'
  'Z. Lin'
  'R. A. [S{\\"a} Ferreira]'
_journal_name_full_name
;
Acta Crystallographica Section E: Crystallographic Communications
;
_journal_volume 63
_journal_year 2007
_journal_page_first i186
_journal_page_last i186
_publ_section_title
;
Refinement of the layered titanosilicate AM-1 from single-crystal X-ray
  ↪ diffraction data
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'NaS_{4}STiS_{2}SSiS_{8}SOS_{22}SHS_{2}SO}_{4} Structure'
_aflow_proto 'A4B2C13D_tP40_90_g_d_cef2g_c'
_aflow_params 'a, c/a, z_{1}, z_{2}, z_{3}, x_{4}, x_{5}, x_{6}, y_{6}, z_{6}, x_{7}, y_{7}, z_{7}, x_{8}, y_{8}, z_{8}'
_aflow_params_values '7.3739946979, 1.45226471387, -0.0654, 0.7769, 0.83072, 0.6476, 0.7846, 0.648, 0.751, 0.001, 0.7502, 0.5354, 0.32757, 0.7289, 0.8811, 0.2635'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP40'

_cell_length_a 7.3739946979
_cell_length_b 7.3739946979
_cell_length_c 10.7089923000
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'P 4 21 2'
_symmetry_Int_Tables_number 90

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x, y, z
  2 x+1/2, -y+1/2, -z
  3 -x+1/2, y+1/2, -z
  4 -x, -y, z
  5 -y, -x, -z
  6 -y+1/2, x+1/2, z
  7 y+1/2, -x+1/2, z
  8 y, x, -z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
```

_atom_site_fract_y							
_atom_site_fract_z							
_atom_site_occupancy							
O1	O	2	c	0.00000	0.50000	-0.06540	1.00000
Ti1	Ti	2	c	0.00000	0.50000	0.77690	1.00000
Na1	Na	4	d	0.00000	0.00000	0.83072	1.00000
O2	O	4	e	0.64760	0.64760	0.00000	1.00000
O3	O	4	f	0.78460	0.78460	0.50000	1.00000
H1	H	8	g	0.64800	0.75100	0.00100	1.00000
O4	O	8	g	0.75020	0.53540	0.32757	1.00000
O5	O	8	g	0.72890	0.88110	0.26350	1.00000

Na<sub>4</sub>Ti<sub>2</sub>Si<sub>8</sub>O<sub>22</sub>[H<sub>2</sub>O]<sub>4</sub>: A4B2C13D\_tP40\_90\_g\_d\_cef2g\_c - POSCAR

```
A4B2C13D_tP40_90_g_d_cef2g_c & a, c/a, z1, z2, z3, x4, x5, x6, y6, z6, x7, y7, z7, x8
  ↪ y8, z8 --params=7.3739946979, 1.45226471387, -0.0654, 0.7769,
  ↪ 0.83072, 0.6476, 0.7846, 0.648, 0.751, 0.001, 0.7502, 0.5354, 0.32757,
  ↪ 0.7289, 0.8811, 0.2635 & P42_{1}2 D_{4}^{2} #90 (c^2defg^3) &
  ↪ tP40 & None & Na4Ti2Si8O22[H2O]4 & S. Ferdov et al., Acta
  ↪ Crystallogr. E 63, i186-i186 (2007)

1.000000000000000
7.37399469790000 0.00000000000000 0.00000000000000
0.00000000000000 7.37399469790000 0.00000000000000
0.00000000000000 0.00000000000000 10.70899230000000

H Na O Ti
8 4 26 2

Direct
0.64800000000000 0.75100000000000 0.00100000000000 H (8g)
-0.64800000000000 -0.75100000000000 0.00100000000000 H (8g)
-0.25100000000000 1.14800000000000 0.00100000000000 H (8g)
1.25100000000000 -0.14800000000000 0.00100000000000 H (8g)
-0.14800000000000 1.25100000000000 -0.00100000000000 H (8g)
1.14800000000000 -0.25100000000000 -0.00100000000000 H (8g)
0.75100000000000 -0.64800000000000 -0.00100000000000 H (8g)
-0.75100000000000 -0.64800000000000 -0.00100000000000 H (8g)
0.00000000000000 0.00000000000000 0.83072000000000 Na (4d)
0.50000000000000 0.50000000000000 0.83072000000000 Na (4d)
0.50000000000000 0.50000000000000 -0.83072000000000 Na (4d)
0.00000000000000 0.00000000000000 -0.83072000000000 Na (4d)
0.00000000000000 0.50000000000000 -0.06540000000000 O (2c)
0.50000000000000 0.00000000000000 0.06540000000000 O (2c)
0.64760000000000 0.64760000000000 0.00000000000000 O (4e)
-0.64760000000000 -0.64760000000000 0.00000000000000 O (4e)
-0.14760000000000 1.14760000000000 0.00000000000000 O (4e)
1.14760000000000 -0.14760000000000 0.00000000000000 O (4e)
0.78460000000000 0.78460000000000 0.50000000000000 O (4f)
-0.78460000000000 -0.78460000000000 0.50000000000000 O (4f)
-0.28460000000000 1.28460000000000 0.50000000000000 O (4f)
1.28460000000000 -0.28460000000000 0.50000000000000 O (4f)
0.75020000000000 0.53540000000000 0.32757000000000 O (8g)
-0.75020000000000 -0.53540000000000 0.32757000000000 O (8g)
-0.03540000000000 1.25020000000000 0.32757000000000 O (8g)
1.03540000000000 -0.25020000000000 0.32757000000000 O (8g)
-0.25020000000000 1.03540000000000 -0.32757000000000 O (8g)
1.25020000000000 -0.03540000000000 -0.32757000000000 O (8g)
0.53540000000000 0.75020000000000 -0.32757000000000 O (8g)
-0.53540000000000 -0.75020000000000 -0.32757000000000 O (8g)
0.72890000000000 0.88110000000000 0.26350000000000 O (8g)
-0.72890000000000 -0.88110000000000 0.26350000000000 O (8g)
-0.38110000000000 1.22890000000000 0.26350000000000 O (8g)
1.38110000000000 -0.22890000000000 0.26350000000000 O (8g)
-0.22890000000000 1.38110000000000 -0.26350000000000 O (8g)
1.22890000000000 -0.38110000000000 -0.26350000000000 O (8g)
0.88110000000000 0.72890000000000 -0.26350000000000 O (8g)
-0.88110000000000 -0.72890000000000 -0.26350000000000 O (8g)
0.00000000000000 0.50000000000000 0.77690000000000 Ti (2c)
0.50000000000000 0.00000000000000 -0.77690000000000 Ti (2c)
```

BaCu<sub>4</sub>[VO][PO<sub>4</sub>]<sub>4</sub>: AB4C17D4E\_tP54\_90\_a\_g\_c4g\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'BaCu4[VO][PO4]4'
_chemical_formula_sum 'Ba Cu4 O17 P4 V'

loop_
  _publ_author_name
  'S. Meyer'
  '{Hk.} {M{\\"u}ller-Buschbaum}'
_journal_name_full_name
;
Zeitschrift fur Anorganische und Allgemeine Chemie
;
_journal_volume 623
_journal_year 1997
_journal_page_first 1693
_journal_page_last 1698
_publ_section_title
;
CuS_{4}SOS_{12}S-Baugruppen aus planaren CuOS_{4}S-Polygonen im
  ↪ Barium-Vanadyl-Oxocuprat (II)-phosphat Ba(VO)Cu_{4}S(POS_{4}S)
  ↪ S_{4}S

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'BaCuS_{4}S[VO][POS_{4}S]_{4} Structure'
_aflow_proto 'AB4C17D4E_tP54_90_a_g_c4g_c'
_aflow_params 'a, c/a, z_{2}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}, x_{7}, y_{7}, z_{7}, x_{8}, y_{8}, z_{8}, x_{9}, y_{9}, z_{9}'
```

```

_aflow_params_values '9.5601062765 , 0.748953974895 , 0.2035 , -0.023 , 0.7639 ,
↳ 0.5152 , 0.407 , 0.6525 , 0.8664 , 0.4465 , 0.8786 , 0.838 , 0.2708 , 0.6666 ,
↳ 0.8964 , 0.0943 , 0.6838 , 0.656 , 0.2468 , 0.7207 , 0.8114 , 0.2609 '
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP54'

_cell_length_a 9.5601062765
_cell_length_b 9.5601062765
_cell_length_c 7.1600795962
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4 21 2"
_symmetry_Int_Tables_number 90

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x+1/2, -y+1/2, -z
3 -x+1/2, y+1/2, -z
4 -x, -y, z
5 -y, -x, -z
6 -y+1/2, x+1/2, z
7 y+1/2, -x+1/2, z
8 y, x, -z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ba1 Ba 2 a 0.00000 0.00000 1.00000
O1 O 2 c 0.00000 0.50000 0.20350 1.00000
V1 V 2 c 0.00000 0.50000 -0.02300 1.00000
Cu1 Cu 8 g 0.76390 0.51520 0.40700 1.00000
O2 O 8 g 0.65250 0.86640 0.44650 1.00000
O3 O 8 g 0.87860 0.83800 0.27080 1.00000
O4 O 8 g 0.66660 0.89640 0.09430 1.00000
O5 O 8 g 0.68380 0.65600 0.24680 1.00000
P1 P 8 g 0.72070 0.81140 0.26090 1.00000

```

BaCu<sub>4</sub>[VO][PO<sub>4</sub>]<sub>4</sub>: AB4C17D4E\_tP54\_90\_a\_g\_c4g\_g\_c - POSCAR

```

AB4C17D4E_tP54_90_a_g_c4g_g_c & a, c/a, z2, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6,
↳ x7, y7, z7, x8, y8, z8, x9, y9, z9 --params=9.5601062765 , 0.748953974895
↳ , 0.2035 , -0.023 , 0.7639 , 0.5152 , 0.407 , 0.6525 , 0.8664 , 0.4465 , 0.8786 ,
↳ 0.838 , 0.2708 , 0.6666 , 0.8964 , 0.0943 , 0.6838 , 0.656 , 0.2468 , 0.7207 ,
↳ 0.8114 , 0.2609 & P4_2_21_2 D_4^2 #90 (ac^2g^6) & tP54 & None
↳ & BaCu4[VO][PO4]4 & S. Meyer and [Hk.] [M["u]]ler-Buschbaum
↳ ], Z. Anorg. Allg. Chem. 623, 1693-1698 (1997)

1.0000000000000000
9.56010627650000 0.00000000000000 0.00000000000000
0.00000000000000 9.56010627650000 0.00000000000000
0.00000000000000 0.00000000000000 7.16007959620000
Ba Cu O P V
2 8 34 8 2
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Ba (2a)
0.50000000000000 0.50000000000000 0.00000000000000 Ba (2a)
0.76390000000000 0.51520000000000 0.40700000000000 Cu (8g)
-0.76390000000000 -0.51520000000000 0.40700000000000 Cu (8g)
-0.01520000000000 1.26390000000000 0.40700000000000 Cu (8g)
1.01520000000000 -0.26390000000000 0.40700000000000 Cu (8g)
-0.26390000000000 1.01520000000000 -0.40700000000000 Cu (8g)
1.26390000000000 -0.01520000000000 -0.40700000000000 Cu (8g)
0.51520000000000 0.76390000000000 -0.40700000000000 Cu (8g)
-0.51520000000000 -0.76390000000000 -0.40700000000000 Cu (8g)
0.00000000000000 0.50000000000000 0.20350000000000 O (2c)
0.50000000000000 0.00000000000000 -0.20350000000000 O (2c)
0.65250000000000 0.86640000000000 0.44650000000000 O (8g)
-0.65250000000000 -0.86640000000000 0.44650000000000 O (8g)
-0.36640000000000 1.15250000000000 0.44650000000000 O (8g)
1.36640000000000 -0.15250000000000 0.44650000000000 O (8g)
-0.15250000000000 1.36640000000000 -0.44650000000000 O (8g)
1.15250000000000 -0.36640000000000 -0.44650000000000 O (8g)
0.86640000000000 0.65250000000000 -0.44650000000000 O (8g)
-0.86640000000000 -0.65250000000000 -0.44650000000000 O (8g)
0.87860000000000 0.83800000000000 0.27080000000000 O (8g)
-0.87860000000000 -0.83800000000000 0.27080000000000 O (8g)
-0.33800000000000 1.37860000000000 0.27080000000000 O (8g)
1.33800000000000 -0.37860000000000 0.27080000000000 O (8g)
-0.37860000000000 1.33800000000000 -0.27080000000000 O (8g)
1.37860000000000 -0.33800000000000 -0.27080000000000 O (8g)
0.83800000000000 0.87860000000000 -0.27080000000000 O (8g)
-0.83800000000000 -0.87860000000000 -0.27080000000000 O (8g)
0.66660000000000 0.89640000000000 0.09430000000000 O (8g)
-0.66660000000000 -0.89640000000000 0.09430000000000 O (8g)
-0.39640000000000 1.16660000000000 0.09430000000000 O (8g)
1.39640000000000 -0.16660000000000 0.09430000000000 O (8g)
-0.16660000000000 1.39640000000000 -0.09430000000000 O (8g)
1.16660000000000 -0.39640000000000 -0.09430000000000 O (8g)
0.89640000000000 0.66660000000000 -0.09430000000000 O (8g)
-0.89640000000000 -0.66660000000000 -0.09430000000000 O (8g)
0.68380000000000 0.65600000000000 0.24680000000000 O (8g)
-0.68380000000000 -0.65600000000000 0.24680000000000 O (8g)
-0.15600000000000 1.18380000000000 0.24680000000000 O (8g)
1.15600000000000 -0.18380000000000 0.24680000000000 O (8g)
-0.18380000000000 1.15600000000000 -0.24680000000000 O (8g)
1.18380000000000 -0.15600000000000 -0.24680000000000 O (8g)

```

```

0.65600000000000 0.68380000000000 -0.24680000000000 O (8g)
-0.65600000000000 -0.68380000000000 -0.24680000000000 O (8g)
0.72070000000000 0.81140000000000 0.26090000000000 P (8g)
-0.72070000000000 -0.81140000000000 0.26090000000000 P (8g)
-0.31140000000000 1.22070000000000 0.26090000000000 P (8g)
1.31140000000000 -0.22070000000000 0.26090000000000 P (8g)
-0.22070000000000 1.31140000000000 -0.26090000000000 P (8g)
1.22070000000000 -0.31140000000000 -0.26090000000000 P (8g)
0.81140000000000 0.72070000000000 -0.26090000000000 P (8g)
-0.81140000000000 -0.72070000000000 -0.26090000000000 P (8g)
0.00000000000000 0.50000000000000 -0.02300000000000 V (2c)
0.50000000000000 0.00000000000000 0.02300000000000 V (2c)

```

ThBC: ABC\_tP24\_91\_d\_d\_d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'ThBC'
_chemical_formula_sum 'B C Th'

loop_
_publ_author_name
'P. Rogl'
_journal_name_full_name
;
Journal of Nuclear Materials
;
_journal_volume 73
_journal_year 1978
_journal_page_first 198
_journal_page_last 203
_publ_section_title
;
The crystal structure of ThBC
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'ThBC Structure'
_aflow_proto 'ABC_tP24_91_d_d_d'
_aflow_params 'a, c/a, x_{1}, y_{1}, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3}'
↳ 3)
_aflow_params_values '3.7620082462 , 6.71079213192 , 0.303 , 0.202 , 0.019 , 0.296
↳ , 0.189 , 0.08 , 0.2975 , 0.1983 , 0.1795 '
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP24'

_cell_length_a 3.7620082462
_cell_length_b 3.7620082462
_cell_length_c 25.2460553388
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 41 2 2"
_symmetry_Int_Tables_number 91

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z+1/2
3 -x, y, -z
4 -x, -y, z+1/2
5 -y, -x, -z+1/4
6 -y, x, z+1/4
7 y, -x, z+3/4
8 y, x, -z+3/4

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
B1 B 8 d 0.30300 0.20200 0.01900 1.00000
C1 C 8 d 0.29600 0.18900 0.08000 1.00000
Th1 Th 8 d 0.29750 0.19830 0.17950 1.00000

```

ThBC: ABC\_tP24\_91\_d\_d\_d - POSCAR

```

ABC_tP24_91_d_d_d & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3 --params=
↳ 3.7620082462 , 6.71079213192 , 0.303 , 0.202 , 0.019 , 0.296 , 0.189 , 0.08 ,
↳ 0.2975 , 0.1983 , 0.1795 & P4_1_2_2 D_4^2 #91 (d^3) & tP24 &
↳ None & ThBC & P. Rogl, J. Nucl. Mat. 73, 198-203 (1978)

1.0000000000000000
3.76200824620000 0.00000000000000 0.00000000000000
0.00000000000000 3.76200824620000 0.00000000000000
0.00000000000000 0.00000000000000 25.24605533880000
B C Th
8 8 8
Direct
0.30300000000000 0.20200000000000 0.01900000000000 B (8d)
-0.30300000000000 -0.20200000000000 0.51900000000000 B (8d)
-0.20200000000000 0.30300000000000 0.26900000000000 B (8d)
0.20200000000000 -0.30300000000000 0.76900000000000 B (8d)
-0.30300000000000 0.20200000000000 -0.01900000000000 B (8d)
0.30300000000000 -0.20200000000000 0.48100000000000 B (8d)
0.20200000000000 0.30300000000000 0.73100000000000 B (8d)

```

-0.20200000000000	-0.30300000000000	0.23100000000000	B	(8d)
0.29600000000000	0.18900000000000	0.08000000000000	C	(8d)
-0.29600000000000	-0.18900000000000	0.58000000000000	C	(8d)
-0.18900000000000	0.29600000000000	0.33000000000000	C	(8d)
0.18900000000000	-0.29600000000000	0.83000000000000	C	(8d)
-0.29600000000000	0.18900000000000	-0.08000000000000	C	(8d)
0.29600000000000	-0.18900000000000	0.42000000000000	C	(8d)
0.18900000000000	0.29600000000000	0.67000000000000	C	(8d)
-0.18900000000000	-0.29600000000000	0.17000000000000	C	(8d)
0.29750000000000	0.19830000000000	0.17950000000000	Th	(8d)
-0.29750000000000	-0.19830000000000	0.67950000000000	Th	(8d)
-0.19830000000000	0.29750000000000	0.42950000000000	Th	(8d)
0.19830000000000	-0.29750000000000	0.92950000000000	Th	(8d)
-0.29750000000000	0.19830000000000	-0.17950000000000	Th	(8d)
0.29750000000000	-0.19830000000000	0.32050000000000	Th	(8d)
0.19830000000000	0.29750000000000	0.57050000000000	Th	(8d)
-0.19830000000000	-0.29750000000000	0.07050000000000	Th	(8d)

AsPh<sub>4</sub>CeSgP<sub>4</sub>Me<sub>8</sub>: AB32CD4E8\_tP184\_93\_i\_16p\_af\_2p\_4p - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'AsPh4CeS8P4Me8'
_chemical_formula_sum 'As C32 Ce P4 S8'

_aflow_title 'AsPh4CeS8P4Me8 Structure'
_aflow_proto 'AB32CD4E8_tP184_93_i_16p_af_2p_4p'
_aflow_params 'a, c/a, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}, x_{7}, y_{7}, z_{7}, x_{8}, y_{8}, z_{8}, x_{9}, y_{9}, z_{9}, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22}, y_{22}, z_{22}, x_{23}, y_{23}, z_{23}, x_{24}, y_{24}, z_{24}, x_{25}, y_{25}, z_{25}'
_aflow_params_values '11.461, 2.92112381119, 0.62279, 0.369, 0.14, 0.5403, 0.251, 0.129, 0.6173, 0.138, 0.647, 0.7882, 0.215, 0.58, 0.8645, 0.138, 0.517, 0.591, 0.132, 0.58, 0.5541, 0.244, 0.605, 0.536, 0.345, 0.554, 0.5495, 0.343, 0.485, 0.5842, 0.237, 0.463, 0.6031, 0.008, 0.366, 0.6554, 0.077, 0.371, 0.6892, 0.082, 0.273, 0.7151, 0.023, 0.17, 0.7031, -0.04, 0.165, 0.6678, -0.05, 0.265, 0.6408, 0.2272, 0.1019, 0.5636, 0.2601, 0.5802, 0.812, 0.1021, 0.205, 0.5436, 0.1936, -0.0676, 0.5558, 0.404, 0.6758, 0.8049, 0.2809, 0.418, 0.7912'
_aflow_Structurbericht 'None'
_aflow_Pearson 'tP184'

_cell_length_a 11.4610000000
_cell_length_b 11.4610000000
_cell_length_c 33.4790000000
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'P 42 2 2'
_symmetry_Int_Tables_number 93

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y, -z
4 -x, -y, z
5 -y, -x, -z+1/2
6 -y, x, z+1/2
7 y, -x, z+1/2
8 y, x, -z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ce1 Ce 2 a 0.00000 0.00000 0.00000 1.00000
Ce2 Ce 2 f 0.50000 0.50000 0.25000 1.00000
As1 As 4 i 0.00000 0.50000 0.62279 1.00000
C1 C 8 p 0.36900 0.14000 0.54030 1.00000
C2 C 8 p 0.25100 0.12900 0.61730 1.00000
C3 C 8 p 0.13800 0.64700 0.78820 1.00000
C4 C 8 p 0.21500 0.58000 0.86450 1.00000
C5 C 8 p 0.13800 0.51700 0.59100 1.00000
C6 C 8 p 0.13200 0.58000 0.55410 1.00000
C7 C 8 p 0.24400 0.60500 0.53600 1.00000
C8 C 8 p 0.34500 0.55400 0.54950 1.00000
C9 C 8 p 0.34300 0.48500 0.58420 1.00000
C10 C 8 p 0.23700 0.46300 0.60310 1.00000
C11 C 8 p 0.00800 0.36600 0.65540 1.00000
C12 C 8 p 0.07700 0.37100 0.68920 1.00000
C13 C 8 p 0.08200 0.27300 0.71510 1.00000
C14 C 8 p 0.02300 0.17000 0.70310 1.00000
C15 C 8 p -0.04000 0.16500 0.66780 1.00000
C16 C 8 p -0.05000 0.26500 0.64080 1.00000
P1 P 8 p 0.22720 0.10190 0.56360 1.00000
P2 P 8 p 0.26010 0.58020 0.81200 1.00000
S1 S 8 p 0.10210 0.20500 0.54360 1.00000
S2 S 8 p 0.19360 -0.06760 0.55580 1.00000
S3 S 8 p 0.40400 0.67580 0.80490 1.00000
S4 S 8 p 0.28090 0.41800 0.79120 1.00000
```

AsPh<sub>4</sub>CeSgP<sub>4</sub>Me<sub>8</sub>: AB32CD4E8\_tP184\_93\_i\_16p\_af\_2p\_4p - POSCAR

```
AB32CD4E8_tP184_93_i_16p_af_2p_4p & a, c/a, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6,
x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12,
x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18,
y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22, x23,
y23, z23, x24, y24, z24, x25, y25, z25 --params=11.461, 2.92112381119,
0.62279, 0.369, 0.14, 0.5403, 0.251, 0.129, 0.6173, 0.138, 0.647, 0.7882
0.215, 0.58, 0.8645, 0.138, 0.517, 0.591, 0.132, 0.58, 0.5541, 0.244,
0.605, 0.536, 0.345, 0.554, 0.5495, 0.343, 0.485, 0.5842, 0.237, 0.463,
0.6031, 0.008, 0.366, 0.6554, 0.077, 0.371, 0.6892, 0.082, 0.273, 0.7151
0.023, 0.17, 0.7031, -0.04, 0.165, 0.6678, -0.05, 0.265, 0.6408, 0.2272
0.1019, 0.5636, 0.2601, 0.5802, 0.812, 0.1021, 0.205, 0.5436, 0.1936, -
0.0676, 0.5558, 0.404, 0.6758, 0.8049, 0.2809, 0.418, 0.7912 & P4_2 & P4_2}
22 D_4^{45} #93 (afip^22) & tP184 & None & AsPh4CeS8P4Me8 & &
1.0000000000000000
11.46100000000000 0.00000000000000 0.00000000000000
0.00000000000000 11.46100000000000 0.00000000000000
0.00000000000000 0.00000000000000 33.47900000000000
As C Ce P S
4 128 4 16 32
Direct
0.00000000000000 0.50000000000000 0.62279000000000 As (4i)
0.50000000000000 0.00000000000000 1.12279000000000 As (4i)
0.00000000000000 0.50000000000000 -0.62279000000000 As (4i)
0.50000000000000 0.00000000000000 -0.12279000000000 As (4i)
0.36900000000000 0.14000000000000 0.54030000000000 C (8p)
-0.36900000000000 -0.14000000000000 0.54030000000000 C (8p)
-0.14000000000000 0.36900000000000 1.04030000000000 C (8p)
0.14000000000000 -0.36900000000000 1.04030000000000 C (8p)
-0.36900000000000 0.14000000000000 -0.54030000000000 C (8p)
0.36900000000000 -0.14000000000000 -0.54030000000000 C (8p)
0.14000000000000 0.36900000000000 -0.04030000000000 C (8p)
-0.14000000000000 -0.36900000000000 -0.04030000000000 C (8p)
0.25100000000000 0.12900000000000 0.61730000000000 C (8p)
-0.25100000000000 -0.12900000000000 0.61730000000000 C (8p)
-0.12900000000000 0.25100000000000 1.11730000000000 C (8p)
0.12900000000000 -0.25100000000000 1.11730000000000 C (8p)
-0.25100000000000 0.12900000000000 -0.61730000000000 C (8p)
0.25100000000000 -0.12900000000000 -0.61730000000000 C (8p)
0.12900000000000 0.25100000000000 -0.11730000000000 C (8p)
-0.12900000000000 -0.25100000000000 -0.11730000000000 C (8p)
0.13800000000000 0.64700000000000 0.78820000000000 C (8p)
-0.13800000000000 -0.64700000000000 0.78820000000000 C (8p)
-0.64700000000000 0.13800000000000 1.28820000000000 C (8p)
0.64700000000000 -0.13800000000000 1.28820000000000 C (8p)
-0.13800000000000 0.64700000000000 -0.78820000000000 C (8p)
0.13800000000000 -0.64700000000000 -0.78820000000000 C (8p)
0.64700000000000 0.13800000000000 -0.28820000000000 C (8p)
-0.64700000000000 -0.13800000000000 -0.28820000000000 C (8p)
0.21500000000000 0.58000000000000 0.86450000000000 C (8p)
-0.21500000000000 -0.58000000000000 0.86450000000000 C (8p)
-0.58000000000000 0.21500000000000 1.36450000000000 C (8p)
0.58000000000000 -0.21500000000000 1.36450000000000 C (8p)
-0.21500000000000 0.58000000000000 -0.86450000000000 C (8p)
0.21500000000000 -0.58000000000000 -0.86450000000000 C (8p)
0.58000000000000 0.21500000000000 -0.36450000000000 C (8p)
-0.58000000000000 -0.21500000000000 -0.36450000000000 C (8p)
0.13800000000000 0.51700000000000 0.59100000000000 C (8p)
-0.13800000000000 -0.51700000000000 0.59100000000000 C (8p)
-0.51700000000000 0.13800000000000 1.09100000000000 C (8p)
0.51700000000000 -0.13800000000000 1.09100000000000 C (8p)
-0.13800000000000 0.51700000000000 -0.59100000000000 C (8p)
0.13800000000000 -0.51700000000000 -0.59100000000000 C (8p)
0.51700000000000 0.13800000000000 -0.09100000000000 C (8p)
-0.51700000000000 -0.13800000000000 -0.09100000000000 C (8p)
0.13200000000000 0.58000000000000 0.55410000000000 C (8p)
-0.13200000000000 -0.58000000000000 0.55410000000000 C (8p)
-0.58000000000000 0.13200000000000 1.05410000000000 C (8p)
0.58000000000000 -0.13200000000000 1.05410000000000 C (8p)
-0.13200000000000 0.58000000000000 -0.55410000000000 C (8p)
0.13200000000000 -0.58000000000000 -0.55410000000000 C (8p)
0.58000000000000 0.13200000000000 -0.05410000000000 C (8p)
-0.58000000000000 -0.13200000000000 -0.05410000000000 C (8p)
0.24400000000000 0.60500000000000 0.53600000000000 C (8p)
-0.24400000000000 -0.60500000000000 0.53600000000000 C (8p)
-0.60500000000000 0.24400000000000 1.03600000000000 C (8p)
0.60500000000000 -0.24400000000000 1.03600000000000 C (8p)
-0.24400000000000 0.60500000000000 -0.53600000000000 C (8p)
0.24400000000000 -0.60500000000000 -0.53600000000000 C (8p)
0.60500000000000 0.24400000000000 0.24400000000000 C (8p)
-0.60500000000000 -0.24400000000000 0.24400000000000 C (8p)
-0.24400000000000 0.60500000000000 0.54950000000000 C (8p)
0.24400000000000 -0.60500000000000 0.54950000000000 C (8p)
-0.54950000000000 0.24400000000000 1.04950000000000 C (8p)
0.54950000000000 -0.24400000000000 1.04950000000000 C (8p)
-0.24400000000000 0.54950000000000 -0.54950000000000 C (8p)
0.24400000000000 -0.54950000000000 -0.54950000000000 C (8p)
0.54950000000000 0.24400000000000 -0.04950000000000 C (8p)
-0.54950000000000 -0.24400000000000 -0.04950000000000 C (8p)
0.34300000000000 0.48500000000000 0.58420000000000 C (8p)
-0.34300000000000 -0.48500000000000 0.58420000000000 C (8p)
-0.48500000000000 0.34300000000000 1.08420000000000 C (8p)
0.48500000000000 -0.34300000000000 1.08420000000000 C (8p)
-0.34300000000000 0.48500000000000 -0.58420000000000 C (8p)
0.34300000000000 -0.48500000000000 -0.58420000000000 C (8p)
-0.48500000000000 0.34300000000000 -0.08420000000000 C (8p)
0.48500000000000 -0.34300000000000 -0.08420000000000 C (8p)
0.23700000000000 0.46300000000000 0.60310000000000 C (8p)
-0.23700000000000 -0.46300000000000 0.60310000000000 C (8p)
-0.46300000000000 0.23700000000000 1.10310000000000 C (8p)
0.46300000000000 -0.23700000000000 1.10310000000000 C (8p)
-0.23700000000000 0.46300000000000 -0.60310000000000 C (8p)
0.23700000000000 -0.46300000000000 -0.60310000000000 C (8p)
0.46300000000000 0.23700000000000 -0.10310000000000 C (8p)
-0.46300000000000 -0.23700000000000 -0.10310000000000 C (8p)
```

```
0.00800000000000 0.36600000000000 0.65540000000000 C (8p)
-0.00800000000000 -0.36600000000000 0.65540000000000 C (8p)
-0.36600000000000 0.00800000000000 1.15540000000000 C (8p)
0.36600000000000 -0.00800000000000 1.15540000000000 C (8p)
-0.00800000000000 0.36600000000000 -0.65540000000000 C (8p)
0.00800000000000 -0.36600000000000 -0.65540000000000 C (8p)
0.36600000000000 0.00800000000000 -0.15540000000000 C (8p)
-0.36600000000000 -0.00800000000000 -0.15540000000000 C (8p)
0.07700000000000 0.37100000000000 0.68920000000000 C (8p)
-0.07700000000000 -0.37100000000000 0.68920000000000 C (8p)
-0.37100000000000 0.07700000000000 1.18920000000000 C (8p)
0.37100000000000 -0.07700000000000 1.18920000000000 C (8p)
-0.07700000000000 0.37100000000000 -0.68920000000000 C (8p)
0.07700000000000 -0.37100000000000 -0.68920000000000 C (8p)
0.37100000000000 0.07700000000000 -0.18920000000000 C (8p)
-0.37100000000000 -0.07700000000000 -0.18920000000000 C (8p)
0.08200000000000 0.27300000000000 0.71510000000000 C (8p)
-0.08200000000000 -0.27300000000000 0.71510000000000 C (8p)
-0.27300000000000 0.08200000000000 1.21510000000000 C (8p)
0.27300000000000 -0.08200000000000 1.21510000000000 C (8p)
-0.08200000000000 0.27300000000000 -0.71510000000000 C (8p)
0.08200000000000 -0.27300000000000 -0.71510000000000 C (8p)
0.27300000000000 0.08200000000000 -0.21510000000000 C (8p)
-0.27300000000000 -0.08200000000000 -0.21510000000000 C (8p)
0.02300000000000 0.17000000000000 0.70310000000000 C (8p)
-0.02300000000000 -0.17000000000000 0.70310000000000 C (8p)
-0.17000000000000 0.02300000000000 1.20310000000000 C (8p)
0.17000000000000 -0.02300000000000 1.20310000000000 C (8p)
-0.02300000000000 0.17000000000000 -0.70310000000000 C (8p)
0.02300000000000 -0.17000000000000 -0.70310000000000 C (8p)
0.17000000000000 0.02300000000000 -0.20310000000000 C (8p)
-0.17000000000000 -0.02300000000000 -0.20310000000000 C (8p)
-0.04000000000000 0.16500000000000 0.66780000000000 C (8p)
0.04000000000000 -0.16500000000000 0.66780000000000 C (8p)
-0.16500000000000 0.04000000000000 1.16780000000000 C (8p)
0.16500000000000 -0.04000000000000 1.16780000000000 C (8p)
0.04000000000000 0.16500000000000 -0.66780000000000 C (8p)
-0.04000000000000 -0.16500000000000 -0.66780000000000 C (8p)
0.16500000000000 0.04000000000000 -0.16780000000000 C (8p)
-0.16500000000000 -0.04000000000000 -0.16780000000000 C (8p)
-0.05000000000000 0.26500000000000 0.64080000000000 C (8p)
0.05000000000000 -0.26500000000000 0.64080000000000 C (8p)
-0.26500000000000 0.05000000000000 1.14080000000000 C (8p)
0.26500000000000 -0.05000000000000 1.14080000000000 C (8p)
0.05000000000000 0.26500000000000 -0.64080000000000 C (8p)
-0.05000000000000 -0.26500000000000 -0.64080000000000 C (8p)
0.26500000000000 0.05000000000000 -0.14080000000000 C (8p)
-0.26500000000000 -0.05000000000000 -0.14080000000000 C (8p)
0.00000000000000 0.00000000000000 0.00000000000000 Ce (2a)
0.00000000000000 0.00000000000000 0.00000000000000 Ce (2a)
0.50000000000000 0.50000000000000 0.25000000000000 Ce (2f)
0.50000000000000 0.50000000000000 0.75000000000000 Ce (2f)
0.22720000000000 0.10190000000000 0.56360000000000 P (8p)
-0.22720000000000 -0.10190000000000 0.56360000000000 P (8p)
0.10190000000000 0.22720000000000 1.06360000000000 P (8p)
-0.10190000000000 -0.22720000000000 1.06360000000000 P (8p)
0.22720000000000 0.10190000000000 -0.56360000000000 P (8p)
-0.22720000000000 -0.10190000000000 -0.56360000000000 P (8p)
0.10190000000000 0.22720000000000 -0.06360000000000 P (8p)
-0.10190000000000 -0.22720000000000 -0.06360000000000 P (8p)
0.26010000000000 0.58020000000000 0.81200000000000 P (8p)
-0.26010000000000 -0.58020000000000 0.81200000000000 P (8p)
-0.58020000000000 0.26010000000000 1.31200000000000 P (8p)
0.58020000000000 -0.26010000000000 1.31200000000000 P (8p)
-0.26010000000000 0.58020000000000 -0.81200000000000 P (8p)
0.26010000000000 -0.58020000000000 -0.81200000000000 P (8p)
0.58020000000000 0.26010000000000 -0.31200000000000 P (8p)
-0.58020000000000 -0.26010000000000 -0.31200000000000 P (8p)
0.10210000000000 0.20500000000000 0.54360000000000 S (8p)
-0.10210000000000 -0.20500000000000 0.54360000000000 S (8p)
-0.20500000000000 0.10210000000000 1.04360000000000 S (8p)
0.20500000000000 -0.10210000000000 1.04360000000000 S (8p)
-0.10210000000000 0.20500000000000 -0.54360000000000 S (8p)
0.10210000000000 -0.20500000000000 -0.54360000000000 S (8p)
0.20500000000000 0.10210000000000 -0.04360000000000 S (8p)
-0.20500000000000 -0.10210000000000 -0.04360000000000 S (8p)
0.19360000000000 -0.06760000000000 0.55580000000000 S (8p)
-0.19360000000000 0.06760000000000 0.55580000000000 S (8p)
0.06760000000000 0.19360000000000 1.05580000000000 S (8p)
-0.06760000000000 -0.19360000000000 1.05580000000000 S (8p)
-0.19360000000000 0.06760000000000 -0.55580000000000 S (8p)
0.19360000000000 -0.06760000000000 -0.55580000000000 S (8p)
0.06760000000000 0.19360000000000 -0.05580000000000 S (8p)
-0.06760000000000 -0.19360000000000 -0.05580000000000 S (8p)
0.40400000000000 0.67580000000000 0.80490000000000 S (8p)
-0.40400000000000 -0.67580000000000 0.80490000000000 S (8p)
-0.67580000000000 0.40400000000000 1.30490000000000 S (8p)
0.67580000000000 -0.40400000000000 1.30490000000000 S (8p)
-0.40400000000000 0.67580000000000 -0.80490000000000 S (8p)
0.40400000000000 -0.67580000000000 -0.80490000000000 S (8p)
0.67580000000000 0.40400000000000 -0.30490000000000 S (8p)
-0.67580000000000 -0.40400000000000 -0.30490000000000 S (8p)
0.28090000000000 0.41800000000000 0.79120000000000 S (8p)
-0.28090000000000 -0.41800000000000 0.79120000000000 S (8p)
-0.41800000000000 0.28090000000000 1.29120000000000 S (8p)
0.41800000000000 -0.28090000000000 1.29120000000000 S (8p)
-0.28090000000000 0.41800000000000 -0.79120000000000 S (8p)
0.28090000000000 -0.41800000000000 -0.79120000000000 S (8p)
0.41800000000000 0.28090000000000 -0.29120000000000 S (8p)
-0.41800000000000 -0.28090000000000 -0.29120000000000 S (8p)
```

Na<sub>5</sub>Fe<sub>3</sub>F<sub>14</sub> (High-temperature): A14B3C5\_tP44\_94\_c3g\_ad\_bg - CIF

```
# CIF file
data_findsym -output
```

```
_audit_creation_method FINDSYM
_chemical_name_mineral 'Na5Fe3F14'
_chemical_formula_sum 'F14 Fe3 Na5'
loop_
  _publ_author_name
    'M. Vlasse'
    'F. Menil'
    'C. Morilliere'
    'J. M. Dance'
    'A. Tressaud'
    'J. Portier'
_journal_name_full_name
  ;
  Journal of Solid State Chemistry
  ;
_journal_volume 17
_journal_year 1976
_journal_page_first 291
_journal_page_last 298
_publ_section_title
  ;
  Etude cristallographique et par effet M(\|")ssbauer du fluorure
  ↳ ferrimagn(\|')e)tique NaS_{5}SFeS_{3}SFS_{14}\gammaS
  ;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013
_aware_title 'NaS_{5}SFeS_{3}SFS_{14}S (High-temperature) Structure'
_aware_proto 'A14B3C5_tP44_94_c3g_ad_bg'
_aware_params 'a,c/a,z_{3},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},y_{7},z_{7},x_{8},y_{8},z_{8}'
_aware_params_values '7.3451315192,1.41592920353,0.8225,-0.0016,0.7086,-
↳ 0.0024,0.6281,-0.0287,0.6575,0.6242,0.54,0.75,0.5448,0.7312,
↳ 0.7348,0.7403'
_aware_strukturbericht 'None'
_aware_pearson 'tP44'
_cell_length_a 7.3451315192
_cell_length_b 7.3451315192
_cell_length_c 10.4001862218
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000
_symmetry_space_group_name_H-M "P 42 21 2"
_symmetry_Int_Tables_number 94
loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x+1/2,y+1/2,-z+1/2
4 -x,-y,z
5 -y,-x,-z
6 -y+1/2,x+1/2,z+1/2
7 y+1/2,-x+1/2,z+1/2
8 y,x,-z
loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Fe1 Fe 2 a 0.0000 0.0000 0.0000 1.0000
Na1 Na 2 b 0.0000 0.0000 0.5000 1.0000
F1 F 4 c 0.0000 0.0000 0.8225 1.0000
Fe2 Fe 4 d 0.0000 0.5000 -0.0016 1.0000
F2 F 8 g 0.7086 -0.0024 0.6281 1.0000
F3 F 8 g -0.0287 0.6575 0.6242 1.0000
F4 F 8 g 0.5400 0.7500 0.5448 1.0000
Na2 Na 8 g 0.7312 0.7348 0.7403 1.0000
```

Na<sub>5</sub>Fe<sub>3</sub>F<sub>14</sub> (High-temperature): A14B3C5\_tP44\_94\_c3g\_ad\_bg - POSCAR

```
A14B3C5_tP44_94_c3g_ad_bg & a,c/a,z3,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8
↳ ,z8 --params=7.3451315192,1.41592920353,0.8225,-0.0016,0.7086,-
↳ 0.0024,0.6281,-0.0287,0.6575,0.6242,0.54,0.75,0.5448,0.7312,
↳ 0.7348,0.7403 & P4_{2}2_{1}2 D_{4}^{(4)} #94 (abcdg^4) & tP44 &
↳ None & Na5Fe3F14 & M. Vlasse et al., J. Solid State Chem. 17
↳ , 291-298 (1976)
1.0000000000000000
7.34513151920000 0.00000000000000 0.00000000000000
0.00000000000000 7.34513151920000 0.00000000000000
0.00000000000000 0.00000000000000 10.40018622180000
F Fe Na
28 6 10
Direct
0.00000000000000 0.00000000000000 0.82250000000000 F (4c)
0.50000000000000 0.50000000000000 1.32250000000000 F (4c)
0.50000000000000 0.50000000000000 -0.32250000000000 F (4c)
0.00000000000000 0.00000000000000 -0.82250000000000 F (4c)
0.70860000000000 -0.00240000000000 0.62810000000000 F (8g)
-0.70860000000000 0.00240000000000 0.62810000000000 F (8g)
0.50240000000000 1.20860000000000 1.12810000000000 F (8g)
0.49760000000000 -0.20860000000000 1.12810000000000 F (8g)
-0.20860000000000 0.49760000000000 -0.12810000000000 F (8g)
1.20860000000000 0.50240000000000 -0.12810000000000 F (8g)
```

```

-0.002400000000000 0.708600000000000 -0.628100000000000 F (8g)
0.002400000000000 -0.708600000000000 -0.628100000000000 F (8g)
-0.028700000000000 0.657500000000000 0.624200000000000 F (8g)
0.028700000000000 -0.657500000000000 0.624200000000000 F (8g)
-0.157500000000000 0.471300000000000 1.124200000000000 F (8g)
1.157500000000000 0.528700000000000 1.124200000000000 F (8g)
0.528700000000000 1.157500000000000 -0.124200000000000 F (8g)
0.471300000000000 -0.157500000000000 -0.124200000000000 F (8g)
0.657500000000000 -0.028700000000000 -0.624200000000000 F (8g)
-0.657500000000000 0.028700000000000 -0.624200000000000 F (8g)
0.540000000000000 0.750000000000000 0.544800000000000 F (8g)
-0.540000000000000 -0.750000000000000 0.544800000000000 F (8g)
-0.250000000000000 1.040000000000000 1.044800000000000 F (8g)
1.250000000000000 -0.040000000000000 1.044800000000000 F (8g)
-0.040000000000000 1.250000000000000 -0.044800000000000 F (8g)
1.040000000000000 -0.250000000000000 -0.044800000000000 F (8g)
0.750000000000000 -0.540000000000000 -0.544800000000000 F (8g)
-0.750000000000000 0.540000000000000 -0.544800000000000 F (8g)
0.000000000000000 -0.000000000000000 0.000000000000000 Fe (2a)
0.500000000000000 0.500000000000000 0.500000000000000 Fe (2a)
0.000000000000000 0.500000000000000 -0.001600000000000 Fe (4d)
0.000000000000000 0.500000000000000 0.498400000000000 Fe (4d)
0.500000000000000 0.000000000000000 0.501600000000000 Fe (4d)
0.500000000000000 0.000000000000000 0.001600000000000 Fe (4d)
0.000000000000000 0.000000000000000 0.500000000000000 Na (2b)
0.500000000000000 0.500000000000000 0.000000000000000 Na (2b)
0.731200000000000 0.734800000000000 0.740300000000000 Na (8g)
-0.731200000000000 -0.734800000000000 0.740300000000000 Na (8g)
-0.234800000000000 1.231200000000000 1.240300000000000 Na (8g)
1.234800000000000 -0.231200000000000 1.240300000000000 Na (8g)
-0.231200000000000 1.234800000000000 -0.240300000000000 Na (8g)
1.231200000000000 -0.234800000000000 -0.240300000000000 Na (8g)
0.734800000000000 0.731200000000000 -0.740300000000000 Na (8g)
-0.734800000000000 -0.731200000000000 -0.740300000000000 Na (8g)

```

**Li<sub>2</sub>MoF<sub>6</sub>: A6B2C\_tP18\_94\_eg\_c\_a - CIF**

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Li2MoF6'
_chemical_formula_sum 'F6 Li2 Mo'

loop_
_publ_author_name
'G. Brunton'
_journal_name_full_name
;
Materials Research Bulletin
;
_journal_volume 6
_journal_year 1971
_journal_page_first 555
_journal_page_last 560
_publ_section_title
;
The crystal structure of LiS_{2}$MoFS_{6}$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'LiS_{2}$MoFS_{6}$ Structure'
_aflow_proto 'A6B2C_tP18_94_eg_c_a'
_aflow_params 'a, c/a, z_{2}, x_{3}, x_{4}, y_{4}, z_{4}'
_aflow_params_values '4.6863209101, 1.96124874637, 0.6623, 0.7093, 0.684,
↳ 0.707, 0.6579'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP18'

_cell_length_a 4.6863209101
_cell_length_b 4.6863209101
_cell_length_c 9.1910410100
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 42 21 2"
_symmetry_Int_Tables_number 94

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x+1/2, -y+1/2, -z+1/2
3 -x+1/2, y+1/2, -z+1/2
4 -x, -y, z
5 -y, -x, -z
6 -y+1/2, x+1/2, z+1/2
7 y+1/2, -x+1/2, z+1/2
8 y, x, -z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mol Mo 2 a 0.00000 0.00000 0.00000 1.00000
Li1 Li 4 c 0.00000 0.00000 0.66230 1.00000
F1 F 4 e 0.70930 0.70930 0.00000 1.00000

```

F2 F 8 g 0.68400 0.70700 0.65790 1.00000

**Li<sub>2</sub>MoF<sub>6</sub>: A6B2C\_tP18\_94\_eg\_c\_a - POSCAR**

```

A6B2C_tP18_94_eg_c_a & a, c/a, z2, x3, x4, y4, z4 --params=4.6863209101,
↳ 1.96124874637, 0.6623, 0.7093, 0.684, 0.707, 0.6579 & P4_{2}_{1}_{2}
↳ D_{4}^{2} #94 (aceg) & tP18 & None & Li2MoF6 & G. Brunton,
↳ Mater. Res. Bull. 6, 555-560 (1971)
1.000000000000000
4.68632091010000 0.00000000000000 0.00000000000000
0.00000000000000 4.68632091010000 0.00000000000000
0.00000000000000 0.00000000000000 9.19104101000000
F Li Mo
12 4 2
Direct
0.709300000000000 0.709300000000000 0.00000000000000 F (4e)
-0.709300000000000 -0.709300000000000 0.00000000000000 F (4e)
-0.209300000000000 1.209300000000000 0.50000000000000 F (4e)
1.209300000000000 -0.209300000000000 0.50000000000000 F (4e)
0.684000000000000 0.707000000000000 0.657900000000000 F (8g)
-0.684000000000000 -0.707000000000000 0.657900000000000 F (8g)
-0.207000000000000 1.184000000000000 1.157900000000000 F (8g)
1.207000000000000 -0.184000000000000 1.157900000000000 F (8g)
-0.184000000000000 1.207000000000000 -0.157900000000000 F (8g)
1.184000000000000 -0.207000000000000 -0.157900000000000 F (8g)
0.707000000000000 0.684000000000000 -0.657900000000000 F (8g)
-0.707000000000000 -0.684000000000000 -0.657900000000000 F (8g)
0.000000000000000 0.000000000000000 0.662300000000000 Li (4c)
0.500000000000000 0.500000000000000 1.162300000000000 Li (4c)
0.500000000000000 0.500000000000000 -0.162300000000000 Li (4c)
0.000000000000000 0.000000000000000 -0.662300000000000 Li (4c)
0.000000000000000 0.000000000000000 0.000000000000000 Mo (2a)
0.500000000000000 0.500000000000000 0.500000000000000 Mo (2a)

```

**ThBC: ABC\_tP24\_95\_d\_d - CIF**

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'ThBC'
_chemical_formula_sum 'B C Th'

_aflow_title 'ThBC Structure'
_aflow_proto 'ABC_tP24_95_d_d'
_aflow_params 'a, c/a, x_{1}, y_{1}, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3}'
↳ 3}
_aflow_params_values '3.7620082462, 6.71079213192, 0.303, 0.202, -0.019,
↳ 0.296, 0.189, -0.08, 0.2975, 0.1983, 0.8205'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP24'

_cell_length_a 3.7620082462
_cell_length_b 3.7620082462
_cell_length_c 25.2460553388
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 43 2 2"
_symmetry_Int_Tables_number 95

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z+1/2
3 -x, y, -z
4 -x, -y, z+1/2
5 -y, -x, -z+3/4
6 -y, x, z+3/4
7 y, -x, z+1/4
8 y, x, -z+1/4

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
B1 B 8 d 0.30300 0.20200 -0.01900 1.00000
C1 C 8 d 0.29600 0.18900 -0.08000 1.00000
Th1 Th 8 d 0.29750 0.19830 0.82050 1.00000

```

**ThBC: ABC\_tP24\_95\_d\_d - POSCAR**

```

ABC_tP24_95_d_d & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3 --params=
↳ 3.7620082462, 6.71079213192, 0.303, 0.202, -0.019, 0.296, 0.189, -0.08
↳ 0.2975, 0.1983, 0.8205 & P4_{3}_{2}_{2} D_{4}^{2} #95 (d^3) & tP24 &
↳ None & ThBC & ThBC &
1.000000000000000
3.76200824620000 0.00000000000000 0.00000000000000
0.00000000000000 3.76200824620000 0.00000000000000
0.00000000000000 0.00000000000000 25.24605533880000
B C Th
8 8 8
Direct
0.303000000000000 0.202000000000000 -0.019000000000000 B (8d)
-0.303000000000000 -0.202000000000000 0.481000000000000 B (8d)
-0.202000000000000 0.303000000000000 0.731000000000000 B (8d)
0.202000000000000 -0.303000000000000 0.231000000000000 B (8d)

```



-0.30300000000000	0.20200000000000	0.01900000000000	B	(8d)
0.30300000000000	-0.20200000000000	0.51900000000000	B	(8d)
0.20200000000000	0.30300000000000	0.26900000000000	B	(8d)
-0.20200000000000	-0.30300000000000	0.76900000000000	B	(8d)
0.29600000000000	0.18900000000000	-0.08000000000000	C	(8d)
-0.29600000000000	-0.18900000000000	0.42000000000000	C	(8d)
0.18900000000000	0.29600000000000	0.67000000000000	C	(8d)
-0.18900000000000	-0.29600000000000	0.17000000000000	C	(8d)
0.29600000000000	0.18900000000000	0.08000000000000	C	(8d)
0.29600000000000	-0.18900000000000	0.58000000000000	C	(8d)
0.18900000000000	0.29600000000000	0.33000000000000	C	(8d)
-0.18900000000000	-0.29600000000000	0.83000000000000	C	(8d)
0.29750000000000	0.19830000000000	0.82050000000000	Th	(8d)
-0.29750000000000	-0.19830000000000	1.32050000000000	Th	(8d)
-0.19830000000000	0.29750000000000	1.57050000000000	Th	(8d)
0.19830000000000	-0.29750000000000	1.07050000000000	Th	(8d)
-0.29750000000000	0.19830000000000	-0.82050000000000	Th	(8d)
0.29750000000000	-0.19830000000000	-0.32050000000000	Th	(8d)
0.19830000000000	0.29750000000000	-0.57050000000000	Th	(8d)
-0.19830000000000	-0.29750000000000	-0.07050000000000	Th	(8d)

NaGdCu<sub>2</sub>F<sub>8</sub>: A2B8CD\_t124\_97\_d\_k\_a\_b - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'NaGdCu2F8'
_chemical_formula_sum 'Cu2 F8 Gd Na'

loop_
  _publ_author_name
    'C. {De Nada|i}'
    'A. Demourgues'
    'L. Lozano'
    'P. Gravereau'
    'J. Grannec'
  _journal_name_full_name
    'Journal of Materials Chemistry'
  _journal_volume 8
  _journal_year 1998
  _journal_page_first 2487
  _journal_page_last 2491
  _publ_section_title
    'Structural investigations of new copper fluorides Na$RE$Cu$_{2}$F$_{8}$'
    ↪ (SRE^{3+}$ = Sm^{3+}$, Eu^{3+}$, Gd^{3+}$, YS^{3+}$, Er^{3+}$, Yb^{3+}$)
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'NaGdCu$_{2}$F$_{8}$ Structure'
_aflow_proto 'A2B8CD_t124_97_d_k_a_b'
_aflow_params 'a,c/a,x_{4},y_{4},z_{4}'
_aflow_params_values '5.4068544677,1.92010356944,0.1697,0.3128,0.1237'
_aflow_strukturbericht 'None'
_aflow_Pearson 'tI24'

_cell_length_a 5.4068544677
_cell_length_b 5.4068544677
_cell_length_c 10.3817205629
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 4 2 2"
_symmetry_Int_Tables_number 97

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
    1 x,y,z
    2 x,-y,-z
    3 -x,y,-z
    4 -x,-y,z
    5 -y,-x,-z
    6 -y,x,z
    7 y,-x,z
    8 y,x,-z
    9 x+1/2,y+1/2,z+1/2
    10 x+1/2,-y+1/2,-z+1/2
    11 -x+1/2,y+1/2,-z+1/2
    12 -x+1/2,-y+1/2,z+1/2
    13 -y+1/2,-x+1/2,-z+1/2
    14 -y+1/2,x+1/2,z+1/2
    15 y+1/2,-x+1/2,z+1/2
    16 y+1/2,x+1/2,-z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
    Gd1 Gd 2 a 0.00000 0.00000 0.50000 1.00000
    Na1 Na 2 b 0.00000 0.00000 0.50000 1.00000
    Cu1 Cu 4 d 0.00000 0.50000 0.25000 1.00000
    F1 F 16 k 0.16970 0.31280 0.12370 1.00000
```

NaGdCu<sub>2</sub>F<sub>8</sub>: A2B8CD\_t124\_97\_d\_k\_a\_b - POSCAR

```
A2B8CD_t124_97_d_k_a_b & a,c/a,x4,y4,z4 --params=5.4068544677,
  ↪ 1.92010356944,0.1697,0.3128,0.1237 & I422 D_{4}^{9} #97 (abdk)
  ↪ & tI24 & None & NaGdCu2F8 & C. {De Nada|i} et al., J.
  ↪ Mater. Chem. 8, 2487-2491 (1998)
1.0000000000000000
-2.70342723385000 2.70342723385000 5.19086028145000
2.70342723385000 -2.70342723385000 5.19086028145000
2.70342723385000 2.70342723385000 -5.19086028145000
Cu F Gd Na
2 8 1 1
Direct
0.750000000000000 0.250000000000000 0.500000000000000 Cu (4d)
0.250000000000000 0.750000000000000 0.500000000000000 Cu (4d)
0.436500000000000 0.293400000000000 0.482500000000000 F (16k)
-0.189100000000000 -0.046000000000000 -0.482500000000000 F (16k)
0.293400000000000 -0.189100000000000 -0.143100000000000 F (16k)
-0.046000000000000 0.436500000000000 0.143100000000000 F (16k)
0.189100000000000 -0.293400000000000 0.143100000000000 F (16k)
-0.436500000000000 0.046000000000000 -0.143100000000000 F (16k)
0.046000000000000 0.189100000000000 0.482500000000000 F (16k)
-0.293400000000000 -0.436500000000000 -0.482500000000000 F (16k)
0.000000000000000 0.000000000000000 0.000000000000000 Gd (2a)
0.500000000000000 0.500000000000000 0.000000000000000 Na (2b)
```

Ta<sub>2</sub>Se<sub>8</sub>I: AB8C2\_t144\_97\_e\_2k\_cd - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ta2Se8I'
_chemical_formula_sum 'I Se8 Ta2'

loop_
  _publ_author_name
    'P. Gressier'
    'A. Meerschaut'
    'L. Guemas'
    'J. Rouxel'
    'P. Monceau'
  _journal_name_full_name
    'Journal of Solid State Chemistry'
  _journal_volume 51
  _journal_year 1984
  _journal_page_first 141
  _journal_page_last 151
  _publ_section_title
    'Characterization of the new series of quasi one-dimensional compounds (
    ↪ $MX_{4}$)_{n}$Y$ ($M$ = Nb, Ta; $SX$ = S, Se; $YS$ = Br, I)
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'Ta$_{2}$Se$_{8}$I Structure'
_aflow_proto 'AB8C2_t144_97_e_2k_cd'
_aflow_params 'a,c/a,z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5}'
_aflow_params_values '9.5317026755,1.33879580768,0.1553,0.0449,0.284,
  ↪ 0.3693,0.312,0.1212,0.1191'
_aflow_strukturbericht 'None'
_aflow_Pearson 'tI44'

_cell_length_a 9.5317026755
_cell_length_b 9.5317026755
_cell_length_c 12.7610035820
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 4 2 2"
_symmetry_Int_Tables_number 97

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
    1 x,y,z
    2 x,-y,-z
    3 -x,y,-z
    4 -x,-y,z
    5 -y,-x,-z
    6 -y,x,z
    7 y,-x,z
    8 y,x,-z
    9 x+1/2,y+1/2,z+1/2
    10 x+1/2,-y+1/2,-z+1/2
    11 -x+1/2,y+1/2,-z+1/2
    12 -x+1/2,-y+1/2,z+1/2
    13 -y+1/2,-x+1/2,-z+1/2
    14 -y+1/2,x+1/2,z+1/2
    15 y+1/2,-x+1/2,z+1/2
    16 y+1/2,x+1/2,-z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
    Ta1 Ta 2 a 0.00000 0.00000 0.50000 1.00000
    Se1 Se 8 b 0.00000 0.00000 0.50000 1.00000
    I1 I 2 c 0.00000 0.50000 0.25000 1.00000
```

```

_atom_site_occupancy
Ta1 Ta 4 c 0.00000 0.50000 0.00000 1.00000
Ta2 Ta 4 d 0.00000 0.50000 0.25000 1.00000
I1 I 4 e 0.00000 0.00000 0.15530 1.00000
Se1 Se 16 k 0.04490 0.28400 0.36930 1.00000
Se2 Se 16 k 0.31200 0.12120 0.11910 1.00000

```

Ta2Seg1: AB8C2\_tI44\_97\_e\_2k\_cd - POSCAR

```

AB8C2_tI44_97_e_2k_cd & a,c/a,z3,x4,y4,z4,x5,y5,z5 --params=9.5317026755
↪ ,1.33879580768,0.1553,0.0449,0.284,0.3693,0.312,0.1212,0.1191 &
↪ I422_D_{4}^{9} #97 (cdek^2) & tI44 & None & Ta2Se8I & & P.
↪ Gressier et al., J. Solid State Chem. 51, 141-151 (1984)
1.000000000000000
-4.76585133775000 4.76585133775000 6.38050179100000
4.76585133775000 -4.76585133775000 6.38050179100000
4.76585133775000 4.76585133775000 -6.38050179100000
I Se Ta
2 16 4
Direct
0.155300000000000 0.155300000000000 0.000000000000000 I (4e)
-0.155300000000000 -0.155300000000000 0.000000000000000 I (4e)
0.653300000000000 0.414200000000000 0.328900000000000 Se (16k)
0.085300000000000 0.324400000000000 -0.328900000000000 Se (16k)
0.414200000000000 0.085300000000000 -0.239100000000000 Se (16k)
0.324400000000000 0.653300000000000 0.239100000000000 Se (16k)
-0.085300000000000 -0.414200000000000 0.239100000000000 Se (16k)
-0.653300000000000 -0.324400000000000 -0.239100000000000 Se (16k)
-0.324400000000000 -0.085300000000000 0.328900000000000 Se (16k)
-0.414200000000000 -0.653300000000000 -0.328900000000000 Se (16k)
0.240300000000000 0.431100000000000 0.433200000000000 Se (16k)
-0.002100000000000 -0.192900000000000 -0.433200000000000 Se (16k)
0.431100000000000 -0.002100000000000 0.190800000000000 Se (16k)
-0.192900000000000 0.240300000000000 -0.190800000000000 Se (16k)
0.002100000000000 -0.431100000000000 -0.190800000000000 Se (16k)
-0.240300000000000 0.192900000000000 0.190800000000000 Se (16k)
0.192900000000000 0.002100000000000 0.433200000000000 Se (16k)
-0.431100000000000 -0.240300000000000 -0.433200000000000 Se (16k)
0.500000000000000 0.000000000000000 0.500000000000000 Ta (4c)
0.000000000000000 0.500000000000000 0.500000000000000 Ta (4c)
0.750000000000000 0.250000000000000 0.500000000000000 Ta (4d)
0.250000000000000 0.750000000000000 0.500000000000000 Ta (4d)

```

CdAs2: A2B\_tI12\_98\_f\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'CdAs2'
_chemical_formula_sum 'As2 Cd'

loop_
_publ_author_name
'V. N. Yakimovich'
'V. A. Rubtsov'
'V. M. Trukhan'
_journal_name_full_name
;
Inorganic Materials
;
_journal_volume 32
_journal_year 1996
_journal_page_first 579
_journal_page_last 582
_publ_section_title
;
Phase Relationships in the CdPS_{4}S-ZnPS_{2}S-CdAs_{2}S-ZnAs_{2}S System
↪ System
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_flow_title 'CdAs_{2}S Structure'
_flow_proto 'A2B_tI12_98_f_a'
_flow_params 'a,c/a,x_{2}'
_flow_params_values '7.953376649,0.587954231111,0.44'
_flow_strukturbericht 'None'
_flow_pearson 'tI12'

_cell_length_a 7.9533766490
_cell_length_b 7.9533766490
_cell_length_c 4.6762214524
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 41 2 2"
_symmetry_Int_Tables_number 98

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y+1/2,-z+1/4
3 -x,y+1/2,-z+1/4
4 -x,-y,z
5 -y,-x,-z
6 -y,x+1/2,z+1/4
7 y,-x+1/2,z+1/4
8 y,x,-z
9 x+1/2,y+1/2,z+1/2
10 x+1/2,-y,-z+3/4
11 -x+1/2,y,-z+3/4

```

```

12 -x+1/2,-y+1/2,z+1/2
13 -y+1/2,-x+1/2,-z+1/2
14 -y+1/2,x,z+3/4
15 y+1/2,-x,z+3/4
16 y+1/2,x+1/2,-z+1/2

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cd1 Cd 4 a 0.00000 0.00000 0.00000 1.00000
As1 As 8 f 0.44000 0.25000 0.12500 1.00000

```

CdAs2: A2B\_tI12\_98\_f\_a - POSCAR

```

A2B_tI12_98_f_a & a,c/a,x2 --params=7.953376649,0.587954231111,0.44 &
↪ I4_{1}22 D_{4}^{10} #98 (af) & tI12 & None & CdAs2 & & V. N.
↪ Yakimovich and V. A. Rubtsov and V. M. Trukhan, Inorg. Mat. 32,
↪ 579-582 (1996)
1.000000000000000
-3.97668832450000 3.97668832450000 2.33811072620000
3.97668832450000 -3.97668832450000 2.33811072620000
3.97668832450000 3.97668832450000 -2.33811072620000
As Cd
4 2
Direct
0.375000000000000 0.565000000000000 0.690000000000000 As (8f)
0.875000000000000 -0.315000000000000 0.310000000000000 As (8f)
1.315000000000000 0.125000000000000 0.690000000000000 As (8f)
0.435000000000000 0.625000000000000 0.310000000000000 As (8f)
0.000000000000000 0.000000000000000 0.000000000000000 Cd (4a)
0.750000000000000 0.250000000000000 0.500000000000000 Cd (4a)

```

Fresnoite (Ba2TiSi2O8): A2B8C2D\_tP26\_100\_c\_abcd\_c\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Fresnoite'
_chemical_formula_sum 'Ba2 O8 Si2 Ti'

loop_
_publ_author_name
'S. A. Markgraf'
'A. Halliya'
'A. S. Bhalla'
'R. E. Newnham'
'C. T. Prewitt'
_journal_name_full_name
;
Ferroelectrics
;
_journal_volume 62
_journal_year 1985
_journal_page_first 17
_journal_page_last 26
_publ_section_title
;
X-ray structure refinement and pyroelectric investigation of fresnoite,
↪ BaS_{2}TiSi_{2}OS_{8}
;

_flow_title 'Fresnoite (BaS_{2}TiSi_{2}OS_{8}) Structure'
_flow_proto 'A2B8C2D_tP26_100_c_abcd_c_a'
_flow_params 'a,c/a,z_{1},z_{2},z_{3},z_{4},z_{5},z_{6},z_{7},z_{8}'
_flow_params_values '8.527,0.611047261639,0.7904,0.4646,0.3707,0.32701,
↪ 0.0,0.1259,0.7949,0.1282,0.4871,0.2924,0.5772,0.3571'
_flow_strukturbericht 'None'
_flow_pearson 'tP26'

_symmetry_space_group_name_H-M "P 4 b m"
_symmetry_Int_Tables_number 100

_cell_length_a 8.52700
_cell_length_b 8.52700
_cell_length_c 5.21040
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x+1/2,y+1/2,z
6 x+1/2,-y+1/2,z
7 y+1/2,x+1/2,z
8 -y+1/2,-x+1/2,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x

```

```

_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 2 a 0.00000 0.00000 0.79040 1.00000
Ti1 Ti 2 a 0.00000 0.00000 0.46460 1.00000
O2 O 2 b 0.50000 0.00000 0.30700 1.00000
Ba1 Ba 4 c 0.32701 0.82701 0.00000 1.00000
O3 O 4 c 0.12590 0.62590 0.79490 1.00000
Si1 Si 4 c 0.12820 0.62820 0.48710 1.00000
O4 O 8 d 0.29240 0.57720 0.35710 1.00000

```

Fresnoite (Ba<sub>2</sub>TiSi<sub>2</sub>O<sub>8</sub>): A2B8C2D\_tP26\_100\_c\_abcd\_c\_a - POSCAR

```

A2B8C2D_tP26_100_c_abcd_c_a & a, c/a, z1, z2, z3, x4, z4, x5, z5, x6, z6, x7, y7, z7
--params=8.527, 0.611047261639, 0.7904, 0.4646, 0.3707, 0.32701, 0.0,
0.1259, 0.7949, 0.1282, 0.4871, 0.2924, 0.5772, 0.3571 & P4bm C_{4v}
)^{2} #100 (a^2bc^3d) & tP26 & None & Ba2TiSi2O8 & Fresnoite &
S. A. Markgraf et al., Ferroelectrics 62, 17-26 (1985)
1.000000000000000
8.527000000000000 0.000000000000000 0.000000000000000
0.000000000000000 8.527000000000000 0.000000000000000
0.000000000000000 0.000000000000000 5.210400000000000
Ba O Si Ti
4 16 4 2
Direct
0.327010000000000 0.827010000000000 0.000000000000000 Ba (4c)
-0.327010000000000 0.172990000000000 0.000000000000000 Ba (4c)
0.172990000000000 0.327010000000000 0.000000000000000 Ba (4c)
0.827010000000000 -0.327010000000000 0.000000000000000 Ba (4c)
0.000000000000000 0.000000000000000 0.790400000000000 O (2a)
0.500000000000000 0.500000000000000 0.790400000000000 O (2a)
0.500000000000000 0.000000000000000 0.370700000000000 O (2b)
0.000000000000000 0.500000000000000 0.370700000000000 O (2b)
0.125900000000000 0.625900000000000 0.794900000000000 O (4c)
-0.125900000000000 0.374100000000000 0.794900000000000 O (4c)
0.374100000000000 0.125900000000000 0.794900000000000 O (4c)
0.625900000000000 -0.125900000000000 0.794900000000000 O (4c)
0.292400000000000 0.577200000000000 0.357100000000000 O (8d)
-0.292400000000000 -0.577200000000000 0.357100000000000 O (8d)
-0.577200000000000 0.292400000000000 0.357100000000000 O (8d)
0.577200000000000 -0.292400000000000 0.357100000000000 O (8d)
0.792400000000000 -0.077200000000000 0.357100000000000 O (8d)
0.207600000000000 1.077200000000000 0.357100000000000 O (8d)
-0.077200000000000 0.207600000000000 0.357100000000000 O (8d)
1.077200000000000 0.792400000000000 0.357100000000000 O (8d)
0.128200000000000 0.628200000000000 0.487100000000000 Si (4c)
-0.128200000000000 0.371800000000000 0.487100000000000 Si (4c)
0.371800000000000 0.128200000000000 0.487100000000000 Si (4c)
0.628200000000000 -0.128200000000000 0.487100000000000 Si (4c)
0.000000000000000 0.000000000000000 0.464600000000000 Ti (2a)
0.500000000000000 0.500000000000000 0.464600000000000 Ti (2a)

```

Ce<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>: A3B11C6\_tP40\_100\_ac\_be2d\_cd - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ce3Si6N11'
_chemical_formula_sum 'Ce3 N11 Si6'

loop_
_publ_author_name
'M. Woike'
'W. Jeitschko'
_journal_name_full_name
;
Inorganic Chemistry
;
_journal_volume 34
_journal_year 1995
_journal_page_first 5105
_journal_page_last 5108
_publ_section_title
;
Preparation and Crystal Structure of the Nitridosilicates $Ln_{3}$Si$_{6}$N$_{11}$
--params={11}$ (Ln$ = La, Ce, Pr, Nd, Sm) and $Ln$Si$_{6}$N$_{11}$}
--$ (Ln$ = Ce, Pr, Nd)
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
Inorganic Compounds, 2013

_aflow_title 'Ce$_{3}$Si$_{6}$N$_{11}$ Structure'
_aflow_proto 'A3B11C6_tP40_100_ac_be2d_cd'
_aflow_params 'a, c/a, z_{1}, z_{2}, x_{3}, z_{3}, x_{4}, z_{4}, x_{5}, z_{5}, x_{6}, z_{6}, x_{7}, z_{7}, x_{8}, z_{8}, y_{8}, z_{8}'
_aflow_params_values '10.1311200179, 0.47843253381, 0.0, 0.0672, 0.18111,
0.0154, 0.6536, 0.6912, 0.6174, 0.0432, 0.5814, 0.678, 0.6402, 0.7288,
0.574, 0.1742, 0.7098, 0.5782, 0.5334'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP40'

_cell_length_a 10.1311200179
_cell_length_b 10.1311200179
_cell_length_c 4.8470574205
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4 b m"
_symmetry_Int_Tables_number 100

loop_
_space_group_symop_id

```

```

_space_group_symop_operation_xyz
1 x, y, z
2 -x, -y, z
3 -y, x, z
4 y, -x, z
5 -x+1/2, y+1/2, z
6 x+1/2, -y+1/2, z
7 y+1/2, x+1/2, z
8 -y+1/2, -x+1/2, z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ce1 Ce 2 a 0.00000 0.00000 0.00000 1.00000
N1 N 2 b 0.50000 0.00000 0.06720 1.00000
Ce2 Ce 4 c 0.18111 0.68111 0.01540 1.00000
N2 N 4 c 0.65360 0.15360 0.69120 1.00000
Si1 Si 4 c 0.61740 0.11740 0.04320 1.00000
N3 N 8 d 0.58140 0.67800 0.64020 1.00000
N4 N 8 d 0.72880 0.57400 0.17420 1.00000
Si2 Si 8 d 0.70980 0.57820 0.53340 1.00000

```

Ce<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>: A3B11C6\_tP40\_100\_ac\_be2d\_cd - POSCAR

```

A3B11C6_tP40_100_ac_be2d_cd & a, c/a, z1, z2, x3, z3, x4, z4, x5, z5, x6, y6, z6, x7,
y7, z7, x8, y8, z8 --params=10.1311200179, 0.47843253381, 0.0, 0.0672,
0.18111, 0.0154, 0.6536, 0.6912, 0.6174, 0.0432, 0.5814, 0.678, 0.6402,
0.7288, 0.574, 0.1742, 0.7098, 0.5782, 0.5334 & P4bm C_{4v}^{2} #100
(abc^3d^3) & tP40 & None & Ce3Si6N11 & M. Woike and W.
Jeitschko, Inorg. Chem. 34, 5105-5108 (1995)
1.000000000000000
10.131120017900000 0.000000000000000 0.000000000000000
0.000000000000000 10.131120017900000 0.000000000000000
0.000000000000000 0.000000000000000 4.847057420500000
Ce N Si
6 22 12
Direct
0.000000000000000 0.000000000000000 0.000000000000000 Ce (2a)
0.500000000000000 0.500000000000000 0.000000000000000 Ce (2a)
0.181110000000000 0.681110000000000 0.015400000000000 Ce (4c)
-0.181110000000000 0.318890000000000 0.015400000000000 Ce (4c)
0.318890000000000 0.181110000000000 0.015400000000000 Ce (4c)
0.681110000000000 -0.181110000000000 0.015400000000000 Ce (4c)
0.500000000000000 0.000000000000000 0.067200000000000 N (2b)
0.000000000000000 0.500000000000000 0.067200000000000 N (2b)
0.653600000000000 1.153600000000000 0.691200000000000 N (4c)
-0.653600000000000 -0.153600000000000 0.691200000000000 N (4c)
-0.153600000000000 0.653600000000000 0.691200000000000 N (4c)
1.153600000000000 -0.653600000000000 0.691200000000000 N (4c)
0.581400000000000 0.678000000000000 0.640200000000000 N (8d)
-0.581400000000000 -0.678000000000000 0.640200000000000 N (8d)
-0.678000000000000 0.581400000000000 0.640200000000000 N (8d)
0.678000000000000 -0.581400000000000 0.640200000000000 N (8d)
1.081400000000000 -0.178000000000000 0.640200000000000 N (8d)
-0.081400000000000 1.178000000000000 0.640200000000000 N (8d)
-0.178000000000000 -0.081400000000000 0.640200000000000 N (8d)
1.178000000000000 1.081400000000000 0.640200000000000 N (8d)
0.728800000000000 0.574000000000000 0.174200000000000 N (8d)
-0.728800000000000 -0.574000000000000 0.174200000000000 N (8d)
-0.574000000000000 0.728800000000000 0.174200000000000 N (8d)
0.574000000000000 -0.728800000000000 0.174200000000000 N (8d)
1.228800000000000 -0.074000000000000 0.174200000000000 N (8d)
-0.228800000000000 1.074000000000000 0.174200000000000 N (8d)
-0.074000000000000 -0.228800000000000 0.174200000000000 N (8d)
1.074000000000000 1.228800000000000 0.174200000000000 N (8d)
0.617400000000000 1.117400000000000 0.043200000000000 Si (4c)
-0.617400000000000 -0.117400000000000 0.043200000000000 Si (4c)
-0.117400000000000 0.617400000000000 0.043200000000000 Si (4c)
1.117400000000000 -0.617400000000000 0.043200000000000 Si (4c)
0.709800000000000 0.578200000000000 0.533400000000000 Si (8d)
-0.709800000000000 -0.578200000000000 0.533400000000000 Si (8d)
-0.578200000000000 0.709800000000000 0.533400000000000 Si (8d)
0.578200000000000 -0.709800000000000 0.533400000000000 Si (8d)
1.209800000000000 -0.078200000000000 0.533400000000000 Si (8d)
-0.209800000000000 1.078200000000000 0.533400000000000 Si (8d)
-0.078200000000000 -0.209800000000000 0.533400000000000 Si (8d)
1.078200000000000 1.209800000000000 0.533400000000000 Si (8d)

```

γ-MgNiSn: A7B7C2\_tP32\_101\_bde\_ade\_d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'gamma-MgNiSn'
_chemical_formula_sum 'M7 Mg7 Ni2'

loop_
_publ_author_name
'M. Boudard'
'P. Bordet'
'H. Vincent'
'F. Audebert'
_journal_name_full_name
;
Journal of Alloys and Compounds
;
_journal_volume 372
_journal_year 2004

```

```
_journal_page_first 121
_journal_page_last 128
_publ_Section_title
;
The structure of the Y-phase in the Mg--Ni--Sn system
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title '$\gamma$MgNiSn Structure'
_aflow_proto 'A7B7C2_tP32_101_bde_ade_d'
_aflow_params 'a,c/a,z_{1},z_{2},x_{3},z_{3},x_{4},z_{4},x_{5},z_{5},x_{6},z_{6},x_{7},z_{7}'
↳ 6,y_{6},z_{6},x_{7},y_{7},z_{7}'
_aflow_params_values '9.8510697809,0.697188102729,0.0,0.4692,0.17136,
↳ 0.73945,0.2254,0.3402,0.30926,0.0086,0.2384,0.5244,0.2259,
↳ 0.0352,0.3449,0.0281'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP32'

_cell_length_a 9.8510697809
_cell_length_b 9.8510697809
_cell_length_c 6.8680486504
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 42 c m"
_symmetry_Int_Tables_number 101

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z+1/2
4 y,-x,z+1/2
5 -x,y,z+1/2
6 x,-y,z+1/2
7 y,x,z
8 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mg1 Mg 2 a 0.00000 0.00000 0.00000 1.00000
M1 M 2 b 0.50000 0.50000 0.46920 1.00000
M2 M 4 d 0.17136 0.17136 0.73945 1.00000
Mg2 Mg 4 d 0.22540 0.22540 0.34020 1.00000
Ni1 Ni 4 d 0.30926 0.30926 0.00860 1.00000
M3 M 8 e 0.23840 0.52440 0.22590 1.00000
Mg3 Mg 8 e 0.03520 0.34490 0.02810 1.00000
```

y-MgNiSn: A7B7C2\_tP32\_101\_bde\_ade\_d - POSCAR

```
A7B7C2_tP32_101_bde_ade_d & a,c/a,z1,z2,x3,z3,x4,z4,x5,z5,x6,y6,z6,x7,y7
↳ z7 --params=9.8510697809,0.697188102729,0.0,0.4692,0.17136,
↳ 0.73945,0.2254,0.3402,0.30926,0.0086,0.2384,0.5244,0.2259,
↳ 0.0352,0.3449,0.0281 & P4_{2}cm C_{4v}^{3} #101 (abd^3e^2) &
↳ tP32 & None & MgNiSn & gamma & M. Boudard et al., J. Alloys
↳ Compd. 372, 121-128 (2004)
1.0000000000000000
9.85106978090000 0.00000000000000 0.00000000000000
0.00000000000000 9.85106978090000 0.00000000000000
0.00000000000000 0.00000000000000 6.86804865040000
M Mg Ni
14 14 4
Direct
0.50000000000000 0.50000000000000 0.46920000000000 M (2b)
0.50000000000000 0.50000000000000 0.96920000000000 M (2b)
0.17136000000000 0.17136000000000 0.73945000000000 M (4d)
-0.17136000000000 -0.17136000000000 0.73945000000000 M (4d)
-0.17136000000000 0.17136000000000 1.23945000000000 M (4d)
0.17136000000000 -0.17136000000000 1.23945000000000 M (4d)
0.23840000000000 0.52440000000000 0.22590000000000 M (8e)
-0.23840000000000 -0.52440000000000 0.22590000000000 M (8e)
-0.52440000000000 0.23840000000000 0.72590000000000 M (8e)
0.52440000000000 -0.23840000000000 0.72590000000000 M (8e)
0.23840000000000 -0.52440000000000 0.72590000000000 M (8e)
-0.23840000000000 0.52440000000000 0.72590000000000 M (8e)
-0.52440000000000 -0.23840000000000 0.22590000000000 M (8e)
0.00000000000000 0.00000000000000 0.00000000000000 Mg (2a)
0.00000000000000 0.00000000000000 0.50000000000000 Mg (2a)
0.22540000000000 0.22540000000000 0.34020000000000 Mg (4d)
-0.22540000000000 -0.22540000000000 0.34020000000000 Mg (4d)
-0.22540000000000 0.22540000000000 0.84020000000000 Mg (4d)
0.22540000000000 -0.22540000000000 0.84020000000000 Mg (4d)
0.03520000000000 0.34490000000000 0.02810000000000 Mg (8e)
-0.03520000000000 -0.34490000000000 0.02810000000000 Mg (8e)
-0.34490000000000 0.03520000000000 0.52810000000000 Mg (8e)
0.34490000000000 -0.03520000000000 0.52810000000000 Mg (8e)
0.03520000000000 -0.34490000000000 0.52810000000000 Mg (8e)
-0.03520000000000 0.34490000000000 0.52810000000000 Mg (8e)
-0.34490000000000 -0.03520000000000 0.02810000000000 Mg (8e)
0.34490000000000 0.03520000000000 0.02810000000000 Mg (8e)
0.30926000000000 0.30926000000000 0.00860000000000 Ni (4d)
-0.30926000000000 -0.30926000000000 0.00860000000000 Ni (4d)
-0.30926000000000 0.30926000000000 0.50860000000000 Ni (4d)
```

0.30926000000000 -0.30926000000000 0.50860000000000 Ni (4d)

Gd3Al2: A2B3\_tP20\_102\_2c\_b2c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Gd3Al2'
_chemical_formula_sum 'Al2 Gd3'

loop_
_publ_author_name
'K. H. J. Buschow'
_journal_name_full_name
;
Journal of the Less-Common Metals
;
_journal_volume 8
_journal_year 1965
_journal_page_first 209
_journal_page_last 212
_publ_Section_title
;
Rare earth-aluminium intermetallic compounds of the form SRSAI and SR_{
↳ 3}SAIS_{2}S
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title 'Gd_{3}Al_{2}S Structure'
_aflow_proto 'A2B3_tP20_102_2c_b2c'
_aflow_params 'a,c/a,z_{1},x_{2},z_{2},x_{3},z_{3},x_{4},z_{4},x_{5},z_{5},z_{6}'
↳ 5)'
_aflow_params_values '8.3289849893,0.909833113223,0.5,0.604,0.439,0.623,
↳ 0.031,0.795,0.725,0.848,0.251'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP20'

_cell_length_a 8.3289849893
_cell_length_b 8.3289849893
_cell_length_c 7.5779863428
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 42 n m"
_symmetry_Int_Tables_number 102

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y+1/2,x+1/2,z+1/2
4 y+1/2,-x+1/2,z+1/2
5 -x+1/2,y+1/2,z+1/2
6 x+1/2,-y+1/2,z+1/2
7 y,x,z
8 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Gd1 Gd 4 b 0.00000 0.50000 1.00000
Al1 Al 4 c 0.60400 0.60400 0.43900 1.00000
Al2 Al 4 c 0.62300 0.62300 0.03100 1.00000
Gd2 Gd 4 c 0.79500 0.79500 0.72500 1.00000
Gd3 Gd 4 c 0.84800 0.84800 0.25100 1.00000
```

Gd3Al2: A2B3\_tP20\_102\_2c\_b2c - POSCAR

```
A2B3_tP20_102_2c_b2c & a,c/a,z1,x2,z2,x3,z3,x4,z4,x5,z5 --params=
↳ 8.3289849893,0.909833113223,0.5,0.604,0.439,0.623,0.031,0.795,
↳ 0.725,0.848,0.251 & P4_{2}nm C_{4v}^{4} #102 (bc^4) & tP20 &
↳ None & Gd3Al2 & K. H. J. Buschow, J. Less-Common Met. 8,
↳ 209-212 (1965)
1.0000000000000000
8.32898498930000 0.00000000000000 0.00000000000000
0.00000000000000 8.32898498930000 0.00000000000000
0.00000000000000 0.00000000000000 7.57798634280000
Al Gd
8 12
Direct
0.60400000000000 0.60400000000000 0.43900000000000 Al (4c)
-0.60400000000000 -0.60400000000000 0.43900000000000 Al (4c)
-0.10400000000000 -0.10400000000000 1.04000000000000 Al (4c)
1.04000000000000 -0.10400000000000 0.93900000000000 Al (4c)
0.62300000000000 0.62300000000000 0.03100000000000 Al (4c)
-0.62300000000000 -0.62300000000000 0.03100000000000 Al (4c)
-0.12300000000000 -0.12300000000000 0.53100000000000 Al (4c)
1.12300000000000 -0.12300000000000 0.53100000000000 Al (4c)
0.00000000000000 0.50000000000000 0.50000000000000 Gd (4b)
0.00000000000000 0.50000000000000 1.00000000000000 Gd (4b)
0.50000000000000 0.00000000000000 1.00000000000000 Gd (4b)
0.50000000000000 0.00000000000000 0.50000000000000 Gd (4b)
0.79500000000000 0.79500000000000 0.72500000000000 Gd (4c)
-0.79500000000000 -0.79500000000000 0.72500000000000 Gd (4c)
```

```

-0.29500000000000 1.29500000000000 1.22500000000000 Gd (4c)
1.29500000000000 -0.29500000000000 1.22500000000000 Gd (4c)
0.84800000000000 0.84800000000000 0.25100000000000 Gd (4c)
-0.84800000000000 -0.84800000000000 0.25100000000000 Gd (4c)
-0.34800000000000 1.34800000000000 0.75100000000000 Gd (4c)
1.34800000000000 -0.34800000000000 0.75100000000000 Gd (4c)

```

NbTe<sub>4</sub>: AB<sub>4</sub>tP10<sub>103</sub>a<sub>d</sub> - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'NbTe4'
_chemical_formula_sum 'Nb Te4'

loop_
_publ_author_name
'H. B{\o}hm'
_journal_name_full_name
;
Zeitschrift f{\u}r Kristallographie - Crystalline Materials
;
_journal_volume 180
_journal_year 1987
_journal_page_first 113
_journal_page_last 122
_publ_section_title
;
The high temperature modification of niobium tetratelluride NbTe_{4}$

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'NbTe_{4}$ Structure'
_aflow_proto 'AB4_tP10_103_a_d'
_aflow_params 'a,c/a,z_{1},x_{2},y_{2},z_{2}'
_aflow_params_values '6.5509768136,1.04518394138,0.0,0.144,0.3276,0.242'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP10'

_cell_length_a 6.5509768136
_cell_length_b 6.5509768136
_cell_length_c 6.8469757659
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4 c c"
_symmetry_Int_Tables_number 103

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z+1/2
6 x,-y,z+1/2
7 y,x,z+1/2
8 -y,-x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Nb1 Nb 2 a 0.00000 0.00000 0.00000 1.00000
Te1 Te 8 d 0.14400 0.32760 0.24200 1.00000

```

NbTe<sub>4</sub>: AB<sub>4</sub>tP10<sub>103</sub>a<sub>d</sub> - POSCAR

```

AB4_tP10_103_a_d & a,c/a,z1,x2,y2,z2 --params=6.5509768136,1.04518394138
↳ ,0.0,0.144,0.3276,0.242 & P4cc C_{4v}^{5} #103 (ad) & tP10 &
↳ None & NbTe4 & H. B{\o}hm, Zeitschrift f{\u}r
↳ Kristallographie - Crystalline Materials 180, 113-122 (1987)
1.00000000000000
6.55097681360000 0.00000000000000 0.00000000000000
0.00000000000000 6.55097681360000 0.00000000000000
0.00000000000000 0.00000000000000 6.84697576590000
Nb Te
2 8
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Nb (2a)
0.00000000000000 0.00000000000000 0.50000000000000 Nb (2a)
0.14400000000000 0.32760000000000 0.24200000000000 Te (8d)
-0.14400000000000 -0.32760000000000 0.24200000000000 Te (8d)
-0.32760000000000 0.14400000000000 0.24200000000000 Te (8d)
0.32760000000000 -0.14400000000000 0.24200000000000 Te (8d)
0.14400000000000 -0.32760000000000 0.74200000000000 Te (8d)
-0.14400000000000 0.32760000000000 0.74200000000000 Te (8d)
-0.32760000000000 -0.14400000000000 0.74200000000000 Te (8d)
0.32760000000000 0.14400000000000 0.74200000000000 Te (8d)

```

Ba<sub>5</sub>In<sub>4</sub>Bi<sub>5</sub>: A5B5C<sub>4</sub>tP28<sub>104</sub>ac<sub>ac</sub>c - CIF

```

# CIF file
data_findsym-output

```

```

_audit_creation_method FINDSYM

_chemical_name_mineral 'Ba5In4Bi5'
_chemical_formula_sum 'Ba5 Bi5 In4'

loop_
_publ_author_name
'S. Ponou'
'T. F. F{\a}ssler'
'G. Tob{\i}as'
'E. Canadell'
'A. Cho'
'S. C. Sevov'
_journal_name_full_name
;
Chemistry - A European Journal
;
_journal_volume 10
_journal_year 2004
_journal_page_first 3615
_journal_page_last 3621
_publ_section_title
;
Synthesis, Characterization, and Electronic Structure of Ba_{5}$In_{4}$
↳ }Bi_{5}$: An Acentric and One-Electron Deficient Phase
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'Ba_{5}$In_{4}$Bi_{5}$ Structure'
_aflow_proto 'A5B5C4_tP28_104_ac_ac_c'
_aflow_params 'a,c/a,z_{1},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5}'
_aflow_params_values '10.6225961282,0.84830508475,0.5,0.8821,0.8116,
↳ 0.6057,0.3261,0.60942,0.80921,0.00978,0.8116,-0.072,0.1681'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP28'

_cell_length_a 10.6225961282
_cell_length_b 10.6225961282
_cell_length_c 9.0112023088
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4 n c"
_symmetry_Int_Tables_number 104

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x+1/2,y+1/2,z+1/2
6 x+1/2,-y+1/2,z+1/2
7 y+1/2,x+1/2,z+1/2
8 -y+1/2,-x+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ba1 Ba 2 a 0.00000 0.00000 0.50000 1.00000
Bi1 Bi 2 a 0.00000 0.00000 0.88210 1.00000
Ba2 Ba 8 c 0.81160 0.60570 0.32610 1.00000
Bi2 Bi 8 c 0.60942 0.80921 0.00978 1.00000
In1 In 8 c 0.81160 -0.07200 0.16810 1.00000

```

Ba<sub>5</sub>In<sub>4</sub>Bi<sub>5</sub>: A5B5C<sub>4</sub>tP28<sub>104</sub>ac<sub>ac</sub>c - POSCAR

```

A5B5C4_tP28_104_ac_ac_c & a,c/a,z1,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5 --
↳ params=10.6225961282,0.84830508475,0.5,0.8821,0.8116,0.6057,
↳ 0.3261,0.60942,0.80921,0.00978,0.8116,-0.072,0.1681 & P4nc C_{
↳ 4v}^{6} #104 (a^2c^3) & tP28 & None & Ba5In4Bi5 & S. Ponou
↳ et al., Chem. Euro. J. 10, 3615-3621 (2004)
1.00000000000000
10.62259612820000 0.00000000000000 0.00000000000000
0.00000000000000 10.62259612820000 0.00000000000000
0.00000000000000 0.00000000000000 9.01120230880000
Ba Bi In
10 10 8
Direct
0.00000000000000 0.00000000000000 0.50000000000000 Ba (2a)
0.50000000000000 0.50000000000000 1.00000000000000 Ba (2a)
0.81160000000000 0.60570000000000 0.32610000000000 Ba (8c)
-0.81160000000000 -0.60570000000000 0.32610000000000 Ba (8c)
-0.60570000000000 0.81160000000000 0.32610000000000 Ba (8c)
0.60570000000000 -0.81160000000000 0.32610000000000 Ba (8c)
1.31160000000000 -0.10570000000000 0.82610000000000 Ba (8c)
-0.31160000000000 1.10570000000000 0.82610000000000 Ba (8c)
-0.10570000000000 -0.31160000000000 0.82610000000000 Ba (8c)
1.10570000000000 1.31160000000000 0.82610000000000 Ba (8c)
0.00000000000000 0.00000000000000 0.88210000000000 Bi (2a)
0.50000000000000 0.50000000000000 1.38210000000000 Bi (2a)
0.60942000000000 0.80921000000000 0.00978000000000 Bi (8c)
-0.60942000000000 -0.80921000000000 0.00978000000000 Bi (8c)
-0.80921000000000 0.60942000000000 0.00978000000000 Bi (8c)

```

0.80921000000000	-0.60942000000000	0.00978000000000	Bi	(8c)
1.10942000000000	-0.30921000000000	0.50978000000000	Bi	(8c)
-0.10942000000000	1.30921000000000	0.50978000000000	Bi	(8c)
-0.30921000000000	-0.10942000000000	0.50978000000000	Bi	(8c)
1.30921000000000	1.10942000000000	0.50978000000000	Bi	(8c)
0.81160000000000	-0.07200000000000	0.16810000000000	In	(8c)
-0.81160000000000	0.07200000000000	0.16810000000000	In	(8c)
0.07200000000000	0.81160000000000	0.16810000000000	In	(8c)
-0.07200000000000	-0.81160000000000	0.16810000000000	In	(8c)
1.31160000000000	0.57200000000000	0.66810000000000	In	(8c)
-0.31160000000000	0.42800000000000	0.66810000000000	In	(8c)
0.57200000000000	-0.31160000000000	0.66810000000000	In	(8c)
0.42800000000000	1.31160000000000	0.66810000000000	In	(8c)

Tl<sub>4</sub>HgI<sub>6</sub>: AB6C<sub>4</sub>tP22\_104\_a\_2ac\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Tl4HgI6'
_chemical_formula_sum 'Hg I6 Tl4'

loop_
_publ_author_name
'D. V. Badikov'
'V. V. Badikov'
'G. M. {Kuz}'micheva'
'V. L. Panyutin'
'V. B. Rybakov'
'V. I. Chizhikov'
'G. S. Shevrydyayeva'
'E. S. Shcherbakova'
_journal_name_full_name
;
Inorganic Materials
;
_journal_volume 40
_journal_year 2004
_journal_page_first 314
_journal_page_last 320
_publ_section_title
;
Growth and X-ray diffraction study of TlS_{4}SHgIS_{6}$ crystals
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'TlS_{4}SHgIS_{6}$ Structure'
_aflow_proto 'AB6C4_tP22_104_a_2ac_c'
_aflow_params 'a, c/a, z_{1}, z_{2}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}'
↪ 5)
_aflow_params_values '9.3940153509, 0.981690440703, 0.786, 0.5, 0.0649,
↪ 0.8297, 0.6458, 0.286, 0.6491, 0.8588, 0.036'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP22'

_cell_length_a 9.3940153509
_cell_length_b 9.3940153509
_cell_length_c 9.2220150698
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4 n c"
_symmetry_Int_Tables_number 104

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -x, -y, z
3 -y, x, z
4 y, -x, z
5 -x+1/2, y+1/2, z+1/2
6 x+1/2, -y+1/2, z+1/2
7 y+1/2, x+1/2, z+1/2
8 -y+1/2, -x+1/2, z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Hg1 Hg 2 a 0.00000 0.00000 0.78600 1.00000
I1 I 2 a 0.00000 0.00000 0.50000 1.00000
I2 I 2 a 0.00000 0.00000 0.06490 1.00000
I3 I 8 c 0.82970 0.64580 0.28600 1.00000
Tl1 Tl 8 c 0.64910 0.85880 0.03600 1.00000
```

Tl<sub>4</sub>HgI<sub>6</sub>: AB6C<sub>4</sub>tP22\_104\_a\_2ac\_c - POSCAR

```
AB6C4_tP22_104_a_2ac_c & a, c/a, z1, z2, z3, x4, y4, z4, x5, y5, z5 --params=
↪ 9.3940153509, 0.981690440703, 0.786, 0.5, 0.0649, 0.8297, 0.6458,
↪ 0.286, 0.6491, 0.8588, 0.036 & P4nc C_{4v}^{6} #104 (a^3c^2) &
↪ tP22 & None & Tl4HgI6 & D. V. Badikov et al., Inorg. Mat. 40
↪ 314-320 (2004)
1.00000000000000
9.3940153509000 0.0000000000000 0.0000000000000
0.0000000000000 9.3940153509000 0.0000000000000
```

0.00000000000000	0.00000000000000	0.00000000000000	9.22201506980000
Hg	I	Tl	
2	12	8	
Direct			
0.00000000000000	0.00000000000000	0.78600000000000	Hg (2a)
0.50000000000000	0.50000000000000	1.28600000000000	Hg (2a)
0.00000000000000	0.00000000000000	0.50000000000000	I (2a)
0.50000000000000	0.50000000000000	1.00000000000000	I (2a)
0.00000000000000	0.00000000000000	0.06490000000000	I (2a)
0.50000000000000	0.50000000000000	0.56490000000000	I (2a)
0.82970000000000	0.64580000000000	0.28600000000000	I (8c)
-0.82970000000000	-0.64580000000000	0.28600000000000	I (8c)
-0.64580000000000	0.82970000000000	0.28600000000000	I (8c)
0.64580000000000	-0.82970000000000	0.28600000000000	I (8c)
1.32970000000000	-0.14580000000000	0.78600000000000	I (8c)
-0.32970000000000	1.14580000000000	0.78600000000000	I (8c)
-0.14580000000000	-0.32970000000000	0.78600000000000	I (8c)
1.14580000000000	1.32970000000000	0.78600000000000	I (8c)
0.64910000000000	0.85880000000000	0.03600000000000	Tl (8c)
-0.64910000000000	-0.85880000000000	0.03600000000000	Tl (8c)
-0.85880000000000	0.64910000000000	0.03600000000000	Tl (8c)
0.85880000000000	-0.64910000000000	0.03600000000000	Tl (8c)
1.14910000000000	-0.35880000000000	0.53600000000000	Tl (8c)
-0.14910000000000	1.35880000000000	0.53600000000000	Tl (8c)
-0.35880000000000	-0.14910000000000	0.53600000000000	Tl (8c)
1.35880000000000	1.14910000000000	0.53600000000000	Tl (8c)

BaGe<sub>2</sub>As<sub>2</sub>: A2BC2\_tP20\_105\_f\_ac\_2e - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'BaGe2As2'
_chemical_formula_sum 'As2 Ba Ge2'

loop_
_publ_author_name
'B. Eisenmann'
'H. Sch{\a}fer'
_journal_name_full_name
;
Zeitschrift f{\u}r Naturforschung B
;
_journal_volume 36
_journal_year 1981
_journal_page_first 415
_journal_page_last 419
_publ_section_title
;
Zintlphasen mit bin{\a}ren Anionen: Zur Kenntnis von BaGeS_{2}$PS_{2}$
↪ und BaGeS_{2}$As_{2}$ / Zintl Phases with Binary Anions:
↪ BaGeS_{2}$PS_{2}$ and BaGeS_{2}$As_{2}$
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'BaGeS_{2}$As_{2}$ Structure'
_aflow_proto 'A2BC2_tP20_105_f_ac_2e'
_aflow_params 'a, c/a, z_{1}, z_{2}, x_{3}, z_{3}, x_{4}, z_{4}, x_{5}, y_{5}, z_{5}'
↪ 5)
_aflow_params_values '7.7858653925, 1.11276650398, 0.0, 0.0241, 0.3351,
↪ 0.3664, 0.1632, 0.6068, 0.3453, 0.229, 0.2558'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP20'

_cell_length_a 7.7858653925
_cell_length_b 7.7858653925
_cell_length_c 8.6638502133
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 42 m c"
_symmetry_Int_Tables_number 105

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -x, -y, z
3 -y, x, z+1/2
4 y, -x, z+1/2
5 -x, y, z
6 x, -y, z
7 y, x, z+1/2
8 -y, -x, z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ba1 Ba 2 a 0.00000 0.00000 0.00000 1.00000
Ba2 Ba 2 c 0.00000 0.50000 0.02410 1.00000
Ge1 Ge 4 e 0.33510 0.50000 0.36640 1.00000
Ge2 Ge 4 e 0.16320 0.50000 0.60680 1.00000
As1 As 8 f 0.34530 0.22900 0.25580 1.00000
```

BaGe<sub>2</sub>As<sub>2</sub>: A2BC2\_tP20\_105\_f\_ac\_2e - POSCAR

```
A2BC2_tP20_105_f_ac_2e & a, c/a, z1, z2, x3, z3, x4, z4, x5, y5, z5 --params=
↳ 7.7858653925, 1.11276650398, 0.0, 0.0241, 0.3351, 0.3664, 0.1632,
↳ 0.6068, 0.3453, 0.229, 0.2558 & P4_2]mc C_{4v}^{[7]} #105 (ace^2f)
↳ & tP20 & None & BaGe2As2 & B. Eisenmann and H. Sch[{}]afer,
↳ Z. Naturforsch. B 36, 415-419 (1981)
1.000000000000000
7.78586539250000 0.00000000000000 0.00000000000000
0.00000000000000 7.78586539250000 0.00000000000000
0.00000000000000 0.00000000000000 8.66385021330000
As Ba Ge
8 4 8
Direct
0.345300000000000 0.229000000000000 0.255800000000000 As (8f)
-0.345300000000000 -0.229000000000000 0.255800000000000 As (8f)
-0.229000000000000 0.345300000000000 0.755800000000000 As (8f)
0.229000000000000 -0.345300000000000 0.755800000000000 As (8f)
0.345300000000000 -0.229000000000000 0.255800000000000 As (8f)
-0.345300000000000 0.229000000000000 0.255800000000000 As (8f)
-0.229000000000000 -0.345300000000000 0.755800000000000 As (8f)
0.229000000000000 0.345300000000000 0.755800000000000 As (8f)
0.000000000000000 0.000000000000000 0.000000000000000 Ba (2a)
0.000000000000000 0.000000000000000 0.500000000000000 Ba (2a)
0.000000000000000 0.500000000000000 0.024100000000000 Ba (2c)
0.500000000000000 0.000000000000000 0.524100000000000 Ba (2c)
0.335100000000000 0.500000000000000 0.366400000000000 Ge (4e)
-0.335100000000000 0.500000000000000 0.366400000000000 Ge (4e)
0.500000000000000 0.000000000000000 0.866400000000000 Ge (4e)
0.500000000000000 -0.335100000000000 0.866400000000000 Ge (4e)
0.500000000000000 0.500000000000000 0.606800000000000 Ge (4e)
-0.163200000000000 0.500000000000000 0.606800000000000 Ge (4e)
-0.163200000000000 0.500000000000000 1.106800000000000 Ge (4e)
0.500000000000000 -0.163200000000000 1.106800000000000 Ge (4e)
0.500000000000000 -0.163200000000000 1.106800000000000 Ge (4e)
```

NaZn[OH]<sub>3</sub>: A3BC3D\_tP64\_106\_3c\_c\_3c\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'NaZn[OH]3'
_chemical_formula_sum 'H3 Na O3 Zn'

loop_
_publ_author_name
'R. Stahl'
'H. Jacobs'
_journal_name_full_name
;
Zeitschrift fur Anorganische und Allgemeine Chemie
;
_journal_volume 624
_journal_year 1998
_journal_page_first 25
_journal_page_last 29
_publ_section_title
;
Synthese und Kristallstruktur von NaZn(OH)3
↳ 3HS_2]SO und NaZn(OH)3]
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'NaZn[OH]3] Structure'
_aflow_proto 'A3BC3D_tP64_106_3c_c_3c_c'
_aflow_params 'a, c/a, x_{1}, y_{1}, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}, x_{7}, y_{7}, z_{7}, x_{8}, y_{8}, z_{8}'
_aflow_params_values '10.8312004139, 0.492105992062, 0.836, 0.614, 0.2, 0.531, 0.845, 0.11, 0.858, 0.825, 0.08, 0.5929, 0.62036, 0.0343, 0.8146, 0.6194, 0.0688, 0.5681, 0.8298, 0.1322, 0.8669, -0.0994, 0.0636, 0.69285, -0.05677, 0.0'
_aflow_strukturbericht 'None'
_aflow_pearson 'tP64'

_cell_length_a 10.8312004139
_cell_length_b 10.8312004139
_cell_length_c 5.3300986249
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'P 42 b c'
_symmetry_Int_Tables_number 106

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -x, -y, z
3 -y, x, z+1/2
4 y, -x, z+1/2
5 -x+1/2, y+1/2, z
6 x+1/2, -y+1/2, z
7 y+1/2, x+1/2, z+1/2
8 -y+1/2, -x+1/2, z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

```
_atom_site_occupancy
H1 H 8 c 0.83600 0.61400 0.20000 1.00000
H2 H 8 c 0.53100 0.84500 0.11000 1.00000
H3 H 8 c 0.85800 0.82500 0.08000 1.00000
Na1 Na 8 c 0.59290 0.62036 0.03430 1.00000
O1 O 8 c 0.81460 0.61940 0.06880 1.00000
O2 O 8 c 0.56810 0.82980 0.13220 1.00000
O3 O 8 c 0.86690 -0.09940 0.06360 1.00000
Zn1 Zn 8 c 0.69285 -0.05677 0.00000 1.00000
```

NaZn[OH]<sub>3</sub>: A3BC3D\_tP64\_106\_3c\_c\_3c\_c - POSCAR

```
A3BC3D_tP64_106_3c_c_3c_c & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5,
y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8 --params=10.8312004139,
0.492105992062, 0.836, 0.614, 0.2, 0.531, 0.845, 0.11, 0.858, 0.825,
0.08, 0.5929, 0.62036, 0.0343, 0.8146, 0.6194, 0.0688, 0.5681, 0.8298,
0.1322, 0.8669, -0.0994, 0.0636, 0.69285, -0.05677, 0.0 & P4_2]bc C_
[4v]^{[8]} #106 (c^8) & tP64 & None & NaZn[OH]3] & R. Stahl and
H. Jacobs, Z. Anorg. Allg. Chem. 624, 25-29 (1998)
1.000000000000000
10.83120041390000 0.00000000000000 0.00000000000000
0.00000000000000 10.83120041390000 0.00000000000000
0.00000000000000 0.00000000000000 5.33009862490000
H Na O Zn
24 8 24 8
Direct
0.836000000000000 0.614000000000000 0.200000000000000 H (8c)
-0.836000000000000 -0.614000000000000 0.200000000000000 H (8c)
-0.614000000000000 0.836000000000000 0.700000000000000 H (8c)
0.614000000000000 -0.836000000000000 0.700000000000000 H (8c)
1.336000000000000 -0.114000000000000 0.200000000000000 H (8c)
-0.336000000000000 1.114000000000000 0.200000000000000 H (8c)
-0.114000000000000 -0.336000000000000 0.700000000000000 H (8c)
1.114000000000000 0.336000000000000 0.700000000000000 H (8c)
0.531000000000000 0.845000000000000 0.110000000000000 H (8c)
-0.531000000000000 -0.845000000000000 0.110000000000000 H (8c)
-0.845000000000000 0.531000000000000 0.610000000000000 H (8c)
0.845000000000000 -0.531000000000000 0.610000000000000 H (8c)
1.031000000000000 -0.345000000000000 0.110000000000000 H (8c)
-0.031000000000000 1.345000000000000 0.110000000000000 H (8c)
-0.345000000000000 -0.031000000000000 0.610000000000000 H (8c)
1.345000000000000 1.031000000000000 0.610000000000000 H (8c)
0.858000000000000 0.825000000000000 0.080000000000000 H (8c)
-0.858000000000000 -0.825000000000000 0.080000000000000 H (8c)
0.825000000000000 -0.858000000000000 0.580000000000000 H (8c)
-0.825000000000000 0.858000000000000 0.580000000000000 H (8c)
1.358000000000000 -0.325000000000000 0.080000000000000 H (8c)
-0.358000000000000 1.325000000000000 0.080000000000000 H (8c)
-0.325000000000000 -0.358000000000000 0.580000000000000 H (8c)
1.325000000000000 1.358000000000000 0.580000000000000 H (8c)
0.592900000000000 0.620360000000000 0.034300000000000 Na (8c)
-0.592900000000000 -0.620360000000000 0.034300000000000 Na (8c)
-0.620360000000000 0.592900000000000 0.534300000000000 Na (8c)
0.620360000000000 -0.592900000000000 0.534300000000000 Na (8c)
1.092900000000000 -0.120360000000000 0.034300000000000 Na (8c)
-0.092900000000000 1.120360000000000 0.034300000000000 Na (8c)
1.120360000000000 1.092900000000000 0.534300000000000 Na (8c)
0.814600000000000 0.619400000000000 0.068800000000000 O (8c)
-0.814600000000000 -0.619400000000000 0.068800000000000 O (8c)
-0.619400000000000 0.814600000000000 0.568800000000000 O (8c)
0.619400000000000 -0.814600000000000 0.568800000000000 O (8c)
1.314600000000000 -0.119400000000000 0.068800000000000 O (8c)
-0.314600000000000 1.119400000000000 0.068800000000000 O (8c)
-0.119400000000000 -0.314600000000000 0.568800000000000 O (8c)
1.119400000000000 1.314600000000000 0.568800000000000 O (8c)
0.568100000000000 0.829800000000000 0.132200000000000 O (8c)
-0.568100000000000 -0.829800000000000 0.132200000000000 O (8c)
-0.829800000000000 0.568100000000000 0.632200000000000 O (8c)
0.829800000000000 -0.568100000000000 0.632200000000000 O (8c)
1.068100000000000 -0.329800000000000 0.132200000000000 O (8c)
-0.068100000000000 1.329800000000000 0.132200000000000 O (8c)
-0.329800000000000 -0.068100000000000 0.632200000000000 O (8c)
1.329800000000000 1.068100000000000 0.632200000000000 O (8c)
0.866900000000000 -0.099400000000000 0.063600000000000 O (8c)
-0.866900000000000 0.099400000000000 0.063600000000000 O (8c)
0.099400000000000 0.866900000000000 0.563600000000000 O (8c)
-0.099400000000000 -0.866900000000000 0.563600000000000 O (8c)
1.366900000000000 0.599400000000000 0.063600000000000 O (8c)
-0.366900000000000 0.400600000000000 0.063600000000000 O (8c)
0.599400000000000 -0.366900000000000 0.563600000000000 O (8c)
0.400600000000000 1.366900000000000 0.563600000000000 O (8c)
0.692850000000000 -0.056770000000000 0.000000000000000 Zn (8c)
-0.692850000000000 0.056770000000000 0.000000000000000 Zn (8c)
0.056770000000000 0.692850000000000 0.500000000000000 Zn (8c)
-0.056770000000000 -0.692850000000000 0.500000000000000 Zn (8c)
1.192850000000000 0.556770000000000 0.000000000000000 Zn (8c)
-0.192850000000000 0.443230000000000 0.000000000000000 Zn (8c)
0.556770000000000 -0.192850000000000 0.500000000000000 Zn (8c)
0.443230000000000 1.192850000000000 0.500000000000000 Zn (8c)
```

Co<sub>5</sub>Ge<sub>7</sub>: A5B7\_t24\_107\_ac\_abd - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Co5Ge7'
_chemical_formula_sum 'Co5 Ge7'

loop_
_publ_author_name
'K. Schubert'
'T. R. Anantharaman'
'H. O. K. Ata'
```

```

'H. G. Meissner '
'M. P{\o}tzschke '
'W. Rossteutscher '
'E. Stolz '
_journal_name_full_name
;
Naturwissenschaften
;
_journal_volume 47
_journal_year 1960
_journal_page_first 512
_journal_page_last 512
_publ_Section_title
;
Einige strukturelle Ergebnisse an metallischen Phasen (6)
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'Co$_{5}$Ge$_{7}$ Structure '
_aflow_proto 'A5B7_tI24_107_ac_abd'
_aflow_params 'a,c/a,z_{1},z_{2},z_{3},x_{4},z_{4},x_{5},z_{5}'
_aflow_params_values '7.6400197048,0.760471204184,0.0,0.056,0.04,0.22,
↪ 0.0,0.243,0.29'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tI24'

_cell_length_a 7.6400197048
_cell_length_b 7.6400197048
_cell_length_c 5.8100149849
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 4 m m"
_symmetry_Int_Tables_number 107

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z
9 x+1/2,y+1/2,z+1/2
10 -x+1/2,-y+1/2,z+1/2
11 -y+1/2,x+1/2,z+1/2
12 y+1/2,-x+1/2,z+1/2
13 -x+1/2,y+1/2,z+1/2
14 x+1/2,-y+1/2,z+1/2
15 y+1/2,x+1/2,z+1/2
16 -y+1/2,-x+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Co1 Co 2 a 0.00000 0.00000 0.00000 1.00000
Ge1 Ge 2 a 0.00000 0.00000 0.05600 1.00000
Ge2 Ge 4 b 0.00000 0.50000 0.04000 1.00000
Co2 Co 8 c 0.22000 0.22000 0.00000 1.00000
Ge3 Ge 8 d 0.24300 0.00000 0.29000 1.00000

```

Co<sub>5</sub>Ge<sub>7</sub>: A5B7\_tI24\_107\_ac\_abd - POSCAR

```

A5B7_tI24_107_ac_abd & a,c/a,z1,z2,z3,x4,z4,x5,z5 --params=7.6400197048,
↪ 0.760471204184,0.0,0.056,0.04,0.22,0.0,0.243,0.29 & 14mm C_{4v}
↪ ]^{(9)} #107 (a^2bcd) & tI24 & None & Co5Ge7 & & K. Schubert et
↪ al., {Naturwissenschaften 47, 512(1960)}
1.000000000000000
-3.82000985240000 3.82000985240000 2.90500749245000
3.82000985240000 -3.82000985240000 2.90500749245000
3.82000985240000 3.82000985240000 -2.90500749245000
Co Ge
5 7
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Co (2a)
0.22000000000000 0.22000000000000 0.44000000000000 Co (8c)
-0.22000000000000 -0.22000000000000 -0.44000000000000 Co (8c)
0.22000000000000 -0.22000000000000 0.00000000000000 Co (8c)
-0.22000000000000 0.22000000000000 0.00000000000000 Co (8c)
0.05600000000000 0.05600000000000 0.00000000000000 Ge (2a)
0.54000000000000 0.04000000000000 0.50000000000000 Ge (4b)
0.04000000000000 0.54000000000000 0.50000000000000 Ge (4b)
0.29000000000000 0.53300000000000 0.24300000000000 Ge (8d)
0.29000000000000 0.04700000000000 -0.24300000000000 Ge (8d)
0.53300000000000 0.29000000000000 0.24300000000000 Ge (8d)
0.04700000000000 0.29000000000000 -0.24300000000000 Ge (8d)

```

GeP (High-pressure, superconducting): AB\_tI4\_107\_a\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Sr5Si3'
_chemical_formula_sum 'Si3 Sr5'
loop_
_publ_author_name
'G. Nagorsen '
'G. Rockt{"a}schel '
'H. Sch{"a}fer '
'A. Weiss '
_journal_name_full_name

```

```

_chemical_name_mineral 'GeP'
_chemical_formula_sum 'Ge P'

loop_
_publ_author_name
'P. C. Donohue '
'H. S. Young '
_journal_name_full_name
;
Journal of Solid State Chemistry
;
_journal_volume 1
_journal_year 1970
_journal_page_first 143
_journal_page_last 149
_publ_Section_title
;
Synthesis, structure, and superconductivity of new high pressure phases
↪ in the systems Ge-P and Ge-As
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'GeP (High-pressure, superconducting) Structure '
_aflow_proto 'AB_tI4_107_a_a'
_aflow_params 'a,c/a,z_{1},z_{2}'
_aflow_params_values '3.5440505103,1.57477426639,0.0,0.427'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tI4'

_cell_length_a 3.5440505103
_cell_length_b 3.5440505103
_cell_length_c 5.5810795424
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 4 m m"
_symmetry_Int_Tables_number 107

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z
9 x+1/2,y+1/2,z+1/2
10 -x+1/2,-y+1/2,z+1/2
11 -y+1/2,x+1/2,z+1/2
12 y+1/2,-x+1/2,z+1/2
13 -x+1/2,y+1/2,z+1/2
14 x+1/2,-y+1/2,z+1/2
15 y+1/2,x+1/2,z+1/2
16 -y+1/2,-x+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ge1 Ge 2 a 0.00000 0.00000 0.00000 1.00000
P1 P 2 a 0.00000 0.00000 0.42700 1.00000

```

GeP (High-pressure, superconducting): AB\_tI4\_107\_a\_a - POSCAR

```

AB_tI4_107_a_a & a,c/a,z1,z2 --params=3.5440505103,1.57477426639,0.0,
↪ 0.427 & 14mm C_{4v}^{(9)} #107 (a^2) & tI4 & None & GeP & & P.
↪ C. Donohue and H. S. Young, J. Solid State Chem. 1, 143-149 (
↪ 1970)
1.000000000000000
-1.77202525515000 1.77202525515000 2.79053977120000
1.77202525515000 -1.77202525515000 2.79053977120000
1.77202525515000 1.77202525515000 -2.79053977120000
Ge P
1 1
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Ge (2a)
0.42700000000000 0.42700000000000 0.00000000000000 P (2a)

```

Sr<sub>5</sub>Si<sub>3</sub>: A3B5\_tI32\_108\_ac\_a2c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Sr5Si3'
_chemical_formula_sum 'Si3 Sr5'
loop_
_publ_author_name
'G. Nagorsen '
'G. Rockt{"a}schel '
'H. Sch{"a}fer '
'A. Weiss '
_journal_name_full_name

```



```

;
Zeitschrift f{"u}r Naturforschung B
;
_journal_volume 22
_journal_year 1967
_journal_page_first 101
_journal_page_last 102
_publ_section_title
;
Die Kristallstruktur der Phase SrS_{5}Si_{3}S
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'SrS_{5}Si_{3}S Structure'
_aflow_proto 'A3B5_t132_108_ac_a2c'
_aflow_params 'a,c/a,z_{1},z_{2},x_{3},z_{3},x_{4},z_{4},x_{5},z_{5}'
_aflow_params_values '8.0549870847,1.94761018001,0.007,0.75,0.109,0.257,
↳ 0.676,0.114,0.676,0.4'
_aflow_strukturbericht 'None'
_aflow_pearson 't132'

_cell_length_a 8.0549870847
_cell_length_b 8.0549870847
_cell_length_c 15.6879748460
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 4 c m"
_symmetry_Int_Tables_number 108

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z+1/2
6 x,-y,z+1/2
7 y,x,z+1/2
8 -y,-x,z+1/2
9 x+1/2,y+1/2,z+1/2
10 -x+1/2,-y+1/2,z+1/2
11 -y+1/2,x+1/2,z+1/2
12 y+1/2,-x+1/2,z+1/2
13 -x+1/2,y+1/2,z
14 x+1/2,-y+1/2,z
15 y+1/2,x+1/2,z
16 -y+1/2,-x+1/2,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Si1 Si 4 a 0.00000 0.00000 0.00700 1.00000
Sr1 Sr 4 a 0.00000 0.00000 0.75000 1.00000
Si2 Si 8 c 0.10900 0.60900 0.25700 1.00000
Sr2 Sr 8 c 0.67600 0.17600 0.11400 1.00000
Sr3 Sr 8 c 0.67600 0.17600 0.40000 1.00000

```

Sr<sub>5</sub>Si<sub>3</sub>: A3B5\_t132\_108\_ac\_a2c - POSCAR

```

A3B5_t132_108_ac_a2c & a,c/a,z1,z2,x3,z3,x4,z4,x5,z5 --params=
↳ 8.0549870847,1.94761018001,0.007,0.75,0.109,0.257,0.676,0.114,
↳ 0.676,0.4 & 14cm C_{4v}^{10} #108 (a^2c^3) & t132 & None &
↳ Sr5Si3 & G. Nagorsen et al., Z. Naturforsch. B 22, 101-102 (
↳ 1967)
1.0000000000000000
-4.02749354235000 4.02749354235000 7.84398742300000
4.02749354235000 -4.02749354235000 7.84398742300000
4.02749354235000 4.02749354235000 -7.84398742300000
Si Sr
6 10
Direct
0.0070000000000000 0.0070000000000000 0.0000000000000000 Si (4a)
0.5070000000000000 0.5070000000000000 0.0000000000000000 Si (4a)
0.8660000000000000 0.3660000000000000 0.7180000000000000 Si (8c)
0.6480000000000000 0.1480000000000000 0.2820000000000000 Si (8c)
0.3660000000000000 0.6480000000000000 0.5000000000000000 Si (8c)
0.1480000000000000 0.8660000000000000 0.5000000000000000 Si (8c)
0.7500000000000000 0.7500000000000000 0.0000000000000000 Sr (4a)
1.2500000000000000 1.2500000000000000 0.0000000000000000 Sr (4a)
1.2900000000000000 0.7900000000000000 1.8520000000000000 Sr (8c)
-0.0620000000000000 -0.5620000000000000 -0.8520000000000000 Sr (8c)
0.7900000000000000 -0.0620000000000000 0.5000000000000000 Sr (8c)
-0.5620000000000000 1.2900000000000000 0.5000000000000000 Sr (8c)
1.5760000000000000 1.0760000000000000 1.8520000000000000 Sr (8c)
0.2240000000000000 -0.2760000000000000 -0.8520000000000000 Sr (8c)
1.0760000000000000 0.2240000000000000 0.5000000000000000 Sr (8c)
-0.2760000000000000 1.5760000000000000 0.5000000000000000 Sr (8c)

```

LaPtSi: ABC\_t112\_109\_a\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

```

```

_chemical_name_mineral 'LaPtSi'
_chemical_formula_sum 'La Pt Si'

loop_
_publ_author_name
'K. Klepp'
'E. Parth{\`e}'
_journal_name_full_name
;
Acta Crystallographica Section B: Structural Science
;
_journal_volume 38
_journal_year 1982
_journal_page_first 1105
_journal_page_last 1108
_publ_section_title
;
SRSPtSi phases (SRS = La, Ce, Pr, Nd, Sm and Gd) with an ordered ThSiS_{2} derivative structure
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'LaPtSi Structure'
_aflow_proto 'ABC_t112_109_a_a_a'
_aflow_params 'a,c/a,z_{1},z_{2},z_{3}'
_aflow_params_values '4.2490694941,3.42174629325,0.081,0.666,0.5'
_aflow_strukturbericht 'None'
_aflow_pearson 't112'

_cell_length_a 4.2490694941
_cell_length_b 4.2490694941
_cell_length_c 14.5392377912
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 41 m d"
_symmetry_Int_Tables_number 109

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x+1/2,z+1/4
4 y,-x+1/2,z+1/4
5 -x,y,z
6 x,-y,z
7 y,x+1/2,z+1/4
8 -y,-x+1/2,z+1/4
9 x+1/2,y+1/2,z+1/2
10 -x+1/2,-y+1/2,z+1/2
11 -y+1/2,x,z+3/4
12 y+1/2,-x,z+3/4
13 -x+1/2,y+1/2,z+1/2
14 x+1/2,-y+1/2,z+1/2
15 y+1/2,x,z+3/4
16 -y+1/2,-x,z+3/4

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
La1 La 4 a 0.00000 0.00000 0.08100 1.00000
Pt1 Pt 4 a 0.00000 0.00000 0.66600 1.00000
Si1 Si 4 a 0.00000 0.00000 0.50000 1.00000

```

LaPtSi: ABC\_t112\_109\_a\_a - POSCAR

```

ABC_t112_109_a_a_a & a,c/a,z1,z2,z3 --params=4.2490694941,3.42174629325,
↳ 0.081,0.666,0.5 & 14_{1}md C_{4v}^{11} #109 (a^3) & t112 & None
↳ & LaPtSi & K. Klepp and E. Parth{\`e}, Acta Crystallogr.
↳ Sect. B Struct. Sci. 38, 1105-1108 (1982)
1.0000000000000000
-2.12453474705000 2.12453474705000 7.26961889560000
2.12453474705000 -2.12453474705000 7.26961889560000
2.12453474705000 2.12453474705000 -7.26961889560000
La Pt Si
2 2 2
Direct
0.0810000000000000 0.0810000000000000 0.0000000000000000 La (4a)
0.8310000000000000 0.3310000000000000 0.5000000000000000 La (4a)
0.6660000000000000 0.6660000000000000 0.0000000000000000 Pt (4a)
1.4160000000000000 0.9160000000000000 0.5000000000000000 Pt (4a)
0.5000000000000000 0.5000000000000000 0.0000000000000000 Si (4a)
1.2500000000000000 0.7500000000000000 0.5000000000000000 Si (4a)

```

NbAs: AB\_t18\_109\_a\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'NbAs'
_chemical_formula_sum 'As Nb'

loop_
_publ_author_name

```

```
'S. Furuseth'
'A. Kjekshus'
_journal_name_full_name
;
Acta Chemica Scandinavica
;
_journal_volume 18
_journal_year 1964
_journal_page_first 1180
_journal_page_last 1195
_publ_Section_title
;
On the Arsenides and Antimonides of Niobium
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'NbAs Structure'
_aflow_proto 'AB_t18_109_a_a'
_aflow_params 'a,c/a,z_{1},z_{2}'
_aflow_params_values '3.4517145504,3.38383984705,0.5416,0.5'
_aflow_Strukturbericht 'None'
_aflow_Pearson 't18'

_cell_length_a 3.4517145504
_cell_length_b 3.4517145504
_cell_length_c 11.6800492363
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I 41 m d"
_symmetry_Int_Tables_number 109

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x+1/2,z+1/4
4 y,-x+1/2,z+1/4
5 -x,y,z
6 x,-y,z
7 y,x+1/2,z+1/4
8 -y,-x+1/2,z+1/4
9 x+1/2,y+1/2,z+1/2
10 -x+1/2,-y+1/2,z+1/2
11 -y+1/2,x,z+3/4
12 y+1/2,-x,z+3/4
13 -x+1/2,y+1/2,z+1/2
14 x+1/2,-y+1/2,z+1/2
15 y+1/2,x,z+3/4
16 -y+1/2,-x,z+3/4

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
As1 As 4 a 0.00000 0.00000 0.54160 1.00000
Nb1 Nb 4 a 0.00000 0.00000 0.50000 1.00000
```

NbAs: AB\_t18\_109\_a\_a - POSCAR

```
AB_t18_109_a_a & a,c/a,z1,z2 --params=3.4517145504,3.38383984705,0.5416,
↳ 0.5 & I4_{1}md C_{4v}^{11} #109 (a^2) & t18 & None & NbAs & &
↳ S. Furuseth and A. Kjekshus, Acta Chem. Scand. 18, 1180-1195 (
↳ 1964)
1.0000000000000000
-1.72585727520000 1.72585727520000 5.84002461815000
1.72585727520000 -1.72585727520000 5.84002461815000
1.72585727520000 1.72585727520000 -5.84002461815000
As Nb
2 2
Direct
0.541600000000000 0.541600000000000 0.000000000000000 As (4a)
1.291600000000000 0.791600000000000 0.500000000000000 As (4a)
0.500000000000000 0.500000000000000 0.000000000000000 Nb (4a)
1.250000000000000 0.750000000000000 0.500000000000000 Nb (4a)
```

Be[BH<sub>4</sub>]<sub>2</sub>: A2BC8\_t176\_110\_2b\_b\_8b - CIF

```
# CIF file# This file was generated by FINDSYM
# Harold T. Stokes, Branton J. Campbell, Dorian M. Hatch
# Brigham Young University, Provo, Utah, USA

data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Be[BH4]2'
_chemical_formula_sum 'B2 Be H8'

loop_
_publ_author_name
'D. S. Marynick'
'W. N. Lipscomb'
_journal_name_full_name
;
Inorganic Chemistry
;
```

```
_journal_volume 11
_journal_year 1972
_journal_page_first 820
_journal_page_last 823
_publ_Section_title
;
Crystal structure of beryllium borohydride
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'Be[BH4]2 Structure'
_aflow_proto 'A2BC8_t176_110_2b_b_8b'
_aflow_params 'a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},
↳ x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},
↳ y_{7},z_{7},x_{8},y_{8},z_{8},x_{9},y_{9},z_{9},x_{10},y_{10},
↳ z_{10},x_{11},y_{11},z_{11}'
_aflow_params_values '13.62003,0.668135092213,0.5491,0.8362,0.259,0.8065
↳ ,0.6386,0.3704,0.1998,0.0869,0.0,0.5687,-0.0955,0.3098,0.6012,
↳ 0.7807,0.2082,0.5033,0.7931,0.3482,0.6413,0.5083,0.4159,0.8436,
↳ 0.6054,0.2752,0.8374,0.7122,0.3904,0.7286,0.645,0.3515,0.815,
↳ 0.5899,0.4761'
_aflow_Strukturbericht 'None'
_aflow_Pearson 't176'

_symmetry_space_group_name_H-M "I 41 c d"
_symmetry_Int_Tables_number 110

_cell_length_a 13.62003
_cell_length_b 13.62003
_cell_length_c 9.10002
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x+1/2,z+1/4
4 y,-x+1/2,z+1/4
5 -x,y,z+1/2
6 x,-y,z+1/2
7 y+1/2,x,z+1/4
8 -y+1/2,-x,z+1/4
9 x+1/2,y+1/2,z+1/2
10 -x+1/2,-y+1/2,z+1/2
11 -y+1/2,x,z+3/4
12 y+1/2,-x,z+3/4
13 -x+1/2,y+1/2,z
14 x+1/2,-y+1/2,z
15 y,x+1/2,z+3/4
16 -y,-x+1/2,z+3/4

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
B1 B 16 b 0.54910 0.83620 0.25900 1.00000
B2 B 16 b 0.80650 0.63860 0.37040 1.00000
Be1 Be 16 b 0.19980 0.08690 0.00000 1.00000
H1 H 16 b 0.56870 -0.09550 0.30980 1.00000
H2 H 16 b 0.60120 0.78070 0.20820 1.00000
H3 H 16 b 0.50330 0.79310 0.34820 1.00000
H4 H 16 b 0.64130 0.50830 0.41590 1.00000
H5 H 16 b 0.84360 0.60540 0.27520 1.00000
H6 H 16 b 0.83740 0.71220 0.39040 1.00000
H7 H 16 b 0.72860 0.64500 0.35150 1.00000
H8 H 16 b 0.81500 0.58990 0.47610 1.00000
```

Be[BH<sub>4</sub>]<sub>2</sub>: A2BC8\_t176\_110\_2b\_b\_8b - POSCAR

```
A2BC8_t176_110_2b_b_8b & a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,
↳ y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11,y11,
↳ z11 --params=13.62003,0.668135092213,0.5491,0.8362,0.259,0.8065
↳ ,0.6386,0.3704,0.1998,0.0869,0.0,0.5687,-0.0955,0.3098,0.6012,
↳ 0.7807,0.2082,0.5033,0.7931,0.3482,0.6413,0.5083,0.4159,0.8436,
↳ 0.6054,0.2752,0.8374,0.7122,0.3904,0.7286,0.645,0.3515,0.815,
↳ 0.5899,0.4761 & I4_{1}cd C_{4v}^{12} #110 (b^11) & t176 & None
↳ & Be[BH4]2 & D. S. Marynick and W. N. Lipscomb, Inorg.
↳ Chem. 11, 820-823 (1972)
1.0000000000000000
-6.810015000000000 6.810015000000000 4.550010000000000
6.810015000000000 -6.810015000000000 4.550010000000000
6.810015000000000 6.810015000000000 -4.550010000000000
B B H
16 8 64
Direct
1.095200000000000 0.808100000000000 1.385300000000000 B (16b)
-0.577200000000000 -0.290100000000000 -1.385300000000000 B (16b)
1.558100000000000 -0.327200000000000 0.212900000000000 B (16b)
0.459900000000000 1.345200000000000 0.787100000000000 B (16b)
-0.077200000000000 1.308100000000000 -0.287100000000000 B (16b)
1.595200000000000 0.209900000000000 0.287100000000000 B (16b)
-0.040100000000000 0.172800000000000 -0.885300000000000 B (16b)
1.058100000000000 1.845200000000000 1.885300000000000 B (16b)
1.009000000000000 1.176900000000000 1.445100000000000 B (16b)
-0.268200000000000 -0.436100000000000 -1.445100000000000 B (16b)
```

```
1.9269000000000000 -0.0182000000000000 0.6679000000000000 B (16b)
0.3139000000000000 1.2590000000000000 0.3321000000000000 B (16b)
0.2318000000000000 1.6769000000000000 0.1679000000000000 B (16b)
1.5090000000000000 0.0639000000000000 -0.1679000000000000 B (16b)
-0.1861000000000000 0.4818000000000000 -0.9451000000000000 B (16b)
1.4269000000000000 1.7590000000000000 1.9451000000000000 B (16b)
0.0869000000000000 0.1998000000000000 0.2867000000000000 Be (16b)
-0.0869000000000000 -0.1998000000000000 -0.2867000000000000 Be (16b)
0.9498000000000000 0.1631000000000000 0.6129000000000000 Be (16b)
0.5502000000000000 0.3369000000000000 0.3871000000000000 Be (16b)
0.4131000000000000 0.6998000000000000 0.1129000000000000 Be (16b)
0.5869000000000000 0.3002000000000000 -0.1129000000000000 Be (16b)
0.0502000000000000 0.6631000000000000 0.2133000000000000 Be (16b)
0.4498000000000000 0.8369000000000000 0.7867000000000000 Be (16b)
0.2143000000000000 0.8785000000000000 0.4732000000000000 H (16b)
0.4053000000000000 -0.2589000000000000 -0.4732000000000000 H (16b)
1.6285000000000000 0.6553000000000000 1.1642000000000000 H (16b)
0.4911000000000000 0.4643000000000000 -0.1642000000000000 H (16b)
0.9053000000000000 1.3785000000000000 0.6642000000000000 H (16b)
0.7143000000000000 0.2411000000000000 -0.6642000000000000 H (16b)
-0.0089000000000000 1.1553000000000000 0.0268000000000000 H (16b)
1.1285000000000000 0.9643000000000000 0.9732000000000000 H (16b)
0.9889000000000000 0.8094000000000000 1.3819000000000000 H (16b)
-0.5725000000000000 -0.3930000000000000 -1.3819000000000000 H (16b)
1.5594000000000000 -0.3225000000000000 0.3205000000000000 H (16b)
0.3570000000000000 1.2389000000000000 0.6795000000000000 H (16b)
-0.0725000000000000 1.3094000000000000 -0.1795000000000000 H (16b)
1.4889000000000000 0.1070000000000000 0.1795000000000000 H (16b)
-0.1430000000000000 0.1775000000000000 -0.8819000000000000 H (16b)
1.0594000000000000 1.7389000000000000 1.8819000000000000 H (16b)
1.1413000000000000 0.8515000000000000 1.2964000000000000 H (16b)
-0.4449000000000000 -0.1551000000000000 -1.2964000000000000 H (16b)
1.6015000000000000 -0.1949000000000000 0.2102000000000000 H (16b)
0.5949000000000000 1.3913000000000000 0.7898000000000000 H (16b)
0.0551000000000000 1.3515000000000000 -0.2898000000000000 H (16b)
1.6413000000000000 0.3449000000000000 0.2898000000000000 H (16b)
0.0949000000000000 0.3051000000000000 -0.7964000000000000 H (16b)
1.1015000000000000 1.8913000000000000 1.7964000000000000 H (16b)
0.9242000000000000 1.0572000000000000 1.1496000000000000 H (16b)
-0.0924000000000000 -0.2254000000000000 -1.1496000000000000 H (16b)
1.8072000000000000 0.1576000000000000 0.6330000000000000 H (16b)
0.5246000000000000 1.1742000000000000 0.3670000000000000 H (16b)
0.4076000000000000 1.1572000000000000 0.1330000000000000 H (16b)
1.4242000000000000 0.2746000000000000 -0.1330000000000000 H (16b)
0.0246000000000000 0.6576000000000000 -0.6496000000000000 H (16b)
1.3072000000000000 1.6742000000000000 1.6496000000000000 H (16b)
0.8806000000000000 1.1188000000000000 1.4490000000000000 H (16b)
-0.3302000000000000 -0.5684000000000000 -1.4490000000000000 H (16b)
1.8688000000000000 -0.0802000000000000 0.7382000000000000 H (16b)
0.1816000000000000 1.1306000000000000 0.2618000000000000 H (16b)
0.1698000000000000 1.6188000000000000 0.2382000000000000 H (16b)
1.3806000000000000 -0.0684000000000000 -0.2382000000000000 H (16b)
-0.3184000000000000 0.4198000000000000 -0.9490000000000000 H (16b)
1.3688000000000000 1.6306000000000000 1.9490000000000000 H (16b)
1.1026000000000000 1.2278000000000000 1.5496000000000000 H (16b)
-0.3218000000000000 -0.4470000000000000 -1.5496000000000000 H (16b)
1.9778000000000000 -0.0718000000000000 0.6252000000000000 H (16b)
0.3030000000000000 1.3526000000000000 0.3748000000000000 H (16b)
0.1782000000000000 0.1727800000000000 0.1252000000000000 H (16b)
1.6026000000000000 0.0530000000000000 -0.1252000000000000 H (16b)
-0.1970000000000000 0.4282000000000000 -1.0496000000000000 H (16b)
1.4778000000000000 1.8526000000000000 2.0496000000000000 H (16b)
0.9965000000000000 1.0801000000000000 1.3736000000000000 H (16b)
-0.2935000000000000 -0.3771000000000000 -1.3736000000000000 H (16b)
1.8301000000000000 -0.0435000000000000 0.5836000000000000 H (16b)
0.3729000000000000 1.2465000000000000 0.4164000000000000 H (16b)
0.2065000000000000 1.5801000000000000 0.0836000000000000 H (16b)
1.4965000000000000 0.1229000000000000 -0.0836000000000000 H (16b)
-0.1271000000000000 0.4565000000000000 -0.8736000000000000 H (16b)
1.3301000000000000 1.7465000000000000 1.8736000000000000 H (16b)
1.0660000000000000 1.2911000000000000 1.4049000000000000 H (16b)
-0.1138000000000000 -0.3389000000000000 -1.4049000000000000 H (16b)
2.0411000000000000 0.1362000000000000 0.7251000000000000 H (16b)
0.4111000000000000 1.3160000000000000 0.2749000000000000 H (16b)
0.3862000000000000 1.7911000000000000 0.2251000000000000 H (16b)
1.5660000000000000 0.1611000000000000 -0.2251000000000000 H (16b)
-0.0889000000000000 0.6362000000000000 -0.9049000000000000 H (16b)
1.5411000000000000 1.8160000000000000 1.9049000000000000 H (16b)
```

MnF<sub>2</sub>: A2B\_tP12\_111\_2n\_adf - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'MnF2'
_chemical_formula_sum 'F2 Mn'

loop_
_publ_author_name
'T. Yagi'
'J. C. Jamieson'
'P. B. Moore'
_journal_name_full_name
;
Journal of Geophysical Research
;
_journal_volume 84
_journal_year 1979
_journal_page_first 1113
_journal_page_last 1115
_publ_section_title
;
Polymorphism in MnFS_{2}$ (rutile type) at high pressures
;
```

```
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'MnFS_{2}$ Structure'
_aflow_proto 'A2B_tP12_111_2n_adf'
_aflow_params 'a,c/a,x_{4},z_{4},x_{5},z_{5}'
_aflow_params_values '5.1219931862,1.02616165562,0.205,0.28,0.301,0.622'
_aflow_Structurbericht 'None'
_aflow_Pearson 'tP12'

_cell_length_a 5.1219931862
_cell_length_b 5.1219931862
_cell_length_c 5.2559930080
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M 'P -4 2 m'
_symmetry_Int_Tables_number 111

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,x,z
6 y,-x,-z
7 -y,x,-z
8 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mn1 Mn 1 a 0.00000 0.00000 1.00000
Mn2 Mn 1 d 0.50000 0.50000 0.00000 1.00000
Mn3 Mn 2 f 0.50000 0.00000 0.50000 1.00000
F1 F 4 n 0.20500 0.20500 0.28000 1.00000
F2 F 4 n 0.30100 0.30100 0.62200 1.00000
```

MnF<sub>2</sub>: A2B\_tP12\_111\_2n\_adf - POSCAR

```
A2B_tP12_111_2n_adf & a,c/a,x4,z4,x5,z5 --params=5.1219931862,
↳ 1.02616165562,0.205,0.28,0.301,0.622 & P-42m D_{2d}^{11} #111 (
↳ adfn^2) & tP12 & None & MnF2 & T. Yagi and J. C. Jamieson
↳ and P. B. Moore, J. Geophys. Res. 84, 1113-1115 (1979)

1.0000000000000000
5.12199318620000 0.00000000000000 0.00000000000000
0.00000000000000 5.12199318620000 0.00000000000000
0.00000000000000 0.00000000000000 5.25599300800000

F Mn
8 4

Direct
0.20500000000000 0.20500000000000 0.28000000000000 F (4n)
-0.20500000000000 -0.20500000000000 0.28000000000000 F (4n)
0.20500000000000 -0.20500000000000 -0.28000000000000 F (4n)
-0.20500000000000 0.20500000000000 -0.28000000000000 F (4n)
0.30100000000000 0.30100000000000 0.62200000000000 F (4n)
-0.30100000000000 -0.30100000000000 0.62200000000000 F (4n)
0.30100000000000 -0.30100000000000 -0.62200000000000 F (4n)
-0.30100000000000 0.30100000000000 -0.62200000000000 F (4n)
0.00000000000000 0.00000000000000 0.00000000000000 Mn (1a)
0.50000000000000 0.50000000000000 0.00000000000000 Mn (1d)
0.50000000000000 0.00000000000000 0.50000000000000 Mn (2f)
0.00000000000000 0.50000000000000 0.50000000000000 Mn (2f)
```

NV (Low-temperature): AB\_tP8\_111\_n\_n - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'VN'
_chemical_formula_sum 'N V'

loop_
_publ_author_name
'F. Kubel'
'W. Lengauer'
'K. Yvon'
'K. Knorr'
'A. Junod'
_journal_name_full_name
;
Physical Review B
;
_journal_volume 38
_journal_year 1988
_journal_page_first 12908
_journal_page_last 12908
_publ_section_title
;
Structural phase transition at 205 K in stoichiometric vanadium nitride
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013
```

```

_aflow_title 'NV (Low-temperature) Structure'
_aflow_proto 'AB_tP8_111_n_n'
_aflow_params 'a,c/a,x_{1},z_{1},x_{2},z_{2}'
_aflow_params_values '4.1305540686,0.998959140196,0.2522,0.7473,0.24415,
↳ 0.24404'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP8'

_cell_length_a 4.1305540686
_cell_length_b 4.1305540686
_cell_length_c 4.1262547409
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P -4 2 m"
_symmetry_Int_Tables_number 111

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,x,z
6 y,-x,-z
7 -y,x,-z
8 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ni N 4 n 0.25220 0.25220 0.74730 1.00000
Vl V 4 n 0.24415 0.24415 0.24404 1.00000

```

NV (Low-temperature): AB\_tP8\_111\_n\_n - POSCAR

```

AB_tP8_111_n_n & a,c/a,x1,z1,x2,z2 --params=4.1305540686,0.998959140196,
↳ 0.2522,0.7473,0.24415,0.24404 & P-42m D_{2d}^{(1)} #111 (n^2) &
↳ tP8 & None & VN & & F. Kubel et al., Phys. Rev. B 38, 12908(
↳ 1988)
1.0000000000000000
4.13055406860000 0.00000000000000 0.00000000000000
0.00000000000000 4.13055406860000 0.00000000000000
0.00000000000000 0.00000000000000 4.12625474090000
N V
4 4
Direct
0.25220000000000 0.25220000000000 0.74730000000000 N (4n)
-0.25220000000000 -0.25220000000000 0.74730000000000 N (4n)
0.25220000000000 -0.25220000000000 -0.74730000000000 N (4n)
-0.25220000000000 0.25220000000000 -0.74730000000000 N (4n)
0.24415000000000 0.24415000000000 0.24404000000000 V (4n)
-0.24415000000000 -0.24415000000000 0.24404000000000 V (4n)
0.24415000000000 -0.24415000000000 -0.24404000000000 V (4n)
-0.24415000000000 0.24415000000000 -0.24404000000000 V (4n)

```

$\alpha$ -CuAlCl<sub>4</sub>: AB4C\_tP12\_112\_b\_n\_e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'alpha-CuAlCl4'
_chemical_formula_sum 'Al Cl4 Cu'

loop_
_publ_author_name
'J. D. Martin'
'B. R. Leafblad'
'R. M. Sullivan'
'P. D. Boyle'
_journal_name_full_name
;
Inorganic Chemistry
;
_journal_volume 37
_journal_year 1998
_journal_page_first 1341
_journal_page_last 1346
_publ_section_title
;
'$\alpha$-and $\beta$-CuAlCl$_4$': Framework Construction Using
↳ Corner-Shared Tetrahedral Metal-Halide Building Blocks
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title '$\alpha$-CuAlCl$_4$ Structure'
_aflow_proto 'AB4C_tP12_112_b_n_e'
_aflow_params 'a,c/a,x_{3},y_{3},z_{3}'
_aflow_params_values '5.4410982776,1.85862633019,0.2334,0.2761,0.6295'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP12'

_cell_length_a 5.4410982776

```

```

_cell_length_b 5.4410982776
_cell_length_c 10.1129685239
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P -4 2 c"
_symmetry_Int_Tables_number 112

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z+1/2
3 -x,y,-z+1/2
4 -x,-y,z
5 y,x,z+1/2
6 y,-x,-z
7 -y,x,-z
8 -y,-x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 2 b 0.50000 0.00000 0.25000 1.00000
Cu1 Cu 2 e 0.00000 0.00000 0.00000 1.00000
Cl1 Cl 8 n 0.23340 0.27610 0.62950 1.00000

```

$\alpha$ -CuAlCl<sub>4</sub>: AB4C\_tP12\_112\_b\_n\_e - POSCAR

```

AB4C_tP12_112_b_n_e & a,c/a,x3,y3,z3 --params=5.4410982776,1.85862633019
↳ 0.2334,0.2761,0.6295 & P-42c D_{2d}^{(2)} #112 (ben) & tP12 &
↳ None & CuAlCl4 & alpha & J. D. Martin et al., Inorg. Chem. 37,
↳ 1341-1346 (1998)
1.0000000000000000
5.44109827760000 0.00000000000000 0.00000000000000
0.00000000000000 5.44109827760000 0.00000000000000
0.00000000000000 0.00000000000000 10.11296852390000
Al Cl Cu
2 8 2
Direct
0.50000000000000 0.00000000000000 0.25000000000000 Al (2b)
0.00000000000000 0.50000000000000 0.75000000000000 Al (2b)
0.23340000000000 0.27610000000000 0.62950000000000 Cl (8n)
-0.23340000000000 -0.27610000000000 0.62950000000000 Cl (8n)
0.27610000000000 -0.23340000000000 -0.62950000000000 Cl (8n)
-0.27610000000000 0.23340000000000 -0.62950000000000 Cl (8n)
-0.23340000000000 0.27610000000000 -0.12950000000000 Cl (8n)
0.23340000000000 -0.27610000000000 -0.12950000000000 Cl (8n)
-0.27610000000000 -0.23340000000000 1.12950000000000 Cl (8n)
0.27610000000000 0.23340000000000 1.12950000000000 Cl (8n)
0.00000000000000 0.00000000000000 0.00000000000000 Cu (2e)
0.00000000000000 0.00000000000000 0.50000000000000 Cu (2e)

```

Akermanite (Ca<sub>2</sub>MgSi<sub>2</sub>O<sub>7</sub>·5S<sub>3</sub>): A2BC7D2\_tP24\_113\_e\_a\_cef\_e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Akermanite'
_chemical_formula_sum 'Ca2 Mg O7 Si2'

loop_
_publ_author_name
'H. Yang'
'R. M. Hazen'
'R. T. Downs'
'L. W. Finger'
_journal_name_full_name
;
Physics and Chemistry of Minerals
;
_journal_volume 24
_journal_year 1997
_journal_page_first 510
_journal_page_last 519
_publ_section_title
;
Structural change associated with the incommensurate-normal phase
↳ transition in akermanite, Ca$_{2}$MgSi$_{2}$S$_{3}$, at high
↳ pressure

_aflow_title 'Akermanite (Ca$_{2}$MgSi$_{2}$S$_{3}$) Structure'
_aflow_proto 'A2BC7D2_tP24_113_e_a_cef_e'
_aflow_params 'a,c/a,z_{2},x_{3},z_{3},x_{4},z_{4},x_{5},z_{5},x_{6},y_{6},z_{6}'
_aflow_params_values '7.8338,0.639306594501,0.8201,0.8324,0.4935,0.6407,
↳ 0.7471,0.6396,0.0642,0.0798,0.1862,0.7856'
_aflow_Strukturbericht '$S_{3}$'
_aflow_Pearson 'tP24'

_symmetry_space_group_name_H-M "P -4 21 m"
_symmetry_Int_Tables_number 113

_cell_length_a 7.83380
_cell_length_b 7.83380
_cell_length_c 5.00820

```

```
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000
```

```
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z
3 -x+1/2,y+1/2,-z
4 -x,-y,z
5 y+1/2,x+1/2,z
6 y,-x,-z
7 -y,x,-z
8 -y+1/2,-x+1/2,z
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mg1 Mg 2 a 0.00000 0.00000 0.00000 1.00000
O1 O 2 c 0.00000 0.50000 0.82010 1.00000
Ca1 Ca 4 e 0.83240 0.33240 0.49350 1.00000
O2 O 4 e 0.64070 0.14070 0.74710 1.00000
Si1 Si 4 e 0.63960 0.13960 0.06420 1.00000
O3 O 8 f 0.07980 0.18620 0.78560 1.00000
```

Akermanite (Ca<sub>2</sub>MgSi<sub>2</sub>O<sub>7</sub>, S<sub>5</sub>): A2BC7D2\_tP24\_113\_e\_a\_cef\_e - POSCAR

```
A2BC7D2_tP24_113_e_a_cef_e & a,c/a,z2,x3,z3,x4,z4,x5,z5,x6,y6,z6 --
params=7.8338,0.639306594501,0.8201,0.8324,0.4935,0.6407,0.7471
↪ ,0.6396,0.0642,0.0798,0.1862,0.7856 & P-42_1m D_{2d}^{(3)} #113
↪ (ace^3f) & tP24 & S5_{(3)} & Ca2MgSi2O7 & Akermanite & H. Yang
↪ et al., Phys. Chem. Miner. 24, 510-519 (1997)
```

```
1.0000000000000000
7.8338000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.8338000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.0082000000000000
Ca Mg O Si
4 2 14 4
Direct
0.8324000000000000 1.3324000000000000 0.4935000000000000 Ca (4e)
-0.8324000000000000 -0.3324000000000000 0.4935000000000000 Ca (4e)
1.3324000000000000 -0.8324000000000000 -0.4935000000000000 Ca (4e)
-0.3324000000000000 0.8324000000000000 -0.4935000000000000 Ca (4e)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Mg (2a)
0.5000000000000000 0.5000000000000000 0.0000000000000000 Mg (2a)
0.0000000000000000 0.5000000000000000 0.8201000000000000 O (2c)
0.5000000000000000 0.0000000000000000 -0.8201000000000000 O (2c)
0.6407000000000000 1.1407000000000000 0.7471000000000000 O (4e)
-0.6407000000000000 -0.1407000000000000 0.7471000000000000 O (4e)
1.1407000000000000 -0.6407000000000000 -0.7471000000000000 O (4e)
-0.1407000000000000 0.6407000000000000 -0.7471000000000000 O (4e)
0.0798000000000000 0.1862000000000000 0.7856000000000000 O (8f)
-0.0798000000000000 -0.1862000000000000 0.7856000000000000 O (8f)
0.1862000000000000 -0.0798000000000000 -0.7856000000000000 O (8f)
-0.1862000000000000 0.0798000000000000 -0.7856000000000000 O (8f)
0.4202000000000000 0.6862000000000000 -0.7856000000000000 O (8f)
0.5798000000000000 0.3138000000000000 -0.7856000000000000 O (8f)
0.3138000000000000 0.4202000000000000 0.7856000000000000 O (8f)
0.6862000000000000 0.5798000000000000 0.7856000000000000 O (8f)
0.6396000000000000 1.1396000000000000 0.0642000000000000 Si (4e)
-0.6396000000000000 -0.1396000000000000 0.0642000000000000 Si (4e)
1.1396000000000000 -0.6396000000000000 -0.0642000000000000 Si (4e)
-0.1396000000000000 0.6396000000000000 -0.0642000000000000 Si (4e)
```

SeO<sub>3</sub>: A3B\_tP32\_114\_3e\_e - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'SeO3'
_chemical_formula_sum 'O3 Se'
```

```
loop_
_publ_author_name
'F. C. Mijlhoff'
'C. H. {MacGillavry}'
_journal_name_full_name
;
Acta Crystallographica
;
_journal_volume 15
_journal_year 1962
_journal_page_first 620
_journal_page_last 620
_publ_section_title
;
Symmetry and unit-cell dimensions of selenium trioxide
;
```

# Found in Pearson's Crystal Data - Crystal Structure Database for  
↪ Inorganic Compounds, 2013

```
_aflow_title 'SeO3_{(3)} Structure'
_aflow_proto 'A3B_tP32_114_3e_e'
_aflow_params 'a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4}'
```

```
_aflow_params_values '9.6362543341,0.547945205485,0.6,0.743,0.809,0.836,
↪ 0.555,0.604,0.881,0.899,0.844,0.5125,0.7273,0.563'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP32'
```

```
_cell_length_a 9.6362543341
_cell_length_b 9.6362543341
_cell_length_c 5.2801393612
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000
```

```
_symmetry_space_group_name_H-M "P -4 21 c"
_symmetry_Int_Tables_number 114
```

```
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x+1/2,y+1/2,-z+1/2
4 -x,-y,z
5 y+1/2,x+1/2,z+1/2
6 y,-x,-z
7 -y,x,-z
8 -y+1/2,-x+1/2,z+1/2
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 8 e 0.60000 0.74300 0.80900 1.00000
O2 O 8 e 0.83600 0.55500 0.60400 1.00000
O3 O 8 e 0.88100 0.89900 0.84400 1.00000
Se1 Se 8 e 0.51250 0.72730 0.56300 1.00000
```

SeO<sub>3</sub>: A3B\_tP32\_114\_3e\_e - POSCAR

```
A3B_tP32_114_3e_e & a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4 --params=
↪ 9.6362543341,0.547945205485,0.6,0.743,0.809,0.836,0.555,0.604,
↪ 0.881,0.899,0.844,0.5125,0.7273,0.563 & P-42_1m D_{2d}^{(4)} #
↪ 114 (e^4) & tP32 & None & SeO3 & F. C. Mijlhoff and C. H. {
↪ MacGillavry}, Acta Cryst. 15, 620-620 (1962)
1.0000000000000000
9.636254334100000 0.0000000000000000 0.0000000000000000
0.0000000000000000 9.636254334100000 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.280139361200000
O Se
24 8
Direct
0.6000000000000000 0.7430000000000000 0.8090000000000000 O (8e)
-0.6000000000000000 -0.7430000000000000 0.8090000000000000 O (8e)
0.7430000000000000 -0.6000000000000000 -0.8090000000000000 O (8e)
-0.7430000000000000 0.6000000000000000 -0.8090000000000000 O (8e)
-1.0000000000000000 1.2430000000000000 -0.3090000000000000 O (8e)
1.1000000000000000 -0.2430000000000000 -0.3090000000000000 O (8e)
-0.2430000000000000 -1.1000000000000000 1.3090000000000000 O (8e)
1.2430000000000000 1.1000000000000000 1.3090000000000000 O (8e)
0.8360000000000000 0.5550000000000000 0.6040000000000000 O (8e)
-0.8360000000000000 -0.5550000000000000 0.6040000000000000 O (8e)
0.5550000000000000 -0.8360000000000000 -0.6040000000000000 O (8e)
-0.5550000000000000 0.8360000000000000 -0.6040000000000000 O (8e)
-0.3360000000000000 1.0550000000000000 -0.1040000000000000 O (8e)
1.3360000000000000 -0.0550000000000000 -0.1040000000000000 O (8e)
-0.0550000000000000 -0.3360000000000000 1.1040000000000000 O (8e)
1.0550000000000000 1.3360000000000000 1.1040000000000000 O (8e)
0.8810000000000000 0.8990000000000000 0.8440000000000000 O (8e)
-0.8810000000000000 -0.8990000000000000 0.8440000000000000 O (8e)
0.8990000000000000 -0.8810000000000000 -0.8440000000000000 O (8e)
-0.8990000000000000 0.8810000000000000 -0.8440000000000000 O (8e)
-0.3810000000000000 1.3990000000000000 -0.3440000000000000 O (8e)
1.3810000000000000 -0.3990000000000000 -0.3440000000000000 O (8e)
-0.3990000000000000 -0.3810000000000000 1.3440000000000000 O (8e)
1.3990000000000000 1.3810000000000000 1.3440000000000000 O (8e)
0.5125000000000000 0.7273000000000000 0.5630000000000000 Se (8e)
-0.5125000000000000 -0.7273000000000000 0.5630000000000000 Se (8e)
0.7273000000000000 -0.5125000000000000 -0.5630000000000000 Se (8e)
-0.7273000000000000 0.5125000000000000 -0.5630000000000000 Se (8e)
-0.0125000000000000 1.2273000000000000 -0.0630000000000000 Se (8e)
1.0125000000000000 -0.2273000000000000 -0.0630000000000000 Se (8e)
-0.2273000000000000 -0.0125000000000000 1.0630000000000000 Se (8e)
1.2273000000000000 1.0125000000000000 1.0630000000000000 Se (8e)
```

Pd<sub>4</sub>Se: A4B\_tP10\_114\_e\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Pd4Se'
_chemical_formula_sum 'Pd4 Se'
```

```
loop_
_publ_author_name
'F. Gr{\o}nvold'
'E. R{\o}st'
_journal_name_full_name
;
Acta Chemica Scandinavica
;
```

```

_journal_volume 10
_journal_year 1956
_journal_page_first 1620
_journal_page_last 1634
_publ_Section_title
;
On the sulfides, selenides and tellurides of palladium
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'Pd$_{4}$Sse Structure'
_aflow_proto 'A4B_tP10_114_e_a'
_aflow_params 'a,c/a,x_{2},y_{2},z_{2}'
_aflow_params_values '5.2323591487,1.07923706139,0.626,0.768,0.846'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP10'

_cell_length_a 5.2323591487
_cell_length_b 5.2323591487
_cell_length_c 5.6469559118
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P -4 21 c"
_symmetry_Int_Tables_number 114

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z+1/2
3 -x+1/2,y+1/2,-z+1/2
4 -x,-y,z
5 y+1/2,x+1/2,z+1/2
6 y,-x,-z
7 -y,x,-z
8 -y+1/2,-x+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Se1 Se 2 a 0.00000 0.00000 0.00000 1.00000
Pd1 Pd 8 e 0.62600 0.76800 0.84600 1.00000

```

Pd<sub>4</sub>Se: A4B\_tP10\_114\_e\_a - POSCAR

```

A4B_tP10_114_e_a & a,c/a,x2,y2,z2 --params=5.2323591487,1.07923706139,
↳ 0.626,0.768,0.846 & P-4_21c D_{2d}^{4} #114 (ae) & tP10 &
↳ None & Pd4Se & F.Gr{\o}nvald and E.R{\o}st, Acta Chem.
↳ Scand. 10, 1620-1634 (1956)
1.0000000000000000
5.23235914870000 0.00000000000000 0.00000000000000
0.00000000000000 5.23235914870000 0.00000000000000
0.00000000000000 0.00000000000000 5.64695591180000
Pd Se
8 2
Direct
0.62600000000000 0.76800000000000 0.84600000000000 Pd (8e)
-0.62600000000000 -0.76800000000000 0.84600000000000 Pd (8e)
0.76800000000000 -0.62600000000000 -0.84600000000000 Pd (8e)
-0.76800000000000 0.62600000000000 -0.84600000000000 Pd (8e)
-0.12600000000000 1.26800000000000 -0.34600000000000 Pd (8e)
1.12600000000000 -0.26800000000000 -0.34600000000000 Pd (8e)
-0.26800000000000 -0.12600000000000 1.34600000000000 Pd (8e)
1.26800000000000 1.12600000000000 1.34600000000000 Pd (8e)
0.00000000000000 0.00000000000000 0.00000000000000 Se (2a)
0.50000000000000 0.50000000000000 0.50000000000000 Se (2a)

```

Rh<sub>3</sub>P<sub>2</sub>: A2B3\_tP5\_115\_g\_ag - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Rh3P2'
_chemical_formula_sum 'P2 Rh3'

loop_
_publ_author_name
'E. H. {El Ghadraoui}'
'R. Guerin'
'M. Sergent'
_journal_name_full_name
;
Acta Crystallographica Section C: Structural Chemistry
;
_journal_volume 39
_journal_year 1983
_journal_page_first 1493
_journal_page_last 1494
_publ_Section_title
;
Diphosphure de trirhodium, Rh$_{3}$SP$_{2}$: premier exemple d'une
↳ structure lacunaire ordonn{\e}e de type {\it anti}-PbFCl
;

```

```

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'Rh$_{3}$SP$_{2}$ Structure'
_aflow_proto 'A2B3_tP5_115_g_ag'
_aflow_params 'a,c/a,z_{2},z_{3}'
_aflow_params_values '3.3269188443,1.84881274424,0.253,0.6308'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP5'

_cell_length_a 3.3269188443
_cell_length_b 3.3269188443
_cell_length_c 6.1508499584
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P -4 m 2"
_symmetry_Int_Tables_number 115

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,-x,-z
4 y,x,-z
5 -x,y,z
6 x,-y,z
7 y,-x,-z
8 -y,x,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Rh1 Rh 1 a 0.00000 0.00000 1.00000
P1 P 2 g 0.00000 0.50000 0.25300 1.00000
Rh2 Rh 2 g 0.00000 0.50000 0.63080 1.00000

```

Rh<sub>3</sub>P<sub>2</sub>: A2B3\_tP5\_115\_g\_ag - POSCAR

```

A2B3_tP5_115_g_ag & a,c/a,z2,z3 --params=3.3269188443,1.84881274424,
↳ 0.253,0.6308 & P-4m2 D_{2d}^{5} #115 (ag^2) & tP5 & None &
↳ Rh3P2 & E. H. {El Ghadraoui} and R. Guerin and M. Sergent,
↳ Acta Crystallogr. C 39, 1493-1494 (1983)
1.0000000000000000
3.32691884430000 0.00000000000000 0.00000000000000
0.00000000000000 3.32691884430000 0.00000000000000
0.00000000000000 0.00000000000000 6.15084995840000
P Rh
2 3
Direct
0.00000000000000 0.50000000000000 0.25300000000000 P (2g)
0.50000000000000 0.00000000000000 -0.25300000000000 P (2g)
0.00000000000000 0.00000000000000 0.00000000000000 Rh (1a)
0.00000000000000 0.50000000000000 0.63080000000000 Rh (2g)
0.50000000000000 0.00000000000000 -0.63080000000000 Rh (2g)

```

Hg<sub>12</sub>: AB2\_tP12\_115\_j\_egi - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Hg12'
_chemical_formula_sum 'Hg 12'

loop_
_publ_author_name
'M. Hostettler'
'H. Birkedal'
'D. Schwarzenbach'
_journal_name_full_name
;
Acta Crystallographica Section B: Structural Science
;
_journal_volume 58
_journal_year 2002
_journal_page_first 903
_journal_page_last 913
_publ_Section_title
;
The structure of orange HgIS_{2}$. I. Polytypic layer structure
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'HgI$_{2}$ Structure'
_aflow_proto 'AB2_tP12_115_j_egi'
_aflow_params 'a,c/a,z_{1},z_{2},x_{3},x_{4},z_{4}'
_aflow_params_values '8.7863400452,0.701854022742,0.0288,0.0315,0.26398,
↳ 0.24918,0.24945'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP12'

_cell_length_a 8.7863400452
_cell_length_b 8.7863400452
_cell_length_c 6.1667281059

```

```

_cell_angle_alpha 90.000000000
_cell_angle_beta 90.000000000
_cell_angle_gamma 90.000000000

_symmetry_space_group_name_H-M "P -4 m 2"
_symmetry_Int_Tables_number 115

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,-x,-z
4 y,x,-z
5 -x,y,z
6 x,-y,z
7 y,-x,-z
8 -y,x,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
I1 I 2 e 0.00000 0.00000 0.02880 1.00000
I2 I 2 g 0.00000 0.50000 0.03150 1.00000
I3 I 4 i 0.26398 0.26398 0.50000 1.00000
Hg1 Hg 4 j 0.24918 0.00000 0.24945 1.00000

```

HgI<sub>2</sub>: AB2\_tP12\_115\_j\_egi - POSCAR

```

AB2_tP12_115_j_egi & a,c/a,z1,z2,x3,x4,z4 --params=8.7863400452,
↪ 0.701854022742,0.0288,0.0315,0.26398,0.24918,0.24945 & P-4m2 D_
↪ [2d]^5 #115 (egij) & tP12 & None & HgI2 & M. Hostettler
↪ and H. Birkedal and D. Schwarzenbach, Acta Crystallogr. Sect. B
↪ Struct. Sci. 58, 903-913 (2002)
1.000000000000000
8.78634004520000 0.00000000000000 0.00000000000000
0.00000000000000 8.78634004520000 0.00000000000000
0.00000000000000 0.00000000000000 6.16672810590000
Hg I
4 8
Direct
0.24918000000000 0.00000000000000 0.24945000000000 Hg (4j)
-0.24918000000000 0.00000000000000 0.24945000000000 Hg (4j)
0.00000000000000 -0.24918000000000 -0.24945000000000 Hg (4j)
0.00000000000000 0.24918000000000 -0.24945000000000 Hg (4j)
0.00000000000000 0.00000000000000 0.02880000000000 I (2e)
0.00000000000000 0.00000000000000 -0.02880000000000 I (2e)
0.00000000000000 0.50000000000000 0.03150000000000 I (2g)
0.50000000000000 0.00000000000000 -0.03150000000000 I (2g)
0.26398000000000 0.26398000000000 0.50000000000000 I (4i)
-0.26398000000000 -0.26398000000000 0.50000000000000 I (4i)
0.26398000000000 -0.26398000000000 0.50000000000000 I (4i)
-0.26398000000000 0.26398000000000 0.50000000000000 I (4i)

```

Ru<sub>2</sub>Sn<sub>3</sub>: A2B3\_tP20\_116\_bci\_fj - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ru2Sn3'
_chemical_formula_sum 'Ru2 Sn3'

loop_
_publ_author_name
'O. Schwomma'
'H. Nowotny'
'A. Wittmann'
_journal_name_full_name
;
'Monatshefte f{"u}r Chemie - Chemical Monthly
;
_journal_volume 95
_journal_year 1964
_journal_page_first 1538
_journal_page_last 1543
_publ_section_title
;
'Untersuchungen im System: Ru--Sn
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'Ru$_{2}$Sn$_{3}$ Structure'
_aflow_proto 'A2B3_tP20_116_bci_fj'
_aflow_params 'a,c/a,x_{3},z_{4},x_{5},y_{5},z_{5}'
_aflow_params_values '6.1720115185,1.606448477,0.177,0.625,0.655,0.216,
↪ 0.582'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP20'

_cell_length_a 6.1720115185
_cell_length_b 6.1720115185
_cell_length_c 9.9150185039
_cell_angle_alpha 90.000000000
_cell_angle_beta 90.000000000
_cell_angle_gamma 90.000000000

```

```

_symmetry_space_group_name_H-M "P -4 c 2"
_symmetry_Int_Tables_number 116

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,-x,-z+1/2
4 y,x,-z+1/2
5 -x,y,z+1/2
6 x,-y,z+1/2
7 y,-x,-z
8 -y,x,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ru1 Ru 2 b 0.50000 0.50000 0.25000 1.00000
Ru2 Ru 2 c 0.00000 0.00000 0.00000 1.00000
Sn1 Sn 4 f 0.17700 0.17700 0.75000 1.00000
Ru3 Ru 4 i 0.00000 0.50000 0.62500 1.00000
Sn2 Sn 8 j 0.65500 0.21600 0.58200 1.00000

```

Ru<sub>2</sub>Sn<sub>3</sub>: A2B3\_tP20\_116\_bci\_fj - POSCAR

```

A2B3_tP20_116_bci_fj & a,c/a,x3,z4,x5,y5,z5 --params=6.1720115185,
↪ 1.606448477,0.177,0.625,0.655,0.216,0.582 & P-4c2 D_{2d}^{6} #
↪ 116 (bcfij) & tP20 & None & Ru2Sn3 & O. Schwomma and H.
↪ Nowotny and A. Wittmann, Monatsh. Chem. 95, 1538-1543 (1964)
1.000000000000000
6.17201151850000 0.00000000000000 0.00000000000000
0.00000000000000 6.17201151850000 0.00000000000000
0.00000000000000 0.00000000000000 9.91501850390000
Ru Sn
8 12
Direct
0.50000000000000 0.50000000000000 0.25000000000000 Ru (2b)
0.50000000000000 0.50000000000000 0.75000000000000 Ru (2b)
0.00000000000000 0.00000000000000 0.00000000000000 Ru (2c)
0.00000000000000 0.00000000000000 0.50000000000000 Ru (2c)
0.00000000000000 0.50000000000000 0.62500000000000 Ru (4i)
0.50000000000000 0.00000000000000 -0.62500000000000 Ru (4i)
0.00000000000000 0.50000000000000 1.12500000000000 Ru (4i)
0.50000000000000 0.00000000000000 -0.12500000000000 Ru (4i)
0.17700000000000 0.17700000000000 0.75000000000000 Sn (4f)
-0.17700000000000 -0.17700000000000 0.75000000000000 Sn (4f)
0.17700000000000 -0.17700000000000 0.25000000000000 Sn (4f)
-0.17700000000000 0.17700000000000 0.25000000000000 Sn (4f)
0.65500000000000 0.21600000000000 0.58200000000000 Sn (8j)
-0.65500000000000 -0.21600000000000 0.58200000000000 Sn (8j)
0.21600000000000 -0.65500000000000 -0.58200000000000 Sn (8j)
-0.21600000000000 0.65500000000000 -0.58200000000000 Sn (8j)
0.65500000000000 -0.21600000000000 1.08200000000000 Sn (8j)
-0.65500000000000 0.21600000000000 1.08200000000000 Sn (8j)
0.21600000000000 0.65500000000000 -0.08200000000000 Sn (8j)
-0.21600000000000 -0.65500000000000 -0.08200000000000 Sn (8j)

```

β-Bi<sub>2</sub>O<sub>3</sub> (High-temperature): A2B3\_tP20\_117\_i\_adgh - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'beta-Bi2O3'
_chemical_formula_sum 'Bi2 O3'

loop_
_publ_author_name
'L. G. Sill{"e}n'
_journal_name_full_name
;
'Arkiv f{"o}r Kemi, Mineralogi och Geologi
;
_journal_volume 12A
_journal_year 1937
_journal_page_first 1
_journal_page_last 15
_publ_section_title
;
'X-ray studies on bismuth trioxide
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title '$\beta$-Bi$_{2}$O$_{3}$ (High-temperature) Structure'
_aflow_proto 'A2B3_tP20_117_i_adgh'
_aflow_params 'a,c/a,x_{3},x_{4},x_{5},y_{5},z_{5}'
_aflow_params_values '7.7289660931,0.727131582349,0.73,0.73,0.75,0.52,
↪ 0.25'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP20'

_cell_length_a 7.7289660931
_cell_length_b 7.7289660931
_cell_length_c 5.6199753452
_cell_angle_alpha 90.000000000
_cell_angle_beta 90.000000000

```

```

_cell_angle_gamma 90.000000000
_symmetry_space_group_name_H-M "P -4 b 2"
_symmetry_Int_Tables_number 117

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y+1/2,-x+1/2,-z
4 y+1/2,x+1/2,-z
5 -x+1/2,y+1/2,z
6 x+1/2,-y+1/2,z
7 y,-x,-z
8 -y,x,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 2 a 0.00000 0.00000 0.00000 1.00000
O2 O 2 d 0.00000 0.50000 0.50000 1.00000
O3 O 4 g 0.73000 0.23000 0.00000 1.00000
O4 O 4 h 0.73000 0.23000 0.50000 1.00000
Bi1 Bi 8 i 0.75000 0.52000 0.25000 1.00000

```

$\beta$ -Bi<sub>2</sub>O<sub>3</sub> (High-temperature): A2B<sub>3</sub>tP<sub>20</sub>117\_i\_adgh - POSCAR

```

A2B3_tP20_117_i_adgh & a,c/a,x3,x4,x5,y5,z5 --params=7.7289660931,
↪ 0.727131582349,0.73,0.73,0.75,0.52,0.25 & P-4b2_D[2d]^{7} #117
↪ (adghi) & tP20 & None & Bi2O3 & beta & L. G. Sill [\`e]n, [Ark.
↪ Kem. Mineral. Geol. 12A, 1-15 (1937)
1.0000000000000000
7.72896609310000 0.00000000000000 0.0000000000000000
0.0000000000000000 7.72896609310000 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.61997534520000
Bi O
8 12
Direct
0.7500000000000000 0.5200000000000000 0.2500000000000000 Bi (8i)
-0.7500000000000000 -0.5200000000000000 0.2500000000000000 Bi (8i)
0.5200000000000000 -0.7500000000000000 -0.2500000000000000 Bi (8i)
-0.5200000000000000 0.7500000000000000 -0.2500000000000000 Bi (8i)
1.2500000000000000 -0.0200000000000000 0.2500000000000000 Bi (8i)
-0.2500000000000000 1.0200000000000000 0.2500000000000000 Bi (8i)
1.0200000000000000 1.2500000000000000 -0.2500000000000000 Bi (8i)
-0.0200000000000000 -0.2500000000000000 -0.2500000000000000 Bi (8i)
0.0000000000000000 0.0000000000000000 0.0000000000000000 O (2a)
0.5000000000000000 0.5000000000000000 0.0000000000000000 O (2a)
0.0000000000000000 0.5000000000000000 0.5000000000000000 O (2d)
0.5000000000000000 0.0000000000000000 0.5000000000000000 O (2d)
0.7300000000000000 1.2300000000000000 0.0000000000000000 O (4g)
-0.7300000000000000 -0.2300000000000000 0.0000000000000000 O (4g)
1.2300000000000000 -0.7300000000000000 0.0000000000000000 O (4g)
-0.2300000000000000 0.7300000000000000 0.0000000000000000 O (4g)
0.7300000000000000 1.2300000000000000 0.5000000000000000 O (4h)
-0.7300000000000000 -0.2300000000000000 0.5000000000000000 O (4h)
1.2300000000000000 -0.7300000000000000 0.5000000000000000 O (4h)
-0.2300000000000000 0.7300000000000000 0.5000000000000000 O (4h)

```

RuIn<sub>3</sub>: A3B\_tP16\_118\_ei\_f - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'RuIn3'
_chemical_formula_sum 'In3 Ru'

loop_
_publ_author_name
'R. B. Roof'
'Z. Fisk'
'J. L. Smith'
_journal_name_full_name
;
Powder Diffraction
;
_journal_volume 1
_journal_year 1986
_journal_page_first 20
_journal_page_last 21
_publ_section_title
;
Crystal data for RuIn_{3}$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'RuIn_{3}$ Structure'
_aflow_proto 'A3B_tP16_118_ei_f'
_aflow_params 'a,c/a,z_{1},x_{2},x_{3},y_{3},z_{3}'
_aflow_params_values '6.9983025398,1.03510852635,0.237,0.15,0.343,0.149,
↪ 0.509'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP16'

_cell_length_a 6.9983025398

```

```

_cell_length_b 6.9983025398
_cell_length_c 7.2440026289
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P -4 n 2"
_symmetry_Int_Tables_number 118

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y+1/2,-x+1/2,-z+1/2
4 y+1/2,x+1/2,-z+1/2
5 -x+1/2,y+1/2,z+1/2
6 x+1/2,-y+1/2,z+1/2
7 y,-x,-z
8 -y,x,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
In1 In 4 e 0.00000 0.00000 0.23700 1.00000
Ru1 Ru 4 f 0.15000 0.35000 0.25000 1.00000
In2 In 8 i 0.34300 0.14900 0.50900 1.00000

```

RuIn<sub>3</sub>: A3B\_tP16\_118\_ei\_f - POSCAR

```

A3B_tP16_118_ei_f & a,c/a,z1,x2,x3,y3,z3 --params=6.9983025398,
↪ 1.03510852635,0.237,0.15,0.343,0.149,0.509 & P-4n2_D[2d]^{8} #
↪ 118 (efi) & tP16 & None & RuIn3 & R. B. Roof and Z. Fisk and
↪ J. L. Smith, Powder Diffraction 1, 20-21 (1986)
1.0000000000000000
6.99830253980000 0.00000000000000 0.0000000000000000
0.0000000000000000 6.99830253980000 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.24400262890000
In Ru
12 4
Direct
0.0000000000000000 0.0000000000000000 0.2370000000000000 In (4e)
0.0000000000000000 0.0000000000000000 -0.2370000000000000 In (4e)
0.5000000000000000 0.5000000000000000 0.7370000000000000 In (4e)
0.5000000000000000 0.5000000000000000 0.2630000000000000 In (4e)
0.3430000000000000 0.1490000000000000 0.5090000000000000 In (8i)
-0.3430000000000000 -0.1490000000000000 0.5090000000000000 In (8i)
0.1490000000000000 -0.3430000000000000 -0.5090000000000000 In (8i)
-0.1490000000000000 0.3430000000000000 -0.5090000000000000 In (8i)
0.8430000000000000 0.3510000000000000 1.0090000000000000 In (8i)
0.1570000000000000 0.6490000000000000 1.0090000000000000 In (8i)
0.6490000000000000 0.8430000000000000 -0.0090000000000000 In (8i)
0.3510000000000000 0.1570000000000000 -0.0090000000000000 In (8i)
0.1500000000000000 0.3500000000000000 0.7500000000000000 Ru (4f)
-0.1500000000000000 0.6500000000000000 0.2500000000000000 Ru (4f)
0.3500000000000000 -0.1500000000000000 0.7500000000000000 Ru (4f)
0.6500000000000000 0.1500000000000000 0.7500000000000000 Ru (4f)

```

Ir<sub>3</sub>Ga<sub>5</sub>: A5B<sub>3</sub>tP<sub>32</sub>118\_g2i\_aceh - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ir3Ga5'
_chemical_formula_sum 'Ga5 Ir3'

loop_
_publ_author_name
'H. V[\"o]llenkle'
'A. Wittmann'
'H. Nowotny'
_journal_name_full_name
;
Monatshefte f[\"u]r Chemie - Chemical Monthly
;
_journal_volume 98
_journal_year 1967
_journal_page_first 176
_journal_page_last 183
_publ_section_title
;
Die Kristallstrukturen von Rh_{10}$Ga_{17}$ und Ir_{3}$Ga_{5}$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'Ir_{3}$Ga_{5}$ Structure'
_aflow_proto 'A5B3_tP32_118_g2i_aceh'
_aflow_params 'a,c/a,z_{3},x_{4},z_{5},x_{6},y_{6},z_{6},x_{7},y_{7},z_{7}'
↪ 7)
_aflow_params_values '5.8229835854,2.43860552978,0.6709,0.675,0.5861,
↪ 0.73,0.85,0.5515,0.84,0.8,0.15'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP32'

_cell_length_a 5.8229835854
_cell_length_b 5.8229835854

```



```

_cell_length_c 14.1999599712
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P -4 n 2"
_symmetry_Int_Tables_number 118

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y+1/2,-x+1/2,-z+1/2
4 y+1/2,x+1/2,-z+1/2
5 -x+1/2,y+1/2,z+1/2
6 x+1/2,-y+1/2,z+1/2
7 y,-x,-z
8 -y,x,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ir1 Ir 2 a 0.00000 0.00000 0.25000 1.00000
Ir2 Ir 2 c 0.00000 0.50000 0.25000 1.00000
Ir3 Ir 4 e 0.00000 0.00000 0.67090 1.00000
Ga1 Ga 4 g 0.67500 0.17500 0.25000 1.00000
Ir4 Ir 4 h 0.00000 0.50000 0.58610 1.00000
Ga2 Ga 8 i 0.73000 0.85000 0.55150 1.00000
Ga3 Ga 8 i 0.84000 0.80000 0.15000 1.00000

```

Ir<sub>3</sub>Ga<sub>5</sub>: A5B<sub>3</sub>tP32\_118\_g2i\_aceh - POSCAR

```

A5B3_tP32_118_g2i_aceh & a,c/a,z3,x4,z5,x6,y6,z6,x7,y7,z7 --params=
↳ 5.8229835854,2.43860552978,0.6709,0.675,0.5861,0.73,0.85,0.5515
↳ 0.84,0.8,0.15 & P-4n2 D_{2d}^{14} #118 (aceghi^2) & tP32 & None
↳ & Ir3Ga5 & H. V[{}o]llenkne and A. Wittmann and H. Nowotny,
↳ Monatsh. Chem. 98, 176-183 (1967)
1.0000000000000000
5.82298358540000 0.00000000000000 0.00000000000000
0.00000000000000 5.82298358540000 0.00000000000000
0.00000000000000 0.00000000000000 14.19995997120000
Ga Ir
20 12
Direct
0.67500000000000 1.17500000000000 0.25000000000000 Ga (4g)
-0.67500000000000 -0.17500000000000 0.25000000000000 Ga (4g)
1.17500000000000 -0.67500000000000 0.75000000000000 Ga (4g)
-0.17500000000000 0.67500000000000 0.75000000000000 Ga (4g)
0.73000000000000 0.85000000000000 0.55150000000000 Ga (8i)
-0.73000000000000 -0.85000000000000 0.55150000000000 Ga (8i)
0.85000000000000 -0.73000000000000 -0.55150000000000 Ga (8i)
-0.85000000000000 0.73000000000000 -0.55150000000000 Ga (8i)
1.23000000000000 -0.35000000000000 1.05150000000000 Ga (8i)
-0.23000000000000 1.35000000000000 1.05150000000000 Ga (8i)
1.35000000000000 1.23000000000000 -0.05150000000000 Ga (8i)
-0.35000000000000 -0.23000000000000 -0.05150000000000 Ga (8i)
0.84000000000000 0.80000000000000 0.15000000000000 Ga (8i)
-0.84000000000000 -0.80000000000000 0.15000000000000 Ga (8i)
0.80000000000000 -0.84000000000000 -0.15000000000000 Ga (8i)
-0.80000000000000 0.84000000000000 -0.15000000000000 Ga (8i)
1.34000000000000 -0.30000000000000 0.65000000000000 Ga (8i)
-0.34000000000000 1.30000000000000 0.65000000000000 Ga (8i)
1.30000000000000 1.34000000000000 0.35000000000000 Ga (8i)
-0.30000000000000 -0.34000000000000 0.35000000000000 Ga (8i)
0.00000000000000 0.00000000000000 0.00000000000000 Ir (2a)
0.50000000000000 0.50000000000000 0.50000000000000 Ir (2a)
0.00000000000000 0.50000000000000 0.25000000000000 Ir (2c)
0.50000000000000 0.00000000000000 0.75000000000000 Ir (2c)
0.00000000000000 0.00000000000000 0.67090000000000 Ir (4e)
0.00000000000000 0.00000000000000 -0.67090000000000 Ir (4e)
0.50000000000000 0.50000000000000 1.17090000000000 Ir (4e)
0.50000000000000 0.50000000000000 -0.17090000000000 Ir (4e)
0.00000000000000 0.50000000000000 0.58610000000000 Ir (4h)
0.50000000000000 0.00000000000000 -0.58610000000000 Ir (4h)
0.50000000000000 0.00000000000000 1.08610000000000 Ir (4h)
0.00000000000000 0.50000000000000 -0.08610000000000 Ir (4h)

```

RbGa<sub>3</sub>: A3B\_tI24\_119\_b2i\_af - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'RbGa3'
_chemical_formula_sum 'Ga3 Rb'

loop_
_publ_author_name
'R. G. Ling'
'C. Belin'
_journal_name_full_name
;
Zeitschrift fur Anorganische und Allgemeine Chemie
;
_journal_volume 480
_journal_year 1981
_journal_page_first 181
_journal_page_last 185

```

```

_publ_section_title
;
Preparation and Crystal Structure Determination of the New
↳ Intermetallic Compound RbGa3_3$
;

# Found in Pearson's Handbook of Crystallographic Data for Intermetallic
↳ Phases, 1991

_afLOW_title 'RbGa3_3$ Structure'
_afLOW_proto 'A3B_tI24_119_b2i_af'
_afLOW_params 'a,c/a,z_{3},x_{4},z_{4},x_{5},z_{5}'
_afLOW_params_values '6.315,2.37529691211,0.372,0.2068,0.2229,0.3067,
↳ 0.3917'
_afLOW_Strukturbericht 'None'
_afLOW_Pearson 'tI24'

_symmetry_space_group_name_H-M "I -4 m 2"
_symmetry_Int_Tables_number 119

_cell_length_a 6.31500
_cell_length_b 6.31500
_cell_length_c 15.00000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,-x,-z
4 y,x,-z
5 -x,y,z
6 x,-y,z
7 y,-x,-z
8 -y,x,-z
9 x+1/2,y+1/2,z+1/2
10 -x+1/2,-y+1/2,z+1/2
11 -y+1/2,-x+1/2,-z+1/2
12 y+1/2,x+1/2,-z+1/2
13 -x+1/2,y+1/2,z+1/2
14 x+1/2,-y+1/2,z+1/2
15 y+1/2,-x+1/2,-z+1/2
16 -y+1/2,x+1/2,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Rb1 Rb 2 a 0.00000 0.00000 0.00000 1.00000
Ga1 Ga 2 b 0.00000 0.00000 0.50000 1.00000
Rb2 Rb 4 f 0.00000 0.50000 0.37200 1.00000
Ga2 Ga 8 i 0.20680 0.00000 0.22290 1.00000
Ga3 Ga 8 i 0.30670 0.00000 0.39170 1.00000

```

RbGa<sub>3</sub>: A3B\_tI24\_119\_b2i\_af - POSCAR

```

A3B_tI24_119_b2i_af & a,c/a,z3,x4,z4,x5,z5 --params=6.315,2.37529691211,
↳ 0.372,0.2068,0.2229,0.3067,0.3917 & I-4m2 D_{2d}^{14} #119 (abfi
↳ ^2) & tI24 & None & RbGa3 & RbGa3 & R. G. Ling and C. Belin, Z.
↳ Anorg. Allg. Chem. 480, 181-185 (1981)
1.0000000000000000
-3.15750000000000 3.15750000000000 7.50000000000000
3.15750000000000 -3.15750000000000 7.50000000000000
3.15750000000000 3.15750000000000 -7.50000000000000
Ga Rb
9 3
Direct
0.50000000000000 0.50000000000000 0.00000000000000 Ga (2b)
0.22290000000000 0.42970000000000 0.20680000000000 Ga (8i)
0.22290000000000 0.01610000000000 -0.20680000000000 Ga (8i)
-0.42970000000000 -0.22290000000000 -0.20680000000000 Ga (8i)
-0.01610000000000 -0.22290000000000 0.20680000000000 Ga (8i)
0.39170000000000 0.69840000000000 0.30670000000000 Ga (8i)
0.39170000000000 0.08500000000000 -0.30670000000000 Ga (8i)
-0.69840000000000 -0.39170000000000 -0.30670000000000 Ga (8i)
-0.08500000000000 -0.39170000000000 0.30670000000000 Ga (8i)
0.00000000000000 0.00000000000000 0.00000000000000 Rb (2a)
0.87200000000000 0.37200000000000 0.50000000000000 Rb (4f)
-0.37200000000000 0.12800000000000 0.50000000000000 Rb (4f)

```

GaSb: AB\_tI4\_119\_c\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'GaSb'
_chemical_formula_sum 'Ga Sb'

loop_
_publ_author_name
'T. R. R. McDonald'
'R. Sard'
'E. Gregory'
_journal_name_full_name
;
Journal of Applied Physics
;

```

```

;
_journal_volume 36
_journal_year 1965
_journal_page_first 1498
_journal_page_last 1499
_publ_section_title
;
Retention of GaSb (II) at low temperatures and one atmosphere pressure
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'GaSb Structure'
_aflow_proto 'AB_tI4_119_c_a'
_aflow_params 'a,c/a'
_aflow_params_values '5.4790101504,0.558496075934'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tI4'

_cell_length_a 5.4790101504
_cell_length_b 5.4790101504
_cell_length_c 3.0600056690
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I -4 m 2"
_symmetry_Int_Tables_number 119

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,-x,-z
4 y,x,-z
5 -x,y,z
6 x,-y,z
7 y,-x,-z
8 -y,x,-z
9 x+1/2,y+1/2,z+1/2
10 -x+1/2,-y+1/2,z+1/2
11 -y+1/2,-x+1/2,-z+1/2
12 y+1/2,x+1/2,-z+1/2
13 -x+1/2,y+1/2,z+1/2
14 x+1/2,-y+1/2,z+1/2
15 y+1/2,-x+1/2,-z+1/2
16 -y+1/2,x+1/2,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Sb1 Sb 2 a 0.00000 0.00000 0.00000 1.00000
Ga1 Ga 2 c 0.00000 0.50000 0.25000 1.00000

```

**GaSb: AB\_tI4\_119\_c\_a - POSCAR**

```

AB_tI4_119_c_a & a,c/a --params=5.4790101504,0.558496075934 & I-4m2 D_{
↳ 2d}^{9} #119 (ac) & tI4 & None & GaSb & & T. R. R. McDonald
↳ and R. Sard and E. Gregory, J. Appl. Phys. 36, 1498-1499 (1965)
1.0000000000000000
-2.73950507520000 2.73950507520000 1.53000283450000
2.73950507520000 -2.73950507520000 1.53000283450000
2.73950507520000 2.73950507520000 -1.53000283450000
Ga Sb
1 1
Direct
0.750000000000000 0.250000000000000 0.500000000000000 Ga (2c)
0.000000000000000 0.000000000000000 0.000000000000000 Sb (2a)

```

**KAu<sub>4</sub>Sn<sub>2</sub>: A4BC2\_tI28\_120\_i\_d\_e - CIF**

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'KAu4Sn2'
_chemical_formula_sum 'Au4 K Sn2'

loop_
_publ_author_name
'H.-D. Sinnen'
'H.-U. Schuster'
_journal_name_full_name
;
Zeitschrift f{"u}r Naturforschung B
;
_journal_volume 33
_journal_year 1978
_journal_page_first 1077
_journal_page_last 1079
_publ_section_title
;
Darstellung und Struktur des KAu_{4}SSn_{2} / Preparation and
↳ Crystal Structure of KAu_{4}SSn_{2}
;

```

```

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'KAu_{4}SSn_{2} Structure'
_aflow_proto 'A4BC2_tI28_120_i_d_e'
_aflow_params 'a,c/a,x_{2},x_{3},y_{3},z_{3}'
_aflow_params_values '8.8470588481,0.924381146154,0.856,0.6452,0.6575,
↳ 0.0851'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tI28'

_cell_length_a 8.8470588481
_cell_length_b 8.8470588481
_cell_length_c 8.1780543981
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "I -4 c 2"
_symmetry_Int_Tables_number 120

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,-x,-z+1/2
4 y,x,-z+1/2
5 -x,y,z+1/2
6 x,-y,z+1/2
7 y,-x,-z
8 -y,x,-z
9 x+1/2,y+1/2,z+1/2
10 -x+1/2,-y+1/2,z+1/2
11 -y+1/2,-x+1/2,-z
12 y+1/2,x+1/2,-z
13 -x+1/2,y+1/2,z
14 x+1/2,-y+1/2,z
15 y+1/2,-x+1/2,-z+1/2
16 -y+1/2,x+1/2,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
K1 K 4 d 0.00000 0.50000 0.00000 1.00000
Sn1 Sn 8 e 0.85600 0.85600 0.25000 1.00000
Au1 Au 16 i 0.64520 0.65750 0.08510 1.00000

```

**KAu<sub>4</sub>Sn<sub>2</sub>: A4BC2\_tI28\_120\_i\_d\_e - POSCAR**

```

A4BC2_tI28_120_i_d_e & a,c/a,x2,x3,y3,z3 --params=8.8470588481,
↳ 0.924381146154,0.856,0.6452,0.6575,0.0851 & I-4c2 D_{2d}^{10} #
↳ 120 (dei) & tI28 & None & KAu4Sn2 & & H.-D. Sinnen and H.-U.
↳ Schuster, Z. Naturforsch. B 33, 1077-1079 (1978)
1.0000000000000000
-4.42352942405000 4.42352942405000 4.08902719905000
4.42352942405000 -4.42352942405000 4.08902719905000
4.42352942405000 4.42352942405000 -4.08902719905000
Au K Sn
8 2 4
Direct
0.742600000000000 0.730300000000000 1.302700000000000 Au (16i)
-0.572400000000000 -0.560100000000000 -1.302700000000000 Au (16i)
-0.730300000000000 0.572400000000000 0.012300000000000 Au (16i)
0.560100000000000 -0.742600000000000 -0.012300000000000 Au (16i)
-0.072400000000000 1.230300000000000 -0.012300000000000 Au (16i)
1.242600000000000 -0.060100000000000 0.012300000000000 Au (16i)
1.060100000000000 1.072400000000000 1.302700000000000 Au (16i)
-0.230300000000000 -0.242600000000000 -1.302700000000000 Au (16i)
0.500000000000000 0.000000000000000 0.500000000000000 K (4d)
0.000000000000000 0.500000000000000 0.500000000000000 K (4d)
1.106000000000000 1.106000000000000 1.712000000000000 Sn (8e)
-0.606000000000000 -0.606000000000000 -1.712000000000000 Sn (8e)
-0.106000000000000 1.606000000000000 0.000000000000000 Sn (8e)
1.606000000000000 -0.106000000000000 0.000000000000000 Sn (8e)

```

**CaRbFe<sub>4</sub>As<sub>4</sub> (Superconducting): A4BC4D\_tP10\_123\_gh\_a\_i\_d - CIF**

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'CsRbFe4As4'
_chemical_formula_sum 'As4 Cs Fe4 Rb'

loop_
_publ_author_name
'A. Iyo'
'K. Kawashima'
'T. Kinjo'
'T. Nishio'
'S. Ishida'
'H. Fujihisa'
'Y. Gotoh'
'K. Kihou'
'H. Eisaki'
'Y. Yoshida'
_journal_name_full_name
;

```

```

Journal of the American Chemical Society
;
_journal_volume 138
_journal_year 2016
_journal_page_first 3410
_journal_page_last 3415
_publ_Section_title
;
New-Structure-Type Fe-Based Superconductors: CaFeS4As4 (A = K
↪ , Rb, Cs) and SrFeS4As4 (A = Rb, Cs)
;
_flow_title 'CaRbFeS4As4 (Superconducting) Structure'
_flow_proto 'A4BC4D_tP10_123_gh_a_i_d'
_flow_params 'a,c/a,z3,z4,z5'
_flow_params_values '3.8757,3.38106664603,0.3336,0.1193,0.2246'
_flow_Strukturbericht 'None'
_flow_Pearson 'tP10'

_symmetry_space_group_name_H-M "P 4/m 2/m 2/m"
_symmetry_Int_Tables_number 123

_cell_length_a 3.87570
_cell_length_b 3.87570
_cell_length_c 13.10400
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 -y,-x,-z
6 -y,x,z
7 y,-x,z
8 y,x,-z
9 -x,-y,-z
10 -x,y,z
11 x,-y,z
12 x,y,-z
13 y,x,z
14 y,-x,-z
15 -y,x,-z
16 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cs1 Cs 1 a 0.00000 0.00000 1.00000
Rb1 Rb 1 d 0.50000 0.50000 0.50000 1.00000
As1 As 2 g 0.00000 0.00000 0.33360 1.00000
As2 As 2 h 0.50000 0.50000 0.11930 1.00000
Fe1 Fe 4 i 0.00000 0.50000 0.22460 1.00000

```

CaRbFe<sub>4</sub>As<sub>4</sub> (Superconducting): A4BC4D\_tP10\_123\_gh\_a\_i\_d - POSCAR

```

A4BC4D_tP10_123_gh_a_i_d & a,c/a,z3,z4,z5 --params=3.8757,3.38106664603,
↪ 0.3336,0.1193,0.2246 & P4/mmm D2{4h}^{1} #123 (adghi) & tP10 &
↪ None & CsRbFe4As4 & CsRbFe4As4 & A. Iyo et al., J. Am. Chem.
↪ Soc. 138, 3410-3415 (2016)
1.0000000000000000
3.8757000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 3.8757000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.1040000000000000
As Cs Fe Rb
4 1 4 1
Direct
0.0000000000000000 0.0000000000000000 0.3336000000000000 As (2g)
0.0000000000000000 0.0000000000000000 -0.3336000000000000 As (2g)
0.5000000000000000 0.5000000000000000 0.1193000000000000 As (2h)
0.5000000000000000 0.5000000000000000 -0.1193000000000000 As (2h)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Cs (1a)
0.0000000000000000 0.5000000000000000 0.2246000000000000 Fe (4i)
0.5000000000000000 0.0000000000000000 0.2246000000000000 Fe (4i)
0.0000000000000000 0.5000000000000000 -0.2246000000000000 Fe (4i)
0.5000000000000000 0.0000000000000000 -0.2246000000000000 Fe (4i)
0.5000000000000000 0.5000000000000000 0.5000000000000000 Rb (1d)

```

Nb<sub>4</sub>CoSi: AB4C\_tP12\_124\_a\_m\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Nb4CoSi'
_chemical_formula_sum 'Co Nb4 Si'

loop_
_publ_author_name
'E. I. Gladyshevskii'
'{Yu}. B. {Kuz'ma}'
_journal_name_full_name
;
Journal of Structural Chemistry
;

```

```

_journal_volume 6
_journal_year 1965
_journal_page_first 60
_journal_page_last 63
_publ_Section_title
;
The compounds NbS4FeSi, NbS4CoSi, NbS4NiSi and their
↪ crystal structures
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_flow_title 'NbS4CoSi Structure'
_flow_proto 'AB4C_tP12_124_a_m_c'
_flow_params 'a,c/a,x3,y3'
_flow_params_values '6.1884808485,0.816448537725,0.162,0.662'
_flow_Strukturbericht 'None'
_flow_Pearson 'tP12'

_cell_length_a 6.1884808485
_cell_length_b 6.1884808485
_cell_length_c 5.0525761395
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4/m 2/c 2/c"
_symmetry_Int_Tables_number 124

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z+1/2
3 -x,y,-z+1/2
4 -x,-y,z
5 -y,-x,-z+1/2
6 -y,x,z
7 y,-x,z
8 y,x,-z+1/2
9 -x,-y,-z
10 -x,y,z+1/2
11 x,-y,z+1/2
12 x,y,-z
13 y,x,z+1/2
14 y,-x,-z
15 -y,x,-z
16 -y,-x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Co1 Co 2 a 0.00000 0.00000 0.25000 1.00000
Si1 Si 2 c 0.50000 0.50000 0.25000 1.00000
Nb1 Nb 8 m 0.16200 0.66200 0.00000 1.00000

```

Nb<sub>4</sub>CoSi: AB4C\_tP12\_124\_a\_m\_c - POSCAR

```

AB4C_tP12_124_a_m_c & a,c/a,x3,y3 --params=6.1884808485,0.816448537725,
↪ 0.162,0.662 & P4/mcc D2{4h}^{2} #124 (acm) & tP12 & None &
↪ Nb4CoSi & E. I. Gladyshevskii and {Yu}. B. {Kuz'ma}, J.
↪ Struct. Chem. 6, 60-63 (1965)
1.0000000000000000
6.188480848500000 0.000000000000000 0.0000000000000000
0.0000000000000000 6.188480848500000 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.052576139500000
Co Nb Si
2 8 2
Direct
0.0000000000000000 0.0000000000000000 0.2500000000000000 Co (2a)
0.0000000000000000 0.0000000000000000 0.7500000000000000 Co (2a)
0.1620000000000000 0.6620000000000000 0.0000000000000000 Nb (8m)
-0.1620000000000000 -0.6620000000000000 0.0000000000000000 Nb (8m)
-0.6620000000000000 0.1620000000000000 0.0000000000000000 Nb (8m)
0.6620000000000000 -0.1620000000000000 0.0000000000000000 Nb (8m)
-0.1620000000000000 0.6620000000000000 0.5000000000000000 Nb (8m)
0.1620000000000000 -0.6620000000000000 0.5000000000000000 Nb (8m)
0.6620000000000000 0.1620000000000000 0.5000000000000000 Nb (8m)
-0.6620000000000000 -0.1620000000000000 0.5000000000000000 Nb (8m)
0.5000000000000000 0.5000000000000000 0.2500000000000000 Si (2c)
0.5000000000000000 0.5000000000000000 0.7500000000000000 Si (2c)

```

NbTe<sub>4</sub>: AB<sub>4</sub>tP10\_124\_a\_m - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'NbTe4'
_chemical_formula_sum 'Nb Te4'

loop_
_publ_author_name
'K. Selte'
'A. Kjekshus'
_journal_name_full_name
;
Acta Chemica Scandinavica
;

```

```

;
_journal_volume 18
_journal_year 1964
_journal_page_first 690
_journal_page_last 696
_publ_Section_title
;
On the crystal structure of NbTe4
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'NbTe4 Structure'
_aflow_proto 'AB4_tP10_124_a_m'
_aflow_params 'a,c/a,x_{2},y_{2}'
_aflow_params_values '6.4989671731,1.05200800123,0.1425,0.3361'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP10'

_cell_length_a 6.4989671731
_cell_length_b 6.4989671731
_cell_length_c 6.8369654658
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4/m 2/c 2/c"
_symmetry_Int_Tables_number 124

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z+1/2
3 -x,y,-z+1/2
4 -x,-y,z
5 -y,-x,-z+1/2
6 -y,x,z
7 y,-x,z
8 y,x,-z+1/2
9 -x,-y,-z
10 -x,y,z+1/2
11 x,-y,z+1/2
12 x,y,-z
13 y,x,z+1/2
14 y,-x,-z
15 -y,x,-z
16 -y,-x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Nb1 Nb 2 a 0.00000 0.00000 0.25000 1.00000
Te1 Te 8 m 0.14250 0.33610 0.00000 1.00000

```

NbTe<sub>4</sub>: AB4\_tP10\_124\_a\_m - POSCAR

```

AB4_tP10_124_a_m & a,c/a,x2,y2 --params=6.4989671731,1.05200800123,
↳ 0.1425,0.3361 & P4/mcc D_{4h}^{2} #124 (am) & tP10 & None &
↳ NbTe4 & K. Selte and A. Kjekshus, Acta Chem. Scand. 18,
↳ 690-696 (1964)
1.0000000000000000
6.49896717310000 0.00000000000000 0.00000000000000
0.00000000000000 6.49896717310000 0.00000000000000
0.00000000000000 0.00000000000000 6.83696546580000
Nb Te
2 8
Direct
0.00000000000000 0.00000000000000 0.25000000000000 Nb (2a)
0.00000000000000 0.00000000000000 0.75000000000000 Nb (2a)
0.14250000000000 0.33610000000000 0.00000000000000 Te (8m)
-0.14250000000000 -0.33610000000000 0.00000000000000 Te (8m)
-0.33610000000000 -0.14250000000000 0.00000000000000 Te (8m)
0.33610000000000 -0.14250000000000 0.00000000000000 Te (8m)
-0.14250000000000 0.33610000000000 0.50000000000000 Te (8m)
0.14250000000000 -0.33610000000000 0.50000000000000 Te (8m)
0.33610000000000 0.14250000000000 0.50000000000000 Te (8m)
-0.33610000000000 -0.14250000000000 0.50000000000000 Te (8m)

```

PtPb<sub>4</sub>: A4B\_tP10\_125\_m\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'PtPb4'
_chemical_formula_sum 'Pb4 Pt'

loop_
_publ_author_name
'R. Graham'
'G. C. S. Waghorn'
'P. T. Davies'
_journal_year 1954
_publ_Section_title
;
An X-ray investigation of the lead-platinum system
;

```

```

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'PtPb4 Structure'
_aflow_proto 'A4B_tP10_125_m_a'
_aflow_params 'a,c/a,x_{2},z_{2}'
_aflow_params_values '6.6398746049,0.899096385539,0.425,0.255'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP10'

_cell_length_a 6.6398746049
_cell_length_b 6.6398746049
_cell_length_c 5.9698872577
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4/n 2/b 2/m (origin choice 2)"
_symmetry_Int_Tables_number 125

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y+1/2,-z
3 -x+1/2,y,-z
4 -x+1/2,-y+1/2,z
5 -y+1/2,-x+1/2,-z
6 -y+1/2,x,z
7 y,-x+1/2,z
8 y,x,-z
9 -x,-y,-z
10 -x,y+1/2,z
11 x+1/2,-y,z
12 x+1/2,y+1/2,-z
13 y+1/2,x+1/2,z
14 y+1/2,-x,-z
15 -y,x+1/2,-z
16 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Pt1 Pt 2 a 0.25000 0.25000 0.00000 1.00000
Pb1 Pb 8 m 0.42500 0.57500 0.25500 1.00000

```

PtPb<sub>4</sub>: A4B\_tP10\_125\_m\_a - POSCAR

```

A4B_tP10_125_m_a & a,c/a,x2,z2 --params=6.6398746049,0.899096385539,
↳ 0.425,0.255 & P4/nbm D_{4h}^{3} #125 (am) & tP10 & None & PtPb4
↳ & R. Graham and G. C. S. Waghorn and P. T. Davies, (1954)
1.0000000000000000
6.63987460490000 0.00000000000000 0.00000000000000
0.00000000000000 6.63987460490000 0.00000000000000
0.00000000000000 0.00000000000000 5.96988725770000
Pb Pt
8 2
Direct
0.42500000000000 -0.42500000000000 0.25500000000000 Pb (8m)
0.07500000000000 0.92500000000000 0.25500000000000 Pb (8m)
0.92500000000000 0.42500000000000 0.25500000000000 Pb (8m)
-0.42500000000000 0.07500000000000 0.25500000000000 Pb (8m)
0.07500000000000 -0.42500000000000 -0.25500000000000 Pb (8m)
0.42500000000000 0.92500000000000 -0.25500000000000 Pb (8m)
-0.42500000000000 0.42500000000000 -0.25500000000000 Pb (8m)
0.92500000000000 0.07500000000000 -0.25500000000000 Pb (8m)
0.25000000000000 0.25000000000000 0.00000000000000 Pt (2a)
0.75000000000000 0.75000000000000 0.00000000000000 Pt (2a)

```

KCeSe<sub>4</sub>: ABC4\_tP12\_125\_a\_b\_m - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'KCeSe4'
_chemical_formula_sum 'Ce K Se4'

loop_
_publ_author_name
'A. C. Sutorik'
'M. G. Kanatzidis'
_journal_name_full_name
;
Angewandte Chemie (International ed.)
;
_journal_volume 31
_journal_year 1992
_journal_page_first 1594
_journal_page_last 1596
_publ_Section_title
;
KCeSe4: A New Solid-State Lanthanide Polychalcogenide
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

```

```

_flow_title 'KCeSe4{4}$ Structure'
_flow_proto 'ABC4_tP12_125_a_b_m'
_flow_params 'a,c/a,x3,z3'
_flow_params_values '6.3759876428,1.30630489336,0.3822,0.2163'
_flow_Strukturbericht 'None'
_flow_Pearson 'tP12'

_cell_length_a 6.3759876428
_cell_length_b 6.3759876428
_cell_length_c 8.3289838578
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4/n 2/b 2/m (origin choice 2)"
_symmetry_Int_Tables_number 125

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y+1/2,-z
3 -x+1/2,y,-z
4 -x+1/2,-y+1/2,z
5 -y+1/2,-x+1/2,-z
6 -y+1/2,x,z
7 y,-x+1/2,z
8 y,x,-z
9 -x,-y,-z
10 -x,y+1/2,z
11 x+1/2,-y,z
12 x+1/2,y+1/2,-z
13 y+1/2,x+1/2,z
14 y+1/2,-x,-z
15 -y,x+1/2,-z
16 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ce1 Ce 2 a 0.25000 0.25000 0.00000 1.00000
K1 K 2 b 0.25000 0.25000 0.50000 1.00000
Se1 Se 8 m 0.38220 0.61780 0.21630 1.00000

```

**KCeSe<sub>4</sub>: ABC4\_tP12\_125\_a\_b\_m - POSCAR**

```

ABC4_tP12_125_a_b_m & a,c/a,x3,z3 --params=6.3759876428,1.30630489336,
↪ 0.3822,0.2163 & P4/nbm D2[4h]{3} #125 (abm) & tP12 & None &
↪ KCeSe4 & A. C. Sutorik and M. G. Kanatzidis, Angew. Chem.
↪ Int. Ed. 31, 1594-1596 (1992)
1.0000000000000000
6.37598764280000 0.00000000000000 0.00000000000000
0.00000000000000 6.37598764280000 0.00000000000000
0.00000000000000 0.00000000000000 8.32898385780000
Ce K Se
2 2 8
Direct
0.25000000000000 0.25000000000000 0.00000000000000 Ce (2a)
0.75000000000000 0.75000000000000 0.00000000000000 Ce (2a)
0.25000000000000 0.25000000000000 0.50000000000000 K (2b)
0.75000000000000 0.75000000000000 0.50000000000000 K (2b)
0.38220000000000 -0.38220000000000 0.21630000000000 Se (8m)
0.11780000000000 0.88220000000000 0.21630000000000 Se (8m)
0.88220000000000 0.38220000000000 0.21630000000000 Se (8m)
-0.38220000000000 0.11780000000000 0.21630000000000 Se (8m)
0.11780000000000 -0.38220000000000 -0.21630000000000 Se (8m)
0.38220000000000 0.88220000000000 -0.21630000000000 Se (8m)
-0.38220000000000 0.38220000000000 -0.21630000000000 Se (8m)
0.88220000000000 0.11780000000000 -0.21630000000000 Se (8m)

```

**BiAl<sub>2</sub>S<sub>4</sub>: A2BC4\_tP28\_126\_cd\_e\_k - CIF**

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'BiAl2S4'
_chemical_formula_sum 'A12 Bi S4'

loop_
_publ_author_name
'H. Kalpen'
'W. H[\"o]nle'
'M. Somer'
'U. Schwarz'
'K. Peters'
'H. G. [von Schnering]'
'R. Blachnik'
_journal_name_full_name
;
Zeitschrift fur Anorganische und Allgemeine Chemie
;
_journal_volume 624
_journal_year 1998
_journal_page_first 1137
_journal_page_last 1147
_publ_section_title
;

```

```

Bismut(II)-chalkogenometallate(III) Bi2M4X8$, Verbindungen
↪ mit Bi2{4+}$-Hanteln ($M$ = Al, Ga; $X$ = S, Se)
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_flow_title 'BiAl2{2}$SS4{4}$ Structure'
_flow_proto 'A2BC4_tP28_126_cd_e_k'
_flow_params 'a,c/a,z3,x4,y4,z4'
_flow_params_values '7.4920241479,1.58609183128,0.11808,0.0865,0.5924,
↪ 0.1254'
_flow_Strukturbericht 'None'
_flow_Pearson 'tP28'

_cell_length_a 7.4920241479
_cell_length_b 7.4920241479
_cell_length_c 11.8830383007
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4/n 2/n 2/c (origin choice 2)"
_symmetry_Int_Tables_number 126

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y+1/2,-z+1/2
3 -x+1/2,y,-z+1/2
4 -x+1/2,-y+1/2,z
5 -y+1/2,-x+1/2,-z+1/2
6 -y+1/2,x,z
7 y,-x+1/2,z
8 y,x,-z+1/2
9 -x,-y,-z
10 -x,y+1/2,z+1/2
11 x+1/2,-y,z+1/2
12 x+1/2,y+1/2,-z
13 y+1/2,x+1/2,z+1/2
14 y+1/2,-x,-z
15 -y,x+1/2,-z
16 -y,-x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 4 c 0.25000 0.75000 1.00000
Al2 Al 4 d 0.25000 0.75000 0.00000 1.00000
Bi1 Bi 4 e 0.25000 0.25000 0.11808 1.00000
S1 S 16 k 0.08650 0.59240 0.12540 1.00000

```

**BiAl<sub>2</sub>S<sub>4</sub>: A2BC4\_tP28\_126\_cd\_e\_k - POSCAR**

```

A2BC4_tP28_126_cd_e_k & a,c/a,z3,x4,y4,z4 --params=7.4920241479,
↪ 1.58609183128,0.11808,0.0865,0.5924,0.1254 & P4/nnc D2[4h]{4}
↪ #126 (cdek) & tP28 & None & BiAl2S4 & H. Kalpen et al., Z.
↪ Anorg. Allg. Chem. 624, 1137-1147 (1998)
1.0000000000000000
7.49202414790000 0.00000000000000 0.00000000000000
0.00000000000000 7.49202414790000 0.00000000000000
0.00000000000000 0.00000000000000 11.88303830070000
Al Bi S
8 4 16
Direct
0.25000000000000 0.75000000000000 0.75000000000000 Al (4c)
0.75000000000000 0.25000000000000 0.25000000000000 Al (4c)
0.75000000000000 0.25000000000000 0.25000000000000 Al (4c)
0.25000000000000 0.75000000000000 0.00000000000000 Al (4d)
0.75000000000000 0.25000000000000 0.50000000000000 Al (4d)
0.75000000000000 0.25000000000000 0.50000000000000 Al (4d)
0.25000000000000 0.25000000000000 0.50000000000000 Al (4d)
0.25000000000000 0.25000000000000 0.11808000000000 Bi (4e)
0.25000000000000 0.25000000000000 0.38192000000000 Bi (4e)
0.75000000000000 0.75000000000000 -0.11808000000000 Bi (4e)
0.75000000000000 0.75000000000000 0.61808000000000 Bi (4e)
0.08650000000000 0.59240000000000 0.12540000000000 S (16k)
0.41350000000000 -0.09240000000000 0.12540000000000 S (16k)
-0.09240000000000 0.08650000000000 0.12540000000000 S (16k)
0.59240000000000 0.41350000000000 0.12540000000000 S (16k)
0.41350000000000 0.59240000000000 0.37460000000000 S (16k)
0.08650000000000 -0.09240000000000 0.37460000000000 S (16k)
0.59240000000000 0.08650000000000 0.37460000000000 S (16k)
-0.09240000000000 0.41350000000000 0.37460000000000 S (16k)
-0.08650000000000 -0.59240000000000 -0.12540000000000 S (16k)
0.58650000000000 1.09240000000000 -0.12540000000000 S (16k)
1.09240000000000 -0.08650000000000 -0.12540000000000 S (16k)
-0.59240000000000 0.58650000000000 -0.12540000000000 S (16k)
0.58650000000000 -0.59240000000000 0.62540000000000 S (16k)
-0.08650000000000 1.09240000000000 0.62540000000000 S (16k)
-0.59240000000000 -0.08650000000000 0.62540000000000 S (16k)
1.09240000000000 0.58650000000000 0.62540000000000 S (16k)

```

**ThB<sub>4</sub>(D<sub>1c</sub>): A4B\_tP20\_127\_chj\_g - CIF**

```

# CIF file
data_findsym-output

```

```

_audit_creation_method FINDSYM
_chemical_name_mineral 'ThB4'
_chemical_formula_sum 'B4 Th'

loop_
  _publ_author_name
  'A. Zalkin'
  'D. H. Templeton'
  _journal_name_full_name
  ;
  Journal of Chemical Physics
  ;
  _journal_volume 18
  _journal_year 1950
  _journal_page_first 391
  _journal_page_last 391
  _publ_section_title
  ;
  The Crystal Structures of CeBS_{4}$, ThBS_{4}$, and UBS_{4}$
  ;
  _aflow_title 'ThBS_{4}$ (SD1{e}$) Structure'
  _aflow_proto 'A4B_tP20_127_ehj_g'
  _aflow_params 'a,c/a,z_{1},x_{2},x_{3},x_{4},y_{4}'
  _aflow_params_values '7.256,0.56684123484,0.2,0.31,0.1,0.2,0.04'
  _aflow_Strukturbericht 'SD1{e}$'
  _aflow_Pearson 'tP20'

_symmetry_space_group_name_H-M "P 4/m 21/b 2/m"
_symmetry_Int_Tables_number 127

_cell_length_a 7.25600
_cell_length_b 7.25600
_cell_length_c 4.11300
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x+1/2,-y+1/2,-z
  3 -x+1/2,y+1/2,-z
  4 -x,-y,z
  5 -y+1/2,-x+1/2,-z
  6 -y,x,z
  7 y,-x,z
  8 y+1/2,x+1/2,-z
  9 -x,-y,-z
  10 -x+1/2,y+1/2,z
  11 x+1/2,-y+1/2,z
  12 x,y,-z
  13 y+1/2,x+1/2,z
  14 y,-x,-z
  15 -y,x,-z
  16 -y+1/2,-x+1/2,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  B1 B 4 e 0.00000 0.00000 0.20000 1.00000
  Th1 Th 4 g 0.31000 0.81000 0.00000 1.00000
  B2 B 4 h 0.10000 0.60000 0.50000 1.00000
  B3 B 8 j 0.20000 0.04000 0.50000 1.00000

```

ThB<sub>4</sub> (D<sub>1c</sub>): A4B\_tP20\_127\_ehj\_g - POSCAR

```

A4B_tP20_127_ehj_g & a,c/a,z1,x2,x3,x4,y4 --params=7.256,0.56684123484,
  ↪ 0.2,0.31,0.1,0.2,0.04 & P4/mbm D_{4h}^{5} #127 (eghj) & tP20 &
  ↪ SD1{e}$ & ThB4 & ThB4 & A. Zalkin and D. H. Templeton, J.
  ↪ Chem. Phys. 18, 391 (1950)
1.0000000000000000
7.2560000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.2560000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.1130000000000000
  B Th
  16 4
Direct
0.0000000000000000 0.0000000000000000 0.2000000000000000 B (4e)
0.5000000000000000 0.5000000000000000 -0.2000000000000000 B (4e)
0.0000000000000000 0.0000000000000000 -0.2000000000000000 B (4e)
0.5000000000000000 0.5000000000000000 0.2000000000000000 B (4e)
0.1000000000000000 0.6000000000000000 0.5000000000000000 B (4h)
-0.1000000000000000 0.4000000000000000 0.5000000000000000 B (4h)
0.4000000000000000 0.1000000000000000 0.5000000000000000 B (4h)
0.6000000000000000 -0.1000000000000000 0.5000000000000000 B (4h)
0.2000000000000000 0.0400000000000000 0.5000000000000000 B (8j)
-0.2000000000000000 -0.0400000000000000 0.5000000000000000 B (8j)
-0.0400000000000000 0.2000000000000000 0.5000000000000000 B (8j)
0.0400000000000000 -0.2000000000000000 0.5000000000000000 B (8j)
0.3000000000000000 0.5400000000000000 0.5000000000000000 B (8j)
0.7000000000000000 0.4600000000000000 0.5000000000000000 B (8j)
0.5400000000000000 0.7000000000000000 0.5000000000000000 B (8j)
0.4600000000000000 0.3000000000000000 0.5000000000000000 B (8j)
0.3100000000000000 0.8100000000000000 0.0000000000000000 Th (4g)
-0.3100000000000000 0.1900000000000000 0.0000000000000000 Th (4g)
0.1900000000000000 0.3100000000000000 0.0000000000000000 Th (4g)

```

0.8100000000000000 -0.3100000000000000 0.0000000000000000 Th (4g)

K<sub>2</sub>SnCl<sub>6</sub> (Low-temperature): A6B2C\_tP18\_128\_eh\_d\_b - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'K2SnCl6'
_chemical_formula_sum 'Cl6 K2 Sn'

loop_
  _publ_author_name
  'H. Boysen'
  'A. W. Hewat'
  _journal_name_full_name
  ;
  Acta Crystallographica Section B: Structural Science
  ;
  _journal_volume 34
  _journal_year 1978
  _journal_page_first 1412
  _journal_page_last 1418
  _publ_section_title
  ;
  A neutron powder investigation of the structural changes in KS_{2}
  ↪ SSnClS_{6}$

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'KS_{2}$SnClS_{6}$ (Low-temperature) Structure'
_aflow_proto 'A6B2C_tP18_128_eh_d_b'
_aflow_params 'a,c/a,z_{3},x_{4},y_{4}'
_aflow_params_values '7.057532571,1.41383170154,0.7523,0.7217,0.2489'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP18'

_cell_length_a 7.0575325710
_cell_length_b 7.0575325710
_cell_length_c 9.9781632835
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4/m 21/n 2/c"
_symmetry_Int_Tables_number 128

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x+1/2,-y+1/2,-z+1/2
  3 -x+1/2,y+1/2,-z+1/2
  4 -x,-y,z
  5 -y+1/2,-x+1/2,-z+1/2
  6 -y,x,z
  7 y,-x,z
  8 y+1/2,x+1/2,-z+1/2
  9 -x,-y,-z
  10 -x+1/2,y+1/2,z+1/2
  11 x+1/2,-y+1/2,z+1/2
  12 x,y,-z
  13 y+1/2,x+1/2,z+1/2
  14 y,-x,-z
  15 -y,x,-z
  16 -y+1/2,-x+1/2,z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Sn1 Sn 2 b 0.00000 0.00000 0.50000 1.00000
  K1 K 4 d 0.00000 0.50000 0.25000 1.00000
  Cl1 Cl 4 e 0.00000 0.00000 0.75230 1.00000
  Cl2 Cl 8 h 0.72170 0.24890 0.00000 1.00000

```

K<sub>2</sub>SnCl<sub>6</sub> (Low-temperature): A6B2C\_tP18\_128\_eh\_d\_b - POSCAR

```

A6B2C_tP18_128_eh_d_b & a,c/a,z3,x4,y4 --params=7.057532571,
  ↪ 1.41383170154,0.7523,0.7217,0.2489 & P4/mnc D_{4h}^{6} #128 (
  ↪ bdeh) & tP18 & None & K2SnCl6 & H. Boysen and A. W. Hewat,
  ↪ Acta Crystallogr. Sect. B Struct. Sci. 34, 1412-1418 (1978)
1.0000000000000000
7.0575325710000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.0575325710000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 9.9781632835000000
  Cl K Sn
  12 4 2
Direct
0.0000000000000000 0.0000000000000000 0.7523000000000000 Cl (4e)
0.5000000000000000 0.5000000000000000 -0.2523000000000000 Cl (4e)
0.0000000000000000 0.0000000000000000 -0.7523000000000000 Cl (4e)
0.5000000000000000 0.5000000000000000 1.2523000000000000 Cl (4e)
0.7217000000000000 0.2489000000000000 0.0000000000000000 Cl (8h)
-0.7217000000000000 -0.2489000000000000 0.0000000000000000 Cl (8h)
-0.2489000000000000 0.7217000000000000 0.0000000000000000 Cl (8h)
0.2489000000000000 -0.7217000000000000 0.0000000000000000 Cl (8h)
-0.2217000000000000 0.7489000000000000 0.5000000000000000 Cl (8h)

```

1.22170000000000	0.25110000000000	0.50000000000000	Cl	(8h)
0.74890000000000	1.22170000000000	0.50000000000000	Cl	(8h)
0.25110000000000	-0.22170000000000	0.50000000000000	Cl	(8h)
0.00000000000000	0.50000000000000	0.25000000000000	K	(4d)
0.50000000000000	0.00000000000000	0.25000000000000	K	(4d)
0.00000000000000	0.50000000000000	0.75000000000000	K	(4d)
0.50000000000000	0.00000000000000	0.75000000000000	K	(4d)
0.00000000000000	0.00000000000000	0.50000000000000	Sn	(2b)
0.50000000000000	0.50000000000000	0.00000000000000	Sn	(2b)

FeCu<sub>2</sub>Al<sub>7</sub> (E<sub>9</sub>): A7B2C\_tP40\_128\_egi\_h\_e - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'FeCu2Al7'
_chemical_formula_sum 'A17 Cu2 Fe'

loop_
_publ_author_name
'M. G. Bown'
'P. J. Brown'
_journal_name_full_name
Acta Crystallographica
;
_journal_volume 9
_journal_year 1956
_journal_page_first 911
_journal_page_last 914
_publ_section_title
The structure of FeCu2{2}Al7{7} and T(CoCuAl)
;
_aflow_title 'FeCu2{2}Al7{7} ($E9_{a})$ Structure'
_aflow_proto 'A7B2C_tP40_128_egi_h_e'
_aflow_params 'a, c/a, z_{1}, z_{2}, x_{3}, x_{4}, y_{4}, x_{5}, y_{5}, z_{5}'
_aflow_params_values '6.336, 2.34690656566, 0.366, 0.2008, 0.165, 0.278, 0.088
↪ 0.198, 0.42, 0.1'
_aflow_Strukturbericht '$E9_{a})$'
_aflow_Pearson 'tP40'

_symmetry_space_group_name_H-M "P 4/m 21/n 2/c"
_symmetry_Int_Tables_number 128

_cell_length_a 6.33600
_cell_length_b 6.33600
_cell_length_c 14.87000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x+1/2, -y+1/2, -z+1/2
3 -x+1/2, y+1/2, -z+1/2
4 -x, -y, z
5 -y+1/2, -x+1/2, -z+1/2
6 -y, x, z
7 y, -x, z
8 y+1/2, x+1/2, -z+1/2
9 -x, -y, -z
10 -x+1/2, y+1/2, z+1/2
11 x+1/2, -y+1/2, z+1/2
12 x, y, -z
13 y+1/2, x+1/2, z+1/2
14 y, -x, -z
15 -y, x, -z
16 -y+1/2, -x+1/2, z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 4 e 0.00000 0.00000 0.36600 1.00000
Fe1 Fe 4 e 0.00000 0.00000 0.20080 1.00000
Al2 Al 8 g 0.16500 0.66500 0.25000 1.00000
Cu1 Cu 8 h 0.27800 0.08800 0.00000 1.00000
Al3 Al 16 i 0.19800 0.42000 0.10000 1.00000
```

FeCu<sub>2</sub>Al<sub>7</sub> (E<sub>9</sub>): A7B2C\_tP40\_128\_egi\_h\_e - POSCAR

```
A7B2C_tP40_128_egi_h_e & a, c/a, z1, z2, x3, x4, y4, x5, y5, z5 --params=6.336,
↪ 2.34690656566, 0.366, 0.2008, 0.165, 0.278, 0.088, 0.198, 0.42, 0.1 &
↪ P4/mnc D_{4h}^{6} #128 (e^2g_{hi}) & tP40 & $E9_{a})$ & FeCu2Al7 &
↪ FeCu2Al7 & M. G. Bown and P. J. Brown, Acta Cryst. 9, 911-914 (
↪ 1956)
1.00000000000000
6.33600000000000 0.00000000000000 0.00000000000000
0.00000000000000 6.33600000000000 0.00000000000000
0.00000000000000 0.00000000000000 14.87000000000000
Al Cu Fe
28 8 4
Direct
0.00000000000000 0.00000000000000 0.36600000000000 Al (4e)
0.50000000000000 0.50000000000000 0.13400000000000 Al (4e)
```

0.00000000000000	0.00000000000000	-0.36600000000000	Al	(4e)
0.50000000000000	0.50000000000000	0.86600000000000	Al	(4e)
0.16500000000000	0.66500000000000	0.25000000000000	Al	(8g)
-0.16500000000000	0.33500000000000	0.25000000000000	Al	(8g)
0.33500000000000	0.16500000000000	0.25000000000000	Al	(8g)
0.66500000000000	-0.16500000000000	0.25000000000000	Al	(8g)
-0.16500000000000	0.33500000000000	0.75000000000000	Al	(8g)
0.16500000000000	0.66500000000000	0.75000000000000	Al	(8g)
0.66500000000000	-0.16500000000000	0.75000000000000	Al	(8g)
0.33500000000000	0.16500000000000	0.75000000000000	Al	(8g)
0.19800000000000	0.42000000000000	0.10000000000000	Al	(16i)
-0.19800000000000	-0.42000000000000	0.10000000000000	Al	(16i)
-0.42000000000000	0.19800000000000	0.10000000000000	Al	(16i)
0.42000000000000	-0.19800000000000	0.10000000000000	Al	(16i)
0.30200000000000	0.92000000000000	0.40000000000000	Al	(16i)
0.69800000000000	0.08000000000000	0.40000000000000	Al	(16i)
0.92000000000000	0.69800000000000	0.40000000000000	Al	(16i)
0.08000000000000	0.30200000000000	0.40000000000000	Al	(16i)
-0.19800000000000	-0.42000000000000	-0.10000000000000	Al	(16i)
0.19800000000000	0.42000000000000	-0.10000000000000	Al	(16i)
-0.42000000000000	0.19800000000000	-0.10000000000000	Al	(16i)
0.69800000000000	0.08000000000000	0.60000000000000	Al	(16i)
0.30200000000000	0.92000000000000	0.60000000000000	Al	(16i)
0.08000000000000	0.30200000000000	0.60000000000000	Al	(16i)
0.92000000000000	0.69800000000000	0.60000000000000	Al	(16i)
0.27800000000000	0.08800000000000	0.00000000000000	Cu	(8h)
-0.27800000000000	-0.08800000000000	0.00000000000000	Cu	(8h)
-0.08800000000000	0.27800000000000	0.00000000000000	Cu	(8h)
0.08800000000000	-0.27800000000000	0.00000000000000	Cu	(8h)
0.22200000000000	0.58800000000000	0.50000000000000	Cu	(8h)
0.77800000000000	0.41200000000000	0.50000000000000	Cu	(8h)
0.58800000000000	0.77800000000000	0.50000000000000	Cu	(8h)
0.41200000000000	0.22200000000000	0.50000000000000	Cu	(8h)
0.00000000000000	0.00000000000000	0.20080000000000	Fe	(4e)
0.50000000000000	0.50000000000000	0.29920000000000	Fe	(4e)
0.00000000000000	0.00000000000000	-0.20080000000000	Fe	(4e)
0.50000000000000	0.50000000000000	0.70080000000000	Fe	(4e)

CuBi<sub>2</sub>O<sub>4</sub>: A2BC4\_tP28\_130\_f\_c\_g - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'CuBi2O4'
_chemical_formula_sum 'Bi2 Cu O4'

loop_
_publ_author_name
'J.-C. Boivin'
'J. Trehoux'
'D. Thomas'
_journal_name_full_name
Bulletin of Research Laboratory of Precision Machinery and Electronics
;
_journal_volume 99
_journal_year 1976
_journal_page_first 193
_journal_page_last 196
_publ_section_title
{\\'E}tude structurale de CuBi2{2}SO4{4}$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'CuBi2{2}SO4{4}$ Structure'
_aflow_proto 'A2BC4_tP28_130_f_c_g'
_aflow_params 'a, c/a, z_{1}, x_{2}, x_{3}, y_{3}, z_{3}'
_aflow_params_values '8.5103337343, 0.683196239716, 0.58, 0.5815, 0.045,
↪ 0.136, 0.597'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP28'

_cell_length_a 8.5103337343
_cell_length_b 8.5103337343
_cell_length_c 5.8142280060
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4/n 21/c 2/c (origin choice 2)"
_symmetry_Int_Tables_number 130

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x+1/2, -y, -z+1/2
3 -x, y+1/2, -z+1/2
4 -x+1/2, -y+1/2, z
5 -y, -x, -z+1/2
6 -y+1/2, x, z
7 y, -x+1/2, z
8 y+1/2, x+1/2, -z+1/2
9 -x, -y, -z
10 -x+1/2, y, z+1/2
11 x, -y+1/2, z+1/2
12 x+1/2, y+1/2, -z
13 y, x, z+1/2
14 y+1/2, -x, -z
15 -y, x+1/2, -z
```

```

16 -y+1/2,-x+1/2,z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Cu1 Cu 4 c 0.25000 0.25000 0.58000 1.00000
Bi1 Bi 8 f 0.58150 0.41850 0.25000 1.00000
O1 O 16 g 0.04500 0.13600 0.59700 1.00000

```

CuBi<sub>2</sub>O<sub>4</sub>: A2BC4\_tP28\_130\_f\_c\_g - POSCAR

```

A2BC4_tP28_130_f_c_g & a,c/a,z1,x2,x3,y3,z3 --params=8.5103337343.
↪ 0.683196239716, 0.58, 0.5815, 0.045, 0.136, 0.597 & P4/ncc D_{4h}^{8}
↪ #130 (cfcg) & tP28 & None & CuBi2O4 & & J.-C. Boivin and J.
↪ Trehoux and D. Thomas, Bull. Soc. fr. Min'eral. Crystallogr. 99
↪ , 193-196 (1976)
1.0000000000000000
8.51033373430000 0.00000000000000 0.00000000000000
0.00000000000000 8.51033373430000 0.00000000000000
0.00000000000000 0.00000000000000 5.81422800600000
Bi Cu O
8 4 16
Direct
0.58150000000000 -0.58150000000000 0.25000000000000 Bi (8f)
-0.08150000000000 -0.08150000000000 0.25000000000000 Bi (8f)
1.08150000000000 0.58150000000000 0.25000000000000 Bi (8f)
-0.58150000000000 -0.08150000000000 0.25000000000000 Bi (8f)
-0.58150000000000 0.58150000000000 0.75000000000000 Bi (8f)
1.08150000000000 -0.08150000000000 0.75000000000000 Bi (8f)
-0.08150000000000 -0.58150000000000 0.75000000000000 Bi (8f)
0.58150000000000 1.08150000000000 0.75000000000000 Bi (8f)
0.25000000000000 0.25000000000000 0.58000000000000 Cu (4c)
0.75000000000000 0.75000000000000 -0.08000000000000 Cu (4c)
0.75000000000000 0.75000000000000 -0.58000000000000 Cu (4c)
0.25000000000000 0.25000000000000 1.08000000000000 Cu (4c)
0.04500000000000 0.13600000000000 0.59700000000000 O (16g)
0.45500000000000 0.36400000000000 0.59700000000000 O (16g)
0.36400000000000 0.04500000000000 0.59700000000000 O (16g)
0.13600000000000 0.45500000000000 0.59700000000000 O (16g)
-0.04500000000000 -0.63600000000000 -0.09700000000000 O (16g)
0.54500000000000 -0.13600000000000 -0.09700000000000 O (16g)
0.63600000000000 0.54500000000000 -0.09700000000000 O (16g)
-0.13600000000000 -0.04500000000000 -0.09700000000000 O (16g)
-0.04500000000000 -0.13600000000000 -0.59700000000000 O (16g)
0.54500000000000 0.63600000000000 -0.59700000000000 O (16g)
0.63600000000000 -0.04500000000000 -0.59700000000000 O (16g)
-0.13600000000000 0.54500000000000 -0.59700000000000 O (16g)
0.04500000000000 0.36400000000000 1.09700000000000 O (16g)
0.45500000000000 0.13600000000000 1.09700000000000 O (16g)
0.36400000000000 0.45500000000000 1.09700000000000 O (16g)
0.13600000000000 0.04500000000000 1.09700000000000 O (16g)

```

Ba<sub>5</sub>Si<sub>3</sub>: A5B3\_tP32\_130\_cg\_cf - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Ba5 Si3'

loop_
  _publ_author_name
  'R. Nesper'
  'F. Z{"u}rcher'
  _journal_name_full_name
  ;
  Zeitschrift f{"u}r Kristallografiya B
  ;
  _journal_volume 214
  _journal_year 1966
  _journal_page_first 20
  _journal_page_last 20
  _publ_section_title
  ;
  Refinement of the crystal structure of pentabarium trisilicide, Ba5{5}
  ↪ $Si$_{3}$
  ;
  _aflow_title 'Ba5{5}$Si$_{3}$ Structure'
  _aflow_proto 'A5B3_tP32_130_cg_cf'
  _aflow_params 'a,c/a,z{1},z{2},x_{3},x_{4},y_{4},z_{4}'
  _aflow_params_values '8.465,1.94329592439,0.2271,0.0095,0.1482,0.57997,
  ↪ 0.07997,0.10688'
  _aflow_Strukturbericht 'None'
  _aflow_Pearson 'tP32'

_symmetry_space_group_name_H-M "P 4/n c c:2"
_symmetry_Int_Tables_number 130

_cell_length_a 8.46500
_cell_length_b 8.46500
_cell_length_c 16.45000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id

```

```

_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y,-z+1/2
3 -x,y+1/2,-z+1/2
4 -x+1/2,-y+1/2,z
5 -y,-x,-z+1/2
6 -y+1/2,x,z
7 y,-x+1/2,z
8 y+1/2,x+1/2,-z+1/2
9 -x,-y,-z
10 -x+1/2,y,z+1/2
11 x,-y+1/2,z+1/2
12 x+1/2,y+1/2,-z
13 y,x,z+1/2
14 y+1/2,-x,-z
15 -y,x+1/2,-z
16 -y+1/2,-x+1/2,z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Ba1 Ba 4 c 0.25000 0.25000 0.22710 1.00000
Si1 Si 4 c 0.25000 0.25000 0.00950 1.00000
Si2 Si 8 f 0.14820 0.85180 0.25000 1.00000
Ba2 Ba 16 g 0.57997 0.07997 0.10688 1.00000

```

Ba<sub>5</sub>Si<sub>3</sub>: A5B3\_tP32\_130\_cg\_cf - POSCAR

```

A5B3_tP32_130_cg_cf & a,c/a,z1,z2,x3,x4,y4,z4 --params=8.465,
↪ 1.94329592439,0.2271,0.0095,0.1482,0.57997,0.07997,0.10688 & P4
↪ /ncc D_{4h}^{8} #130 (c^2fg) & tP32 & None & Ba5Si3 & & R.
↪ Nesper and F. Z{"u}rcher, Z. Kristallogr. B 214, 20(1966)
1.0000000000000000
8.46500000000000 0.00000000000000 0.00000000000000
0.00000000000000 8.46500000000000 0.00000000000000
0.00000000000000 0.00000000000000 16.45000000000000
Ba Si
20 12
Direct
0.25000000000000 0.25000000000000 0.22710000000000 Ba (4c)
0.75000000000000 0.75000000000000 0.27290000000000 Ba (4c)
0.75000000000000 0.75000000000000 -0.22710000000000 Ba (4c)
0.25000000000000 0.25000000000000 0.72710000000000 Ba (4c)
0.57997000000000 0.07997000000000 0.10688000000000 Ba (16g)
-0.07997000000000 0.42003000000000 0.10688000000000 Ba (16g)
0.42003000000000 0.57997000000000 0.10688000000000 Ba (16g)
0.07997000000000 -0.07997000000000 0.10688000000000 Ba (16g)
-0.57997000000000 0.57997000000000 0.39312000000000 Ba (16g)
0.07997000000000 -0.07997000000000 0.39312000000000 Ba (16g)
0.57997000000000 1.07997000000000 0.39312000000000 Ba (16g)
-0.07997000000000 -0.57997000000000 0.39312000000000 Ba (16g)
-0.57997000000000 -0.07997000000000 -0.10688000000000 Ba (16g)
1.07997000000000 0.57997000000000 -0.10688000000000 Ba (16g)
0.57997000000000 -0.57997000000000 -0.10688000000000 Ba (16g)
-0.07997000000000 1.07997000000000 -0.10688000000000 Ba (16g)
0.57997000000000 0.42003000000000 0.60688000000000 Ba (16g)
-0.07997000000000 0.07997000000000 0.60688000000000 Ba (16g)
0.42003000000000 -0.07997000000000 0.60688000000000 Ba (16g)
0.07997000000000 0.57997000000000 0.60688000000000 Ba (16g)
0.25000000000000 0.25000000000000 0.00950000000000 Si (4c)
0.75000000000000 0.75000000000000 0.49050000000000 Si (4c)
0.75000000000000 0.75000000000000 -0.00950000000000 Si (4c)
0.25000000000000 0.25000000000000 0.50950000000000 Si (4c)
0.14820000000000 -0.14820000000000 0.25000000000000 Si (8f)
0.35180000000000 0.35180000000000 0.25000000000000 Si (8f)
0.64820000000000 0.14820000000000 0.25000000000000 Si (8f)
-0.14820000000000 0.35180000000000 0.25000000000000 Si (8f)
-0.14820000000000 0.14820000000000 0.75000000000000 Si (8f)
0.64820000000000 0.35180000000000 0.75000000000000 Si (8f)
0.35180000000000 -0.14820000000000 0.75000000000000 Si (8f)
0.14820000000000 0.64820000000000 0.75000000000000 Si (8f)

```

Rb<sub>2</sub>TiCu<sub>2</sub>S<sub>4</sub>: A2B2C4D\_tP18\_132\_e\_i\_o\_d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Rb2TiCu2Se4'
_chemical_formula_sum 'Cu2 Rb2 S4 Ti'

loop_
  _publ_author_name
  'F. Q. Huang'
  'J. A. Ibers'
  _journal_name_full_name
  ;
  Inorganic Chemistry
  ;
  _journal_volume 40
  _journal_year 2001
  _journal_page_first 2602
  _journal_page_last 2607
  _publ_section_title
  ;
  New Layered Materials: Syntheses, Structures, and Optical Properties of
  ↪ KS{2}STiCuS{2}SSS{4}$, RbS{2}STiCuS{2}SSS{4}$, RbS{2}
  ↪ STiAgS{2}SSS{4}$, CsS{2}STiAgS{2}SSS{4}$, and CsS{2}
  ↪ STiCuS{2}SSS{4}$

```



```

;
_aflow_title 'RbS_{2}TiCuS_{2}SSS_{4}$ Structure '
_aflow_proto 'A2B2C4D_tP18_132_e_i_o_d'
_aflow_params 'a,c/a,x_{3},x_{4},z_{4}'
_aflow_params_values '5.6046,2.34700067801,0.2369,0.26316,0.34803'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP18'

_symmetry_space_group_name_H-M "P 42/m 2/c 2/m"
_symmetry_Int_Tables_number 132

_cell_length_a 5.60460
_cell_length_b 5.60460
_cell_length_c 13.15400
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z+1/2
3 -x,y,-z+1/2
4 -x,-y,z
5 -y,-x,-z
6 -y,x,z+1/2
7 y,-x,z+1/2
8 y,x,-z
9 -x,-y,-z
10 -x,y,z+1/2
11 x,-y,z+1/2
12 x,y,-z
13 y,x,z
14 y,-x,-z+1/2
15 -y,x,-z+1/2
16 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ti1 Ti 2 d 0.50000 0.50000 0.25000 1.00000
Cu1 Cu 4 e 0.00000 0.50000 0.25000 1.00000
Rb1 Rb 4 i 0.23690 0.23690 0.00000 1.00000
S1 S 8 o 0.26316 0.26316 0.34803 1.00000

```

Rb<sub>2</sub>TiCu<sub>2</sub>S<sub>4</sub>: A2B2C4D\_tP18\_132\_e\_i\_o\_d - POSCAR

```

A2B2C4D_tP18_132_e_i_o_d & a,c/a,x3,x4,z4 --params=5.6046,2.34700067801,
↪ 0.2369,0.26316,0.34803 & P4_{2}/mcm D_{4h}^{10} #132 (deio) &
↪ tP18 & None & Rb2TiCu2Se4 & Rb2TiCu2Se4 & F. Q. Huang and J. A.
↪ Ibers, Inorg. Chem. 40, 2602-2607 (2001)
1.0000000000000000
5.6046000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.6046000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.1540000000000000
Cu Rb S
4 4 8 2
Direct
0.0000000000000000 0.5000000000000000 0.2500000000000000 Cu (4e)
0.5000000000000000 0.0000000000000000 0.7500000000000000 Cu (4e)
0.0000000000000000 0.5000000000000000 0.7500000000000000 Cu (4e)
0.5000000000000000 0.0000000000000000 0.2500000000000000 Cu (4e)
0.2369000000000000 0.2369000000000000 0.0000000000000000 Rb (4i)
-0.2369000000000000 -0.2369000000000000 0.0000000000000000 Rb (4i)
-0.2369000000000000 0.2369000000000000 0.5000000000000000 Rb (4i)
0.2369000000000000 -0.2369000000000000 0.5000000000000000 Rb (4i)
0.2631600000000000 0.2631600000000000 0.3480300000000000 S (8o)
-0.2631600000000000 -0.2631600000000000 0.3480300000000000 S (8o)
-0.2631600000000000 0.2631600000000000 0.8480300000000000 S (8o)
0.2631600000000000 -0.2631600000000000 0.1519700000000000 S (8o)
0.2631600000000000 -0.2631600000000000 0.1519700000000000 S (8o)
0.2631600000000000 0.2631600000000000 -0.3480300000000000 S (8o)
-0.2631600000000000 -0.2631600000000000 -0.3480300000000000 S (8o)
0.5000000000000000 0.5000000000000000 0.2500000000000000 Ti (2d)
0.5000000000000000 0.5000000000000000 0.7500000000000000 Ti (2d)

```

AgUF<sub>6</sub>: AB6C\_tP16\_132\_d\_io\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'AgUF6'
_chemical_formula_sum 'Ag F6 U'

loop_
_publ_author_name
'P. Charpin'
_journal_name_full_name
;
Comptes Rendus Hebdomadaires des S{\`e}ances de l'Acad{\`e}mie des
↪ Sciences
;
_journal_volume 260
_journal_year 1965
_journal_page_first 1914

```

```

_journal_page_last 1916
_publ_section_title
;
Structure cristalline des hexafluorures complexes d\'uranium V et d\'
↪ argent de potassium d\'ammonium de rubidium ou de thallium
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'AgUF6_{6}$ Structure '
_aflow_proto 'AB6C_tP16_132_d_io_a'
_aflow_params 'a,c/a,x_{3},x_{4},z_{4}'
_aflow_params_values '5.4229923801,1.46597824081,0.3,0.2,0.333'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP16'

_cell_length_a 5.4229923801
_cell_length_b 5.4229923801
_cell_length_c 7.9499888293
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 42/m 2/c 2/m"
_symmetry_Int_Tables_number 132

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z+1/2
3 -x,y,-z+1/2
4 -x,-y,z
5 -y,-x,-z
6 -y,x,z+1/2
7 y,-x,z+1/2
8 y,x,-z
9 -x,-y,-z
10 -x,y,z+1/2
11 x,-y,z+1/2
12 x,y,-z
13 y,x,z
14 y,-x,-z+1/2
15 -y,x,-z+1/2
16 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
U1 U 2 a 0.00000 0.00000 0.00000 1.00000
Ag1 Ag 2 d 0.50000 0.50000 0.25000 1.00000
F1 F 4 i 0.30000 0.30000 0.00000 1.00000
F2 F 8 o 0.20000 0.20000 0.33300 1.00000

```

AgUF<sub>6</sub>: AB6C\_tP16\_132\_d\_io\_a - POSCAR

```

AB6C_tP16_132_d_io_a & a,c/a,x3,x4,z4 --params=5.4229923801,
↪ 1.46597824081,0.3,0.2,0.333 & P4_{2}/mcm D_{4h}^{10} #132 (adio
↪ ) & tP16 & None & AgUF6 & P. Charpin, {C. R. Hebd. S{\`e}
↪ ances Acad. Sci. 260, 1914-1916 (1965)
1.0000000000000000
5.42299238010000 0.00000000000000 0.0000000000000000
0.00000000000000 5.42299238010000 0.0000000000000000
0.00000000000000 0.00000000000000 7.94998882930000
Ag F U
2 12 2
Direct
0.5000000000000000 0.5000000000000000 0.2500000000000000 Ag (2d)
0.5000000000000000 0.5000000000000000 0.7500000000000000 Ag (2d)
0.3000000000000000 0.3000000000000000 0.0000000000000000 F (4i)
-0.3000000000000000 -0.3000000000000000 0.0000000000000000 F (4i)
-0.3000000000000000 0.3000000000000000 0.5000000000000000 F (4i)
0.3000000000000000 -0.3000000000000000 0.5000000000000000 F (4i)
0.2000000000000000 0.2000000000000000 0.3330000000000000 F (8o)
-0.2000000000000000 -0.2000000000000000 0.3330000000000000 F (8o)
-0.2000000000000000 0.2000000000000000 0.8330000000000000 F (8o)
0.2000000000000000 -0.2000000000000000 0.8330000000000000 F (8o)
-0.2000000000000000 0.2000000000000000 0.1670000000000000 F (8o)
0.2000000000000000 -0.2000000000000000 0.1670000000000000 F (8o)
0.2000000000000000 0.2000000000000000 -0.3330000000000000 F (8o)
-0.2000000000000000 -0.2000000000000000 -0.3330000000000000 F (8o)
0.0000000000000000 0.0000000000000000 0.0000000000000000 U (2a)
0.0000000000000000 0.0000000000000000 0.5000000000000000 U (2a)

```

β-V<sub>3</sub>S: AB3\_tP32\_133\_h\_i2j - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'beta-V3S'
_chemical_formula_sum 'S V3'

loop_
_publ_author_name
'B. Pedersen'
_journal_name_full_name
'F. Gr{\`o}nvold'
_journal_name_full_name

```

```

;
Acta Crystallographica
;
_journal_volume 12
_journal_year 1959
_journal_page_first 1022
_journal_page_last 1027
_publ_section_title
;
The crystal structures of  $\alpha$ -V3S5 and  $\beta$ -V3S5
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title ' $\beta$ -V3S5 Structure'
_aflow_proto 'AB3_tP32_133_h_i2j'
_aflow_params 'a,c/a,x_{1},x_{2},x_{3},x_{4}'
_aflow_params_values '9.3810096033,0.497068542799,-0.0329,0.8986,0.658,
  ↳ 0.0472'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP32'

_cell_length_a 9.3810096033
_cell_length_b 9.3810096033
_cell_length_c 4.6630047735
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 42/n 2/b 2/c (origin choice 2)"
_symmetry_Int_Tables_number 133

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y+1/2,-z
3 -x+1/2,y,-z
4 -x+1/2,-y+1/2,z
5 -y+1/2,-x+1/2,-z+1/2
6 -y+1/2,x,z+1/2
7 y,-x+1/2,z+1/2
8 y,x,-z+1/2
9 -x,-y,-z
10 -x,y+1/2,z
11 x+1/2,-y,z
12 x+1/2,y+1/2,-z
13 y+1/2,x+1/2,z+1/2
14 y+1/2,-x,-z+1/2
15 -y,x+1/2,-z+1/2
16 -y,-x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
S1 S 8 h -0.03290 0.25000 0.00000 1.00000
V1 V 8 i 0.89860 0.25000 0.50000 1.00000
V2 V 8 j 0.65800 0.65800 0.25000 1.00000
V3 V 8 j 0.04720 0.04720 0.25000 1.00000

```

$\beta$ -V<sub>3</sub>S<sub>5</sub>: AB3\_tP32\_133\_h\_i2j - POSCAR

```

AB3_tP32_133_h_i2j & a,c/a,x1,x2,x3,x4 --params=9.3810096033,
  ↳ 0.497068542799,-0.0329,0.8986,0.658,0.0472 & P4_2_1/nbc D_4h
  ↳ ]^11] #133 (hij^2) & tP32 & None & V3S & beta & B. Pedersen
  ↳ and F. Gr{\o}nvold, Acta Cryst. 12, 1022-1027 (1959)
1.0000000000000000
9.38100960330000 0.00000000000000 0.00000000000000
0.00000000000000 9.38100960330000 0.00000000000000
0.00000000000000 0.00000000000000 4.66300477350000
S V
8 24
Direct
-0.03290000000000 0.25000000000000 0.00000000000000 S (8h)
0.53290000000000 0.25000000000000 0.00000000000000 S (8h)
0.25000000000000 -0.03290000000000 0.50000000000000 S (8h)
0.25000000000000 0.53290000000000 0.50000000000000 S (8h)
0.03290000000000 0.75000000000000 0.00000000000000 S (8h)
0.46710000000000 0.75000000000000 0.00000000000000 S (8h)
0.75000000000000 0.03290000000000 0.50000000000000 S (8h)
0.75000000000000 0.46710000000000 0.50000000000000 S (8h)
0.89860000000000 0.25000000000000 0.50000000000000 V (8i)
-0.39860000000000 0.25000000000000 0.50000000000000 V (8i)
0.25000000000000 0.89860000000000 0.00000000000000 V (8i)
0.25000000000000 -0.39860000000000 0.00000000000000 V (8i)
-0.89860000000000 0.75000000000000 0.50000000000000 V (8i)
1.39860000000000 0.75000000000000 0.50000000000000 V (8i)
0.75000000000000 -0.89860000000000 0.00000000000000 V (8i)
0.75000000000000 1.39860000000000 0.00000000000000 V (8i)
0.65800000000000 0.65800000000000 0.25000000000000 V (8j)
-0.15800000000000 -0.15800000000000 0.25000000000000 V (8j)
-0.15800000000000 0.65800000000000 0.75000000000000 V (8j)
0.65800000000000 -0.15800000000000 0.75000000000000 V (8j)
-0.65800000000000 -0.65800000000000 0.75000000000000 V (8j)
1.15800000000000 1.15800000000000 0.75000000000000 V (8j)
-0.15800000000000 -0.65800000000000 0.25000000000000 V (8j)
-0.65800000000000 1.15800000000000 0.25000000000000 V (8j)
0.04720000000000 0.04720000000000 0.25000000000000 V (8j)

```

```

0.45280000000000 0.45280000000000 0.25000000000000 V (8j)
0.45280000000000 0.04720000000000 0.75000000000000 V (8j)
0.04720000000000 0.45280000000000 0.75000000000000 V (8j)
-0.04720000000000 -0.04720000000000 0.75000000000000 V (8j)
0.54720000000000 0.54720000000000 0.75000000000000 V (8j)
0.54720000000000 -0.04720000000000 0.25000000000000 V (8j)
-0.04720000000000 0.54720000000000 0.25000000000000 V (8j)

```

Downeyite (SeO<sub>2</sub>, C47): A2B\_tP24\_135\_gh\_h - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Downeyite'
_chemical_formula_sum 'O2 Se'

loop_
_publ_author_name
'K. St{\aa}hl'
'J. P. Legros'
'J. Galy'
_journal_name_full_name
;
Kristallografiya, English title: Crystallography Reports
;
_journal_volume 202
_journal_year 1992
_journal_page_first 99
_journal_page_last 107
_publ_section_title
;
The crystal structure of SeO2 at 139 and 286 K
;
# Found in The American Mineralogist Crystal Structure Database, 2003

_aflow_title 'Downeyite (SeO2), SC47S' Structure'
_aflow_proto 'A2B_tP24_135_gh_h'
_aflow_params 'a,c/a,x_{1},x_{2},y_{2},x_{3},y_{3}'
_aflow_params_values '8.3218,0.607332548247,0.36248,-0.05789,0.17358,
  ↳ 0.13396,0.20929'
_aflow_Strukturbericht 'SC47S'
_aflow_Pearson 'tP24'

_symmetry_space_group_name_H-M "P 42/m 21/b 2/c"
_symmetry_Int_Tables_number 135

_cell_length_a 8.32180
_cell_length_b 8.32180
_cell_length_c 5.05410
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z
3 -x+1/2,y+1/2,-z
4 -x,-y,z
5 -y+1/2,-x+1/2,-z+1/2
6 -y,x,z+1/2
7 y,-x,z+1/2
8 y+1/2,x+1/2,-z+1/2
9 -x,-y,-z
10 -x+1/2,y+1/2,z
11 x+1/2,-y+1/2,z
12 x,y,-z
13 y+1/2,x+1/2,z+1/2
14 y,-x,-z+1/2
15 -y,x,-z+1/2
16 -y+1/2,-x+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 8 g 0.36248 0.86248 0.25000 1.00000
O2 O 8 h -0.05789 0.17358 0.00000 1.00000
Se1 Se 8 h 0.13396 0.20929 0.00000 1.00000

```

Downeyite (SeO<sub>2</sub>, C47): A2B\_tP24\_135\_gh\_h - POSCAR

```

A2B_tP24_135_gh_h & a,c/a,x1,x2,y2,x3,y3 --params=8.3218,0.607332548247,
  ↳ 0.36248,-0.05789,0.17358,0.13396,0.20929 & P4_2_1/nbc D_4h^1
  ↳ 13] #135 (gh^2) & tP24 & SC47S & SeO2 & Downeyite & K. St{\aa}hl
  ↳ and J. P. Legros and J. Galy, Kristallografiya 202, 99-107 (
  ↳ 1992)
1.00000000000000
8.32180000000000 0.00000000000000 0.00000000000000
0.00000000000000 8.32180000000000 0.00000000000000
0.00000000000000 0.00000000000000 5.05410000000000
O Se
16 8
Direct
0.36248000000000 0.86248000000000 0.25000000000000 O (8g)
-0.36248000000000 0.17352000000000 0.25000000000000 O (8g)
0.13752000000000 0.36248000000000 0.75000000000000 O (8g)

```

0.86248000000000	-0.36248000000000	0.75000000000000	O	(8g)
-0.36248000000000	0.13752000000000	0.75000000000000	O	(8g)
0.36248000000000	0.86248000000000	0.75000000000000	O	(8g)
0.86248000000000	-0.36248000000000	0.25000000000000	O	(8g)
0.13752000000000	0.36248000000000	0.25000000000000	O	(8g)
-0.05789000000000	0.17358000000000	0.00000000000000	O	(8h)
0.05789000000000	-0.17358000000000	0.00000000000000	O	(8h)
-0.17358000000000	-0.05789000000000	0.50000000000000	O	(8h)
0.17358000000000	0.05789000000000	0.50000000000000	O	(8h)
0.55789000000000	0.67358000000000	0.00000000000000	O	(8h)
0.44211000000000	0.32642000000000	0.00000000000000	O	(8h)
0.67358000000000	0.44211000000000	0.50000000000000	O	(8h)
0.32642000000000	0.55789000000000	0.50000000000000	O	(8h)
0.13396000000000	0.20929000000000	0.00000000000000	Se	(8h)
-0.13396000000000	-0.20929000000000	0.00000000000000	Se	(8h)
-0.20929000000000	0.13396000000000	0.50000000000000	Se	(8h)
0.20929000000000	-0.13396000000000	0.50000000000000	Se	(8h)
0.36604000000000	0.70929000000000	0.00000000000000	Se	(8h)
0.63396000000000	0.29071000000000	0.00000000000000	Se	(8h)
0.70929000000000	0.63396000000000	0.50000000000000	Se	(8h)
0.29071000000000	0.36604000000000	0.50000000000000	Se	(8h)

ZnSb<sub>2</sub>O<sub>4</sub>: A4B2C\_tP28\_135\_gh\_h\_d - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'ZnSb2O4'
_chemical_formula_sum 'O4 Sb2 Zn'

loop_
  _publ_author_name
    'S. St{\aa}hl'
  _journal_name_full_name
    ;
  ;
  Arkiv f{\o}r Kemi, Mineralogi och Geologi
  ;
  ;
  _journal_volume 17B
  _journal_year 1943
  _journal_page_first 1
  _journal_page_last 7
  _publ_section_title
    ;
  The crystal structure of ZnSb_{2}SO_{4}S and isomorphous compounds
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'ZnSb_{2}SO_{4}S Structure'
_aflow_proto 'A4B2C_tP28_135_gh_h_d'
_aflow_params 'a,c/a,x_{2},x_{3},y_{3},x_{4},y_{4}'
_aflow_params_values '8.4909023894,0.697208809336,0.169,0.114,0.386,
  ↪ 0.167,0.175'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP28'

_cell_length_a 8.4909023894
_cell_length_b 8.4909023894
_cell_length_c 5.9199319451
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 42/m 21/b 2/c"
_symmetry_Int_Tables_number 135

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x+1/2,-y+1/2,-z
  3 -x+1/2,y+1/2,-z
  4 -x,-y,z
  5 -y+1/2,-x+1/2,-z+1/2
  6 -y,x,z+1/2
  7 y,-x,z+1/2
  8 y+1/2,x+1/2,-z+1/2
  9 -x,-y,-z
  10 -x+1/2,y+1/2,z
  11 x+1/2,-y+1/2,z
  12 x,y,-z
  13 y+1/2,x+1/2,z+1/2
  14 y,-x,-z+1/2
  15 -y,x,-z+1/2
  16 -y+1/2,-x+1/2,z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Zn1 Zn 4 d 0.00000 0.50000 0.25000 1.00000
  O1 O 8 g 0.16900 0.66900 0.25000 1.00000
  O2 O 8 h 0.11400 0.38600 0.00000 1.00000
  Sb1 Sb 8 h 0.16700 0.17500 0.00000 1.00000
```

ZnSb<sub>2</sub>O<sub>4</sub>: A4B2C\_tP28\_135\_gh\_h\_d - POSCAR

```
A4B2C_tP28_135_gh_h_d & a,c/a,x2,x3,y3,x4,y4 --params=8.4909023894,
  ↪ 0.697208809336,0.169,0.114,0.386,0.167,0.175 & P4_{2}/mbc_D_{4h}
  ↪ }^{13} #135 (dgh^2) & tP28 & None & ZnSb2O4 & & S. St{\aa}hl,
  ↪ {Ark. Kem. Mineral. Geol. 17B, 1-7 (1943)}
1.0000000000000000
8.49090238940000 0.00000000000000 0.00000000000000
0.00000000000000 8.49090238940000 0.00000000000000
0.00000000000000 0.00000000000000 5.91993194510000
O Sb Zn
16 8 4
Direct
0.16900000000000 0.66900000000000 0.25000000000000 O (8g)
-0.16900000000000 0.33100000000000 0.25000000000000 O (8g)
0.33100000000000 0.16900000000000 0.75000000000000 O (8g)
0.66900000000000 -0.16900000000000 0.75000000000000 O (8g)
-0.16900000000000 0.33100000000000 0.75000000000000 O (8g)
0.16900000000000 0.66900000000000 0.75000000000000 O (8g)
0.66900000000000 -0.16900000000000 0.25000000000000 O (8g)
0.33100000000000 0.16900000000000 0.25000000000000 O (8g)
0.11400000000000 0.38600000000000 0.00000000000000 O (8h)
-0.11400000000000 -0.38600000000000 0.00000000000000 O (8h)
-0.38600000000000 0.11400000000000 0.50000000000000 O (8h)
0.38600000000000 -0.11400000000000 0.50000000000000 O (8h)
0.38600000000000 0.88600000000000 0.00000000000000 O (8h)
0.61400000000000 0.11400000000000 0.00000000000000 O (8h)
0.88600000000000 0.61400000000000 0.50000000000000 O (8h)
0.11400000000000 0.38600000000000 0.50000000000000 O (8h)
0.16700000000000 0.17500000000000 0.00000000000000 Sb (8h)
-0.16700000000000 -0.17500000000000 0.00000000000000 Sb (8h)
-0.17500000000000 0.16700000000000 0.50000000000000 Sb (8h)
0.17500000000000 -0.16700000000000 0.50000000000000 Sb (8h)
0.33300000000000 0.67500000000000 0.00000000000000 Sb (8h)
0.66700000000000 0.32500000000000 0.00000000000000 Sb (8h)
0.67500000000000 0.66700000000000 0.50000000000000 Sb (8h)
0.32500000000000 0.33300000000000 0.50000000000000 Sb (8h)
0.00000000000000 0.50000000000000 0.25000000000000 Zn (4d)
0.50000000000000 0.00000000000000 0.75000000000000 Zn (4d)
0.00000000000000 0.50000000000000 0.75000000000000 Zn (4d)
0.50000000000000 0.00000000000000 0.25000000000000 Zn (4d)
```

Zn<sub>3</sub>P<sub>2</sub> (D5<sub>9</sub>): A2B3\_tP40\_137\_cdf\_3g - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Zn3P2'
_chemical_formula_sum 'P2 Zn3'

loop_
  _publ_author_name
    'M. v. Stackelberg'
    'R. Paulu'
  _journal_name_full_name
    ;
    ;
    Zeitschrift f{\u}r Physikalische Chemie B
  ;
  ;
  _journal_volume 28
  _journal_year 1935
  _journal_page_first 427
  _journal_page_last 460
  _publ_section_title
    ;
    Untersuchungen an den Phosphiden und Arseniden des Zinks und Cadmiums.
    ↪ Das Zn_{3}SP_{2}-Gitter
  ;

# Found in The American Mineralogist Crystal Structure Database, 2003

_aflow_title 'Zn_{3}SP_{2}S (SD5_{9}) Structure'
_aflow_proto 'A2B3_tP40_137_cdf_3g'
_aflow_params 'a,c/a,z_{1},z_{2},x_{3},y_{4},z_{4},y_{5},z_{5},y_{6},z_{6}'
  ↪ 6)
_aflow_params_values '8.097,1.41410398913,0.0,0.011,0.511,0.533,0.147,
  ↪ 0.467,0.864,0.5,0.603'
_aflow_Strukturbericht 'SD5_{9}'
_aflow_Pearson 'tP40'

_symmetry_space_group_name_H-M "P 42/n 21/m 2/c (origin choice 2)"
_symmetry_Int_Tables_number 137

_cell_length_a 8.09700
_cell_length_b 8.09700
_cell_length_c 11.45000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x+1/2,-y,-z
  3 -x,y+1/2,-z
  4 -x+1/2,-y+1/2,z
  5 -y,-x,-z+1/2
  6 -y+1/2,x,z+1/2
  7 y,-x+1/2,z+1/2
  8 y+1/2,x+1/2,-z+1/2
  9 -x,-y,-z
  10 -x+1/2,y,z
  11 x,-y+1/2,z
  12 x+1/2,y+1/2,-z
  13 y,x,z+1/2
  14 y+1/2,-x,-z+1/2
```

```
15 -y, x+1/2, -z+1/2
16 -y+1/2, -x+1/2, z+1/2
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
P1 P 4 c 0.75000 0.25000 0.00000 1.00000
P2 P 4 d 0.25000 0.25000 0.01100 1.00000
P3 P 8 f 0.51100 0.48900 0.25000 1.00000
Zn1 Zn 8 g 0.25000 0.53300 0.14700 1.00000
Zn2 Zn 8 g 0.25000 0.46700 0.86400 1.00000
Zn3 Zn 8 g 0.25000 0.50000 0.60300 1.00000
```

#### Zn<sub>3</sub>P<sub>2</sub> (D<sub>5g</sub>): A2B<sub>3</sub>tP4<sub>0</sub>\_137\_cdf\_3g - POSCAR

```
A2B3_tP40_137_cdf_3g & a, c/a, z1, z2, x3, y4, z4, y5, z5, y6, z6 --params=8.097,
↪ 1.41410398913, 0.0, 0.011, 0.511, 0.533, 0.147, 0.467, 0.864, 0.5, 0.603
↪ & P4_{2}/nmc D_{4h}^{15} #137 (cdfg^3) & tP40 & $D5_{9}$ &
↪ Zn3P2 & Zn3P2 & M. v. Stackelberg and R. Paulu, Z. Phys. Chem.
↪ B 28, 427-460 (1935)
```

```
1.0000000000000000
8.097000000000000 0.000000000000000 0.000000000000000
0.000000000000000 8.097000000000000 0.000000000000000
0.000000000000000 0.000000000000000 11.450000000000000
P Zn
16 24
Direct
0.750000000000000 0.250000000000000 0.000000000000000 P (4c)
0.250000000000000 0.750000000000000 0.500000000000000 P (4c)
0.250000000000000 0.750000000000000 0.000000000000000 P (4c)
0.750000000000000 0.250000000000000 0.500000000000000 P (4c)
0.250000000000000 0.250000000000000 0.011000000000000 P (4d)
0.250000000000000 0.250000000000000 0.511000000000000 P (4d)
0.750000000000000 0.750000000000000 -0.011000000000000 P (4d)
0.750000000000000 0.750000000000000 0.489000000000000 P (4d)
0.511000000000000 -0.511000000000000 0.250000000000000 P (8f)
-0.101000000000000 1.011000000000000 0.250000000000000 P (8f)
1.011000000000000 0.511000000000000 0.750000000000000 P (8f)
-0.511000000000000 -0.011000000000000 0.750000000000000 P (8f)
-0.511000000000000 0.511000000000000 0.750000000000000 P (8f)
1.011000000000000 -0.011000000000000 0.750000000000000 P (8f)
-0.011000000000000 -0.511000000000000 0.250000000000000 P (8f)
0.511000000000000 1.011000000000000 0.250000000000000 P (8f)
0.250000000000000 0.533000000000000 0.147000000000000 Zn (8g)
0.250000000000000 -0.033000000000000 0.147000000000000 Zn (8g)
-0.033000000000000 0.250000000000000 0.647000000000000 Zn (8g)
0.533000000000000 0.250000000000000 0.647000000000000 Zn (8g)
0.750000000000000 1.033000000000000 -0.147000000000000 Zn (8g)
0.750000000000000 -0.533000000000000 -0.147000000000000 Zn (8g)
1.033000000000000 0.750000000000000 0.353000000000000 Zn (8g)
-0.533000000000000 0.750000000000000 0.353000000000000 Zn (8g)
0.250000000000000 0.467000000000000 0.864000000000000 Zn (8g)
0.250000000000000 0.033000000000000 0.864000000000000 Zn (8g)
0.033000000000000 0.250000000000000 1.364000000000000 Zn (8g)
0.467000000000000 0.250000000000000 1.364000000000000 Zn (8g)
0.750000000000000 0.967000000000000 -0.864000000000000 Zn (8g)
0.750000000000000 -0.467000000000000 -0.864000000000000 Zn (8g)
0.967000000000000 0.750000000000000 -0.364000000000000 Zn (8g)
-0.467000000000000 0.750000000000000 -0.364000000000000 Zn (8g)
0.250000000000000 0.500000000000000 0.603000000000000 Zn (8g)
0.250000000000000 0.000000000000000 0.603000000000000 Zn (8g)
0.000000000000000 0.250000000000000 1.103000000000000 Zn (8g)
0.500000000000000 0.250000000000000 1.103000000000000 Zn (8g)
0.750000000000000 1.000000000000000 -0.603000000000000 Zn (8g)
0.750000000000000 -0.500000000000000 -0.603000000000000 Zn (8g)
1.000000000000000 0.750000000000000 -0.103000000000000 Zn (8g)
-0.500000000000000 0.750000000000000 -0.103000000000000 Zn (8g)
```

#### ZrO<sub>2</sub> (High-temperature): A2B\_tP6\_137\_d\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'ZrO2'
_chemical_formula_sum 'O2 Zr'
loop_
_publ_author_name
'G. Teufer'
_journal_name_full_name
;
Acta Crystallographica
;
_journal_volume 15
_journal_year 1962
_journal_page_first 1187
_journal_page_last 1187
_publ_section_title
;
The crystal structure of tetragonal ZrO2
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013
_aflow_title 'ZrO2(2) (High-temperature) Structure'
_aflow_proto 'A2B_tP6_137_d_a'
_aflow_params 'a, c/a, z_{2}'
```

```
_aflow_params_values '3.64008007, 1.4478021978, 0.565'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP6'
_cell_length_a 3.6400800700
_cell_length_b 3.6400800700
_cell_length_c 5.2701159255
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000
_symmetry_space_group_name_H-M "P 42/n 21/m 2/c (origin choice 2)"
_symmetry_Int_Tables_number 137
```

```
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x+1/2, -y, -z
3 -x, y+1/2, -z
4 -x+1/2, -y+1/2, z
5 -y, -x, -z+1/2
6 -y+1/2, x, z+1/2
7 y, -x+1/2, z+1/2
8 y+1/2, x+1/2, -z+1/2
9 -x, -y, -z
10 -x+1/2, y, z
11 x, -y+1/2, z
12 x+1/2, y+1/2, -z
13 y, x, z+1/2
14 y+1/2, -x, -z+1/2
15 -y, x+1/2, -z+1/2
16 -y+1/2, -x+1/2, z+1/2
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Zr1 Zr 2 a 0.75000 0.25000 0.75000 1.00000
O1 O 4 d 0.25000 0.25000 0.56500 1.00000
```

#### ZrO<sub>2</sub> (High-temperature): A2B\_tP6\_137\_d\_a - POSCAR

```
A2B_tP6_137_d_a & a, c/a, z2 --params=3.64008007, 1.4478021978, 0.565 & P4_{
↪ 2}/nmc D_{4h}^{15} #137 (ad) & tP6 & None & ZrO2 & G. Teufer
↪, Acta Cryst. 15, 1187-1187 (1962)
1.0000000000000000
3.640080070000000 0.000000000000000 0.000000000000000
0.000000000000000 3.640080070000000 0.000000000000000
0.000000000000000 0.000000000000000 5.270115925500000
O Zr
4 2
Direct
0.250000000000000 0.250000000000000 0.565000000000000 O (4d)
0.250000000000000 0.250000000000000 1.065000000000000 O (4d)
0.750000000000000 0.750000000000000 -0.565000000000000 O (4d)
0.750000000000000 0.750000000000000 -0.065000000000000 O (4d)
0.750000000000000 0.250000000000000 0.750000000000000 Zr (2a)
0.250000000000000 0.750000000000000 0.250000000000000 Zr (2a)
```

#### CeCo<sub>4</sub>B<sub>4</sub>: A4BC4\_tP18\_137\_g\_b\_g - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'CeCo4B4'
_chemical_formula_sum 'B4 Ce Co4'
loop_
_publ_author_name
'Y. B. Kuzma'
'N. S. Bilonizhko'
_journal_name_full_name
;
Soviet Physics Crystallography
;
_journal_volume 16
_journal_year 1972
_journal_page_first 897
_journal_page_last 898
_publ_section_title
;
Crystal structure of the compounds CeCo4{4}SBS4 and its analogs
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013
_aflow_title 'CeCo4{4}SBS4 Structure'
_aflow_proto 'A4BC4_tP18_137_g_b_g'
_aflow_params 'a, c/a, y_{2}, z_{2}, y_{3}, z_{3}'
_aflow_params_values '5.0593101041, 1.39612571654, 0.08, 0.1, 0.503, 0.384'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP18'
_cell_length_a 5.0593101041
_cell_length_b 5.0593101041
_cell_length_c 7.0634329443
_cell_angle_alpha 90.0000000000
```

```

_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000
_symmetry_space_group_name_H-M "P 42/n 21/m 2/c (origin choice 2)"
_symmetry_Int_Tables_number 137

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x+1/2, -y, -z
3 -x, y+1/2, -z
4 -x+1/2, -y+1/2, z
5 -y, -x, -z+1/2
6 -y+1/2, x, z+1/2
7 y, -x+1/2, z+1/2
8 y+1/2, x+1/2, -z+1/2
9 -x, -y, -z
10 -x+1/2, y, z
11 x, -y+1/2, z
12 x+1/2, y+1/2, -z
13 y, x, z+1/2
14 y+1/2, -x, -z+1/2
15 -y, x+1/2, -z+1/2
16 -y+1/2, -x+1/2, z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ce1 Ce 2 b 0.75000 0.25000 1.00000
B1 B 8 g 0.25000 0.08000 0.10000 1.00000
Co1 Co 8 g 0.25000 0.50300 0.38400 1.00000

```

CeCo<sub>4</sub>B<sub>4</sub>: A4BC4\_tP18\_137\_g\_b\_g - POSCAR

```

A4BC4_tP18_137_g_b_g & a, c/a, y2, z2, y3, z3 --params=5.0593101041,
↳ 1.39612571654, 0.08, 0.1, 0.503, 0.384 & P4_{2}/nmc D_{4h}^{15} #
↳ 137 (bg^2) & tP18 & None & CeCo4B4 & & Y. B. Kuzma and N. S.
↳ Bilonizhko, Sov. Phys. Crystallogr. 16, 897-898 (1972)
1.0000000000000000
5.05931010410000 0.000000000000000 0.000000000000000
0.000000000000000 5.05931010410000 0.000000000000000
0.000000000000000 0.000000000000000 7.06343294430000
B Ce Co
8 2 8
Direct
0.250000000000000 0.080000000000000 0.100000000000000 B (8g)
0.250000000000000 0.420000000000000 0.100000000000000 B (8g)
0.420000000000000 0.250000000000000 0.600000000000000 B (8g)
0.080000000000000 0.250000000000000 0.600000000000000 B (8g)
0.750000000000000 0.580000000000000 -0.100000000000000 B (8g)
0.750000000000000 -0.080000000000000 -0.100000000000000 B (8g)
0.580000000000000 0.750000000000000 0.400000000000000 B (8g)
-0.080000000000000 0.750000000000000 0.400000000000000 B (8g)
0.750000000000000 0.250000000000000 0.250000000000000 Ce (2b)
0.250000000000000 0.750000000000000 0.750000000000000 Ce (2b)
0.250000000000000 0.503000000000000 0.384000000000000 Co (8g)
0.250000000000000 -0.003000000000000 0.384000000000000 Co (8g)
-0.003000000000000 0.250000000000000 0.884000000000000 Co (8g)
0.503000000000000 0.250000000000000 0.884000000000000 Co (8g)
0.750000000000000 1.003000000000000 -0.384000000000000 Co (8g)
0.750000000000000 -0.503000000000000 -0.384000000000000 Co (8g)
1.003000000000000 0.750000000000000 0.116000000000000 Co (8g)
-0.503000000000000 0.750000000000000 0.116000000000000 Co (8g)

```

Hg<sub>2</sub> (C13): AB2\_tP6\_137\_a\_d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Hg I2'

loop_
_publ_author_name
'D. Schwarzenbach'
'H. Birkedal'
'M. Hostettler'
'P. Fischer'
_journal_name_full_name
;
Acta Crystallographica Section B: Structural Science
;
_journal_volume 63
_journal_year 2007
_journal_page_first 826
_journal_page_last 835
_publ_section_title
;
Neutron diffraction investigation of the temperature dependence of
↳ crystal structure and thermal motions of red HgI2
;

# Found in The American Mineralogist Crystal Structure Database, 2003
_aflow_title 'HgI2(C13) (SC13$) Structure'
_aflow_proto 'AB2_tP6_137_a_d'
_aflow_params 'a, c/a, z_{2}'

```

```

_aflow_params_values '4.3675, 2.8551803091, 0.389'
_aflow_Strukturbericht 'SC13$'
_aflow_Pearson 'tP6'

_symmetry_space_group_name_H-M "P 42/n 21/m 2/c (origin choice 2)"
_symmetry_Int_Tables_number 137

_cell_length_a 4.36750
_cell_length_b 4.36750
_cell_length_c 12.47000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x+1/2, -y, -z
3 -x, y+1/2, -z
4 -x+1/2, -y+1/2, z
5 -y, -x, -z+1/2
6 -y+1/2, x, z+1/2
7 y, -x+1/2, z+1/2
8 y+1/2, x+1/2, -z+1/2
9 -x, -y, -z
10 -x+1/2, y, z
11 x, -y+1/2, z
12 x+1/2, y+1/2, -z
13 y, x, z+1/2
14 y+1/2, -x, -z+1/2
15 -y, x+1/2, -z+1/2
16 -y+1/2, -x+1/2, z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Hg1 Hg 2 a 0.75000 0.25000 0.75000 1.00000
I1 I 4 d 0.25000 0.25000 0.38900 1.00000

```

Hg<sub>2</sub> (C13): AB2\_tP6\_137\_a\_d - POSCAR

```

AB2_tP6_137_a_d & a, c/a, z2 --params=4.3675, 2.8551803091, 0.389 & P4_{2}/
↳ nmc D_{4h}^{15} #137 (ad) & tP6 & SC13$ & HgI2 & & D.
↳ Schwarzenbach et al., Acta Crystallogr. Sect. B Struct. Sci. 63
↳ , 826-835 (2007)
1.0000000000000000
4.367500000000000 0.000000000000000 0.000000000000000
0.000000000000000 4.367500000000000 0.000000000000000
0.000000000000000 0.000000000000000 12.470000000000000
Hg I
2 4
Direct
0.750000000000000 0.250000000000000 0.750000000000000 Hg (2a)
0.250000000000000 0.750000000000000 0.250000000000000 Hg (2a)
0.250000000000000 0.250000000000000 0.389000000000000 I (4d)
0.250000000000000 0.250000000000000 0.889000000000000 I (4d)
0.750000000000000 0.750000000000000 -0.389000000000000 I (4d)
0.750000000000000 0.750000000000000 0.111000000000000 I (4d)

```

C (T12 Group IV): A\_tP12\_138\_bi - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'T12'
_chemical_formula_sum 'C'

loop_
_publ_author_name
'Z. Zhao'
'F. Tian'
'X. Dong'
'Q. Li'
'Q. Wang'
'H. Wang'
'X. Zhong'
'B. Xu'
'D. Yu'
'J. He'
'H.-T. Wang'
'Y. Ma'
'Y. Tian'
_journal_name_full_name
;
Journal of the American Chemical Society
;
_journal_volume 134
_journal_year 2012
_journal_page_first 12362
_journal_page_last 12365
_publ_section_title
;
Tetragonal Allotrope of Group 14 Elements
;

_aflow_title 'C (T12 Group IV) Structure'
_aflow_proto 'A_tP12_138_bi'

```

```

_aflow_params 'a,c/a,x_{2},z_{2}'
_aflow_params_values '3.388,1.77420306966,0.086,0.107'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tP12'

_symmetry_space_group_name_H-M "P 42/n 21/c 2/m (origin choice 2)"
_symmetry_Int_Tables_number 138

_cell_length_a 3.38800
_cell_length_b 3.38800
_cell_length_c 6.01100
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y,-z+1/2
3 -x,y+1/2,-z+1/2
4 -x+1/2,-y+1/2,z
5 -y,-x,-z
6 -y+1/2,x,z+1/2
7 y,-x+1/2,z+1/2
8 y+1/2,x+1/2,-z
9 -x,-y,-z
10 -x+1/2,y,z+1/2
11 x,-y+1/2,z+1/2
12 x+1/2,y+1/2,-z
13 y,x,z
14 y+1/2,-x,-z+1/2
15 -y,x+1/2,-z+1/2
16 -y+1/2,-x+1/2,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
C1 C 4 b 0.75000 0.25000 1.00000
C2 C 8 i 0.08600 0.08600 0.10700 1.00000

```

C (T12 Group IV): A\_tP12\_138\_bi - POSCAR

```

A_tP12_138_bi & a,c/a,x2,z2 --params=3.388,1.77420306966,0.086,0.107 &
↳ P4_{2}/ncm D_{4h}^{16} #138 (bi) & tP12 & None & C & T12 & Z.
↳ Zhao et al., J. Am. Chem. Soc. 134, 12362-12365 (2012)
1.0000000000000000
3.3880000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 3.3880000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.0110000000000000
C
12
Direct
0.7500000000000000 0.2500000000000000 0.7500000000000000 C (4b)
0.2500000000000000 0.7500000000000000 0.2500000000000000 C (4b)
0.2500000000000000 0.7500000000000000 0.7500000000000000 C (4b)
0.7500000000000000 0.2500000000000000 0.2500000000000000 C (4b)
0.0860000000000000 0.0860000000000000 0.1070000000000000 C (8i)
0.4140000000000000 0.4140000000000000 0.1070000000000000 C (8i)
0.4140000000000000 0.0860000000000000 0.6070000000000000 C (8i)
0.0860000000000000 0.4140000000000000 0.6070000000000000 C (8i)
-0.0860000000000000 0.5860000000000000 0.3930000000000000 C (8i)
0.5860000000000000 -0.0860000000000000 0.3930000000000000 C (8i)
0.5860000000000000 -0.1070000000000000 C (8i)
-0.0860000000000000 -0.0860000000000000 -0.1070000000000000 C (8i)

```

Calomel (Hg<sub>2</sub>Cl<sub>2</sub>, D<sub>3h</sub>): AB\_tI8\_139\_e\_e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Calomel'
_chemical_formula_sum 'Cl Hg'

loop_
_publ_author_name
'N. J. Calos'
'C. H. L. Kennard'
'R. L. Davis'
_journal_name_full_name
;
Zeitschrift f{"u}r Kristallografiya
;
_journal_volume 187
_journal_year 1989
_journal_page_first 305
_journal_page_last 307
_publ_section_title
;
The structure of calomel, Hg_{2}Cl_{2}, derived from neutron powder
↳ data
;

# Found in The American Mineralogist Crystal Structure Database, 2003

_aflow_title 'Calomel (Hg_{2}Cl_{2}), $D3_{1}$ Structure'
_aflow_proto 'AB_tI8_139_e_e'
_aflow_params 'a,c/a,z_{1},z_{2}'

```

```

_aflow_params_values '4.4795,2.43451278044,0.3356,0.119'
_aflow_Strukturbericht '$D3_{1}$'
_aflow_Pearson 'tI8'

_symmetry_space_group_name_H-M "I 4/m 2/m 2/m"
_symmetry_Int_Tables_number 139

_cell_length_a 4.47950
_cell_length_b 4.47950
_cell_length_c 10.90540
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 -y,-x,-z
6 -y,x,z
7 y,-x,z
8 y,x,-z
9 -x,-y,-z
10 -x,y,z
11 x,-y,z
12 x,y,-z
13 y,x,z
14 y,-x,-z
15 -y,x,-z
16 -y,-x,z
17 x+1/2,y+1/2,z+1/2
18 x+1/2,-y+1/2,-z+1/2
19 -x+1/2,y+1/2,-z+1/2
20 -x+1/2,-y+1/2,z+1/2
21 -y+1/2,-x+1/2,-z+1/2
22 -y+1/2,x+1/2,z+1/2
23 y+1/2,-x+1/2,z+1/2
24 y+1/2,x+1/2,-z+1/2
25 -x+1/2,-y+1/2,-z+1/2
26 -x+1/2,y+1/2,z+1/2
27 x+1/2,-y+1/2,z+1/2
28 x+1/2,y+1/2,-z+1/2
29 y+1/2,x+1/2,z+1/2
30 y+1/2,-x+1/2,-z+1/2
31 -y+1/2,x+1/2,-z+1/2
32 -y+1/2,-x+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cl1 Cl 4 e 0.00000 0.00000 0.33560 1.00000
Hg1 Hg 4 e 0.00000 0.00000 0.11900 1.00000

```

Calomel (Hg<sub>2</sub>Cl<sub>2</sub>, D<sub>3h</sub>): AB\_tI8\_139\_e\_e - POSCAR

```

AB_tI8_139_e_e & a,c/a,z1,z2 --params=4.4795,2.43451278044,0.3356,0.119
↳ I4/mmm D_{4h}^{17} #139 (e^2) & tI8 & $D3_{1}$ & Hg2Cl2 &
↳ Calomel & N. J. Calos and C. H. L. Kennard and R. L. Davis, Z.
↳ Kristallogr. 187, 305-307 (1989)
1.0000000000000000
-2.2397500000000000 2.2397500000000000 5.4527000000000000
2.2397500000000000 -2.2397500000000000 5.4527000000000000
2.2397500000000000 2.2397500000000000 -5.4527000000000000
Cl Hg
2 2
Direct
0.3356000000000000 0.3356000000000000 0.0000000000000000 Cl (4e)
-0.3356000000000000 -0.3356000000000000 0.0000000000000000 Cl (4e)
0.1190000000000000 0.1190000000000000 0.0000000000000000 Hg (4e)
-0.1190000000000000 -0.1190000000000000 0.0000000000000000 Hg (4e)

```

W<sub>5</sub>Si<sub>3</sub> (D<sub>8h</sub>): A3B<sub>5</sub>tI32\_140\_ah\_bk - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'W5Si3'
_chemical_formula_sum 'Si3 W5'

loop_
_publ_author_name
'B. Aronsson'
_journal_name_full_name
;
Acta Chemica Scandinavica
;
_journal_volume 9
_journal_year 1955
_journal_page_first 1107
_journal_page_last 1110
_publ_section_title
;
The Crystal Structure of Mo_{5}Si_{3} and W_{5}Si_{3}
;

```

```

_aflow_title 'W5_{5}$Si_{3}$ (SD8_{m})$ Structure '
_aflow_proto 'A3B5_tI32_140_ah_bk'
_aflow_params 'a,c/a,x_{3},x_{4},y_{4}'
_aflow_params_values '9.64,0.515560165975,0.17,0.074,0.223'
_aflow_Strukturbericht 'SD8_{m}$'
_aflow_Pearson 'tI32'

```

```

_symmetry_space_group_name_H-M "I 4/m 2/c 2/m"
_symmetry_Int_Tables_number 140
_cell_length_a 9.64000
_cell_length_b 9.64000
_cell_length_c 4.97000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

```

```

loop_
_space_group_symop_id
_space_group_symop_operation_xyz

```

```

1 x,y,z
2 x,-y,-z+1/2
3 -x,y,-z+1/2
4 -x,-y,z
5 -y,-x,-z+1/2
6 -y,x,z
7 y,-x,z
8 y,x,-z+1/2
9 -x,-y,-z
10 -x,y,z+1/2
11 x,-y,z+1/2
12 x,y,-z
13 y,x,z+1/2
14 y,-x,-z
15 -y,x,-z
16 -y,-x,z+1/2
17 x+1/2,y+1/2,z+1/2
18 x+1/2,-y+1/2,-z
19 -x+1/2,y+1/2,-z
20 -x+1/2,-y+1/2,z+1/2
21 -y+1/2,-x+1/2,-z
22 -y+1/2,x+1/2,z+1/2
23 y+1/2,-x+1/2,z+1/2
24 y+1/2,x+1/2,-z
25 -x+1/2,-y+1/2,-z+1/2
26 -x+1/2,y+1/2,z
27 x+1/2,-y+1/2,z
28 x+1/2,y+1/2,-z+1/2
29 y+1/2,x+1/2,z
30 y+1/2,-x+1/2,-z+1/2
31 -y+1/2,x+1/2,-z+1/2
32 -y+1/2,-x+1/2,z

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Si1 Si 4 a 0.00000 0.00000 0.25000 1.00000
W1 W 4 b 0.00000 0.50000 0.25000 1.00000
Si2 Si 8 h 0.17000 0.67000 0.00000 1.00000
W2 W 16 k 0.07400 0.22300 0.00000 1.00000

```

W<sub>5</sub>Si<sub>3</sub> (D<sub>8m</sub>): A3B5\_tI32\_140\_ah\_bk - POSCAR

```

A3B5_tI32_140_ah_bk & a,c/a,x3,x4,y4 --params=9.64,0.515560165975,0.17,
↪ 0.074,0.223 & I4/mcm D_{4h}^{18} #140 (abhk) & tI32 & SD8_{m}$
↪ & W5Si3 & W5Si3 & B. Aronsson, Acta Chem. Scand. 9, 1107-1110 (
↪ 1955)

```

```

1.0000000000000000
-4.8200000000000000 4.8200000000000000 2.4850000000000000
4.8200000000000000 -4.8200000000000000 2.4850000000000000
4.8200000000000000 4.8200000000000000 -2.4850000000000000
Si W
6 10
Direct
0.2500000000000000 0.2500000000000000 0.0000000000000000 Si (4a)
0.7500000000000000 0.7500000000000000 0.0000000000000000 Si (4a)
0.6700000000000000 0.1700000000000000 0.8400000000000000 Si (8h)
0.3300000000000000 -0.1700000000000000 0.1600000000000000 Si (8h)
0.1700000000000000 0.3300000000000000 0.5000000000000000 Si (8h)
-0.1700000000000000 0.6700000000000000 0.5000000000000000 Si (8h)
0.7500000000000000 0.2500000000000000 0.5000000000000000 W (4b)
0.2500000000000000 0.7500000000000000 0.5000000000000000 W (4b)
0.2230000000000000 0.0740000000000000 0.2970000000000000 W (16k)
-0.2230000000000000 -0.0740000000000000 -0.2970000000000000 W (16k)
0.0740000000000000 -0.2230000000000000 -0.1490000000000000 W (16k)
-0.0740000000000000 0.2230000000000000 0.1490000000000000 W (16k)
0.2730000000000000 0.4260000000000000 0.1490000000000000 W (16k)
0.2770000000000000 0.5740000000000000 -0.1490000000000000 W (16k)
0.5740000000000000 0.7230000000000000 0.2970000000000000 W (16k)
0.4260000000000000 0.2770000000000000 -0.2970000000000000 W (16k)

```

Cr<sub>5</sub>B<sub>3</sub> (D<sub>8</sub>): A3B5\_tI32\_140\_ah\_cl - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Cr5B3'
_chemical_formula_sum 'B3 Cr5'

```

```

loop_
_publ_author_name
'F. Bertaut'
'P. Blum'
_journal_name_full_name
;
Comptes Rendus Hebdomadaires des S(\eances de l'Acad(\e)mie des
↪ Sciences

```

```

_journal_volume 236
_journal_year 1953
_journal_page_first 1055
_journal_page_last 1056
_publ_section_title
;
Etude des borures de chrome
;

```

# Found in The American Mineralogist Crystal Structure Database, 2003

```

_aflow_title 'Cr5_{5}$B3_{3}$ (SD8_{1})$ Structure '
_aflow_proto 'A3B5_tI32_140_ah_cl'
_aflow_params 'a,c/a,x_{3},x_{4},z_{4}'
_aflow_params_values '5.46,1.91575091575,0.625,0.166,0.15'
_aflow_Strukturbericht 'SD8_{1}$'
_aflow_Pearson 'tI32'

```

```

_symmetry_space_group_name_H-M "I 4/m 2/c 2/m"
_symmetry_Int_Tables_number 140

```

```

_cell_length_a 5.46000
_cell_length_b 5.46000
_cell_length_c 10.46000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

```

```

loop_
_space_group_symop_id
_space_group_symop_operation_xyz

```

```

1 x,y,z
2 x,-y,-z+1/2
3 -x,y,-z+1/2
4 -x,-y,z
5 -y,-x,-z+1/2
6 -y,x,z
7 y,-x,z
8 y,x,-z+1/2
9 -x,-y,-z
10 -x,y,z+1/2
11 x,-y,z+1/2
12 x,y,-z
13 y,x,z+1/2
14 y,-x,-z
15 -y,x,-z
16 -y,-x,z+1/2
17 x+1/2,y+1/2,z+1/2
18 x+1/2,-y+1/2,-z
19 -x+1/2,y+1/2,-z
20 -x+1/2,-y+1/2,z+1/2
21 -y+1/2,-x+1/2,-z
22 -y+1/2,x+1/2,z+1/2
23 y+1/2,-x+1/2,z+1/2
24 y+1/2,x+1/2,-z
25 -x+1/2,-y+1/2,-z+1/2
26 -x+1/2,y+1/2,z
27 x+1/2,-y+1/2,z
28 x+1/2,y+1/2,-z+1/2
29 y+1/2,x+1/2,z
30 y+1/2,-x+1/2,-z+1/2
31 -y+1/2,x+1/2,-z+1/2
32 -y+1/2,-x+1/2,z

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
B1 B 4 a 0.00000 0.00000 0.25000 1.00000
Cr1 Cr 4 c 0.00000 0.00000 0.00000 1.00000
B2 B 8 h 0.62500 0.12500 0.00000 1.00000
Cr2 Cr 16 l 0.16600 0.66600 0.15000 1.00000

```

Cr<sub>5</sub>B<sub>3</sub> (D<sub>8</sub>): A3B5\_tI32\_140\_ah\_cl - POSCAR

```

A3B5_tI32_140_ah_cl & a,c/a,x3,x4,z4 --params=5.46,1.91575091575,0.625,
↪ 0.166,0.15 & I4/mcm D_{4h}^{18} #140 (achl) & tI32 & SD8_{1}$ &
↪ Cr5B3 & Cr5B3 & F. Bertaut and P. Blum, {C. R. Hebd. S(\e)
↪ ances Acad. Sci. 236, 1055-1056 (1953)

```

```

1.0000000000000000
-2.7300000000000000 2.7300000000000000 5.2300000000000000
2.7300000000000000 -2.7300000000000000 5.2300000000000000
2.7300000000000000 2.7300000000000000 -5.2300000000000000
B Cr
6 10
Direct
0.2500000000000000 0.2500000000000000 0.0000000000000000 B (4a)
0.7500000000000000 0.7500000000000000 0.0000000000000000 B (4a)
1.1250000000000000 0.6250000000000000 1.7500000000000000 B (8h)
-0.1250000000000000 -0.6250000000000000 -0.7500000000000000 B (8h)
0.6250000000000000 -0.1250000000000000 0.5000000000000000 B (8h)

```

-0.62500000000000	1.12500000000000	0.50000000000000	B	(8h)
0.00000000000000	0.00000000000000	0.00000000000000	Cr	(4c)
0.50000000000000	0.50000000000000	0.00000000000000	Cr	(4c)
0.81600000000000	0.31600000000000	0.83200000000000	Cr	(16i)
0.48400000000000	-0.01600000000000	0.16800000000000	Cr	(16i)
0.31600000000000	0.48400000000000	0.50000000000000	Cr	(16i)
-0.01600000000000	0.81600000000000	0.50000000000000	Cr	(16i)
0.01600000000000	0.18400000000000	0.50000000000000	Cr	(16i)
-0.31600000000000	0.51600000000000	0.50000000000000	Cr	(16i)
0.51600000000000	0.01600000000000	0.83200000000000	Cr	(16i)
0.18400000000000	-0.31600000000000	0.16800000000000	Cr	(16i)

$\alpha$ -ThSi<sub>2</sub> (C<sub>2</sub>): A2B\_tI12\_141\_e\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '$\alpha$-ThSi$_{2}$'
_chemical_formula_sum 'Si2 Th'

loop_
  _publ_author_name
    'G. Brauer'
    'A. Mitius'
  _journal_name_full_name
    ;
  Zeitschrift fur Anorganische und Allgemeine Chemie
  ;
  _journal_volume 249
  _journal_year 1942
  _journal_page_first 325
  _journal_page_last 339
  _publ_section_title
    ;
  Die Kristallstruktur des Thoriumsilicids ThSi$_{2}$S
  ;

# Found in The Crystal Chemistry and Physics of Metals and Alloys, 1972

_aflow_title '$\alpha$-ThSi$_{2}$ (SC$_{c}$) Structure'
_aflow_proto 'A2B_tI12_141_e_a'
_aflow_params 'a, c/a, z, z_{2}'
_aflow_params_values '4.126, 3.47697527872, 0.2915'
_aflow_Strukturbericht 'SC$_{c}$'
_aflow_Pearson 'tI12'

_symmetry_space_group_name_H-M "I 41/a 2/m 2/d"
_symmetry_Int_Tables_number 141

_cell_length_a 4.12600
_cell_length_b 4.12600
_cell_length_c 14.34600
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x, y, z
  2 x, -y, -z
  3 -x, y+1/2, -z
  4 -x, -y+1/2, z
  5 -y+1/4, -x+1/4, -z+3/4
  6 -y+1/4, x+3/4, z+1/4
  7 y+3/4, -x+3/4, z+1/4
  8 y+3/4, x+1/4, -z+3/4
  9 -x, -y, -z
  10 -x, y, z
  11 x, -y+1/2, z
  12 x, y+1/2, -z
  13 y+3/4, x+3/4, z+1/4
  14 y+3/4, -x+1/4, -z+3/4
  15 -y+1/4, x+1/4, -z+3/4
  16 -y+1/4, -x+3/4, z+1/4
  17 x+1/2, y+1/2, z+1/2
  18 x+1/2, -y+1/2, -z+1/2
  19 -x+1/2, y, -z+1/2
  20 -x+1/2, -y, z+1/2
  21 -y+3/4, -x+3/4, -z+1/4
  22 -y+3/4, x+1/4, z+3/4
  23 y+1/4, -x+1/4, z+3/4
  24 y+1/4, x+3/4, -z+1/4
  25 -x+1/2, -y+1/2, -z+1/2
  26 -x+1/2, y+1/2, z+1/2
  27 x+1/2, -y, z+1/2
  28 x+1/2, y, -z+1/2
  29 y+1/4, x+1/4, z+3/4
  30 y+1/4, -x+3/4, -z+1/4
  31 -y+3/4, x+3/4, -z+1/4
  32 -y+3/4, -x+1/4, z+3/4

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Th1 Th 4 a 0.00000 0.75000 0.12500 1.00000
  Si1 Si 8 e 0.00000 0.25000 0.29150 1.00000
```

$\alpha$ -ThSi<sub>2</sub> (C<sub>2</sub>): A2B\_tI12\_141\_e\_a - POSCAR

```
A2B_tI12_141_e_a & a, c/a, z2 --params=4.126, 3.47697527872, 0.2915 & I4_{1
  ↪ }/amd D_{4h}^{19} #141 (ae) & tI12 & SC_{c}$ & ThSi2 & $
  ↪ alpha$-ThSi$_{2}$ & G. Brauer and A. Mitius, Z. Anorg. Allg.
  ↪ Chem. 249, 325-339 (1942)
  1.0000000000000000
-2.0630000000000000 2.0630000000000000 7.1730000000000000
2.0630000000000000 -2.0630000000000000 7.1730000000000000
2.0630000000000000 2.0630000000000000 -7.1730000000000000
Si Th
  4 2
Direct
0.5415000000000000 0.2915000000000000 0.2500000000000000 Si (8e)
0.2915000000000000 0.5415000000000000 0.7500000000000000 Si (8e)
0.4585000000000000 -0.2915000000000000 0.7500000000000000 Si (8e)
-0.2915000000000000 0.4585000000000000 0.2500000000000000 Si (8e)
0.8750000000000000 0.1250000000000000 0.7500000000000000 Th (4a)
0.1250000000000000 0.8750000000000000 0.2500000000000000 Th (4a)
```

S-III: A\_tI16\_142\_f - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'S-III'
_chemical_formula_sum 'S'

loop_
  _publ_author_name
    'Olga Degtyareva'
    'Eugene Gregoryanz'
    'Maddury Somayazulu'
    'Przemyslaw Dera'
    'Ho-kwang Mao'
    'Russell J. Hemley'
  _journal_name_full_name
    ;
  Nature Materials
  ;
  _journal_volume 4
  _journal_year 2005
  _journal_page_first 152
  _journal_page_last 155
  _publ_section_title
    ;
  Novel chain structures in group VI elements
  ;

_aflow_title 'S-III Structure'
_aflow_proto 'A_tI16_142_f'
_aflow_params 'a, c/a, x_{1}'
_aflow_params_values '8.5939, 0.420984651904, 0.1405'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'tI16'

_symmetry_space_group_name_H-M "I 41/a 2/c 2/d (origin choice 2)"
_symmetry_Int_Tables_number 142

_cell_length_a 8.59390
_cell_length_b 8.59390
_cell_length_c 3.61790
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x, y, z
  2 x+1/2, -y+1/2, -z
  3 -x+1/2, y, -z
  4 -x, -y+1/2, z
  5 -y+1/4, -x+1/4, -z+1/4
  6 -y+1/4, x+3/4, z+1/4
  7 y+3/4, -x+3/4, z+1/4
  8 y+3/4, x+1/4, -z+1/4
  9 -x, -y, -z
  10 -x, y, z+1/2
  11 x, -y+1/2, z+1/2
  12 x, y+1/2, -z
  13 y+1/4, x+1/4, z+1/4
  14 y+3/4, -x+1/4, -z+3/4
  15 -y+1/4, x+1/4, -z+3/4
  16 -y+3/4, -x+1/4, z+1/4
  17 x+1/2, y+1/2, z+1/2
  18 x, -y, -z+1/2
  19 -x, y+1/2, -z+1/2
  20 -x+1/2, -y, z+1/2
  21 -y+3/4, -x+3/4, -z+3/4
  22 -y+3/4, x+1/4, z+3/4
  23 y+1/4, -x+1/4, z+3/4
  24 y+1/4, x+3/4, -z+3/4
  25 -x+1/2, -y+1/2, -z+1/2
  26 -x+1/2, y+1/2, z
  27 x+1/2, -y, z
  28 x+1/2, y, -z+1/2
  29 y+3/4, x+3/4, z+3/4
  30 y+1/4, -x+3/4, -z+1/4
  31 -y+3/4, x+3/4, -z+1/4
  32 -y+1/4, -x+3/4, z+3/4

loop_
  _atom_site_label
```



```

_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
SI S 16 f 0.14050 0.39050 0.12500 1.00000

```

S-III: A\_tI16\_142\_f - POSCAR

```

A_tI16_142_f & a, c/a, x1 --params=8.5939, 0.420984651904, 0.1405 & I4_{1}/
↳ acd D_{4h}^{20} #142 (f) & tI16 & None & S & S-III & Olga
↳ Degtyareva et al., Nat. Mater. 4, 152-155 (2005)
1.0000000000000000
-4.2969500000000000 4.2969500000000000 1.8089500000000000
4.2969500000000000 -4.2969500000000000 1.8089500000000000
4.2969500000000000 4.2969500000000000 -1.8089500000000000
S
8
Direct
0.5155000000000000 0.2655000000000000 0.5310000000000000 S (16f)
0.2345000000000000 -0.0155000000000000 -0.0310000000000000 S (16f)
0.2655000000000000 0.2345000000000000 0.7500000000000000 S (16f)
-0.0155000000000000 0.5155000000000000 0.7500000000000000 S (16f)
0.4845000000000000 0.7345000000000000 0.4690000000000000 S (16f)
0.7655000000000000 1.0155000000000000 1.0310000000000000 S (16f)
0.7345000000000000 0.7655000000000000 0.2500000000000000 S (16f)
1.0155000000000000 0.4845000000000000 0.2500000000000000 S (16f)

```

Simpsonite (Ta<sub>3</sub>Al<sub>4</sub>O<sub>13</sub>[OH]): A4B14C3\_hP21\_143\_bd\_ac4d\_d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ta3Al4O13[OH]'
_chemical_formula_sum 'A14 O14 Ta3'

loop_
_publ_author_name
'T. S. Ercit'
'F. C. Hawthorne'
'P. Cerny'
_journal_name_full_name
;
Canadian Mineralogist
;
_journal_volume 30
_journal_year 1992
_journal_page_first 653
_journal_page_last 662
_publ_section_title
;
The crystal structure of almotantite; its relation to the structures
↳ of simpsonite and the (Al, Ga)(Ta, Nb) OS_{4}S compounds
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'Simpsonite (Ta_{3}Al_{4}OS_{13}[OH]) Structure'
_aflow_proto 'A4B14C3_hP21_143_bd_ac4d_d'
_aflow_params 'a, c/a, z_{1}, z_{2}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5},
↳ x_{6}, y_{6}, z_{6}, x_{7}, y_{7}, z_{7}, x_{8}, y_{8}, z_{8}, x_{9},
↳ y_{9}, z_{9}'
_aflow_params_values '7.3813879247, 0.611841213925, 0.0, 0.305, 0.497, 0.453,
↳ 0.09, 0.302, 0.087, 0.605, 0.536, 0.253, 0.059, 0.583, 0.141, 0.429, 0.08
↳ 0.444, 0.296, 0.071, 0.2215, 0.2757, 0.806'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP21'

_cell_length_a 7.3813879247
_cell_length_b 7.3813879247
_cell_length_c 4.5162373483
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M 'P 3'
_symmetry_Int_Tables_number 143

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 1 a 0.00000 0.00000 0.00000 1.00000
Al1 Al 1 b 0.33333 0.66667 0.30500 1.00000
O2 O 1 c 0.66667 0.33333 0.49700 1.00000
Al2 Al 3 d 0.45300 0.09000 0.30200 1.00000
O3 O 3 d 0.08700 0.60500 0.53600 1.00000
O4 O 3 d 0.25300 0.05900 0.58300 1.00000
O5 O 3 d 0.14100 0.42900 0.08000 1.00000

```

```

O6 O 3 d 0.44400 0.29600 0.07100 1.00000
Ta1 Ta 3 d 0.22150 0.27570 0.80600 1.00000

```

Simpsonite (Ta<sub>3</sub>Al<sub>4</sub>O<sub>13</sub>[OH]): A4B14C3\_hP21\_143\_bd\_ac4d\_d - POSCAR

```

A4B14C3_hP21_143_bd_ac4d_d & a, c/a, z1, z2, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6.
↳ x7, y7, z7, x8, y8, z8, x9, y9, z9 --params=7.3813879247, 0.611841213925
↳ 0.0, 0.305, 0.497, 0.453, 0.09, 0.302, 0.087, 0.605, 0.536, 0.253, 0.059
↳ 0.583, 0.141, 0.429, 0.08, 0.444, 0.296, 0.071, 0.2215, 0.2757, 0.806 &
↳ P3 C_{3}^{1} #143 (abcd^6) & hP21 & None & Ta3Al4O13[OH] & &
↳ T. S. Ercit and F. C. Hawthorne and P. Cerny, Can. Mineral. 30,
↳ 653-662 (1992)
1.0000000000000000
3.69069396235000 -6.39246945797790 0.0000000000000000
3.69069396235000 6.39246945797790 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.51623734830000
Al O Ta
4 14 3
Direct
0.333333333333333 0.666666666666667 0.305000000000000 Al (1b)
0.453000000000000 0.090000000000000 0.302000000000000 Al (3d)
-0.090000000000000 0.363000000000000 0.302000000000000 Al (3d)
-0.363000000000000 -0.453000000000000 0.302000000000000 Al (3d)
0.000000000000000 0.000000000000000 0.000000000000000 O (1a)
0.666666666666667 0.333333333333333 0.497000000000000 O (1c)
0.087000000000000 0.605000000000000 0.536000000000000 O (3d)
-0.605000000000000 -0.518000000000000 0.536000000000000 O (3d)
0.518000000000000 -0.087000000000000 0.536000000000000 O (3d)
0.253000000000000 0.059000000000000 0.583000000000000 O (3d)
-0.059000000000000 0.194000000000000 0.583000000000000 O (3d)
-0.194000000000000 -0.253000000000000 0.583000000000000 O (3d)
0.141000000000000 0.429000000000000 0.080000000000000 O (3d)
-0.429000000000000 -0.288000000000000 0.080000000000000 O (3d)
0.288000000000000 -0.141000000000000 0.080000000000000 O (3d)
0.444000000000000 0.296000000000000 0.071000000000000 O (3d)
-0.296000000000000 0.148000000000000 0.071000000000000 O (3d)
-0.148000000000000 -0.444000000000000 0.071000000000000 O (3d)
0.221500000000000 0.275700000000000 0.806000000000000 Ta (3d)
-0.275700000000000 -0.054200000000000 0.806000000000000 Ta (3d)
0.054200000000000 -0.221500000000000 0.806000000000000 Ta (3d)

```

ScRh<sub>6</sub>P<sub>4</sub>: A4B6C\_hP11\_143\_bd\_2d\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'ScRh6P4'
_chemical_formula_sum 'P4 Rh6 Sc'

loop_
_publ_author_name
'U. Pfannenschmidt'
'U. C. Rodewald'
'R. P[{}o]ttgen'
_journal_name_full_name
;
Monatshefte f[{}u]r Chemie - Chemical Monthly
;
_journal_volume 142
_journal_year 2011
_journal_page_first 219
_journal_page_last 224
_publ_section_title
;
Bismuth flux crystal growth of SRESRh_{6}SP_{4}S (SRES = Sc, Yb, Lu):
↳ new phosphides with a superstructure of the LiCoS_{6}SP_{4}S
↳ type
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'ScRh_{6}SP_{4}S Structure'
_aflow_proto 'A4B6C_hP11_143_bd_2d_a'
_aflow_params 'a, c/a, z_{1}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5},
↳ y_{5}, z_{5}'
_aflow_params_values '6.9672687469, 0.526119402977, 0.0004, -0.0007, 0.8181,
↳ 0.1915, 0.4998, 0.5475, 0.48, 0.0003, 0.1859, 0.799, 0.5002'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP11'

_cell_length_a 6.9672687469
_cell_length_b 6.9672687469
_cell_length_c 3.6656152735
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M 'P 3'
_symmetry_Int_Tables_number 143

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x

```

```

_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Sc1 Sc 1 a 0.00000 0.00000 0.00040 1.00000
P1 P 1 b 0.33333 0.66667 -0.00070 1.00000
P2 P 3 d 0.81810 0.19150 0.49980 1.00000
Rh1 Rh 3 d 0.54750 0.48000 0.00030 1.00000
Rh2 Rh 3 d 0.18590 0.79900 0.50020 1.00000

```

ScRh<sub>6</sub>P<sub>4</sub>: A4B6C\_hP11\_143\_bd\_2d\_a - POSCAR

```

A4B6C_hP11_143_bd_2d_a & a, c/a, z1, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5 --params
↳ =6.9672687469, 0.526119402977, 0.0004, -0.0007, 0.8181, 0.1915,
↳ 0.4998, 0.5475, 0.48, 0.0003, 0.1859, 0.799, 0.5002 & P3 C_{3}^{1} #
↳ 143 (abd^3) & hP11 & None & ScRh6P4 & U. Pfannenschmidt and
↳ U. C. Rodewald and R. P.{}ttgen, Monatsh. Chem. 142, 219-224
↳ (2011)
1.000000000000000
3.48363437345000 -6.03383172980877 0.000000000000000
3.48363437345000 6.03383172980877 0.000000000000000
0.000000000000000 0.000000000000000 3.66561527350000
P Rh Sc
4 6 1
Direct
0.33333333333333 0.66666666666667 -0.00070000000000 P (1b)
0.81810000000000 0.19150000000000 0.49980000000000 P (3d)
-0.19150000000000 0.62660000000000 0.49980000000000 P (3d)
-0.62660000000000 -0.81810000000000 0.49980000000000 P (3d)
0.54750000000000 0.48000000000000 0.00030000000000 Rh (3d)
-0.48000000000000 0.06750000000000 0.00030000000000 Rh (3d)
-0.06750000000000 -0.54750000000000 0.00030000000000 Rh (3d)
0.18590000000000 0.79900000000000 0.50020000000000 Rh (3d)
-0.79900000000000 -0.61310000000000 0.50020000000000 Rh (3d)
0.61310000000000 -0.18590000000000 0.50020000000000 Rh (3d)
0.00000000000000 0.00000000000000 0.00040000000000 Sc (1a)

```

MoS<sub>2</sub>: AB2\_hP12\_143\_cd\_ab2d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'MoS2'
_chemical_formula_sum 'Mo S2'

loop_
_publ_author_name
'K. E. Dungey'
'M. D. Curtis'
'J. E. {Penner-Hahn}'
_journal_name_full_name
;
Chemistry of Materials
;
_journal_volume 10
_journal_year 1998
_journal_page_first 2152
_journal_page_last 2161
_publ_section_title
;
Structural characterization and thermal stability of MoSS_{2}$
↳ intercalation compounds
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'MoSS_{2}$ Structure'
_aflow_proto 'AB2_hP12_143_cd_ab2d'
_aflow_params 'a, c/a, z_{1}, z_{2}, z_{3}, x_{3}, y_{3}, z_{4}, x_{4}, y_{4}, z_{5}, x_{5}, y_{5}, z_{6}, x_{6}, y_{6}, z_{6}'
_aflow_params_values '6.5003859369, 0.944615384626, 0.0, 0.5, 0.25, 0.0548,
↳ 0.2679, 0.25, 0.33333, 0.16667, 0.5, 0.0, 0.5, 0.0'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP12'

_cell_length_a 6.5003859369
_cell_length_b 6.5003859369
_cell_length_c 6.1403645620
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 3"
_symmetry_Int_Tables_number 143

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
S1 S 1 a 0.00000 0.00000 0.00000 1.00000
S2 S 1 b 0.33333 0.66667 0.50000 1.00000
Mol Mo 1 c 0.66667 0.33333 0.25000 1.00000

```

```

Mo2 Mo 3 d 0.05480 0.26790 0.25000 1.00000
S3 S 3 d 0.33333 0.16667 0.50000 1.00000
S4 S 3 d 0.00000 0.50000 0.00000 1.00000

```

MoS<sub>2</sub>: AB2\_hP12\_143\_cd\_ab2d - POSCAR

```

AB2_hP12_143_cd_ab2d & a, c/a, z1, z2, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6 --
↳ params=6.5003859369, 0.944615384626, 0.0, 0.5, 0.25, 0.0548, 0.2679,
↳ 0.25, 0.33333, 0.16667, 0.5, 0.0, 0.5, 0.0 & P3 C_{3}^{1} #143 (abcd^
↳ 3) & hP12 & None & MoS2 & K. E. Dungey and M. D. Curtis and
↳ J. E. {Penner-Hahn}, Chem. Mater. 10, 2152-2161 (1998)
1.000000000000000
3.25019296845000 -5.62949935575851 0.000000000000000
3.25019296845000 5.62949935575851 0.000000000000000
0.000000000000000 0.000000000000000 6.14036456200000
Mo S
4 8
Direct
0.66666666666667 0.33333333333333 0.25000000000000 Mo (1c)
0.05480000000000 0.26790000000000 0.25000000000000 Mo (3d)
-0.26790000000000 -0.21310000000000 0.25000000000000 Mo (3d)
0.21310000000000 -0.05480000000000 0.25000000000000 Mo (3d)
0.00000000000000 0.00000000000000 0.00000000000000 S (1a)
0.33333333333333 0.66666666666667 0.50000000000000 S (1b)
0.33333000000000 0.16667000000000 0.50000000000000 S (3d)
-0.16667000000000 0.16666000000000 0.50000000000000 S (3d)
-0.16666000000000 -0.33333000000000 0.50000000000000 S (3d)
0.00000000000000 0.50000000000000 0.00000000000000 S (3d)
-0.50000000000000 -0.50000000000000 0.00000000000000 S (3d)
0.50000000000000 0.00000000000000 0.00000000000000 S (3d)

```

IrGe<sub>4</sub>: A4B\_hP15\_144\_4a\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'IrGe4'
_chemical_formula_sum 'Ge4 Ir'

loop_
_publ_author_name
'K. Schubert'
'S. Bhan'
'T. K. Biswas'
'K. Frank'
'P. K. Panday'
_journal_name_full_name
;
Naturwissenschaften
;
_journal_volume 55
_journal_year 1968
_journal_page_first 542
_journal_page_last 543
_publ_section_title
;
Einige Strukturdaten metallischer Phasen
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'IrGeS_{4}$ Structure'
_aflow_proto 'A4B_hP15_144_4a_a'
_aflow_params 'a, c/a, x_{1}, y_{1}, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}'
_aflow_params_values '6.2151204722, 1.25245374096, 0.4904, 0.2194, 0.2268,
↳ 0.2226, 0.4873, 0.1142, 0.0775, 0.0012, 0.0, 0.6097, 0.0014, 0.0018,
↳ 0.3178, 0.0008, 0.5062'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP15'

_cell_length_a 6.2151204722
_cell_length_b 6.2151204722
_cell_length_c 7.7841508859
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 31"
_symmetry_Int_Tables_number 144

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z+1/3
3 -x+y, -x, z+2/3

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ge1 Ge 3 a 0.49040 0.21940 0.22680 1.00000
Ge2 Ge 3 a 0.22260 0.48730 0.11420 1.00000
Ge3 Ge 3 a 0.07750 0.00120 0.00000 1.00000
Ge4 Ge 3 a 0.60970 0.00140 0.00180 1.00000
Ir1 Ir 3 a 0.31780 0.00080 0.50620 1.00000

```

IrGe<sub>4</sub>: A4B\_hP15\_144\_4a\_a - POSCAR

A4B\_hP15\_144\_4a\_a & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5
--params=6.2151204722, 1.25245374096, 0.4904, 0.2194, 0.2268, 0.2226
0.4873, 0.1142, 0.0775, 0.0012, 0.0, 0.6097, 0.0014, 0.0018, 0.3178,
0.0008, 0.5062 & P3\_{1} C\_{3}^{2} #144 (a^5) & hP15 & None &
IrGe4 & K. Schubert et al., {Naturwissenschaften 55, 542-543
(1968)
1.0000000000000000
3.10756023610000 -5.38245221650594 0.0000000000000000
3.10756023610000 5.38245221650594 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.7841508859000000
Ge Ir
12 3
Direct
0.4904000000000000 0.2194000000000000 0.2268000000000000 Ge (3a)
-0.2194000000000000 0.2710000000000000 0.5601333333333333 Ge (3a)
-0.2710000000000000 -0.4904000000000000 0.8934666666666667 Ge (3a)
0.2226000000000000 0.4873000000000000 0.1142000000000000 Ge (3a)
-0.4873000000000000 -0.2647000000000000 0.4475333333333333 Ge (3a)
0.2647000000000000 -0.2226000000000000 0.7808666666666667 Ge (3a)
0.0775000000000000 0.0012000000000000 0.0000000000000000 Ge (3a)
-0.0012000000000000 0.0763000000000000 0.3333333333333333 Ge (3a)
-0.0763000000000000 -0.0775000000000000 0.6666666666666667 Ge (3a)
0.6097000000000000 0.0014000000000000 0.0018000000000000 Ge (3a)
-0.0014000000000000 0.6083000000000000 0.3351333333333333 Ge (3a)
-0.6083000000000000 -0.6097000000000000 0.6684666666666667 Ge (3a)
0.3178000000000000 0.0008000000000000 0.5062000000000000 Ir (3a)
-0.0008000000000000 0.3170000000000000 0.8395333333333333 Ir (3a)
-0.3170000000000000 -0.3178000000000000 1.1728666666666667 Ir (3a)

TeZn (High-pressure): AB\_hP6\_144\_a\_a - CIF

# CIF file
data\_findsym-output
\_audit\_creation\_method FINDSYM
\_chemical\_name\_mineral 'ZnTe'
\_chemical\_formula\_sum 'Te Zn'
loop\_
\_publ\_author\_name
'K. Kusaba'
'D. J. Weidner'
\_journal\_year 1994
\_publ\_section\_title
Structure of high pressure phase I in ZnTe
# Found in Pearson's Crystal Data - Crystal Structure Database for
Inorganic Compounds, 2013
\_aflow\_title 'TeZn (High-pressure) Structure'
\_aflow\_proto 'AB\_hP6\_144\_a\_a'
\_aflow\_params 'a, c/a, x\_{1}, y\_{1}, z\_{1}, x\_{2}, y\_{2}, z\_{2}'
\_aflow\_params\_values '4.0452497415, 2.30951792334, 0.33, 0.16, 0.197, 0.13,
0.32, 0.0'
\_aflow\_strukturbericht 'None'
\_aflow\_pearson 'hP6'
\_cell\_length\_a 4.0452497415
\_cell\_length\_b 4.0452497415
\_cell\_length\_c 9.3425767824
\_cell\_angle\_alpha 90.0000000000
\_cell\_angle\_beta 90.0000000000
\_cell\_angle\_gamma 120.0000000000
\_symmetry\_space\_group\_name\_H-M 'P 31'
\_symmetry\_Int\_Tables\_number 144
loop\_
\_space\_group\_symop\_id
\_space\_group\_symop\_operation\_xyz
1 x, y, z
2 -y, x-y, z+1/3
3 -x+y, -x, z+2/3
loop\_
\_atom\_site\_label
\_atom\_site\_type\_symbol
\_atom\_site\_symmetry\_multiplicity
\_atom\_site\_Wyckoff\_label
\_atom\_site\_fract\_x
\_atom\_site\_fract\_y
\_atom\_site\_fract\_z
\_atom\_site\_occupancy
Te1 Te 3 a 0.33000 0.16000 0.19700 1.00000
Zn1 Zn 3 a 0.13000 0.32000 0.00000 1.00000

TeZn (High-pressure): AB\_hP6\_144\_a\_a - POSCAR

AB\_hP6\_144\_a\_a & a, c/a, x1, y1, z1, x2, y2, z2 --params=4.0452497415,
2.30951792334, 0.33, 0.16, 0.197, 0.13, 0.32, 0.0 & P3\_{1} C\_{3}^{2}
#144 (a^2) & hP6 & None & ZnTe & K. Kusaba and D. J. Weidner
(1994)
1.0000000000000000
2.02262487075000 -3.50328904079143 0.0000000000000000
2.02262487075000 3.50328904079143 0.0000000000000000
0.0000000000000000 0.0000000000000000 9.34257678240000
Te Zn
3 3
Direct
0.3300000000000000 0.1600000000000000 0.1970000000000000 Te (3a)
-0.1600000000000000 0.1700000000000000 0.5303333333333333 Te (3a)

-0.1700000000000000 -0.3300000000000000 0.8636666666666667 Te (3a)
0.1300000000000000 0.3200000000000000 0.0000000000000000 Zn (3a)
-0.3200000000000000 -0.1900000000000000 0.3333333333333333 Zn (3a)
0.1900000000000000 -0.1300000000000000 0.6666666666666667 Zn (3a)

Sheldrickite (NaCa<sub>3</sub>[CO<sub>3</sub>]<sub>2</sub>F<sub>3</sub>(H<sub>2</sub>O)): A2B3C3DE7\_hP48\_145\_2a\_3a\_7a - CIF

# CIF file
\_chemical\_name\_mineral 'Sheldrickite'
data\_findsym-output
\_audit\_creation\_method FINDSYM
\_chemical\_name\_mineral 'Sheldrickite'
\_chemical\_formula\_sum 'C2 Ca3 F3 Na O7'
loop\_
\_publ\_author\_name
'J. D. Grice'
'R. A. Gault'
'J. {Van Velthuizen}'
\_journal\_name\_full\_name
Canadian Mineralogist
\_journal\_volume 35
\_journal\_year 1997
\_journal\_page\_first 181
\_journal\_page\_last 187
\_publ\_section\_title
Sheldrickite, a new sodium-calcium-fluorocarbonate mineral species from
Mont Saint-Hilaire, Quebec
# Found in Pearson's Crystal Data - Crystal Structure Database for
Inorganic Compounds, 2013
\_aflow\_title 'Sheldrickite (NaCa<sub>3</sub>[CO<sub>3</sub>]<sub>2</sub>F<sub>3</sub>(H<sub>2</sub>O)) Structure'
\_aflow\_proto 'A2B3C3DE7\_hP48\_145\_2a\_3a\_7a'
\_aflow\_params 'a, c/a, x\_{1}, y\_{1}, z\_{1}, x\_{2}, y\_{2}, z\_{2}, x\_{3}, y\_{3}, z\_{3}, x\_{4}, y\_{4}, z\_{4}, x\_{5}, y\_{5}, z\_{5}, x\_{6}, y\_{6}, z\_{6}, x\_{7}, y\_{7}, z\_{7}, x\_{8}, y\_{8}, z\_{8}, x\_{9}, y\_{9}, z\_{9}, x\_{10}, y\_{10}, z\_{10}, x\_{11}, y\_{11}, z\_{11}, x\_{12}, y\_{12}, z\_{12}, x\_{13}, y\_{13}, z\_{13}, x\_{14}, y\_{14}, z\_{14}, x\_{15}, y\_{15}, z\_{15}, x\_{16}, y\_{16}, z\_{16}'
\_aflow\_params\_values '6.7260126433, 2.23669342849, 0.567, 0.317, 0.168, 0.432, 0.752, 0.169, 0.6161, -0.0009, 0.0, -0.0011, 0.6284, 0.0045, 0.3706, 0.371, -0.0043, -0.003, 0.266, 0.01, 0.271, 0.002, -0.005, 0.73, 0.734, 0.02, 0.001, 0.297, 0.165, 0.664, 0.348, 0.09, 0.668, 0.333, 0.238, 0.353, 0.273, 0.167, 0.321, 0.654, -0.092, 0.336, 0.666, 0.761, 0.646, -0.079, 0.165, 0.203, 0.202, 0.831'
\_aflow\_strukturbericht 'None'
\_aflow\_pearson 'hP48'
\_cell\_length\_a 6.7260126433
\_cell\_length\_b 6.7260126433
\_cell\_length\_c 15.0440282792
\_cell\_angle\_alpha 90.0000000000
\_cell\_angle\_beta 90.0000000000
\_cell\_angle\_gamma 120.0000000000
\_symmetry\_space\_group\_name\_H-M 'P 32'
\_symmetry\_Int\_Tables\_number 145
loop\_
\_space\_group\_symop\_id
\_space\_group\_symop\_operation\_xyz
1 x, y, z
2 -y, x-y, z+2/3
3 -x+y, -x, z+1/3
loop\_
\_atom\_site\_label
\_atom\_site\_type\_symbol
\_atom\_site\_symmetry\_multiplicity
\_atom\_site\_Wyckoff\_label
\_atom\_site\_fract\_x
\_atom\_site\_fract\_y
\_atom\_site\_fract\_z
\_atom\_site\_occupancy
C1 C 3 a 0.56700 0.31700 0.16800 1.00000
C2 C 3 a 0.43200 0.75200 0.16900 1.00000
Ca1 Ca 3 a 0.61610 -0.00090 0.00000 1.00000
Ca2 Ca 3 a -0.00110 0.62840 0.00450 1.00000
Ca3 Ca 3 a 0.37060 0.37100 -0.00430 1.00000
F1 F 3 a -0.00300 0.26600 0.01000 1.00000
F2 F 3 a 0.27100 0.00200 -0.00500 1.00000
F3 F 3 a 0.73000 0.73400 -0.02000 1.00000
Na1 Na 3 a 0.00100 0.29700 0.16500 1.00000
O1 O 3 a 0.66400 0.34800 0.09000 1.00000
O2 O 3 a 0.66800 0.33300 0.23800 1.00000
O3 O 3 a 0.35300 0.27300 0.16700 1.00000
O4 O 3 a 0.32100 0.65400 -0.09200 1.00000
O5 O 3 a 0.33600 0.66600 0.76100 1.00000
O6 O 3 a 0.64600 -0.07900 0.16500 1.00000
O7 O 3 a 0.20300 0.20200 0.83100 1.00000
Sheldrickite (NaCa<sub>3</sub>[CO<sub>3</sub>]<sub>2</sub>F<sub>3</sub>(H<sub>2</sub>O)): A2B3C3DE7\_hP48\_145\_2a\_3a\_7a - POSCAR
A2B3C3DE7\_hP48\_145\_2a\_3a\_7a & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4,
y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10,
x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16,
y16, z16 --params=6.7260126433, 2.23669342849, 0.567, 0.317, 0.168,

```

↪ 0.432, 0.752, 0.169, 0.6161, -0.0009, 0.0, -0.0011, 0.6284, 0.0045,
↪ 0.3706, 0.371, -0.0043, -0.003, 0.266, 0.01, 0.271, 0.002, -0.005, 0.73,
↪ 0.734, -0.02, 0.001, 0.297, 0.165, 0.664, 0.348, 0.09, 0.668, 0.333,
↪ 0.238, 0.353, 0.273, 0.167, 0.321, 0.654, -0.092, 0.336, 0.666, 0.761,
↪ 0.646, -0.079, 0.165, 0.203, 0.202, 0.831 & P3_{2} C_{3}^{4} #145 (a
↪ ^16) & hP48 & None & NaCa3[CO3]2F3[HO] & Sheldrickite & J. D.
↪ Grice and R. A. Gault and J. {Van Velthuizen}, Can. Mineral. 35
↪ , 181-187 (1997)
1.000000000000000
3.36300632165000 -5.82489781527312 0.000000000000000
3.36300632165000 5.82489781527312 0.000000000000000
0.000000000000000 0.000000000000000 15.04402827920000
C Ca F Na O
6 9 9 3 21
Direct
0.567000000000000 0.317000000000000 0.168000000000000 C (3a)
-0.317000000000000 0.250000000000000 0.834666666666667 C (3a)
-0.250000000000000 -0.567000000000000 0.501333333333333 C (3a)
0.432000000000000 0.752000000000000 0.169000000000000 C (3a)
-0.752000000000000 -0.320000000000000 0.835666666666667 C (3a)
0.320000000000000 -0.432000000000000 0.502333333333333 C (3a)
0.616100000000000 -0.000900000000000 0.000000000000000 Ca (3a)
0.000900000000000 0.617000000000000 0.666666666666667 Ca (3a)
-0.617000000000000 -0.616100000000000 0.333333333333333 Ca (3a)
-0.001100000000000 0.628400000000000 0.004500000000000 Ca (3a)
-0.628400000000000 -0.629500000000000 0.671166666666667 Ca (3a)
0.629500000000000 0.001100000000000 0.337833333333333 Ca (3a)
0.370600000000000 -0.371000000000000 -0.004300000000000 Ca (3a)
-0.371000000000000 -0.000400000000000 0.662366666666667 Ca (3a)
0.000400000000000 -0.370600000000000 0.329033333333333 Ca (3a)
-0.003000000000000 0.266000000000000 0.010000000000000 F (3a)
-0.266000000000000 -0.269000000000000 0.676666666666667 F (3a)
0.269000000000000 0.003000000000000 0.343333333333333 F (3a)
0.271000000000000 0.002000000000000 -0.005000000000000 F (3a)
-0.002000000000000 0.269000000000000 0.661666666666667 F (3a)
-0.269000000000000 -0.271000000000000 0.328333333333333 F (3a)
0.730000000000000 0.734000000000000 -0.020000000000000 F (3a)
-0.734000000000000 -0.004000000000000 0.646666666666667 F (3a)
0.004000000000000 -0.730000000000000 0.313333333333333 F (3a)
0.001000000000000 0.297000000000000 0.165000000000000 Na (3a)
-0.297000000000000 -0.296000000000000 0.831666666666667 Na (3a)
0.296000000000000 -0.001000000000000 0.498333333333333 Na (3a)
0.664000000000000 0.348000000000000 0.090000000000000 O (3a)
-0.348000000000000 0.316000000000000 0.756666666666667 O (3a)
-0.316000000000000 -0.664000000000000 0.423333333333333 O (3a)
0.668000000000000 0.333000000000000 0.238000000000000 O (3a)
-0.333000000000000 0.335000000000000 0.904666666666667 O (3a)
-0.335000000000000 -0.668000000000000 0.571333333333333 O (3a)
0.353000000000000 0.273000000000000 0.167000000000000 O (3a)
-0.273000000000000 0.080000000000000 0.833666666666667 O (3a)
-0.080000000000000 -0.353000000000000 0.500333333333333 O (3a)
0.321000000000000 0.654000000000000 -0.092000000000000 O (3a)
-0.654000000000000 -0.333000000000000 0.574666666666667 O (3a)
0.333000000000000 -0.321000000000000 0.241333333333333 O (3a)
0.336000000000000 0.666000000000000 0.761000000000000 O (3a)
-0.666000000000000 -0.330000000000000 1.427666666666667 O (3a)
0.330000000000000 -0.336000000000000 1.094333333333333 O (3a)
0.646000000000000 -0.079000000000000 0.165000000000000 O (3a)
0.079000000000000 0.725000000000000 0.831666666666667 O (3a)
-0.725000000000000 -0.646000000000000 0.498333333333333 O (3a)
0.203000000000000 0.202000000000000 0.831000000000000 O (3a)
-0.202000000000000 0.001000000000000 1.497666666666667 O (3a)
-0.001000000000000 -0.203000000000000 1.164333333333333 O (3a)

```

$\gamma$ -Ag<sub>3</sub>SI (Low-temperature): A3BC\_hR5\_146\_b\_a\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'gamma-Ag3SI'
_chemical_formula_sum 'Ag3 I S'

loop_
_publ_author_name
'S. Hoshino'
'T. Sakuma'
'Y. Fujii'
_journal_name_full_name
;
Journal of the Physical Society of Japan
;
_journal_volume 47
_journal_year 1979
_journal_page_first 1252
_journal_page_last 1259
_publ_section_title
;
A Structural Phase Transition in Superionic Conductor Ag3SI
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title '$\gamma$-Ag3SI (Low-temperature) Structure'
_aflow_proto 'A3BC_hR5_146_b_a_a'
_aflow_params 'a, c/a, x_{1}, x_{2}, x_{3}, y_{3}, z_{3}'
_aflow_params_values '6.8858547087, 1.22475238897, 0.47, 0.0, 0.49, -0.002, -
↪ 0.14399'
_aflow_strukturbericht 'None'
_aflow_pearson 'hR5'

_cell_length_a 6.8858547087
_cell_length_b 6.8858547087
_cell_length_c 8.4334670046

```

```

_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "R 3 (hexagonal axes)"
_symmetry_Int_Tables_number 146

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 x+1/3, y+2/3, z+2/3
5 -y+1/3, x-y+2/3, z+2/3
6 -x+y+1/3, -x+2/3, z+2/3
7 x+2/3, y+1/3, z+1/3
8 -y+2/3, x-y+1/3, z+1/3
9 -x+y+2/3, -x+1/3, z+1/3

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
I1 I 3 a 0.00000 0.00000 0.47000 1.00000
S1 S 3 a 0.00000 0.00000 0.00000 1.00000
Ag1 Ag 9 b 0.37533 0.11667 0.11467 1.00000

```

$\gamma$ -Ag<sub>3</sub>SI (Low-temperature): A3BC\_hR5\_146\_b\_a\_a - POSCAR

```

A3BC_hR5_146_b_a_a & a, c/a, x1, x2, x3, y3, z3 --params=6.8858547087,
↪ 1.22475238897, 0.47, 0.0, 0.49, -0.002, -0.14399 & R3 C_{3}^{4} #146
↪ (a^2b) & hR5 & None & Ag3SI & gamma & S. Hoshino and T. Sakuma
↪ and Y. Fujii, J. Phys. Soc. Jpn. 47, 1252-1259 (1979)

1.000000000000000
3.44292735435000 -1.98777503483430 2.81115566820000
0.000000000000000 3.97555006966860 2.81115566820000
-3.44292735435000 -1.98777503483430 2.81115566820000

Ag I S
3 1 1

Direct
0.490000000000000 -0.002000000000000 -0.143990000000000 Ag (3b)
-0.143990000000000 0.490000000000000 -0.002000000000000 Ag (3b)
-0.002000000000000 -0.143990000000000 0.490000000000000 Ag (3b)
0.470000000000000 0.470000000000000 0.470000000000000 I (1a)
0.000000000000000 0.000000000000000 0.000000000000000 S (1a)

```

FePSe<sub>3</sub>: ABC3\_hR10\_146\_2a\_2a\_2b - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'FePSe3'
_chemical_formula_sum 'Fe P Se3'

loop_
_publ_author_name
'W. Klingen'
'G. Eulenberger'
'H. Hahn'
_journal_name_full_name
;
Zeitschrift fur Anorganische und Allgemeine Chemie
;
_journal_volume 401
_journal_year 1973
_journal_page_first 97
_journal_page_last 112
_publ_section_title
;
Uber die Kristallstrukturen von Fe2SP2Se6 und Fe2SP2Se6
↪ {2}SSS_{6}$
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'FePSe3 Structure'
_aflow_proto 'ABC3_hR10_146_2a_2a_2b'
_aflow_params 'a, c/a, x_{1}, x_{2}, x_{3}, x_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}'
_aflow_params_values '6.2648898445, 3.16041500397, 0.3911, 0.7256, 0.1132,
↪ 0.0, 0.1454, -0.1886, 0.474, 0.6151, -0.0128, 0.3247'
_aflow_strukturbericht 'None'
_aflow_pearson 'hR10'

_cell_length_a 6.2648898445
_cell_length_b 6.2648898445
_cell_length_c 19.7996518628
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "R 3 (hexagonal axes)"
_symmetry_Int_Tables_number 146

loop_
_space_group_symop_id
_space_group_symop_operation_xyz

```

```
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 x+1/3,y+2/3,z+2/3
5 -y+1/3,x-y+2/3,z+2/3
6 -x+y+1/3,-x+2/3,z+2/3
7 x+2/3,y+1/3,z+1/3
8 -y+2/3,x-y+1/3,z+1/3
9 -x+y+2/3,-x+1/3,z+1/3
```

```
loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Fe1 Fe 3 a 0.00000 0.00000 0.39110 1.00000
Fe2 Fe 3 a 0.00000 0.00000 0.72560 1.00000
P1 P 3 a 0.00000 0.00000 0.11320 1.00000
P2 P 3 a 0.00000 0.00000 0.00000 1.00000
Se1 Se 9 b 0.00180 0.33220 0.14360 1.00000
Se2 Se 9 b 0.30610 0.32180 0.30900 1.00000
```

FePSe<sub>3</sub>: ABC3\_hr10\_146\_2a\_2a\_2b - POSCAR

```
ABC3_hr10_146_2a_2a_2b & a, c/a, x1, x2, x3, x4, x5, y5, z5, x6, y6, z6 --params=
↳ 6.2648898445, 3.16041500397, 0.39111, 0.7256, 0.1132, 0.0, 0.1454, -
↳ 0.1886, 0.474, 0.6151, -0.0128, 0.3247 & R3 C_{3}^{4} #146 (a^4b^2)
↳ & hr10 & None & FePSe3 & W. Klingen and G. Eulenberger and
↳ H. Hahn, Z. Anorg. Allg. Chem. 401, 97-112 (1973)
```

```
1.0000000000000000
3.13244492225000 -1.80851791908271 6.59988395426667
0.0000000000000000 3.61703583816543 6.59988395426667
-3.13244492225000 -1.80851791908271 6.59988395426667
Fe P Se
2 2 6
Direct
0.391100000000000 0.391100000000000 0.391100000000000 Fe (1a)
0.725600000000000 0.725600000000000 0.725600000000000 Fe (1a)
0.113200000000000 0.113200000000000 0.113200000000000 P (1a)
0.000000000000000 0.000000000000000 0.000000000000000 P (1a)
0.145400000000000 -0.188600000000000 0.474000000000000 Se (3b)
0.474000000000000 0.145400000000000 -0.188600000000000 Se (3b)
-0.188600000000000 0.474000000000000 0.145400000000000 Se (3b)
0.615100000000000 -0.012800000000000 0.324700000000000 Se (3b)
0.324700000000000 0.615100000000000 -0.012800000000000 Se (3b)
-0.012800000000000 0.324700000000000 0.615100000000000 Se (3b)
```

Phenakite (Be<sub>2</sub>SiO<sub>4</sub>, S<sub>13</sub>): A2B4C\_hr42\_148\_2f\_4f\_f - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Phenakite'
_chemical_formula_sum 'Be2 O4 Si'
loop_
  _publ_author_name
  'R. M. Hazen'
  'L. W. Finger'
  _journal_name_full_name
  'Physics and Chemistry of Minerals'
  _journal_volume 14
  _journal_year 1987
  _journal_page_first 426
  _journal_page_last 434
  _publ_section_title
  'High-Temperature Crystal Chemistry of Phenakite (Be2S2SiO4) and
  ↳ Chrysoberyl (BeAl2S2O4)'
  _aflow_title 'Phenakite (Be2S2SiO4, SS1_{3}) Structure'
  _aflow_proto 'A2B4C_hr42_148_2f_4f_f'
  _aflow_params 'a, c/a, x_{1}, y_{1}, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}, x_{7}, y_{7}, z_{7}'
  _aflow_params_values '12.4401, 0.661634552777, 0.20546, -0.56835, 0.60961,
  ↳ 0.87265, 0.10211, -0.72078, 0.66221, -0.37042, -0.03997, 0.41696, -
  ↳ 0.2507, 0.0834, 0.70548, 0.00275, 0.03736, 0.37614, -0.32772, 0.70785,
  ↳ 0.53815, -0.23404, -0.05466'
  _aflow_Strukturbericht '$S1_{3}$'
  _aflow_Pearson 'hR42'
_symmetry_space_group_name_H-M 'R -3 (hexagonal axes)'
_symmetry_Int_Tables_number 148
_cell_length_a 12.44010
_cell_length_b 12.44010
_cell_length_c 8.23080
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000
loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
```

```
3 -x+y,-x,z
4 -x,-y,-z
5 y,-x+y,-z
6 x-y,x,-z
7 x+1/3,y+2/3,z+2/3
8 -y+1/3,x-y+2/3,z+2/3
9 -x+y+1/3,-x+2/3,z+2/3
10 -x+1/3,-y+2/3,-z+2/3
11 y+1/3,-x+y+2/3,-z+2/3
12 x-y+1/3,x+2/3,-z+2/3
13 x+2/3,y+1/3,z+1/3
14 -y+2/3,x-y+1/3,z+1/3
15 -x+y+2/3,-x+1/3,z+1/3
16 -x+2/3,-y+1/3,-z+1/3
17 y+2/3,-x+y+1/3,-z+1/3
18 x-y+2/3,x+1/3,-z+1/3
```

```
loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Be1 Be 18 f 0.12322 0.65059 0.08224 1.00000
Be2 Be 18 f 0.78799 -0.01745 0.08466 1.00000
O1 O 18 f 0.57827 0.45436 0.08394 1.00000
O2 O 18 f 0.33374 0.33392 0.08322 1.00000
O3 O 18 f 0.45695 0.24578 0.24853 1.00000
O4 O 18 f 0.12405 0.57981 0.25209 1.00000
Si1 Si 18 f 0.45500 0.31719 0.08315 1.00000
```

Phenakite (Be<sub>2</sub>SiO<sub>4</sub>, S<sub>13</sub>): A2B4C\_hr42\_148\_2f\_4f\_f - POSCAR

```
A2B4C_hr42_148_2f_4f_f & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5,
↳ z5, x6, y6, z6, x7, y7, z7 --params=12.4401, 0.661634552777, 0.20546, -
↳ 0.56835, 0.60961, 0.87265, 0.10211, -0.72078, 0.66221, -0.37042, -
↳ 0.03997, 0.41696, -0.2507, 0.0834, 0.70548, 0.00275, 0.03736, 0.37614
↳ -0.32772, 0.70785, 0.53815, -0.23404, -0.05466 & R-3 C_{3i}^{2} #
↳ 148 (f^7) & hR42 & SS1_{3}$ & Be2SiO4 & Phenakite & R. M. Hazen
↳ and L. W. Finger, Phys. Chem. Miner. 14, 426-434 (1987)
```

```
1.0000000000000000
6.220050000000000 -3.59114754187293 2.743600000000000
0.000000000000000 7.18229508374586 2.743600000000000
-6.220050000000000 -3.59114754187293 2.743600000000000
Be O Si
12 24 6
Direct
0.205460000000000 -0.568350000000000 0.609610000000000 Be (6f)
0.609610000000000 0.205460000000000 -0.568350000000000 Be (6f)
-0.568350000000000 0.609610000000000 0.205460000000000 Be (6f)
-0.205460000000000 0.568350000000000 -0.609610000000000 Be (6f)
-0.609610000000000 -0.205460000000000 0.568350000000000 Be (6f)
0.568350000000000 -0.609610000000000 -0.205460000000000 Be (6f)
0.872650000000000 0.102110000000000 -0.720780000000000 Be (6f)
-0.720780000000000 0.872650000000000 0.102110000000000 Be (6f)
0.102110000000000 -0.720780000000000 0.872650000000000 Be (6f)
-0.872650000000000 -0.102110000000000 0.720780000000000 Be (6f)
0.720780000000000 -0.872650000000000 -0.102110000000000 Be (6f)
-0.102110000000000 0.720780000000000 -0.872650000000000 Be (6f)
0.662210000000000 -0.370420000000000 -0.039970000000000 O (6f)
-0.039970000000000 0.662210000000000 -0.370420000000000 O (6f)
-0.370420000000000 -0.039970000000000 0.662210000000000 O (6f)
-0.662210000000000 0.370420000000000 0.039970000000000 O (6f)
0.039970000000000 -0.662210000000000 0.370420000000000 O (6f)
0.370420000000000 0.039970000000000 -0.662210000000000 O (6f)
0.416960000000000 -0.250700000000000 0.083400000000000 O (6f)
0.083400000000000 0.416960000000000 -0.250700000000000 O (6f)
-0.250700000000000 0.083400000000000 0.416960000000000 O (6f)
-0.416960000000000 0.250700000000000 -0.083400000000000 O (6f)
-0.083400000000000 -0.416960000000000 0.250700000000000 O (6f)
0.250700000000000 -0.083400000000000 -0.416960000000000 O (6f)
0.705480000000000 0.002750000000000 0.037360000000000 O (6f)
0.037360000000000 0.705480000000000 0.002750000000000 O (6f)
0.002750000000000 0.037360000000000 0.705480000000000 O (6f)
-0.705480000000000 -0.002750000000000 -0.037360000000000 O (6f)
-0.037360000000000 -0.705480000000000 -0.002750000000000 O (6f)
-0.002750000000000 -0.037360000000000 -0.705480000000000 O (6f)
0.376140000000000 -0.327720000000000 0.707850000000000 O (6f)
0.707850000000000 0.376140000000000 -0.327720000000000 O (6f)
-0.327720000000000 0.707850000000000 0.376140000000000 O (6f)
-0.376140000000000 -0.327720000000000 0.707850000000000 O (6f)
-0.707850000000000 -0.376140000000000 0.327720000000000 O (6f)
0.327720000000000 -0.707850000000000 -0.376140000000000 O (6f)
0.538150000000000 -0.234040000000000 -0.054660000000000 Si (6f)
-0.054660000000000 0.538150000000000 -0.234040000000000 Si (6f)
-0.234040000000000 -0.054660000000000 0.538150000000000 Si (6f)
-0.538150000000000 0.234040000000000 0.054660000000000 Si (6f)
0.054660000000000 -0.538150000000000 -0.234040000000000 Si (6f)
0.234040000000000 0.054660000000000 -0.538150000000000 Si (6f)
```

β-PdCl<sub>2</sub>: A2B\_hr18\_148\_2f\_f - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral '$\beta$PdCl2'
_chemical_formula_sum 'Cl2 Pd'
loop_
  _publ_author_name
  'D. B. {Dell\`Amico}'
```

```
'F. Calderazzo'
'F. Marchetti'
'S. Ramello'
_journal_name_full_name
;
Angewandte Chemie (International ed.)
;
_journal_volume 35
_journal_year 1996
_journal_page_first 1331
_journal_page_last 1333
_publ_section_title
;
Molecular Structure of [Pd3{C12}] in Single Crystals
↳ Chemically Grown at Room Temperature
;
_aflow_title '$\beta$-PdCl2 Structure'
_aflow_proto 'A2B_hr18_148_2f_f'
_aflow_params 'a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3'
↳ '3'
_aflow_params_values '13.0471, 0.659280606418, 0.7407, -0.76315, 0.0238,
↳ 1.14609, 0.38403, -0.59217, 0.08714, 0.06386, 0.3263'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hR18'

_symmetry_space_group_name_H-M "R -3 (hexagonal axes)"
_symmetry_Int_Tables_number 148

_cell_length_a 13.04710
_cell_length_b 13.04710
_cell_length_c 8.60170
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 -x, -y, -z
5 y, -x+y, -z
6 x-y, x, -z
7 x+1/3, y+2/3, z+2/3
8 -y+1/3, x-y+2/3, z+2/3
9 -x+y+1/3, -x+2/3, z+2/3
10 -x+1/3, -y+2/3, -z+2/3
11 y+1/3, -x+y+2/3, -z+2/3
12 x-y+1/3, x+2/3, -z+2/3
13 x+2/3, y+1/3, z+1/3
14 -y+2/3, x-y+1/3, z+1/3
15 -x+y+2/3, -x+1/3, z+1/3
16 -x+2/3, -y+1/3, -z+1/3
17 y+2/3, -x+y+1/3, -z+1/3
18 x-y+2/3, x+1/3, -z+1/3

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cl1 Cl 18 f 0.74025 0.76360 0.00045 1.00000
Cl2 Cl 18 f 0.83344 -0.07138 0.31265 1.00000
Pd1 Pd 18 f -0.07196 0.09524 0.15910 1.00000
```

$\beta$ -PdCl<sub>2</sub>: A2B\_hr18\_148\_2f\_f - POSCAR

```
A2B_hr18_148_2f_f & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3 --params=13.0471,
↳ 0.659280606418, 0.7407, -0.76315, 0.0238, 1.14609, 0.38403, -0.59217,
↳ 0.08714, 0.06386, 0.3263 & R-3 C3i^2 #148 (Fh) & hR18 &
↳ None & PdCl2 & $\beta$-PdCl2 & D. B. {Dell'Amico} et al.,
↳ Angew. Chem. Int. Ed. 35, 1331-1333 (1996)
1.0000000000000000
6.5235500000000000 -3.76637334857198 2.867233333333333
0.0000000000000000 7.53274669714397 2.867233333333333
-6.5235500000000000 -3.76637334857198 2.867233333333333
Cl Pd
12 6
Direct
0.7407000000000000 -0.7631500000000000 0.0238000000000000 Cl (6f)
0.0238000000000000 0.7407000000000000 -0.7631500000000000 Cl (6f)
-0.7631500000000000 0.0238000000000000 0.7407000000000000 Cl (6f)
-0.7407000000000000 0.7631500000000000 -0.0238000000000000 Cl (6f)
0.7631500000000000 -0.0238000000000000 -0.7407000000000000 Cl (6f)
1.1460900000000000 0.3840300000000000 -0.5921700000000000 Cl (6f)
-0.5921700000000000 1.1460900000000000 0.3840300000000000 Cl (6f)
0.3840300000000000 -0.5921700000000000 1.1460900000000000 Cl (6f)
-1.1460900000000000 -0.3840300000000000 0.5921700000000000 Cl (6f)
0.5921700000000000 -1.1460900000000000 -0.3840300000000000 Cl (6f)
-0.3840300000000000 0.5921700000000000 -1.1460900000000000 Cl (6f)
0.0871400000000000 0.0638600000000000 0.3263000000000000 Pd (6f)
0.3263000000000000 0.0871400000000000 0.0638600000000000 Pd (6f)
0.0638600000000000 0.3263000000000000 0.0871400000000000 Pd (6f)
-0.0871400000000000 -0.0638600000000000 -0.3263000000000000 Pd (6f)
-0.3263000000000000 -0.0871400000000000 -0.0638600000000000 Pd (6f)
-0.0638600000000000 -0.3263000000000000 -0.0871400000000000 Pd (6f)
```

Ti<sub>3</sub>O (Room-temperature): AB3\_hp24\_149\_acgi\_3l - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ti3O'
_chemical_formula_sum 'O Ti3'

loop_
_publ_author_name
'A. Jostsons'
'A. S. Malin'
_journal_name_full_name
;
Acta Crystallographica Section B: Structural Science
;
_journal_volume 24
_journal_year 1968
_journal_page_first 211
_journal_page_last 213
_publ_section_title
;
The ordered structure of Ti3SO

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'Ti3SO (Room-temperature) Structure'
_aflow_proto 'AB3_hp24_149_acgi_3l'
_aflow_params 'a, c/a, z3, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7'
↳ '7', y7, z7'
_aflow_params_values '5.1418156677, 2.78268310709, 0.33333, 0.33333, 0.0,
↳ 0.33333, 0.421, 0.33333, 0.33333, 0.246, 0.0, 0.33333, 0.088'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP24'

_cell_length_a 5.1418156677
_cell_length_b 5.1418156677
_cell_length_c 14.3080435983
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 3 1 2"
_symmetry_Int_Tables_number 149

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 x, x-y, -z
5 -x+y, y, -z
6 -y, -x, -z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 1 a 0.00000 0.00000 1.00000
O2 O 1 c 0.33333 0.66667 0.00000 1.00000
O3 O 2 g 0.00000 0.00000 0.33333 1.00000
O4 O 2 i 0.66667 0.33333 0.33333 1.00000
Ti1 Ti 6 l 0.00000 0.33333 0.42100 1.00000
Ti2 Ti 6 l 0.33333 0.33333 0.24600 1.00000
Ti3 Ti 6 l 0.00000 0.33333 0.08800 1.00000
```

Ti<sub>3</sub>O (Room-temperature): AB3\_hp24\_149\_acgi\_3l - POSCAR

```
AB3_hp24_149_acgi_3l & a, c/a, z3, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7 --params=
↳ 5.1418156677, 2.78268310709, 0.33333, 0.33333, 0.0, 0.33333, 0.421,
↳ 0.33333, 0.33333, 0.246, 0.0, 0.33333, 0.088 & P312 D3i^1 #149 (
↳ acgi1^3) & hP24 & None & Ti3O & A. Jostsons and A. S. Malin,
↳ Acta Crystallogr. Sect. B Struct. Sci. 24, 211-213 (1968)
1.0000000000000000
2.57090783385000 -4.45294298980505 0.0000000000000000
2.57090783385000 4.45294298980505 0.0000000000000000
0.0000000000000000 0.0000000000000000 14.30804359830000
O Ti
6 18
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 O (1a)
0.3333333333333333 0.6666666666666667 0.0000000000000000 O (1c)
0.0000000000000000 0.0000000000000000 0.3333300000000000 O (2g)
0.0000000000000000 0.0000000000000000 -0.3333300000000000 O (2g)
0.6666666666666667 0.3333333333333333 0.3333300000000000 O (2i)
0.6666666666666667 0.3333333333333333 -0.3333300000000000 O (2i)
0.0000000000000000 0.3333300000000000 0.4210000000000000 Ti (6i)
-0.3333300000000000 -0.3333300000000000 0.4210000000000000 Ti (6i)
0.3333300000000000 0.0000000000000000 0.4210000000000000 Ti (6i)
-0.3333300000000000 0.0000000000000000 -0.4210000000000000 Ti (6i)
0.0000000000000000 0.3333300000000000 -0.4210000000000000 Ti (6i)
0.0000000000000000 -0.3333300000000000 -0.4210000000000000 Ti (6i)
0.3333300000000000 0.3333300000000000 0.2460000000000000 Ti (6i)
-0.3333300000000000 0.0000000000000000 0.2460000000000000 Ti (6i)
0.0000000000000000 -0.3333300000000000 0.2460000000000000 Ti (6i)
-0.3333300000000000 -0.3333300000000000 -0.2460000000000000 Ti (6i)
0.0000000000000000 0.3333300000000000 -0.2460000000000000 Ti (6i)
0.3333300000000000 0.0000000000000000 -0.2460000000000000 Ti (6i)
```

```

0.00000000000000 0.33333000000000 0.08800000000000 Ti (6l)
-0.33333000000000 -0.33333000000000 0.08800000000000 Ti (6l)
0.33333000000000 0.00000000000000 0.08800000000000 Ti (6l)
-0.33333000000000 0.00000000000000 -0.08800000000000 Ti (6l)
0.33333000000000 0.33333000000000 -0.08800000000000 Ti (6l)
0.00000000000000 -0.33333000000000 -0.08800000000000 Ti (6l)

```

CrCl<sub>3</sub>: A3B\_hP24\_153\_3c\_2b - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'CrCl3'
_chemical_formula_sum 'Cl3 Cr'

_aflow_title 'CrCl3_{3} Structure'
_aflow_proto 'A3B_hP24_153_3c_2b'
_aflow_params 'a,c/a,x_{1},x_{2},x_{3},y_{3},z_{3},x_{4},y_{4},z_{4},x_{5},y_{5},z_{5}'
_aflow_params_values '6.017,2.87518697025,0.1111,0.4444,0.1111,0.2222,0.09357,0.4444,0.8888,0.09357,0.77778,0.55558,0.09357'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP24'

_cell_length_a 6.0170000000
_cell_length_b 6.0170000000
_cell_length_c 17.3000000000
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 32 1 2"
_symmetry_Int_Tables_number 153

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z+2/3
3 -x+y,-x,z+1/3
4 x,x-y,-z
5 -x+y,y,-z+2/3
6 -y,-x,-z+1/3

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cr1 Cr 3 b 0.11110 0.88890 0.16667 1.00000
Cr2 Cr 3 b 0.44440 0.55560 0.16667 1.00000
Cl1 Cl 6 c 0.11110 0.22220 0.09357 1.00000
Cl2 Cl 6 c 0.44440 0.88880 0.09357 1.00000
Cl3 Cl 6 c 0.77778 0.55558 0.09357 1.00000

```

CrCl<sub>3</sub>: A3B\_hP24\_153\_3c\_2b - POSCAR

```

A3B_hP24_153_3c_2b & a,c/a,x1,x2,x3,y3,z3,x4,y4,z4,x5,y5,z5 --params=
6.017,2.87518697025,0.1111,0.4444,0.1111,0.2222,0.09357,0.4444,
0.8888,0.09357,0.77778,0.55558,0.09357 & P3_{2}12 D_{3}^{5} #
153 (b^2c^3) & hP24 & None & CrCl3 & CrCl3 &

1.00000000000000
3.00850000000000 -5.21087485457097 0.00000000000000
3.00850000000000 5.21087485457097 0.00000000000000
0.00000000000000 0.00000000000000 17.30000000000000
Cl Cr
18 6
Direct
0.11110000000000 0.22220000000000 0.09357000000000 Cl (6c)
-0.22220000000000 -0.11110000000000 0.76023666666667 Cl (6c)
0.11110000000000 -0.11110000000000 0.42690333333333 Cl (6c)
-0.22220000000000 -0.11110000000000 0.23976333333333 Cl (6c)
0.11110000000000 0.22220000000000 0.57309666666667 Cl (6c)
0.11110000000000 -0.11110000000000 -0.09357000000000 Cl (6c)
0.44440000000000 0.88880000000000 0.09357000000000 Cl (6c)
-0.88880000000000 -0.44440000000000 0.76023666666667 Cl (6c)
0.44440000000000 -0.44440000000000 0.42690333333333 Cl (6c)
-0.88880000000000 -0.44440000000000 0.23976333333333 Cl (6c)
0.44440000000000 0.88880000000000 0.57309666666667 Cl (6c)
0.44440000000000 -0.44440000000000 -0.09357000000000 Cl (6c)
0.77778000000000 0.55558000000000 0.09357000000000 Cl (6c)
-0.55558000000000 0.22220000000000 0.76023666666667 Cl (6c)
-0.22220000000000 -0.77778000000000 0.42690333333333 Cl (6c)
-0.55558000000000 -0.77778000000000 0.23976333333333 Cl (6c)
-0.22220000000000 0.55558000000000 0.57309666666667 Cl (6c)
0.77778000000000 0.22220000000000 -0.09357000000000 Cl (6c)
0.11110000000000 -0.11110000000000 0.16666666666667 Cr (3b)
0.11110000000000 0.22220000000000 0.83333333333333 Cr (3b)
-0.22220000000000 -0.11110000000000 0.50000000000000 Cr (3b)
0.44440000000000 -0.44440000000000 0.16666666666667 Cr (3b)
0.44440000000000 0.88880000000000 0.83333333333333 Cr (3b)
-0.88880000000000 -0.44440000000000 0.50000000000000 Cr (3b)

```

S-II: A\_hP9\_154\_bc - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'CdI2'
_chemical_formula_sum 'Cd I2'

loop_
_publ_author_name
'R. S. Mitchell'
_journal_name_full_name
;
Zeitschrift f{"u}r Kristallographie - Crystalline Materials
;
_journal_volume 108
_journal_year 1956
_journal_page_first 296
_journal_page_last 315

```

```

_chemical_name_mineral 'S-II'
_chemical_formula_sum 'S'

loop_
_publ_author_name
'O. Degtyareva'
'E. Gregoryanz'
'M. Somayazulu'
'P. Dera'
'H. Mao'
'R. J. Hemley'
_journal_name_full_name
;
Nature Materials
;
_journal_volume 4
_journal_year 2005
_journal_page_first 152
_journal_page_last 155
_publ_section_title
;
Novel chain structures in group VI elements
;

_aflow_title 'S-II Structure'
_aflow_proto 'A_hP9_154_bc'
_aflow_params 'a,c/a,x_{1},x_{2},y_{2},z_{2}'
_aflow_params_values '6.9082,0.616557134999,0.876,0.23,0.534,0.051'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP9'

_symmetry_space_group_name_H-M "P 32 2 1"
_symmetry_Int_Tables_number 154

_cell_length_a 6.90820
_cell_length_b 6.90820
_cell_length_c 4.25930
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z+2/3
3 -x+y,-x,z+1/3
4 x-y,-y,-z+1/3
5 y,x,-z
6 -x,-x+y,-z+2/3

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
S1 S 3 b 0.87600 0.00000 0.16667 1.00000
S2 S 6 c 0.23000 0.53400 0.05100 1.00000

```

S-II: A\_hP9\_154\_bc - POSCAR

```

A_hP9_154_bc & a,c/a,x1,x2,y2,z2 --params=6.9082,0.616557134999,0.876,
0.23,0.534,0.051 & P3_{2}12 D_{3}^{5} #154 (bc) & hP9 & None &
S & S-II & O. Degtyareva et al., Nat. Mater. 4, 152-155 (2005)
1.00000000000000
3.45410000000000 -5.98267669442366 0.00000000000000
3.45410000000000 5.98267669442366 0.00000000000000
0.00000000000000 0.00000000000000 4.25930000000000
S
9
Direct
0.87600000000000 0.00000000000000 0.16666666666667 S (3b)
0.00000000000000 0.87600000000000 0.83333333333333 S (3b)
-0.87600000000000 -0.87600000000000 0.50000000000000 S (3b)
0.23000000000000 0.53400000000000 0.05100000000000 S (6c)
-0.53400000000000 -0.30400000000000 0.71766666666667 S (6c)
0.30400000000000 -0.23000000000000 0.38433333333333 S (6c)
0.53400000000000 0.23000000000000 -0.05100000000000 S (6c)
-0.30400000000000 -0.53400000000000 0.28233333333333 S (6c)
-0.23000000000000 0.30400000000000 0.61566666666667 S (6c)

```

CdI<sub>2</sub> (Polytype 6H<sub>1</sub>): AB2\_hP9\_156\_b2c\_3a2bc - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'CdI2'
_chemical_formula_sum 'Cd I2'

loop_
_publ_author_name
'R. S. Mitchell'
_journal_name_full_name
;
Zeitschrift f{"u}r Kristallographie - Crystalline Materials
;
_journal_volume 108
_journal_year 1956
_journal_page_first 296
_journal_page_last 315

```

```

_publ_Section_title
:
Polytypism of Cadmium Iodide and its Relationship to Screw Dislocations
↪ : I. Cadmium Iodide Polytypes
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'CdI2 (Polytype 6H1) Structure'
_aflow_proto 'AB2hP9156_b2c_3a2bc'
_aflow_params 'a,c/a,z1,z2,z3,z4,z5,z6,z7,z8,z9'
↪ 9)
_aflow_params_values '4.239807232,4.83608490569,0.0,0.66667,0.33333,0.75
↪ ,0.16667,0.5,0.08333,0.41667,0.83333'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP9'

_cell_length_a 4.2398072320
_cell_length_b 4.2398072320
_cell_length_c 20.5040677577
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 3 m 1"
_symmetry_Int_Tables_number 156

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 -x+y,y,z
5 -y,-x,z
6 x,x-y,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
I1 I 1 a 0.00000 0.00000 0.00000 1.00000
I2 I 1 a 0.00000 0.00000 0.66667 1.00000
I3 I 1 a 0.00000 0.00000 0.33333 1.00000
Cd1 Cd 1 b 0.33333 0.66667 0.75000 1.00000
I4 I 1 b 0.33333 0.66667 0.16667 1.00000
I5 I 1 b 0.33333 0.66667 0.50000 1.00000
Cd2 Cd 1 c 0.66667 0.33333 0.08333 1.00000
Cd3 Cd 1 c 0.66667 0.33333 0.41667 1.00000
I6 I 1 c 0.66667 0.33333 0.83333 1.00000

```

CdI<sub>2</sub> (Polytype 6H<sub>1</sub>): AB<sub>2</sub>hP<sub>9</sub>156\_b2c\_3a2bc - POSCAR

```

AB2_hP9_156_b2c_3a2bc & a,c/a,z1,z2,z3,z4,z5,z6,z7,z8,z9 --params=
↪ 4.239807232,4.83608490569,0.0,0.66667,0.33333,0.75,0.16667,0.5,
↪ 0.08333,0.41667,0.83333 & P3m1 C3v[1] #156 (a4b3c6) &
↪ hP9 & None & CdI2 & & R. S. Mitchell, 'Zeitschrift f"ur
↪ Kristallographie - Crystalline Materials 108, 296-315 (1956)
1.0000000000000000
2.11990361600000 -3.67178077006098 0.0000000000000000
2.11990361600000 3.67178077006098 0.0000000000000000
0.00000000000000 0.00000000000000 20.50406775770000
Cd I
3 6
Direct
0.33333333333333 0.66666666666667 0.75000000000000 Cd (1b)
0.66666666666667 0.33333333333333 0.08333000000000 Cd (1c)
0.66666666666667 0.33333333333333 0.41667000000000 Cd (1c)
0.00000000000000 0.00000000000000 0.00000000000000 I (1a)
0.00000000000000 0.00000000000000 0.66667000000000 I (1a)
0.00000000000000 0.00000000000000 0.33333000000000 I (1a)
0.33333333333333 0.66666666666667 0.16667000000000 I (1b)
0.33333333333333 0.66666666666667 0.50000000000000 I (1b)
0.66666666666667 0.33333333333333 0.83333000000000 I (1c)

```

CuI: AB<sub>2</sub>hP<sub>12</sub>156\_2ab3c\_2ab3c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'CuI'
_chemical_formula_sum 'Cu I'

loop_
_publ_author_name
'R. N. Kurdyumova'
'R. V. Baranova'
_journal_name_full_name
:
Soviet Physics Crystallography
;
_journal_volume 6
_journal_year 1961
_journal_page_first 318
_journal_page_last 321
_publ_Section_title
:
An electron diffraction study of thin films of cuprous iodide

```

```

;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'CuI Structure'
_aflow_proto 'AB2hP12156_2ab3c_2ab3c'
_aflow_params 'a,c/a,z1,z2,z3,z4,z5,z6,z7,z8,z9,z10,z11,z12'
↪ 9),z10,z11,z12'
_aflow_params_values '4.2499813346,4.90823529409,0.375,0.70833,0.5,
↪ 0.83333,0.04167,0.16667,0.45833,0.79167,0.125,0.33333,0.66667,
↪ 0.0'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP12'

_cell_length_a 4.2499813346
_cell_length_b 4.2499813346
_cell_length_c 20.8599083857
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 3 m 1"
_symmetry_Int_Tables_number 156

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 -x+y,y,z
5 -y,-x,z
6 x,x-y,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cu1 Cu 1 a 0.00000 0.00000 0.37500 1.00000
Cu2 Cu 1 a 0.00000 0.00000 0.70833 1.00000
I1 I 1 a 0.00000 0.00000 0.50000 1.00000
I2 I 1 a 0.00000 0.00000 0.83333 1.00000
Cu3 Cu 1 b 0.33333 0.66667 0.04167 1.00000
I3 I 1 b 0.33333 0.66667 0.16667 1.00000
Cu4 Cu 1 c 0.66667 0.33333 0.45833 1.00000
Cu5 Cu 1 c 0.66667 0.33333 0.79167 1.00000
Cu6 Cu 1 c 0.66667 0.33333 0.12500 1.00000
I4 I 1 c 0.66667 0.33333 0.33333 1.00000
I5 I 1 c 0.66667 0.33333 0.66667 1.00000
I6 I 1 c 0.66667 0.33333 0.00000 1.00000

```

CuI: AB<sub>2</sub>hP<sub>12</sub>156\_2ab3c\_2ab3c - POSCAR

```

AB_hP12_156_2ab3c_2ab3c & a,c/a,z1,z2,z3,z4,z5,z6,z7,z8,z9,z10,z11,z12
↪ --params=4.2499813346,4.90823529409,0.375,0.70833,0.5,0.83333,
↪ 0.04167,0.16667,0.45833,0.79167,0.125,0.33333,0.66667,0.0 &
↪ P3m1 C3v[1] #156 (a4b4c6) & hP12 & None & CuI & & R. N.
↪ Kurdyumova and R. V. Baranova, Sov. Phys. Crystallogr. 6,
↪ 318-321 (1961)
1.0000000000000000
2.12499066730000 -3.68059180137329 0.0000000000000000
2.12499066730000 3.68059180137329 0.0000000000000000
0.00000000000000 0.00000000000000 20.85990838570000
Cu I
6 6
Direct
0.00000000000000 0.00000000000000 0.37500000000000 Cu (1a)
0.00000000000000 0.00000000000000 0.70833000000000 Cu (1a)
0.33333333333333 0.66666666666667 0.04167000000000 Cu (1b)
0.66666666666667 0.33333333333333 0.45833000000000 Cu (1c)
0.66666666666667 0.33333333333333 0.79167000000000 Cu (1c)
0.66666666666667 0.33333333333333 0.12500000000000 Cu (1c)
0.00000000000000 0.00000000000000 0.50000000000000 I (1a)
0.00000000000000 0.00000000000000 0.83333000000000 I (1a)
0.33333333333333 0.66666666666667 0.16667000000000 I (1b)
0.66666666666667 0.33333333333333 0.33333000000000 I (1c)
0.66666666666667 0.33333333333333 0.66667000000000 I (1c)
0.66666666666667 0.33333333333333 0.00000000000000 I (1c)

```

β-CuI: AB<sub>2</sub>hP<sub>4</sub>156\_ac-ac - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'beta-CuI'
_chemical_formula_sum 'Cu I'

loop_
_publ_author_name
'T. Sakuma'
_journal_name_full_name
:
Journal of the Physical Society of Japan
;
_journal_volume 57
_journal_year 1988
_journal_page_first 565
_journal_page_last 569

```



```

_publ_Section_title
:
Crystal structure of  $\beta$ -CuI
:
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title '$\beta$-CuI Structure'
_aflow_proto 'AB_hP4_156_ac'
_aflow_params 'a,c/a,z_{1},z_{2},z_{3},z_{4}'
_aflow_params_values '4.2794836776,1.67515774714,0.104,0.5,0.364,0.0'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP4'

_cell_length_a 4.2794836776
_cell_length_b 4.2794836776
_cell_length_c 7.1688102363
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 3 m 1"
_symmetry_Int_Tables_number 156

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 -x+y,y,z
5 -y,-x,z
6 x,x-y,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cu1 Cu 1 a 0.00000 0.00000 0.10400 1.00000
I1 I 1 a 0.00000 0.00000 0.50000 1.00000
Cu2 Cu 1 c 0.66667 0.33333 0.36400 1.00000
I2 I 1 c 0.66667 0.33333 0.00000 1.00000

```

$\beta$ -CuI: AB\_hP4\_156\_ac - POSCAR

```

AB_hP4_156_ac & a,c/a,z1,z2,z3,z4 --params=4.2794836776,1.67515774714
↪ 0.104,0.5,0.364,0.0 & P3m1 C_{3v}^{1} #156 (a^2c^2) & hP4 &
↪ None & CuI & beta & T. Sakuma, J. Phys. Soc. Jpn. 57, 565-569 (
↪ 1988)
1.0000000000000000
2.13974183880000 -3.70614157988245 0.0000000000000000
2.13974183880000 3.70614157988245 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.16881023630000
Cu I
2 2
Direct
0.0000000000000000 0.0000000000000000 0.1040000000000000 Cu (1a)
0.666666666666667 0.333333333333333 0.3640000000000000 Cu (1c)
0.0000000000000000 0.0000000000000000 0.5000000000000000 I (1a)
0.666666666666667 0.333333333333333 0.0000000000000000 I (1c)

```

Ag<sub>5</sub>Pb<sub>2</sub>O<sub>6</sub>: A5B6C2\_hP13\_157\_2ac\_2c\_b - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ag5Pb2O6'
_chemical_formula_sum 'Ag5 O6 Pb2'

_aflow_title 'Ag$_{5}$Pb$_{2}$O$_{6}$ Structure'
_aflow_proto 'A5B6C2_hP13_157_2ac_2c_b'
_aflow_params 'a,c/a,z_{1},z_{2},z_{3},x_{4},z_{4},x_{5},z_{5},x_{6},z_{6}'
↪ 6)
_aflow_params_values '5.939,1.08233709379,0.264,0.736,0.022,0.5,0.522,
↪ 0.603,0.215,0.397,0.829'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP13'

_cell_length_a 5.9390000000
_cell_length_b 5.9390000000
_cell_length_c 6.4280000000
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 3 1 m"
_symmetry_Int_Tables_number 157

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 -x,-x+y,z
5 x-y,-y,z
6 y,x,z

```

$\beta$ -RuCl<sub>3</sub>: A3B\_hP8\_158\_d\_a - POSCAR

```

A3B_hP8_158_d_a & a,c/a,z1,x2,y2,z2 --params=6.12,0.924509803922,0.0,
↪ 0.318,0.027,0.237 & P3c1 C_{3v}^{3} #158 (ad) & hP8 & None &
↪ RuCl3 & beta &
1.0000000000000000
3.0600000000000000 -5.30007547116076 0.0000000000000000
3.0600000000000000 5.30007547116076 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.6580000000000000
Cl Ru
6 2
Direct
0.3180000000000000 0.0270000000000000 0.2370000000000000 Cl (6d)

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1 Ag 1 a 0.00000 0.00000 0.26400 1.00000
Ag2 Ag 1 a 0.00000 0.00000 0.73600 1.00000
Pb1 Pb 2 b 0.33333 0.66667 0.02200 1.00000
Ag3 Ag 3 c 0.50000 0.00000 0.52200 1.00000
O1 O 3 c 0.60300 0.00000 0.21500 1.00000
O2 O 3 c 0.39700 0.00000 0.82900 1.00000

```

Ag<sub>5</sub>Pb<sub>2</sub>O<sub>6</sub>: ASB6C2\_hP13\_157\_2ac\_2c\_b - POSCAR

```

A5B6C2_hP13_157_2ac_2c_b & a,c/a,z1,z2,z3,x4,z4,x5,z5,x6,z6 --params=
↪ 5.939,1.08233709379,0.264,0.736,0.022,0.5,0.522,0.603,0.215,
↪ 0.397,0.829 & P3m1 C_{3v}^{1} #157 (a^2bc^3) & hP13 & None &
↪ Ag5Pb2O6 &
1.0000000000000000
2.9695000000000000 -5.14332487307578 0.0000000000000000
2.9695000000000000 5.14332487307578 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.4280000000000000
Ag O Pb
5 6 2
Direct
0.0000000000000000 0.0000000000000000 0.2640000000000000 Ag (1a)
0.0000000000000000 0.0000000000000000 0.7360000000000000 Ag (1a)
0.5000000000000000 0.0000000000000000 0.5220000000000000 Ag (3c)
0.0000000000000000 0.5000000000000000 0.5220000000000000 Ag (3c)
-0.5000000000000000 -0.5000000000000000 0.2150000000000000 O (3c)
0.6030000000000000 0.0000000000000000 0.2150000000000000 O (3c)
0.0000000000000000 0.6030000000000000 0.2150000000000000 O (3c)
-0.6030000000000000 -0.6030000000000000 0.2150000000000000 O (3c)
0.3970000000000000 0.0000000000000000 0.8290000000000000 O (3c)
0.0000000000000000 0.3970000000000000 0.8290000000000000 O (3c)
-0.3970000000000000 -0.3970000000000000 0.8290000000000000 O (3c)
0.333333333333333 0.666666666666667 0.0220000000000000 Pb (2b)
0.666666666666667 0.333333333333333 0.0220000000000000 Pb (2b)

```

$\beta$ -RuCl<sub>3</sub>: A3B\_hP8\_158\_d\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'beta-RuCl3'
_chemical_formula_sum 'Cl3 Ru'

_aflow_title '$\beta$-RuCl3 Structure'
_aflow_proto 'A3B_hP8_158_d_a'
_aflow_params 'a,c/a,z_{1},x_{2},y_{2},z_{2}'
_aflow_params_values '6.12,0.924509803922,0.0,0.318,0.027,0.237'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP8'

_cell_length_a 6.1200000000
_cell_length_b 6.1200000000
_cell_length_c 5.6580000000
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 3 c 1"
_symmetry_Int_Tables_number 158

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 -x+y,y,z+1/2
5 -y,-x,z+1/2
6 x,x-y,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ru1 Ru 2 a 0.00000 0.00000 0.00000 1.00000
Cl1 Cl 6 d 0.31800 0.02700 0.23700 1.00000

```

$\beta$ -RuCl<sub>3</sub>: A3B\_hP8\_158\_d\_a - POSCAR

```

A3B_hP8_158_d_a & a,c/a,z1,x2,y2,z2 --params=6.12,0.924509803922,0.0,
↪ 0.318,0.027,0.237 & P3c1 C_{3v}^{3} #158 (ad) & hP8 & None &
↪ RuCl3 & beta &
1.0000000000000000
3.0600000000000000 -5.30007547116076 0.0000000000000000
3.0600000000000000 5.30007547116076 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.6580000000000000
Cl Ru
6 2
Direct
0.3180000000000000 0.0270000000000000 0.2370000000000000 Cl (6d)

```

-0.02700000000000	0.29100000000000	0.23700000000000	Cl	(6d)
-0.29100000000000	-0.31800000000000	0.23700000000000	Cl	(6d)
-0.02700000000000	-0.31800000000000	0.73700000000000	Cl	(6d)
-0.29100000000000	0.02700000000000	0.73700000000000	Cl	(6d)
0.31800000000000	0.29100000000000	0.73700000000000	Cl	(6d)
0.00000000000000	0.00000000000000	0.00000000000000	Ru	(2a)
0.00000000000000	0.00000000000000	0.50000000000000	Ru	(2a)

Bi<sub>2</sub>O<sub>3</sub> (High-pressure): A2B3\_hp20\_159\_bc\_2c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Bi2O3'
_chemical_formula_sum 'Bi2 O3'

loop_
  _publ_author_name
    'T. Locherer'
    'D. L. V. K. Prasad'
    'R. Dinnebier'
    'U. Wedig'
    'M. Jansen'
    'G. Garbarino'
    'T. Hansen'
  _journal_name_full_name
  ;
  Physical Review B
  ;
  _journal_volume 83
  _journal_year 2011
  _journal_page_first 214102
  _journal_page_last 214102
  _publ_section_title
  ;
  High-pressure structural evolution of HP-Bi$_{2}$O$_{3}$
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title 'Bi$_{2}$O$_{3}$ (High-pressure) Structure'
_aflow_proto 'A2B3_hp20_159_bc_2c'
_aflow_params 'a, c/a, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}'
↳ 4), z_{4}'
_aflow_params_values '7.7488577892, 0.813266227893, 0.0, 0.337, 0.154, 0.021,
↳ 0.451, 0.061, 0.287, 0.149, 0.282, 0.083'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP20'

_cell_length_a 7.7488577892
_cell_length_b 7.7488577892
_cell_length_c 6.3018843447
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 3 1 c"
_symmetry_Int_Tables_number 159

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x, y, z
  2 -y, x-y, z
  3 -x+y, -x, z
  4 -x, -x+y, z+1/2
  5 x-y, -y, z+1/2
  6 y, x, z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Bi1 Bi 2 b 0.33333 0.66667 0.00000 1.00000
  Bi2 Bi 6 c 0.33700 0.15400 0.02100 1.00000
  O1 O 6 c 0.45100 0.06100 0.28700 1.00000
  O2 O 6 c 0.14900 0.28200 0.08300 1.00000
```

Bi<sub>2</sub>O<sub>3</sub> (High-pressure): A2B3\_hp20\_159\_bc\_2c - POSCAR

```
A2B3_hp20_159_bc_2c & a, c/a, z1, z2, z3, z4, z5, z6 --params=
↳ 7.7488577892, 0.813266227893, 0.0, 0.337, 0.154, 0.021, 0.451, 0.061,
↳ 0.287, 0.149, 0.282, 0.083 & P31c C_{3v}^{4} #159 (bc^3) & hP20 &
↳ None & Bi2O3 & T. Locherer et al., Phys. Rev. B 83, 214102 (
↳ 2011)
1.00000000000000
3.87442889460000 -6.71070769576012 0.00000000000000
3.87442889460000 6.71070769576012 0.00000000000000
0.00000000000000 0.00000000000000 6.30188434470000
Bi O
8 12
Direct
0.33333333333333 0.66666666666667 0.00000000000000 Bi (2b)
0.66666666666667 0.33333333333333 0.50000000000000 Bi (2b)
0.33700000000000 0.15400000000000 0.02100000000000 Bi (6c)
-0.15400000000000 0.18300000000000 0.02100000000000 Bi (6c)
-0.18300000000000 -0.33700000000000 0.02100000000000 Bi (6c)
0.15400000000000 0.33700000000000 0.52100000000000 Bi (6c)
```

0.18300000000000	-0.15400000000000	0.52100000000000	Bi	(6c)
-0.33700000000000	-0.18300000000000	0.52100000000000	Bi	(6c)
0.45100000000000	0.06100000000000	0.28700000000000	O	(6c)
-0.06100000000000	0.39000000000000	0.28700000000000	O	(6c)
-0.39000000000000	-0.45100000000000	0.28700000000000	O	(6c)
0.06100000000000	0.45100000000000	0.78700000000000	O	(6c)
0.39000000000000	-0.06100000000000	0.78700000000000	O	(6c)
-0.45100000000000	-0.39000000000000	0.78700000000000	O	(6c)
0.14900000000000	0.28200000000000	0.08300000000000	O	(6c)
-0.28200000000000	-0.13300000000000	0.08300000000000	O	(6c)
0.13300000000000	-0.14900000000000	0.08300000000000	O	(6c)
0.28200000000000	0.14900000000000	0.78700000000000	O	(6c)
-0.13300000000000	-0.28200000000000	0.58300000000000	O	(6c)
-0.14900000000000	0.13300000000000	0.58300000000000	O	(6c)

Nierite (α-Si<sub>3</sub>N<sub>4</sub>): A4B3\_hp28\_159\_ab2c\_2c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'alpha-Si3N4'
_chemical_formula_sum 'N4 Si3'

loop_
  _publ_author_name
    'D. Hardie'
    'K. H. Jack'
  _journal_name_full_name
  ;
  Nature
  ;
  _journal_volume 180
  _journal_year 1957
  _journal_page_first 332
  _journal_page_last 333
  _publ_section_title
  ;
  Crystal structures of silicon nitride
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title 'Nierite (S\alpha-Si$_{3}$N$_{4}$) Structure'
_aflow_proto 'A4B3_hp28_159_ab2c_2c'
_aflow_params 'a, c/a, z_{1}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}'
↳ 5), y_{5}, z_{5}, x_{6}, y_{6}, z_{6}'
_aflow_params_values '7.7479899913, 0.724961280333, 0.0, 0.3649, 0.0424,
↳ 0.3891, 0.0408, 0.3169, 0.3198, 0.2712, 0.0821, 0.5089, 0.3172, 0.1712,
↳ 0.2563, 0.0274'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP28'

_cell_length_a 7.7479899913
_cell_length_b 7.7479899913
_cell_length_c 5.6169927441
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 3 1 c"
_symmetry_Int_Tables_number 159

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x, y, z
  2 -y, x-y, z
  3 -x+y, -x, z
  4 -x, -x+y, z+1/2
  5 x-y, -y, z+1/2
  6 y, x, z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  N1 N 2 a 0.00000 0.00000 1.00000
  N2 N 2 b 0.33333 0.66667 0.36490 1.00000
  N3 N 6 c 0.04240 0.38910 0.04080 1.00000
  N4 N 6 c 0.31690 0.31980 0.27120 1.00000
  Si1 Si 6 c 0.08210 0.50890 0.31720 1.00000
  Si2 Si 6 c 0.17120 0.25630 0.02740 1.00000
```

Nierite (α-Si<sub>3</sub>N<sub>4</sub>): A4B3\_hp28\_159\_ab2c\_2c - POSCAR

```
A4B3_hp28_159_ab2c_2c & a, c/a, z1, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6
--params=7.7479899913, 0.724961280333, 0.0, 0.3649, 0.0424, 0.3891,
↳ 0.0408, 0.3169, 0.3198, 0.2712, 0.0821, 0.5089, 0.3172, 0.1712, 0.2563,
↳ 0.0274 & P31c C_{3v}^{4} #159 (abc^4) & hP28 & None & Si3N4 &
↳ alpha & D. Hardie and K. H. Jack, Nature 180, 332-333 (1957)
1.00000000000000
3.87399499565000 -6.70995616073337 0.00000000000000
3.87399499565000 6.70995616073337 0.00000000000000
0.00000000000000 0.00000000000000 5.61699274410000
N Si
16 12
Direct
0.00000000000000 0.00000000000000 0.00000000000000 N (2a)
```

0.0000000000000	0.0000000000000	0.5000000000000	N	(2a)
0.3333333333333	0.6666666666667	0.3649000000000	N	(2b)
0.6666666666667	0.3333333333333	0.8649000000000	N	(2b)
0.0424000000000	0.3891000000000	0.0408000000000	N	(6c)
-0.3891000000000	-0.3467000000000	0.0408000000000	N	(6c)
0.3467000000000	-0.0424000000000	0.0408000000000	N	(6c)
0.3891000000000	0.0424000000000	0.5408000000000	N	(6c)
-0.3467000000000	-0.3891000000000	0.5408000000000	N	(6c)
-0.0424000000000	0.3467000000000	0.5408000000000	N	(6c)
0.3169000000000	0.3198000000000	0.2712000000000	N	(6c)
-0.3198000000000	-0.0029000000000	0.2712000000000	N	(6c)
0.0029000000000	-0.3169000000000	0.2712000000000	N	(6c)
0.3198000000000	0.3169000000000	0.7712000000000	N	(6c)
-0.0029000000000	-0.3198000000000	0.7712000000000	N	(6c)
-0.3169000000000	0.0029000000000	0.7712000000000	N	(6c)
0.0821000000000	0.5089000000000	0.3172000000000	Si	(6c)
-0.5089000000000	-0.4268000000000	0.3172000000000	Si	(6c)
0.4268000000000	-0.0821000000000	0.3172000000000	Si	(6c)
0.5089000000000	0.0821000000000	0.8172000000000	Si	(6c)
-0.4268000000000	-0.5089000000000	0.8172000000000	Si	(6c)
-0.0821000000000	0.4268000000000	0.8172000000000	Si	(6c)
0.1712000000000	0.2563000000000	0.0274000000000	Si	(6c)
-0.2563000000000	-0.0851000000000	0.0274000000000	Si	(6c)
0.0851000000000	-0.1712000000000	0.0274000000000	Si	(6c)
0.2563000000000	0.1712000000000	0.5274000000000	Si	(6c)
-0.0851000000000	-0.2563000000000	0.5274000000000	Si	(6c)
-0.1712000000000	0.0851000000000	0.5274000000000	Si	(6c)

YbBaCo<sub>4</sub>O<sub>7</sub>: AB4C7D\_hp26\_159\_b\_ac\_a2c\_b - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'YbBaCo4O7'
_chemical_formula_sum 'Ba Co4 O7 Y'

loop_
_publ_author_name
'A. Huq'
'J. F. Mitchell'
'H. Zheng'
'L. C. Chapon'
'P. G. Radaelli'
'K. S. Knight'
'P. W. Stephens'
_journal_name_full_name
:
Journal of Solid State Chemistry
:
_journal_volume 179
_journal_year 2006
_journal_page_first 1136
_journal_page_last 1145
_publ_section_title
:
Structural and magnetic properties of the Kagom{\e} antiferromagnet
↪ YbBaCo_{4}SO_{7}S

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'YbBaCo_{4}SO_{7}S Structure'
_aflow_proto 'AB4C7D_hp26_159_b_ac_a2c_b'
_aflow_params 'a,c/a,z_{1},z_{2},z_{3},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},y_{7},z_{7}'
↪ 6},z_{6},x_{7},y_{7},z_{7}'
_aflow_params_values '6.2653109789,1.6324735851,0.0,0.3057,0.0613,0.4379
↪ ,0.3425,0.1575,0.2472,0.0015,0.5149,0.3102,0.3347,0.1157,0.0618
↪ ,
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP26'

_cell_length_a 6.2653109789
_cell_length_b 6.2653109789
_cell_length_c 10.2279546755
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 3 1 c"
_symmetry_Int_Tables_number 159

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 -x,-x+y,z+1/2
5 x-y,-y,z+1/2
6 y,x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Co1 Co 2 a 0.00000 0.00000 0.00000 1.00000
O1 O 2 a 0.00000 0.00000 0.30570 1.00000
Ba1 Ba 2 b 0.33333 0.66667 0.06130 1.00000
```

Y1	Y	2	b	0.33333	0.66667	0.43790	1.00000
Co2	Co	6	c	0.34250	0.15750	0.24720	1.00000
O2	O	6	c	0.00150	0.51490	0.31020	1.00000
O3	O	6	c	0.33470	0.11570	0.06180	1.00000

YbBaCo<sub>4</sub>O<sub>7</sub>: AB4C7D\_hp26\_159\_b\_ac\_a2c\_b - POSCAR

```
AB4C7D_hp26_159_b_ac_a2c_b & a,c/a,z1,z2,z3,z4,x5,y5,z5,x6,y6,z6,x7,y7,
↪ z7 --params=6.2653109789,1.6324735851,0.0,0.3057,0.0613,0.4379,
↪ 0.3425,0.1575,0.2472,0.0015,0.5149,0.3102,0.3347,0.1157,0.0618
↪ & P31c_C_{3v}^{4} #159 (a^2b^2c^3) & hP26 & None & YbBaCo4O7 &
↪ & A. Huq et al., J. Solid State Chem. 179, 1136-1145 (2006)

1.0000000000000
3.13265548945000 -5.42591847033695 0.00000000000000
3.13265548945000 5.42591847033695 0.00000000000000
0.00000000000000 0.00000000000000 10.22795467550000

Ba Co O Y
2 8 14 2

Direct
0.3333333333333 0.6666666666667 0.0613000000000 Ba (2b)
0.6666666666667 0.3333333333333 0.5613000000000 Ba (2b)
0.0000000000000 0.0000000000000 0.0000000000000 Co (2a)
0.0000000000000 0.0000000000000 0.5000000000000 Co (2a)
0.3425000000000 0.1575000000000 0.2472000000000 Co (6c)
-0.1575000000000 0.1850000000000 0.2472000000000 Co (6c)
-0.1850000000000 -0.3425000000000 0.2472000000000 Co (6c)
0.1575000000000 0.3425000000000 0.7472000000000 Co (6c)
0.1850000000000 -0.1575000000000 0.7472000000000 Co (6c)
-0.3425000000000 -0.1850000000000 0.7472000000000 Co (6c)
0.0000000000000 0.0000000000000 0.3057000000000 O (2a)
0.0000000000000 0.0000000000000 0.8057000000000 O (2a)
0.0015000000000 0.5149000000000 0.3102000000000 O (6c)
-0.5149000000000 -0.5134000000000 0.3102000000000 O (6c)
0.5134000000000 -0.0015000000000 0.3102000000000 O (6c)
0.5149000000000 0.0015000000000 0.8102000000000 O (6c)
-0.5134000000000 -0.5149000000000 0.8102000000000 O (6c)
-0.0015000000000 0.5134000000000 0.8102000000000 O (6c)
0.3347000000000 0.1157000000000 0.0618000000000 O (6c)
-0.1157000000000 0.2190000000000 0.0618000000000 O (6c)
-0.2190000000000 -0.3347000000000 0.0618000000000 O (6c)
0.1157000000000 0.3347000000000 0.5618000000000 O (6c)
0.2190000000000 -0.1157000000000 0.5618000000000 O (6c)
-0.3347000000000 -0.2190000000000 0.5618000000000 O (6c)
0.3333333333333 0.6666666666667 0.4379000000000 Y (2b)
0.6666666666667 0.3333333333333 0.9379000000000 Y (2b)
```

H<sub>3</sub>S (130 GPa): A3B\_hR4\_160\_b\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'H3S'
_chemical_formula_sum 'H3 S'

loop_
_publ_author_name
'D. Duan'
'Y. Liu'
'F. Tian'
'D. Li'
'X. Huang'
'Z. Zhao'
'H. Yu'
'B. Liu'
'W. Tian'
'T. Cui'
_journal_name_full_name
:
Scientific Reports
:
_journal_volume 4
_journal_year 2014
_journal_page_first 6968
_journal_page_last 6968
_publ_section_title
:
Pressure-induced metallization of dense (HS_{2SS})_{2SHS_{2S}} with
↪ high-TS_{cS} superconductivity

_aflow_title 'HS_{3}SS (130-GPa) Structure'
_aflow_proto 'A3B_hR4_160_b_a'
_aflow_params 'a,c/a,x_{1},x_{2},z_{2}'
_aflow_params_values '4.405,0.610442678774,0.0,0.52073,-0.02217'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hR4'

_symmetry_space_group_name_H-M "R 3 m (hexagonal axes)"
_symmetry_Int_Tables_number 160

_cell_length_a 4.40500
_cell_length_b 4.40500
_cell_length_c 2.68900
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 -y,-x,z
```

```

5 x,x-y,z
6 -x+y,y,z
7 x+1/3,y+2/3,z+2/3
8 -y+1/3,x-y+2/3,z+2/3
9 -x+y+1/3,-x+2/3,z+2/3
10 -y+1/3,-x+2/3,z+2/3
11 x+1/3,x-y+2/3,z+2/3
12 -x+y+1/3,y+2/3,z+2/3
13 x+2/3,y+1/3,z+1/3
14 -y+2/3,x-y+1/3,z+1/3
15 -x+y+2/3,-x+1/3,z+1/3
16 -y+2/3,-x+1/3,z+1/3
17 x+2/3,x-y+1/3,z+1/3
18 -x+y+2/3,y+1/3,z+1/3

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
S1 S 3 a 0.00000 0.00000 0.00000 1.00000
H1 H 9 b 0.51430 0.48570 0.00643 1.00000

```

H<sub>3</sub>S (130 GPa): A3B\_hR4\_160\_b\_a - POSCAR

```

A3B_hR4_160_b_a & a,c/a,x1,x2,z2 --params=4.405,0.610442678774,0.0,
↪ 0.52073,-0.02217 & R3m C_{3v}^{15} #160 (ab) & hR4 & None & H3S
↪ & H3S & D. Duan et al., Sci. Rep. 4, 6968(2014)
1.0000000000000000
2.2025000000000000 -1.27161396789015 0.8963333333333333
0.0000000000000000 2.54322793578030 0.8963333333333333
-2.2025000000000000 -1.27161396789015 0.8963333333333333
H S
3 1
Direct
0.5207300000000000 0.5207300000000000 -0.0221700000000000 H (3b)
-0.0221700000000000 0.5207300000000000 0.5207300000000000 H (3b)
0.5207300000000000 -0.0221700000000000 0.5207300000000000 H (3b)
0.0000000000000000 0.0000000000000000 0.0000000000000000 S (1a)

```

AlCr<sub>5</sub> (D8<sub>10</sub>): A8B5\_hR26\_160\_a3bc\_a3b - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Al8 Cr5'

loop_
_publ_author_name
'A. J. Bradley'
'S. S. Lu'
_journal_name_full_name
';
Zeitschrift f{"u}r Kristallografiya
;
_journal_volume 96
_journal_year 1937
_journal_page_first 20
_journal_page_last 37
_publ_section_title
;
The Crystal Structures of Cr_{2}Al and Cr_{5}Al_{8}
;

# Found in Crystal Data, 2014 Found in Crystal Data, {
↪ Crystallography-online.com},

_aflow_title 'Al_{8}Cr_{5} (SD8_{10}) Structure'
_aflow_proto 'A8B5_hR26_160_a3bc_a3b'
_aflow_params 'a,c/a,x_{1},x_{2},x_{3},z_{3},x_{4},z_{4},x_{5},z_{5},x_{6},z_{6},x_{7},z_{7},x_{8},z_{8},x_{9},z_{9}'
↪ 6,z_{6},x_{7},z_{7},x_{8},z_{8},x_{9},z_{9}'
_aflow_params_values '12.71838,0.624030733474,0.672,0.194,0.654,0.01201,
↪ 0.349,0.58199,0.722,0.35601,1.003,-0.20599,0.998,-0.66,0.355,
↪ 1.00601,1.033,-0.339,0.28799'
_aflow_Strukturbericht 'SD8_{10}'
_aflow_Pearson 'hR26'

_symmetry_space_group_name_H-M 'R 3 m (hexagonal axes)'
_symmetry_Int_Tables_number 160

_cell_length_a 12.71838
_cell_length_b 12.71838
_cell_length_c 7.93666
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 -y,-x,z
5 x,x-y,z
6 -x+y,y,z
7 x+1/3,y+2/3,z+2/3
8 -y+1/3,x-y+2/3,z+2/3
9 -x+y+1/3,-x+2/3,z+2/3

```

```

10 -y+1/3,-x+2/3,z+2/3
11 x+1/3,x-y+2/3,z+2/3
12 -x+y+1/3,y+2/3,z+2/3
13 x+2/3,y+1/3,z+1/3
14 -y+2/3,x-y+1/3,z+1/3
15 -x+y+2/3,-x+1/3,z+1/3
16 -y+2/3,-x+1/3,z+1/3
17 x+2/3,x-y+1/3,z+1/3
18 -x+y+2/3,y+1/3,z+1/3

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 3 a 0.00000 0.00000 0.67200 1.00000
Cr1 Cr 3 a 0.00000 0.00000 0.19400 1.00000
Al2 Al 9 b 0.54733 0.45267 0.10667 1.00000
Al3 Al 9 b 0.25567 0.74433 0.09333 1.00000
Al4 Al 9 b 0.45533 0.54467 0.26667 1.00000
Cr2 Cr 9 b 0.73633 0.26367 0.26667 1.00000
Cr3 Cr 9 b 0.88600 0.11400 0.11200 1.00000
Cr4 Cr 9 b 0.11633 0.88367 0.23867 1.00000
Al5 Al 18 c 0.70567 0.66633 0.32733 1.00000

```

AlCr<sub>5</sub> (D8<sub>10</sub>): A8B5\_hR26\_160\_a3bc\_a3b - POSCAR

```

A8B5_hR26_160_a3bc_a3b & a,c/a,x1,x2,x3,z3,x4,z4,x5,z5,x6,z6,x7,z7,x8,z8
↪ ,x9,y9,z9 --params=12.71838,0.624030733474,0.672,0.194,0.654,
↪ 0.01201,0.349,0.58199,0.722,0.35601,1.003,-0.20599,0.998,-0.66,
↪ 0.355,1.00601,1.033,-0.339,0.28799 & R3m C_{3v}^{15} #160 (a^2b^2
↪ 6c) & hR26 & SD8_{10} & Al8Cr5 & A. J. Bradley and S. S. Lu
↪ , Z. Kristallogr. 96, 20-37 (1937)
1.0000000000000000
6.3591900000000000 -3.67148005832798 2.6455533333333333
0.0000000000000000 7.34296011665595 2.6455533333333333
-6.3591900000000000 -3.67148005832798 2.6455533333333333
Al Cr
16 10
Direct
0.6720000000000000 0.6720000000000000 0.6720000000000000 Al (1a)
0.6540000000000000 0.6540000000000000 0.0120100000000000 Al (3b)
0.0120100000000000 0.6540000000000000 0.6540000000000000 Al (3b)
0.6540000000000000 0.0120100000000000 0.6540000000000000 Al (3b)
0.3490000000000000 0.3490000000000000 0.5819900000000000 Al (3b)
0.5819900000000000 0.3490000000000000 0.3490000000000000 Al (3b)
0.3490000000000000 0.5819900000000000 0.3490000000000000 Al (3b)
0.7220000000000000 0.7220000000000000 0.3560100000000000 Al (3b)
0.3560100000000000 0.7220000000000000 0.7220000000000000 Al (3b)
0.7220000000000000 0.3560100000000000 0.7220000000000000 Al (3b)
1.0330000000000000 -0.3390000000000000 0.2879900000000000 Al (6c)
0.2879900000000000 1.0330000000000000 -0.3390000000000000 Al (6c)
-0.3390000000000000 0.2879900000000000 1.0330000000000000 Al (6c)
0.2879900000000000 -0.3390000000000000 1.0330000000000000 Al (6c)
-0.3390000000000000 1.0330000000000000 0.2879900000000000 Al (6c)
1.0330000000000000 0.2879900000000000 -0.3390000000000000 Al (6c)
0.1940000000000000 0.1940000000000000 0.1940000000000000 Cr (1a)
1.0030000000000000 1.0030000000000000 -0.2059900000000000 Cr (3b)
-0.2059900000000000 1.0030000000000000 1.0030000000000000 Cr (3b)
1.0030000000000000 -0.2059900000000000 1.0030000000000000 Cr (3b)
0.9980000000000000 0.9980000000000000 -0.6600000000000000 Cr (3b)
-0.6600000000000000 0.9980000000000000 0.9980000000000000 Cr (3b)
0.9980000000000000 -0.6600000000000000 0.9980000000000000 Cr (3b)
0.3550000000000000 0.3550000000000000 1.0060100000000000 Cr (3b)
1.0060100000000000 0.3550000000000000 0.3550000000000000 Cr (3b)
0.3550000000000000 1.0060100000000000 0.3550000000000000 Cr (3b)

```

Carbonyl Sulphide (COS, F0<sub>2</sub>): ABC\_hR3\_160\_a\_a\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Carbonyl Sulphide'
_chemical_formula_sum 'C O S'

loop_
_publ_author_name
'J. S. W. Overall'
'G. S. Pawley'
'B. M. Powell'
_journal_name_full_name
;
Acta Crystallographica Section B: Structural Science
;
_journal_volume 38
_journal_year 1982
_journal_page_first 1121
_journal_page_last 1123
_publ_section_title
;
Powder refinement of carbonyl sulphide
;

_aflow_title 'Carbonyl Sulphide (COS, SF0_{2}) Structure'
_aflow_proto 'ABC_hR3_160_a_a_a'
_aflow_params 'a,c/a,x_{1},x_{2},x_{3}'
_aflow_params_values '6.1703,0.949908432329,0.0,0.79356,0.25763'
_aflow_Strukturbericht 'SF0_{2}'
_aflow_Pearson 'hR3'

```

```

_symmetry_space_group_name_H-M "R 3 m (hexagonal axes)"
_symmetry_Int_Tables_number 160

_cell_length_a 6.17030
_cell_length_b 6.17030
_cell_length_c 5.86122
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 -y, -x, z
5 x, x-y, z
6 -x+y, y, z
7 x+1/3, y+2/3, z+2/3
8 -y+1/3, x-y+2/3, z+2/3
9 -x+y+1/3, -x+2/3, z+2/3
10 -y+1/3, -x+2/3, z+2/3
11 x+1/3, x-y+2/3, z+2/3
12 -x+y+1/3, y+2/3, z+2/3
13 x+2/3, y+1/3, z+1/3
14 -y+2/3, x-y+1/3, z+1/3
15 -x+y+2/3, -x+1/3, z+1/3
16 -y+2/3, -x+1/3, z+1/3
17 x+2/3, x-y+1/3, z+1/3
18 -x+y+2/3, y+1/3, z+1/3

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
C1 C 3 a 0.00000 0.00000 1.00000
O1 O 3 a 0.00000 0.00000 0.79356 1.00000
S1 S 3 a 0.00000 0.00000 0.25763 1.00000

```

Carbonyl Sulphide (COS, F02): ABC\_hr3\_160\_a\_a - POSCAR

```

ABC_hr3_160_a_a_a & a, c/a, x1, x2, x3 --params=6.1703, 0.949908432329, 0.0,
↪ 0.79356, 0.25763 & R3m C_{3v}^{[5]} #160 (a^3) & hR3 & SF0_{2}S &
↪ COS & Carbonyl Sulphide & J. S. W. Overell and G. S. Pawley and
↪ B. M. Powell, Acta Crystallogr. Sect. B Struct. Sci. 38,
↪ 1121-1123 (1982)
1.0000000000000000
3.0851500000000000 -1.78121218299037 1.9537400000000000
0.0000000000000000 3.56242436598075 1.9537400000000000
-3.0851500000000000 -1.78121218299037 1.9537400000000000
C O S
1 1 1
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 C (1a)
0.7935600000000000 0.7935600000000000 0.7935600000000000 O (1a)
0.2576300000000000 0.2576300000000000 0.2576300000000000 S (1a)

```

Moissanite-15R (SiC, B7): AB\_hr10\_160\_5a\_5a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Moissanite-15R'
_chemical_formula_sum 'C Si'

loop_
_publ_author_name
'N. W. Thibault'
_journal_name_full_name
:
American Mineralogist
;
_journal_volume 29
_journal_year 1944
_journal_page_first 327
_journal_page_last 362
_publ_section_title
:
Morphological and Structural Crystallography and Optical Properties of
↪ Silicon Carbide (SiC) Part II: Structural Crystallography and
↪ Optical Properties
;

# Found in Properties of Silicon Carbide, 1995
_aflow_title 'Moissanite-15R (SiC, SB7S) Structure'
_aflow_proto 'AB_hr10_160_5a_5a'
_aflow_params 'a, c/a, x_{1}, x_{2}, x_{3}, x_{4}, x_{5}, x_{6}, x_{7}, x_{8}, x_{9}, x_{10}'
↪ 9, x_{10}'
_aflow_params_values '3.09, 12.2653721683, 0.0, 0.13333, 0.4, 0.6, 0.86667,
↪ 0.05, 0.18333, 0.45, 0.65, -0.08333'
_aflow_Strukturbericht 'SB7S'
_aflow_Pearson 'hR10'

_symmetry_space_group_name_H-M "R 3 m (hexagonal axes)"
_symmetry_Int_Tables_number 160

_cell_length_a 3.09000

```

```

_cell_length_b 3.09000
_cell_length_c 37.90000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 -y, -x, z
5 x, x-y, z
6 -x+y, y, z
7 x+1/3, y+2/3, z+2/3
8 -y+1/3, x-y+2/3, z+2/3
9 -x+y+1/3, -x+2/3, z+2/3
10 -y+1/3, -x+2/3, z+2/3
11 x+1/3, x-y+2/3, z+2/3
12 -x+y+1/3, y+2/3, z+2/3
13 x+2/3, y+1/3, z+1/3
14 -y+2/3, x-y+1/3, z+1/3
15 -x+y+2/3, -x+1/3, z+1/3
16 -y+2/3, -x+1/3, z+1/3
17 x+2/3, x-y+1/3, z+1/3
18 -x+y+2/3, y+1/3, z+1/3

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
C1 C 3 a 0.00000 0.00000 0.00000 1.00000
C2 C 3 a 0.00000 0.00000 0.13333 1.00000
C3 C 3 a 0.00000 0.00000 0.40000 1.00000
C4 C 3 a 0.00000 0.00000 0.60000 1.00000
C5 C 3 a 0.00000 0.00000 0.86667 1.00000
Si1 Si 3 a 0.00000 0.00000 0.05000 1.00000
Si2 Si 3 a 0.00000 0.00000 0.18333 1.00000
Si3 Si 3 a 0.00000 0.00000 0.45000 1.00000
Si4 Si 3 a 0.00000 0.00000 0.65000 1.00000
Si5 Si 3 a 0.00000 0.00000 -0.08333 1.00000

```

Moissanite-15R (SiC, B7): AB\_hr10\_160\_5a\_5a - POSCAR

```

AB_hr10_160_5a_5a & a, c/a, x1, x2, x3, x4, x5, x6, x7, x8, x9, x10 --params=3.09,
↪ 12.2653721683, 0.0, 0.13333, 0.4, 0.6, 0.86667, 0.05, 0.18333, 0.45,
↪ 0.65, -0.08333 & R3m C_{3v}^{[5]} #160 (a^10) & hR10 & SB7S & SiC
↪ & Moissanite-15R & N. W. Thibault, Am. Mineral. 29, 327-362 (
↪ 1944)
1.0000000000000000
1.5450000000000000 -0.89200616589797 12.633333333333330
0.0000000000000000 1.78401233179594 12.633333333333330
-1.5450000000000000 -0.89200616589797 12.633333333333330
C Si
5 5
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 C (1a)
0.1333300000000000 0.1333300000000000 0.1333300000000000 C (1a)
0.4000000000000000 0.4000000000000000 0.4000000000000000 C (1a)
0.6000000000000000 0.6000000000000000 0.6000000000000000 C (1a)
0.8666700000000000 0.8666700000000000 0.8666700000000000 C (1a)
0.0500000000000000 0.0500000000000000 0.0500000000000000 Si (1a)
0.1833300000000000 0.1833300000000000 0.1833300000000000 Si (1a)
0.4500000000000000 0.4500000000000000 0.4500000000000000 Si (1a)
0.6500000000000000 0.6500000000000000 0.6500000000000000 Si (1a)
-0.0833300000000000 -0.0833300000000000 -0.0833300000000000 Si (1a)

```

La2O3 (D52): A2B3\_hp5\_164\_d\_ad - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'La2 O3'

loop_
_publ_author_name
'P. Aldebert'
'J. P. Traverse'
_journal_name_full_name
:
Materials Research Bulletin
;
_journal_volume 14
_journal_year 1979
_journal_page_first 303
_journal_page_last 323
_publ_section_title
:
Etude par diffraction neutronique des structures de haute temperature
↪ de La_{2}SO_{3} et Nd_{2}SO_{3}
;

_aflow_title 'La_{2}SO_{3} (SD5_{2}) Structure'
_aflow_proto 'A2B3_hp5_164_d_ad'
_aflow_params 'a, c/a, z_{2}, z_{3}'
_aflow_params_values '3.9381, 1.55813717275, 0.2467, 0.647'
_aflow_Strukturbericht 'SD5_{2}'

```

```

_aflow_Pearson 'hP5'

_symmetry_space_group_name_H-M "P -3 2/m 1"
_symmetry_Int_Tables_number 164

_cell_length_a 3.93810
_cell_length_b 3.93810
_cell_length_c 6.13610
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 x-y, -y, -z
5 y, x, -z
6 -x, -x+y, -z
7 -x, -y, -z
8 y, -x+y, -z
9 x-y, x, -z
10 -x+y, y, z
11 -y, -x, z
12 x, x-y, z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 1 a 0.00000 0.00000 0.00000 1.00000
La1 La 2 d 0.33333 0.66667 0.24670 1.00000
O2 O 2 d 0.33333 0.66667 0.64700 1.00000

```

La<sub>2</sub>O<sub>3</sub> (D<sub>5</sub><sub>2</sub>): A2B3\_hP5\_164\_d\_ad - POSCAR

```

A2B3_hP5_164_d_ad & a, c/a, z2, z3 --params=3.9381, 1.55813717275, 0.2467,
↳ 0.647 & P-3m1 D_{3d}^{3} #164 (ad^2) & hP5 & SD5_{2} & LaO3 &
↳ & P. Aldebert and J. P. Traverse, Mater. Res. Bull. 14,
↳ 303-323 (1979)
1.0000000000000000
1.9690500000000000 -3.41049464264350 0.0000000000000000
1.9690500000000000 3.41049464264350 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.1361000000000000
La O
2 3
Direct
0.3333333333333333 0.6666666666666667 0.2467000000000000 La (2d)
0.6666666666666667 0.3333333333333333 -0.2467000000000000 La (2d)
0.0000000000000000 0.0000000000000000 0.0000000000000000 O (1a)
0.3333333333333333 0.6666666666666667 0.6470000000000000 O (2d)
0.6666666666666667 0.3333333333333333 -0.6470000000000000 O (2d)

```

$\delta_H^{\text{II}}$ -NW<sub>2</sub>: AB2\_hP9\_164\_bd\_c2d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '$\delta_{H}^{\text{II}}$-NWS_2S'
_chemical_formula_sum 'N W2'

loop_
_publ_author_name
'V. I. Khitrova'
'Z. G. Pinkser'
_journal_name_full_name
;
Soviet Physics Crystallography
;
_journal_volume 6
_journal_year 1962
_journal_page_first 712
_journal_page_last 719
_publ_section_title
;
Chemical Crystallography of Tungsten Nitrides and of Some Other
↳ Interstitial Phases
;

_aflow_title '$\delta_{H}^{\text{II}}$-NWS_2S Structure'
_aflow_proto 'AB2_hP9_164_bd_c2d'
_aflow_params 'a, c/a, z_{2}, z_{3}, z_{4}, z_{5}'
_aflow_params_values '2.89, 7.90657439446, 0.0607, 0.154, 0.27263, 0.39403'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP9'

_symmetry_space_group_name_H-M "P -3 2/m 1"
_symmetry_Int_Tables_number 164

_cell_length_a 2.89000
_cell_length_b 2.89000
_cell_length_c 22.85000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_

```

```

_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 x-y, -y, -z
5 y, x, -z
6 -x, -x+y, -z
7 -x, -y, -z
8 y, -x+y, -z
9 x-y, x, -z
10 -x+y, y, z
11 -y, -x, z
12 x, x-y, z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
N1 N 1 b 0.00000 0.00000 0.50000 1.00000
W1 W 2 c 0.00000 0.00000 0.06070 1.00000
N2 N 2 d 0.33333 0.66667 0.15400 1.00000
W2 W 2 d 0.33333 0.66667 0.27263 1.00000
W3 W 2 d 0.33333 0.66667 0.39403 1.00000

```

$\delta_H^{\text{II}}$ -NW<sub>2</sub>: AB2\_hP9\_164\_bd\_c2d - POSCAR

```

AB2_hP9_164_bd_c2d & a, c/a, z2, z3, z4, z5 --params=2.89, 7.90657439446,
↳ 0.0607, 0.154, 0.27263, 0.39403 & P-3m1 D_{3d}^{3} #164 (bcd^3) &
↳ hP9 & None & NW2 & $\delta_{H}^{\text{II}}$-NWS_2S & V. I. Khitrova
↳ and Z. G. Pinkser, Sov. Phys. Crystallogr. 6, 712-719 (1962)
1.0000000000000000
1.4450000000000000 -2.50281341693703 0.0000000000000000
1.4450000000000000 2.50281341693703 0.0000000000000000
0.0000000000000000 0.0000000000000000 22.8500000000000000
N W
3 6
Direct
0.0000000000000000 0.0000000000000000 0.5000000000000000 N (1b)
0.3333333333333333 0.6666666666666667 0.1540000000000000 N (2d)
0.6666666666666667 0.3333333333333333 -0.1540000000000000 N (2d)
0.0000000000000000 0.0000000000000000 0.0607000000000000 W (2c)
0.0000000000000000 0.0000000000000000 -0.0607000000000000 W (2c)
0.3333333333333333 0.6666666666666667 0.2726300000000000 W (2d)
0.6666666666666667 0.3333333333333333 -0.2726300000000000 W (2d)
0.3333333333333333 0.6666666666666667 0.3940300000000000 W (2d)
0.6666666666666667 0.3333333333333333 -0.3940300000000000 W (2d)

```

CuNiSb<sub>2</sub>: ABC2\_hP4\_164\_a\_b\_d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Cu Ni Sb2'

loop_
_publ_author_name
'R. L. Kift'
_journal_year 2010
_publ_section_title
;
Intermetallic Compounds by Reductive Annealing
;

_aflow_title 'CuNiSb_{2} Structure'
_aflow_proto 'ABC2_hP4_164_a_b_d'
_aflow_params 'a, c/a, z_{3}'
_aflow_params_values '4.0482, 1.26777333136, 0.271'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP4'

_symmetry_space_group_name_H-M "P -3 2/m 1"
_symmetry_Int_Tables_number 164

_cell_length_a 4.04820
_cell_length_b 4.04820
_cell_length_c 5.13220
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 x-y, -y, -z
5 y, x, -z
6 -x, -x+y, -z
7 -x, -y, -z
8 y, -x+y, -z
9 x-y, x, -z
10 -x+y, y, z
11 -y, -x, z
12 x, x-y, z

loop_

```

```

_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cu1 Cu 1 a 0.00000 0.00000 0.00000 1.00000
Ni1 Ni 1 b 0.00000 0.00000 0.50000 1.00000
Sb1 Sb 2 d 0.33333 0.66667 0.27100 1.00000

```

CuNiSb<sub>2</sub>: ABC2\_hP4\_164\_a\_b\_d - POSCAR

```

ABC2_hP4_164_a_b_d & a,c/a,z3 --params=4.0482,1.26777333136,0.271 &
↳ P-3m1 D_{3d}^{4} #164 (abd) & hP4 & None & CuNiSb2 & & R. L.
↳ Kift, (2010)
1.0000000000000000
2.0241000000000000 -3.50584403960016 0.0000000000000000
2.0241000000000000 3.50584403960016 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.1322000000000000
Cu Ni Sb
1 1 2
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 Cu (1a)
0.0000000000000000 0.0000000000000000 0.5000000000000000 Ni (1b)
0.3333333333333333 0.6666666666666667 0.2710000000000000 Sb (2d)
0.6666666666666667 0.3333333333333333 -0.2710000000000000 Sb (2d)

```

Cu<sub>3</sub>P (D0<sub>21</sub>): A3B\_hP24\_165\_bdg\_f - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral ''
_chemical_formula_sum 'Cu3 P'
loop_
_publ_author_name
'B. Steenberg'
_journal_name_full_name
;
Arkiv f{"o"}r Kemi, Mineralogi och Geologi
;
_journal_volume A12
_journal_year 1938
_journal_page_first 1
_journal_page_last 15
_publ_section_title
;
The Crystal Structure of Cu_{3}SAs and Cu_{3}SP
;
# Found in A Handbook of Lattice Spacings and Structures of Metals and
↳ Alloys, 1958
_aflow_title 'Cu_{3}SP (SD0_{21}S) Structure'
_aflow_proto 'A3B_hP24_165_bdg_f'
_aflow_params 'a,c/a,z_{2},x_{3},x_{4},y_{4},z_{4}'
_aflow_params_values '7.07,1.00919377652,0.17,0.38,0.69,0.07,0.08'
_aflow_Strukturbericht 'SD0_{21}S'
_aflow_Pearson 'hP24'
_symmetry_space_group_name_H-M "P -3 2/c 1"
_symmetry_Int_Tables_number 165
_cell_length_a 7.07000
_cell_length_b 7.07000
_cell_length_c 7.13500
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 x-y,-y,-z+1/2
5 y,x,-z+1/2
6 -x,-x+y,-z+1/2
7 -x,-y,-z
8 y,-x+y,-z
9 x-y,x,-z
10 -x+y,y,z+1/2
11 -y,-x,z+1/2
12 x,x-y,z+1/2
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cu1 Cu 2 b 0.00000 0.00000 0.00000 1.00000
Cu2 Cu 4 d 0.33333 0.66667 0.17000 1.00000
P1 P 6 f 0.38000 0.00000 0.25000 1.00000
Cu3 Cu 12 g 0.69000 0.07000 0.08000 1.00000

```

Cu<sub>3</sub>P (D0<sub>21</sub>): A3B\_hP24\_165\_bdg\_f - POSCAR

```

A3B_hP24_165_bdg_f & a,c/a,z2,x3,x4,y4,z4 --params=7.07,1.00919377652,
↳ 0.17,0.38,0.69,0.07,0.08 & P-3c1 D_{3d}^{4} #165 (bdfg) & hP24
↳ & SD0_{21}S & Cu3P & & B. Steenberg, {Ark. Kem. Mineral. Geol.
↳ A12, 1-15 (1938)
1.0000000000000000
3.5350000000000000 -6.12279960475598 0.0000000000000000
3.5350000000000000 6.12279960475598 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.1350000000000000
Cu P
18 6
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 Cu (2b)
0.0000000000000000 0.0000000000000000 0.5000000000000000 Cu (2b)
0.3333333333333333 0.6666666666666667 0.1700000000000000 Cu (4d)
0.6666666666666667 0.3333333333333333 0.3300000000000000 Cu (4d)
0.6666666666666667 0.3333333333333333 -0.1700000000000000 Cu (4d)
0.3333333333333333 0.6666666666666667 0.6700000000000000 Cu (4d)
0.6900000000000000 0.0700000000000000 0.0800000000000000 Cu (12g)
-0.0700000000000000 0.6200000000000000 0.0800000000000000 Cu (12g)
-0.6200000000000000 -0.6900000000000000 0.0800000000000000 Cu (12g)
0.0700000000000000 0.6900000000000000 0.4200000000000000 Cu (12g)
0.6200000000000000 -0.0700000000000000 0.4200000000000000 Cu (12g)
-0.6900000000000000 -0.6200000000000000 0.4200000000000000 Cu (12g)
-0.6900000000000000 -0.0700000000000000 -0.0800000000000000 Cu (12g)
0.0700000000000000 -0.6200000000000000 -0.0800000000000000 Cu (12g)
0.6200000000000000 0.6900000000000000 -0.0800000000000000 Cu (12g)
-0.0700000000000000 -0.6900000000000000 0.5800000000000000 Cu (12g)
-0.6200000000000000 0.0700000000000000 0.5800000000000000 Cu (12g)
0.6900000000000000 0.6200000000000000 0.5800000000000000 Cu (12g)
0.3800000000000000 0.0000000000000000 0.2500000000000000 P (6f)
0.0000000000000000 0.3800000000000000 0.2500000000000000 P (6f)
-0.3800000000000000 -0.3800000000000000 0.2500000000000000 P (6f)
-0.3800000000000000 0.0000000000000000 0.7500000000000000 P (6f)
0.0000000000000000 -0.3800000000000000 0.7500000000000000 P (6f)
0.3800000000000000 0.3800000000000000 0.7500000000000000 P (6f)

```

Al<sub>4</sub>C<sub>3</sub> (D7<sub>1</sub>): A4B3\_hR7\_166\_2c\_ac - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral ''
_chemical_formula_sum 'Al4 C3'
loop_
_publ_author_name
'T. M. Gesing'
'W. Jeitschko'
_journal_name_full_name
;
Zeitschrift f{"u"}r Naturforschung B
;
_journal_volume 50
_journal_year 1995
_journal_page_first 196
_journal_page_last 200
_publ_section_title
;
The Crystal Structure and Chemical Properties of US_{2}SAIS_{3}SCS_{4}S
↳ and Structure Refinement of Al_{4}SCS_{3}S
;
_aflow_title 'Al_{4}SCS_{3}S (SD7_{1}S) Structure'
_aflow_proto 'A4B3_hR7_166_2c_ac'
_aflow_params 'a,c/a,x_{2},x_{3},x_{4}'
_aflow_params_values '3.335,7.48635682159,0.29422,0.12967,0.2168'
_aflow_Strukturbericht 'SD7_{1}S'
_aflow_Pearson 'hR7'
_symmetry_space_group_name_H-M "R -3 2/m (hexagonal axes)"
_symmetry_Int_Tables_number 166
_cell_length_a 3.33500
_cell_length_b 3.33500
_cell_length_c 24.96700
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 y,x,-z
5 -x,-x+y,-z
6 x-y,-y,-z
7 -x,-y,-z
8 y,-x+y,-z
9 x-y,x,-z
10 -y,-x,z
11 x,x-y,z
12 -x+y,y,z
13 x+1/3,y+2/3,z+2/3
14 -y+1/3,x-y+2/3,z+2/3
15 -x+y+1/3,-x+2/3,z+2/3
16 y+1/3,x+2/3,-z+2/3
17 -x+1/3,-x+y+2/3,-z+2/3
18 x-y+1/3,-y+2/3,-z+2/3
19 -x+1/3,-y+2/3,-z+2/3
20 y+1/3,-x+y+2/3,-z+2/3
21 x-y+1/3,x+2/3,-z+2/3
22 -y+1/3,-x+2/3,z+2/3

```

```

23 x+1/3, x-y+2/3, z+2/3
24 -x+y+1/3, y+2/3, z+2/3
25 x+2/3, y+1/3, z+1/3
26 -y+2/3, x-y+1/3, z+1/3
27 -x+y+2/3, -x+1/3, z+1/3
28 y+2/3, x+1/3, -z+1/3
29 -x+2/3, -x+y+1/3, -z+1/3
30 x-y+2/3, -y+1/3, -z+1/3
31 -x+2/3, -y+1/3, -z+1/3
32 y+2/3, -x+y+1/3, -z+1/3
33 x-y+2/3, x+1/3, -z+1/3
34 -y+2/3, -x+1/3, z+1/3
35 x+2/3, x-y+1/3, z+1/3
36 -x+y+2/3, y+1/3, z+1/3

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
C1 C 3 a 0.00000 0.00000 0.00000 1.00000
Al1 Al 6 c 0.00000 0.00000 0.29422 1.00000
Al2 Al 6 c 0.00000 0.00000 0.12967 1.00000
C2 C 6 c 0.00000 0.00000 0.21680 1.00000

```

Al<sub>4</sub>C<sub>3</sub> (D7<sub>1</sub>): A4B3\_hR7\_166\_2c\_ac - POSCAR

```

A4B3_hR7_166_2c_ac & a, c/a, x2, x3, x4 --params=3.335, 7.48635682159, 0.29422
↪ 0.12967, 0.2168 & R-3m D_{3d}^{5} #166 (ac^3) & hR7 & SD7_{1}$
↪ & Al4C3 & T. M. Gesing and W. Jeitschko, Z. Naturforsch. B
↪ 50, 196-200 (1995)
1.0000000000000000
1.6675000000000000 -0.96273157387370 8.322333333333333
0.0000000000000000 1.92546314774740 8.322333333333333
-1.6675000000000000 -0.96273157387370 8.322333333333333
Al C
4 3
Direct
0.2942200000000000 0.2942200000000000 0.2942200000000000 Al (2c)
-0.2942200000000000 -0.2942200000000000 -0.2942200000000000 Al (2c)
0.1296700000000000 0.1296700000000000 0.1296700000000000 Al (2c)
-0.1296700000000000 -0.1296700000000000 -0.1296700000000000 Al (2c)
0.0000000000000000 0.0000000000000000 0.0000000000000000 C (1a)
0.2168000000000000 0.2168000000000000 0.2168000000000000 C (2c)
-0.2168000000000000 -0.2168000000000000 -0.2168000000000000 C (2c)

```

SmSI: ABC\_hR6\_166\_c\_c\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'SmSI'
_chemical_formula_sum 'I S Sm'
loop_
_publ_author_name
'H. P. Beck'
'C. Strobel'
_journal_name_full_name
;
Zeitschrift fur Anorganische und Allgemeine Chemie
;
_journal_volume 535
_journal_year 1986
_journal_page_first 222
_journal_page_last 239
_publ_section_title
;
Zur Hochdruckpolymorphie der Seltenerdsulfidiodide LnSI
;
# Found in Crystal structure of $\beta$-SmSxSx ($Sx = Zr, Hf; $Sx = Cl,
↪ Br), 1998
_aflow_title 'SmSI Structure'
_aflow_proto 'ABC_hR6_166_c_c_c'
_aflow_params 'a, c/a, x_{1}, x_{2}, x_{3}'
_aflow_params_values '3.8548, 7.95397945419, 0.1159, 0.3017, 0.3815'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hR6'
_symmetry_space_group_name_H-M "R -3 2/m:H"
_symmetry_Int_Tables_number 166
_cell_length_a 3.85480
_cell_length_b 3.85480
_cell_length_c 30.66100
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 y, x, -z
5 -x, -x+y, -z
6 x-y, -y, -z

```

```

7 -x, -y, -z
8 y, -x+y, -z
9 x-y, x, -z
10 -y, -x, z
11 x, x-y, z
12 -x+y, y, z
13 x+1/3, y+2/3, z+2/3
14 -y+1/3, x-y+2/3, z+2/3
15 -x+y+1/3, -x+2/3, z+2/3
16 y+1/3, x+2/3, -z+2/3
17 -x+1/3, -x+y+2/3, -z+2/3
18 x-y+1/3, -y+2/3, -z+2/3
19 -x+1/3, -y+2/3, -z+2/3
20 y+1/3, -x+y+2/3, -z+2/3
21 x-y+1/3, x+2/3, -z+2/3
22 -y+1/3, -x+2/3, z+2/3
23 x+1/3, x-y+2/3, z+2/3
24 -x+y+1/3, y+2/3, z+2/3
25 x+2/3, y+1/3, z+1/3
26 -y+2/3, x-y+1/3, z+1/3
27 -x+y+2/3, -x+1/3, z+1/3
28 y+2/3, x+1/3, -z+1/3
29 -x+2/3, -x+y+1/3, -z+1/3
30 x-y+2/3, -y+1/3, -z+1/3
31 -x+2/3, -y+1/3, -z+1/3
32 y+2/3, -x+y+1/3, -z+1/3
33 x-y+2/3, x+1/3, -z+1/3
34 -y+2/3, -x+1/3, z+1/3
35 x+2/3, x-y+1/3, z+1/3
36 -x+y+2/3, y+1/3, z+1/3

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
I1 I 6 c 0.00000 0.00000 0.11590 1.00000
S1 S 6 c 0.00000 0.00000 0.30170 1.00000
Sm1 Sm 6 c 0.00000 0.00000 0.38150 1.00000

```

SmSI: ABC\_hR6\_166\_c\_c\_c - POSCAR

```

ABC_hR6_166_c_c_c & a, c/a, x1, x2, x3 --params=3.8548, 7.95397945419, 0.1159,
↪ 0.3017, 0.3815 & R-3m D_{3d}^{5} #166 (c^3) & hR6 & None & SmSI
↪ & SmSI & H. P. Beck and C. Strobel, Z. Anorg. Allg. Chem. 535,
↪ 222-239 (1986)
1.0000000000000000
1.9274000000000000 -1.11278490883608 10.220333333333330
0.0000000000000000 2.22556981767217 10.220333333333330
-1.9274000000000000 -1.11278490883608 10.220333333333330
I S Sm
2 2 2
Direct
0.1159000000000000 0.1159000000000000 0.1159000000000000 I (2c)
-0.1159000000000000 -0.1159000000000000 -0.1159000000000000 I (2c)
0.3017000000000000 0.3017000000000000 0.3017000000000000 S (2c)
-0.3017000000000000 -0.3017000000000000 -0.3017000000000000 S (2c)
0.3815000000000000 0.3815000000000000 0.3815000000000000 Sm (2c)
-0.3815000000000000 -0.3815000000000000 -0.3815000000000000 Sm (2c)

```

PrNiO<sub>3</sub>: AB3C\_hR10\_167\_b\_e\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'PrNiO3'
_chemical_formula_sum 'Ni O3 Pr'
loop_
_publ_author_name
'T. C. Huang'
'W. Parrish'
'H. Toraya'
'P. Lacorre'
'J. B. Torrance'
_journal_name_full_name
;
Materials Research Bulletin
;
_journal_volume 25
_journal_year 1990
_journal_page_first 1091
_journal_page_last 1098
_publ_section_title
;
High-Temperature Crystal Structures of Orthorhombic and Rhombohedral
↪ PrNiO_{3}$
;
_aflow_title 'PrNiO_{3}$ Structure'
_aflow_proto 'AB3C_hR10_167_b_e_a'
_aflow_params 'a, c/a, x_{3}'
_aflow_params_values '5.4577, 2.40134122433, 0.6946'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hR10'
_symmetry_space_group_name_H-M "R -3 2/c (hexagonal axes)"
_symmetry_Int_Tables_number 167
_cell_length_a 5.45770

```



```

_cell_length_b 5.45770
_cell_length_c 13.10580
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 y, x, -z+1/2
5 -x, -x+y, -z+1/2
6 x-y, -y, -z+1/2
7 -x, -y, -z
8 y, -x+y, -z
9 x-y, x, -z
10 -y, -x, z+1/2
11 x, x-y, z+1/2
12 -x+y, y, z+1/2
13 x+1/3, y+2/3, z+2/3
14 -y+1/3, x-y+2/3, z+2/3
15 -x+y+1/3, -x+2/3, z+2/3
16 y+1/3, x+2/3, -z+1/6
17 -x+1/3, -x+y+2/3, -z+1/6
18 x-y+1/3, -y+2/3, -z+1/6
19 -x+1/3, -y+2/3, -z+2/3
20 y+1/3, -x+y+2/3, -z+2/3
21 x-y+1/3, x+2/3, -z+2/3
22 -y+1/3, -x+2/3, z+1/6
23 x+1/3, x-y+2/3, z+1/6
24 -x+y+1/3, y+2/3, z+1/6
25 x+2/3, y+1/3, z+1/3
26 -y+2/3, x-y+1/3, z+1/3
27 -x+y+2/3, -x+1/3, z+1/3
28 y+2/3, x+1/3, -z+5/6
29 -x+2/3, -x+y+1/3, -z+5/6
30 x-y+2/3, -y+1/3, -z+5/6
31 -x+2/3, -y+1/3, -z+1/3
32 y+2/3, -x+y+1/3, -z+1/3
33 x-y+2/3, x+1/3, -z+1/3
34 -y+2/3, -x+1/3, z+5/6
35 x+2/3, x-y+1/3, z+5/6
36 -x+y+2/3, y+1/3, z+5/6

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Pr1 Pr 6 a 0.00000 0.00000 0.25000 1.00000
Ni1 Ni 6 b 0.00000 0.00000 0.00000 1.00000
O1 O 18 e 0.44460 0.00000 0.25000 1.00000

```

PrNiO<sub>3</sub>: AB3C\_hR10\_167\_b\_e\_a - POSCAR

```

AB3C_hR10_167_b_e_a & a, c/a, x3 --params=5.4577, 2.40134122433, 0.6946 &
↪ R=3c D_{3d}^{6} #167 (abe) & hR10 & None & PrNiO3 & PrNiO3 & T.
↪ C. Huang et al., Mater. Res. Bull. 25, 1091-1098 (1990)
1.0000000000000000
2.7288500000000000 -1.57550228207811 4.3686000000000000
0.0000000000000000 3.15100456415622 4.3686000000000000
-2.7288500000000000 -1.57550228207811 4.3686000000000000
Ni O Pr
2 6 2
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 Ni (2b)
0.5000000000000000 0.5000000000000000 0.5000000000000000 Ni (2b)
0.6946000000000000 -0.1946000000000000 0.2500000000000000 O (6e)
0.2500000000000000 0.6946000000000000 -0.1946000000000000 O (6e)
-0.1946000000000000 0.2500000000000000 0.6946000000000000 O (6e)
-0.6946000000000000 1.1946000000000000 0.7500000000000000 O (6e)
0.7500000000000000 -0.6946000000000000 1.1946000000000000 O (6e)
1.1946000000000000 0.7500000000000000 -0.6946000000000000 O (6e)
0.2500000000000000 0.2500000000000000 0.2500000000000000 Pr (2a)
0.7500000000000000 0.7500000000000000 0.7500000000000000 Pr (2a)

```

KBO<sub>2</sub> (F5<sub>13</sub>): ABC2\_hR24\_167\_e\_e\_2e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'KBO2'
_chemical_formula_sum 'B K O2'

loop_
_publ_author_name
'W. Schneider'
'G. B. Carpenter'
_journal_name_full_name
;
Acta Crystallographica Section B: Structural Science
;
_journal_volume 26
_journal_year 1970
_journal_page_first 1189
_journal_page_last 1191
_publ_section_title
;

```

```

Bond lengths and thermal parameters of potassium metaborate, KS_{3}BS_{6}
↪ {3}SOS_{6}$
;

# Found in Landolt-B{\o}rnstein - Group III Condensed Matter (Numerical
↪ Data and Functional Relationships in Science and Technology),
↪ 2007

_aflow_title 'KBOS_{2}$ (SF5_{13}$) Structure'
_aflow_proto 'ABC2_hR24_167_e_e_2e'
_aflow_params 'a, c/a, x_{1}, x_{2}, x_{3}, x_{4}'
_aflow_params_values '12.76, 0.575235109718, 1.1389, 0.8113, 1.0343, 0.3584'
_aflow_Strukturbericht 'SF5_{13}$'
_aflow_Pearson 'hR24'

_symmetry_space_group_name_H-M 'R -3 2/c (hexagonal axes)'
_symmetry_Int_Tables_number 167

_cell_length_a 12.76000
_cell_length_b 12.76000
_cell_length_c 7.34000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 y, x, -z+1/2
5 -x, -x+y, -z+1/2
6 x-y, -y, -z+1/2
7 -x, -y, -z
8 y, -x+y, -z
9 x-y, x, -z
10 -y, -x, z+1/2
11 x, x-y, z+1/2
12 -x+y, y, z+1/2
13 x+1/3, y+2/3, z+2/3
14 -y+1/3, x-y+2/3, z+2/3
15 -x+y+1/3, -x+2/3, z+2/3
16 y+1/3, x+2/3, -z+1/6
17 -x+1/3, -x+y+2/3, -z+1/6
18 x-y+1/3, -y+2/3, -z+1/6
19 -x+1/3, -y+2/3, -z+2/3
20 y+1/3, -x+y+2/3, -z+2/3
21 x-y+1/3, x+2/3, -z+2/3
22 -y+1/3, -x+2/3, z+1/6
23 x+1/3, x-y+2/3, z+1/6
24 -x+y+1/3, y+2/3, z+1/6
25 x+2/3, y+1/3, z+1/3
26 -y+2/3, x-y+1/3, z+1/3
27 -x+y+2/3, -x+1/3, z+1/3
28 y+2/3, x+1/3, -z+5/6
29 -x+2/3, -x+y+1/3, -z+5/6
30 x-y+2/3, -y+1/3, -z+5/6
31 -x+2/3, -y+1/3, -z+1/3
32 y+2/3, -x+y+1/3, -z+1/3
33 x-y+2/3, x+1/3, -z+1/3
34 -y+2/3, -x+1/3, z+5/6
35 x+2/3, x-y+1/3, z+5/6
36 -x+y+2/3, y+1/3, z+5/6

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
B1 B 18 e 0.88890 0.00000 0.25000 1.00000
K1 K 18 e 0.56130 0.00000 0.25000 1.00000
O1 O 18 e 0.78430 0.00000 0.25000 1.00000
O2 O 18 e 0.10840 0.00000 0.25000 1.00000

```

KBO<sub>2</sub> (F5<sub>13</sub>): ABC2\_hR24\_167\_e\_e\_2e - POSCAR

```

ABC2_hR24_167_e_e_2e & a, c/a, x1, x2, x3, x4 --params=12.76, 0.575235109718,
↪ 1.1389, 0.8113, 1.0343, 0.3584 & R=3c D_{3d}^{6} #167 (e^4) & hR24
↪ & SF5_{13}$ & KBO2 & KBO2 & W. Schneider and G. B. Carpenter,
↪ Acta Crystallogr. Sect. B Struct. Sci. 26, 1189-1191 (1970)
1.0000000000000000
6.3800000000000000 -3.68349471742981 2.446666666666667
0.0000000000000000 7.36698943485963 2.446666666666667
-6.3800000000000000 -3.68349471742981 2.446666666666667
B K O
6 6 12
Direct
1.1389000000000000 -0.6389000000000000 0.2500000000000000 B (6e)
0.2500000000000000 1.1389000000000000 -0.6389000000000000 B (6e)
-0.6389000000000000 0.2500000000000000 1.1389000000000000 B (6e)
-1.1389000000000000 1.6389000000000000 0.7500000000000000 B (6e)
0.7500000000000000 -1.1389000000000000 1.6389000000000000 B (6e)
1.6389000000000000 0.7500000000000000 -1.1389000000000000 B (6e)
0.8113000000000000 -0.3113000000000000 0.2500000000000000 K (6e)
0.2500000000000000 0.8113000000000000 -0.3113000000000000 K (6e)
-0.3113000000000000 0.2500000000000000 0.8113000000000000 K (6e)
-0.8113000000000000 1.3113000000000000 0.7500000000000000 K (6e)
0.7500000000000000 -0.8113000000000000 1.3113000000000000 K (6e)
1.3113000000000000 0.7500000000000000 -0.8113000000000000 K (6e)
1.0343000000000000 -0.5343000000000000 0.2500000000000000 O (6e)

```

0.25000000000000	1.03430000000000	-0.53430000000000	O	(6e)
-0.53430000000000	0.25000000000000	1.03430000000000	O	(6e)
-1.03430000000000	1.53430000000000	0.75000000000000	O	(6e)
0.75000000000000	-1.03430000000000	1.53430000000000	O	(6e)
1.53430000000000	0.75000000000000	-1.03430000000000	O	(6e)
0.35840000000000	0.14160000000000	0.25000000000000	O	(6e)
0.25000000000000	0.35840000000000	0.14160000000000	O	(6e)
0.14160000000000	0.25000000000000	0.35840000000000	O	(6e)
-0.35840000000000	0.85840000000000	0.75000000000000	O	(6e)
0.75000000000000	-0.35840000000000	0.85840000000000	O	(6e)
0.85840000000000	0.75000000000000	-0.35840000000000	O	(6e)

K<sub>2</sub>Ta<sub>4</sub>O<sub>9</sub>F<sub>4</sub>: A2B13C4\_hP57\_168\_d\_c6d\_2d - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'K2Ta4O9F4'
_chemical_formula_sum 'K2 O13 Ta4'

loop_
  _publ_author_name
  'A. Boukhari'
  'J. P. Chaminade'
  'M. Vlasse'
  'M. Pouchard'
_journal_name_full_name
;
Acta Crystallographica Section B: Structural Science
;
_journal_volume 35
_journal_year 1979
_journal_page_first 1983
_journal_page_last 1986
_publ_section_title
;
Structure cristalline de l'oxyfluore de tantalate et de potassium, K2
→ {2}$Ta_{4}$F_{4}$O_{13}$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
→ Inorganic Compounds, 2013

_aflow_title 'K2{2}$Ta_{4}$O_{13}$F_{4}$ Structure'
_aflow_proto 'A2B13C4_hP57_168_d_c6d_2d'
_aflow_params 'a, c/a, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, y4, z4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12'
→ 4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12'
_aflow_params_values '15.9361426085, 0.244226907628, 0.0, 0.4965, 0.179,
→ 0.555, 0.035, 0.187, 0.007, 0.349, 0.034, 0.018, 0.168, 0.388, 0.01,
→ 0.195, 0.569, 0.02, 0.093, 0.454, 0.539, 0.273, 0.095, 0.555, 0.2634,
→ 0.09, 0.086, 0.0789, 0.4368, 0.071'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP57'

_cell_length_a 15.9361426085
_cell_length_b 15.9361426085
_cell_length_c 3.8920348288
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M 'P 6'
_symmetry_int_tables_number 168

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x, y, z
  2 x-y, x, z
  3 -y, x-y, z
  4 -x, -y, z
  5 -x+y, -x, z
  6 y, -x+y, z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  O1 O 3 c 0.50000 0.00000 0.00000 1.00000
  K1 K 6 d 0.49650 0.17900 0.55500 1.00000
  O2 O 6 d 0.03500 0.18700 0.00700 1.00000
  O3 O 6 d 0.34900 0.03400 0.01800 1.00000
  O4 O 6 d 0.16800 0.38800 0.01000 1.00000
  O5 O 6 d 0.19500 0.56900 0.02000 1.00000
  O6 O 6 d 0.09300 0.45400 0.53900 1.00000
  O7 O 6 d 0.27300 0.09500 0.55500 1.00000
  Ta1 Ta 6 d 0.26340 0.09000 0.08600 1.00000
  Ta2 Ta 6 d 0.07890 0.43680 0.07100 1.00000
```

K<sub>2</sub>Ta<sub>4</sub>O<sub>9</sub>F<sub>4</sub>: A2B13C4\_hP57\_168\_d\_c6d\_2d - POSCAR

```
A2B13C4_hP57_168_d_c6d_2d & a, c/a, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5
→ x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10 --params=
→ 15.9361426085, 0.244226907628, 0.0, 0.4965, 0.179, 0.555, 0.035, 0.187
→ 0.007, 0.349, 0.034, 0.018, 0.168, 0.388, 0.01, 0.195, 0.569, 0.02,
→ 0.093, 0.454, 0.539, 0.273, 0.095, 0.555, 0.2634, 0.09, 0.086, 0.0789,
→ 0.4368, 0.071 & P6 C6^1 #168 (cd^9) & hP57 & None &
```

→ K2Ta4O9F4 & A. Boukhari et al., Acta Crystallogr. Sect. B  
→ Struct. Sci. 35, 1983-1986 (1979)

1.00000000000000				
7.9687130425000	-13.80110433729260	0.00000000000000		
7.96807130425000	13.80110433729260	0.00000000000000		
0.00000000000000	0.00000000000000	3.89203482880000		
K	O	Ta		
6	39	12		

Direct

0.49650000000000	0.17900000000000	0.55500000000000	K	(6d)
-0.17900000000000	0.31750000000000	0.55500000000000	K	(6d)
-0.31750000000000	-0.49650000000000	0.55500000000000	K	(6d)
-0.49650000000000	-0.17900000000000	0.55500000000000	K	(6d)
0.17900000000000	-0.31750000000000	0.55500000000000	K	(6d)
0.31750000000000	0.49650000000000	0.55500000000000	K	(6d)
0.50000000000000	0.00000000000000	0.00000000000000	O	(3c)
0.00000000000000	0.50000000000000	0.00000000000000	O	(3c)
0.50000000000000	0.50000000000000	0.00000000000000	O	(3c)
0.03500000000000	0.18700000000000	0.00700000000000	O	(6d)
-0.18700000000000	-0.15200000000000	0.00700000000000	O	(6d)
0.15200000000000	-0.03500000000000	0.00700000000000	O	(6d)
-0.03500000000000	-0.18700000000000	0.00700000000000	O	(6d)
0.18700000000000	0.15200000000000	0.00700000000000	O	(6d)
-0.15200000000000	0.03500000000000	0.00700000000000	O	(6d)
0.34900000000000	0.03400000000000	0.01800000000000	O	(6d)
-0.03400000000000	0.31500000000000	0.01800000000000	O	(6d)
-0.31500000000000	-0.34900000000000	0.01800000000000	O	(6d)
-0.34900000000000	-0.03400000000000	0.01800000000000	O	(6d)
0.03400000000000	-0.31500000000000	0.01800000000000	O	(6d)
0.31500000000000	0.34900000000000	0.01800000000000	O	(6d)
0.16800000000000	0.38800000000000	0.01000000000000	O	(6d)
-0.38800000000000	-0.22000000000000	0.01000000000000	O	(6d)
0.22000000000000	-0.16800000000000	0.01000000000000	O	(6d)
-0.16800000000000	-0.38800000000000	0.01000000000000	O	(6d)
0.38800000000000	0.22000000000000	0.01000000000000	O	(6d)
-0.22000000000000	0.16800000000000	0.01000000000000	O	(6d)
0.19500000000000	0.56900000000000	0.02000000000000	O	(6d)
-0.56900000000000	-0.37400000000000	0.02000000000000	O	(6d)
0.37400000000000	-0.19500000000000	0.02000000000000	O	(6d)
-0.19500000000000	-0.56900000000000	0.02000000000000	O	(6d)
0.56900000000000	0.37400000000000	0.02000000000000	O	(6d)
-0.37400000000000	0.19500000000000	0.02000000000000	O	(6d)
0.09300000000000	0.45400000000000	0.53900000000000	O	(6d)
-0.45400000000000	-0.36100000000000	0.53900000000000	O	(6d)
0.36100000000000	-0.09300000000000	0.53900000000000	O	(6d)
-0.09300000000000	-0.45400000000000	0.53900000000000	O	(6d)
0.45400000000000	0.36100000000000	0.53900000000000	O	(6d)
-0.36100000000000	0.09300000000000	0.53900000000000	O	(6d)
0.27300000000000	0.09500000000000	0.55500000000000	O	(6d)
-0.09500000000000	0.17800000000000	0.55500000000000	O	(6d)
-0.17800000000000	-0.27300000000000	0.55500000000000	O	(6d)
-0.27300000000000	-0.09500000000000	0.55500000000000	O	(6d)
0.09500000000000	-0.17800000000000	0.55500000000000	O	(6d)
0.17800000000000	0.27300000000000	0.55500000000000	O	(6d)
0.26340000000000	0.09000000000000	0.08600000000000	Ta	(6d)
-0.09000000000000	0.17340000000000	0.08600000000000	Ta	(6d)
-0.17340000000000	-0.26340000000000	0.08600000000000	Ta	(6d)
-0.26340000000000	-0.09000000000000	0.08600000000000	Ta	(6d)
0.09000000000000	-0.17340000000000	0.08600000000000	Ta	(6d)
0.17340000000000	0.26340000000000	0.08600000000000	Ta	(6d)
0.07890000000000	0.43680000000000	0.07100000000000	Ta	(6d)
-0.43680000000000	-0.35790000000000	0.07100000000000	Ta	(6d)
0.35790000000000	-0.07890000000000	0.07100000000000	Ta	(6d)
-0.07890000000000	-0.43680000000000	0.07100000000000	Ta	(6d)
0.43680000000000	0.35790000000000	0.07100000000000	Ta	(6d)
-0.35790000000000	0.07890000000000	0.07100000000000	Ta	(6d)

Al[PO<sub>4</sub>]: AB4C\_hP72\_168\_2d\_8d\_2d - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Al[PO4]'
_chemical_formula_sum 'Al O4 P'

loop_
  _publ_author_name
  'J. W. {Richardson Jnr}'
  'J. J. Pluth'
  'J. V. Smith'
_journal_name_full_name
;
Acta Crystallographica Section C: Structural Chemistry
;
_journal_volume 43
_journal_year 1987
_journal_page_first 1469
_journal_page_last 1472
_publ_section_title
;
Aluminophosphate number 5: time-of-flight neutron powder diffraction
→ study of calcined powder at 295 K
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
→ Inorganic Compounds, 2013

_aflow_title 'Al[PO4]{4}$ Structure'
_aflow_proto 'AB4C_hP72_168_2d_8d_2d'
_aflow_params 'a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12'
→ 3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12'
_aflow_params_values '13.759939558, 0.609738372094, 0.4498, 0.113, 0.6253,
```

```

↪ 0.1278, 0.466, 0.1246, 0.4154, 0.2053, 0.0456, 0.2066, 0.4189, 0.5576,
↪ 0.4218, 0.0894, 0.8248, 0.1514, 0.4907, 0.3249, 0.3746, 0.0106, 0.0948,
↪ 0.0083, 0.3667, 0.4879, 0.5693, 0.1616, 0.0357, 0.1505, 0.5625, 0.5943,
↪ 0.4451, 0.1173, 0.0, 0.1291, 0.4589, 0.4993
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP72'

_cell_length_a 13.7599395580
_cell_length_b 13.7599395580
_cell_length_c 8.3899631462
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 6"
_symmetry_Int_Tables_number 168

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x-y, x, z
3 -y, x-y, z
4 -x, -y, z
5 -x+y, -x, z
6 y, -x+y, z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 6 d 0.44980 0.11300 0.62530 1.00000
Al2 Al 6 d 0.12780 0.46600 0.12460 1.00000
O1 O 6 d 0.41540 0.20530 0.04560 1.00000
O2 O 6 d 0.20660 0.41890 0.55760 1.00000
O3 O 6 d 0.42180 0.08940 0.82480 1.00000
O4 O 6 d 0.15140 0.49070 0.32490 1.00000
O5 O 6 d 0.37460 0.01060 0.09480 1.00000
O6 O 6 d 0.00830 0.36670 0.48790 1.00000
O7 O 6 d 0.56930 0.16160 0.03570 1.00000
O8 O 6 d 0.15050 0.56250 0.59430 1.00000
P1 P 6 d 0.44510 0.11730 0.00000 1.00000
P2 P 6 d 0.12910 0.45890 0.49930 1.00000

```

Al[PO<sub>4</sub>]: AB4C\_hP72\_168\_2d\_8d\_2d - POSCAR

```

AB4C_hP72_168_2d_8d_2d & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5
↪ z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11
↪ x12, y12, z12 --params=13.759939558, 0.609738372094, 0.4498, 0.113,
↪ 0.6253, 0.1278, 0.466, 0.1246, 0.4154, 0.2053, 0.0456, 0.2066, 0.4189,
↪ 0.5576, 0.4218, 0.0894, 0.8248, 0.1514, 0.4907, 0.3249, 0.3746, 0.0106,
↪ 0.0948, 0.0083, 0.3667, 0.4879, 0.5693, 0.1616, 0.0357, 0.1505, 0.5625,
↪ 0.5943, 0.4451, 0.1173, 0.0, 0.1291, 0.4589, 0.4993 & P6 C6{1} #
↪ 168 (dh12) & hP72 & None & Al[PO4] & & J. W. {Richardson Jr}
↪ and J. J. Pluth and J. V. Smith, Acta Crystallogr. C 43,
↪ 1469-1472 (1987)
1.0000000000000000
6.87996977900000 -11.91645721176640 0.00000000000000
6.87996977900000 11.91645721176640 0.00000000000000
0.00000000000000 0.00000000000000 8.38996314620000
Al O P
12 48 12
Direct
0.44980000000000 0.11300000000000 0.62530000000000 Al (6d)
-0.11300000000000 0.33680000000000 0.62530000000000 Al (6d)
-0.33680000000000 -0.44980000000000 0.62530000000000 Al (6d)
-0.44980000000000 -0.11300000000000 0.62530000000000 Al (6d)
0.11300000000000 -0.33680000000000 0.62530000000000 Al (6d)
0.33680000000000 0.44980000000000 0.62530000000000 Al (6d)
0.12780000000000 0.46600000000000 0.12460000000000 Al (6d)
-0.46600000000000 -0.33820000000000 0.12460000000000 Al (6d)
0.33820000000000 -0.12780000000000 0.12460000000000 Al (6d)
-0.12780000000000 -0.46600000000000 0.12460000000000 Al (6d)
0.46600000000000 0.33820000000000 0.12460000000000 Al (6d)
-0.33820000000000 0.12780000000000 0.12460000000000 Al (6d)
0.41540000000000 0.20530000000000 0.04560000000000 O (6d)
-0.20530000000000 0.21010000000000 0.04560000000000 O (6d)
-0.21010000000000 -0.41540000000000 0.04560000000000 O (6d)
-0.41540000000000 -0.20530000000000 0.04560000000000 O (6d)
0.20530000000000 -0.21010000000000 0.04560000000000 O (6d)
0.21010000000000 0.41540000000000 0.04560000000000 O (6d)
0.20660000000000 0.41890000000000 0.55760000000000 O (6d)
-0.41890000000000 -0.21230000000000 0.55760000000000 O (6d)
0.21230000000000 -0.20660000000000 0.55760000000000 O (6d)
-0.20660000000000 -0.41890000000000 0.55760000000000 O (6d)
0.41890000000000 0.21230000000000 0.55760000000000 O (6d)
-0.21230000000000 0.20660000000000 0.55760000000000 O (6d)
0.42180000000000 0.08940000000000 0.82480000000000 O (6d)
-0.08940000000000 0.33240000000000 0.82480000000000 O (6d)
-0.33240000000000 -0.42180000000000 0.82480000000000 O (6d)
-0.42180000000000 -0.08940000000000 0.82480000000000 O (6d)
0.08940000000000 -0.33240000000000 0.82480000000000 O (6d)
0.33240000000000 0.42180000000000 0.82480000000000 O (6d)
0.15140000000000 0.49070000000000 0.32490000000000 O (6d)
-0.49070000000000 -0.33930000000000 0.32490000000000 O (6d)
0.33930000000000 -0.15140000000000 0.32490000000000 O (6d)
-0.15140000000000 -0.49070000000000 0.32490000000000 O (6d)
0.49070000000000 0.33930000000000 0.32490000000000 O (6d)
-0.33930000000000 0.15140000000000 0.32490000000000 O (6d)
0.37460000000000 0.01060000000000 0.09480000000000 O (6d)

```

```

-0.01060000000000 0.36400000000000 0.09480000000000 O (6d)
-0.36400000000000 -0.37460000000000 0.09480000000000 O (6d)
-0.37460000000000 -0.01060000000000 0.09480000000000 O (6d)
0.01060000000000 -0.36400000000000 0.09480000000000 O (6d)
0.36400000000000 0.37460000000000 0.09480000000000 O (6d)
0.00830000000000 0.36670000000000 0.48790000000000 O (6d)
-0.36670000000000 -0.35840000000000 0.48790000000000 O (6d)
0.35840000000000 -0.00830000000000 0.48790000000000 O (6d)
-0.00830000000000 -0.36670000000000 0.48790000000000 O (6d)
0.36670000000000 0.35840000000000 0.48790000000000 O (6d)
-0.35840000000000 0.00830000000000 0.48790000000000 O (6d)
0.56930000000000 0.16160000000000 0.03570000000000 O (6d)
-0.16160000000000 0.40770000000000 0.03570000000000 O (6d)
-0.40770000000000 -0.56930000000000 0.03570000000000 O (6d)
-0.56930000000000 -0.16160000000000 0.03570000000000 O (6d)
0.16160000000000 -0.40770000000000 0.03570000000000 O (6d)
0.40770000000000 0.56930000000000 0.03570000000000 O (6d)
0.15050000000000 0.56250000000000 0.59430000000000 O (6d)
-0.56250000000000 -0.41200000000000 0.59430000000000 O (6d)
0.41200000000000 -0.15050000000000 0.59430000000000 O (6d)
-0.15050000000000 -0.56250000000000 0.59430000000000 O (6d)
0.56250000000000 0.41200000000000 0.59430000000000 O (6d)
-0.41200000000000 0.15050000000000 0.59430000000000 O (6d)
0.44510000000000 0.11730000000000 0.00000000000000 P (6d)
-0.11730000000000 0.32780000000000 0.00000000000000 P (6d)
-0.32780000000000 -0.44510000000000 0.00000000000000 P (6d)
-0.44510000000000 -0.11730000000000 0.00000000000000 P (6d)
0.11730000000000 -0.32780000000000 0.00000000000000 P (6d)
0.32780000000000 0.44510000000000 0.00000000000000 P (6d)
0.12910000000000 0.45890000000000 0.49930000000000 P (6d)
-0.45890000000000 -0.32980000000000 0.49930000000000 P (6d)
0.32980000000000 -0.12910000000000 0.49930000000000 P (6d)
-0.12910000000000 -0.45890000000000 0.49930000000000 P (6d)
0.45890000000000 0.32980000000000 0.49930000000000 P (6d)
-0.32980000000000 0.12910000000000 0.49930000000000 P (6d)

```

α-Al<sub>2</sub>S<sub>3</sub>: A2B3\_hP30\_169\_2a\_3a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'alpha-Al2S3'
_chemical_formula_sum 'Al2 S3'

loop_
_publ_author_name
'B. Eisenmann'
_journal_name_full_name
;
Zeitschrift f{"u}r Kristallografiya
;
_journal_volume 198
_journal_year 1992
_journal_page_first 307
_journal_page_last 308
_publ_section_title
;
Crystal structure of $\alpha$-dialuminum trisulfide, Al2{2}SS3{3}$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title '$\alpha$-Al2{2}SS3{3}$ Structure'
_aflow_proto 'A2B3_hP30_169_2a_3a'
_aflow_params 'a, c/a, x_{1}, y_{1}, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}'
↪ 3), x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}'
_aflow_params_values '6.4300116544, 2.78071539658, 0.013, 0.3579, 0.12736,
↪ 0.3339, 0.3226, 0.29886, 0.3347, 0.0, 0.004, 0.0119, 0.3343, 0.0, 0.338,
↪ 0.0064, 0.33823'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP30'

_cell_length_a 6.4300116544
_cell_length_b 6.4300116544
_cell_length_c 17.8800324076
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 61"
_symmetry_Int_Tables_number 169

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x-y, x, z+1/6
3 -y, x-y, z+1/3
4 -x, -y, z+1/2
5 -x+y, -x, z+2/3
6 y, -x+y, z+5/6

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 6 a 0.01300 0.35790 0.12736 1.00000
Al2 Al 6 a 0.33390 0.32260 0.29886 1.00000

```

```
S1 S 6 a 0.33470 0.00000 0.00400 1.00000
S2 S 6 a 0.01190 0.33430 0.00000 1.00000
S3 S 6 a 0.33800 0.00640 0.33823 1.00000
```

$\alpha$ -Al<sub>2</sub>S<sub>3</sub>: A2B3\_hP30\_169\_2a\_3a - POSCAR

```
A2B3_hP30_169_2a_3a & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5
--params=6.4300116544, 2.78071539658, 0.013, 0.3579, 0.12736,
0.3339, 0.3226, 0.29886, 0.3347, 0.0, 0.004, 0.0119, 0.3343, 0.0, 0.338,
0.0064, 0.33823 & P6_{1} C_{6}^{12} #169 (a^5) & hP30 & None &
Al2S3 & alpha & B. Eisenmann, Z. Kristallogr. 198, 307-308 (
1992)
1.0000000000000000
3.21500582720000 -5.56855343934041 0.0000000000000000
3.21500582720000 5.56855343934041 0.0000000000000000
0.00000000000000 0.00000000000000 17.88003240760000
Al S
12 18
Direct
0.01300000000000 0.35790000000000 0.12736000000000 Al (6a)
-0.35790000000000 -0.34490000000000 0.46069333333333 Al (6a)
0.34490000000000 -0.01300000000000 0.79402666666666 Al (6a)
-0.01300000000000 -0.35790000000000 0.62736000000000 Al (6a)
0.35790000000000 0.34490000000000 0.96069333333333 Al (6a)
-0.34490000000000 0.01300000000000 0.29402666666666 Al (6a)
0.33900000000000 0.32260000000000 0.29886000000000 Al (6a)
-0.32260000000000 0.01130000000000 0.63219333333333 Al (6a)
-0.01130000000000 -0.33900000000000 0.96526666666666 Al (6a)
-0.33900000000000 -0.32260000000000 0.79886000000000 Al (6a)
0.32260000000000 -0.01130000000000 1.13219333333333 Al (6a)
0.01130000000000 0.33900000000000 0.46526666666666 Al (6a)
0.33470000000000 0.00000000000000 0.00400000000000 S (6a)
0.00000000000000 0.33470000000000 0.33733333333333 S (6a)
-0.33470000000000 -0.33470000000000 0.67066666666666 S (6a)
-0.33470000000000 0.00000000000000 0.50400000000000 S (6a)
0.00000000000000 -0.33470000000000 0.83733333333333 S (6a)
0.33470000000000 0.33470000000000 0.17066666666666 S (6a)
0.01190000000000 0.33430000000000 0.00000000000000 S (6a)
-0.33430000000000 -0.32240000000000 0.33333333333333 S (6a)
0.32240000000000 -0.01190000000000 0.66666666666666 S (6a)
-0.01190000000000 -0.33430000000000 0.50000000000000 S (6a)
0.33430000000000 0.32240000000000 0.83333333333333 S (6a)
-0.32240000000000 0.01190000000000 0.16666666666666 S (6a)
0.33800000000000 0.00640000000000 0.33823000000000 S (6a)
-0.00640000000000 0.33160000000000 0.67156333333333 S (6a)
-0.33160000000000 -0.33800000000000 1.00489666666666 S (6a)
-0.33800000000000 -0.00640000000000 0.83823000000000 S (6a)
0.00640000000000 -0.33160000000000 1.17156333333333 S (6a)
0.33160000000000 0.33800000000000 0.50489666666666 S (6a)
```

Al<sub>2</sub>S<sub>3</sub>: A2B3\_hP30\_170\_2a\_3a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Al2S3'
_chemical_formula_sum 'Al2 S3'
_aflow_title 'AlS_{2}SSS_{3}$ Structure'
_aflow_proto 'A2B3_hP30_170_2a_3a'
_aflow_params 'a, c/a, x_{1}, y_{1}, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}'
_aflow_params_values '6.4300116544, 2.78071539658, 0.013, 0.3579, 0.87264,
0.3339, 0.3226, 0.70114, 0.3347, 0.0, -0.004, 0.0119, 0.3343, 0.0, 0.338,
0.0064, 0.66177'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP30'
_cell_length_a 6.4300116544
_cell_length_b 6.4300116544
_cell_length_c 17.8800324076
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000
_symmetry_space_group_name_H-M "P 65"
_symmetry_Int_Tables_number 170
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x-y, x, z+5/6
3 -y, x-y, z+2/3
4 -x, -y, z+1/2
5 -x+y, -x, z+1/3
6 y, -x+y, z+1/6
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 6 a 0.01300 0.35790 0.87264 1.00000
Al2 Al 6 a 0.33390 0.32260 0.70114 1.00000
S1 S 6 a 0.33470 0.00000 -0.00400 1.00000
S2 S 6 a 0.01190 0.33430 0.00000 1.00000
S3 S 6 a 0.33800 0.00640 0.66177 1.00000
```

Al<sub>2</sub>S<sub>3</sub>: A2B3\_hP30\_170\_2a\_3a - POSCAR

```
A2B3_hP30_170_2a_3a & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5
--params=6.4300116544, 2.78071539658, 0.013, 0.3579, 0.87264,
0.3339, 0.3226, 0.70114, 0.3347, 0.0, -0.004, 0.0119, 0.3343, 0.0, 0.338,
0.0064, 0.66177 & P6_{5} C_{6}^{13} #170 (a^5) & hP30 & None &
Al2S3 & Al2S3 &
1.0000000000000000
3.21500582720000 -5.56855343934041 0.0000000000000000
3.21500582720000 5.56855343934041 0.0000000000000000
0.00000000000000 0.00000000000000 17.88003240760000
Al S
12 18
Direct
0.01300000000000 0.35790000000000 0.87264000000000 Al (6a)
-0.35790000000000 -0.34490000000000 1.53930666666666 Al (6a)
0.34490000000000 -0.01300000000000 1.20597333333333 Al (6a)
-0.01300000000000 -0.35790000000000 1.37264000000000 Al (6a)
0.35790000000000 0.34490000000000 1.03930666666666 Al (6a)
-0.34490000000000 0.01300000000000 1.70597333333333 Al (6a)
0.33900000000000 0.32260000000000 0.70114000000000 Al (6a)
-0.32260000000000 0.01130000000000 1.36780666666666 Al (6a)
-0.01130000000000 -0.33900000000000 1.03447333333333 Al (6a)
-0.33900000000000 -0.32260000000000 1.20114000000000 Al (6a)
0.32260000000000 -0.01130000000000 0.86780666666666 Al (6a)
0.01130000000000 0.33900000000000 1.53447333333333 Al (6a)
0.33470000000000 0.00000000000000 -0.00400000000000 S (6a)
0.00000000000000 0.33470000000000 0.62666666666666 S (6a)
-0.33470000000000 -0.33470000000000 0.32933333333333 S (6a)
-0.33470000000000 0.00000000000000 0.49600000000000 S (6a)
0.00000000000000 -0.33470000000000 1.62666666666666 S (6a)
0.33470000000000 0.33470000000000 0.82933333333333 S (6a)
0.01190000000000 0.33430000000000 0.00000000000000 S (6a)
-0.33430000000000 -0.32240000000000 0.66666666666666 S (6a)
0.32240000000000 -0.01190000000000 0.33333333333333 S (6a)
-0.01190000000000 -0.33430000000000 0.50000000000000 S (6a)
0.33430000000000 0.32240000000000 0.16666666666666 S (6a)
-0.32240000000000 0.01190000000000 0.83333333333333 S (6a)
0.33800000000000 0.00640000000000 0.66177000000000 S (6a)
-0.00640000000000 0.33160000000000 1.32843666666666 S (6a)
-0.33160000000000 -0.33800000000000 0.99510333333333 S (6a)
-0.33800000000000 -0.00640000000000 1.16177000000000 S (6a)
0.00640000000000 -0.33160000000000 0.82843666666666 S (6a)
0.33160000000000 0.33800000000000 1.49510333333333 S (6a)
```

Sr[S<sub>2</sub>O<sub>6</sub>](H<sub>2</sub>O)<sub>4</sub>: A10B2C\_hP39\_171\_5c\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Sr[S2O6][H2O]4'
_chemical_formula_sum 'O10 S2 Sr'
loop_
_publ_author_name
'R. N. Hargreaves'
'E. Stanley'
_journal_name_full_name
Zeitschrift f{"u}r Kristallographie - Crystalline Materials
_journal_volume 135
_journal_year 1972
_journal_page_first 399
_journal_page_last 407
_publ_section_title
The structure of strontium dithionate tetrahydrate
# Found in Pearson's Crystal Data - Crystal Structure Database for
Inorganic Compounds, 2013
_aflow_title 'Sr[SS_{2}SO_{6}]_{4}[HS_{2}SO]_{4}$ Structure'
_aflow_proto 'A10B2C_hP39_171_5c_a'
_aflow_params 'a, c/a, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4}, z_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}, x_{7}, y_{7}, z_{7}'
_aflow_params_values '6.3199906634, 3.05221518986, 0.0, -0.004, 0.253,
0.23633, 0.015, 0.248, 0.11034, 0.681, 0.192, 0.16733, 0.448, 0.188,
0.29533, 0.449, 0.25, 0.048, 0.373, 0.065, 0.50467'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP39'
_cell_length_a 6.3199906634
_cell_length_b 6.3199906634
_cell_length_c 19.2899715026
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000
_symmetry_space_group_name_H-M "P 62"
_symmetry_Int_Tables_number 171
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x-y, x, z+1/3
3 -y, x-y, z+2/3
4 -x, -y, z
5 -x+y, -x, z+1/3
6 y, -x+y, z+2/3
loop_
_atom_site_label
_atom_site_type_symbol
```

```

_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Sr1 Sr 3 a 0.00000 0.00000 1.00000
O1 O 6 c -0.00400 0.25300 0.23633 1.00000
O2 O 6 c 0.01500 0.24800 0.11034 1.00000
O3 O 6 c 0.68100 0.19200 0.16733 1.00000
O4 O 6 c 0.44800 0.18800 0.29533 1.00000
O5 O 6 c 0.44900 0.25000 0.04800 1.00000
S1 S 6 c 0.37300 0.06500 0.50467 1.00000

```

Sr[S<sub>2</sub>O<sub>6</sub>](H<sub>2</sub>O)<sub>4</sub>: A10B2C\_hP39\_171\_5c\_c\_a - POSCAR

```

A10B2C_hP39_171_5c_c_a & a, c/a, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6
↳ , y6, z6, x7, y7, z7 --params=6.3199906634, 3.05221518986, 0.0, -0.004,
↳ 0.253, 0.23633, 0.015, 0.248, 0.11034, 0.681, 0.192, 0.16733, 0.448,
↳ 0.188, 0.29533, 0.449, 0.25, 0.048, 0.373, 0.065, 0.50467 & P6_4 C_
↳ 6]^4 #171 (ac^6) & hP39 & None & Sr[S2O6][H2O]4 & R. N.
↳ Hargreaves and E. Stanley, Zeitschrift f"ur Kristallographie
↳ - Crystalline Materials 135, 399-407 (1972)
1.000000000000000
3.15999533170000 -5.47327246618487 0.000000000000000
3.15999533170000 5.47327246618487 0.000000000000000
0.000000000000000 0.000000000000000 19.28997150260000
O S Sr
30 6 3
Direct
-0.004000000000000 0.253000000000000 0.236330000000000 O (6c)
-0.253000000000000 -0.257000000000000 0.902996666666667 O (6c)
0.257000000000000 0.004000000000000 0.569663333333333 O (6c)
0.004000000000000 -0.253000000000000 0.236330000000000 O (6c)
0.253000000000000 0.257000000000000 0.902996666666667 O (6c)
-0.257000000000000 -0.004000000000000 0.569663333333333 O (6c)
0.015000000000000 0.248000000000000 0.110340000000000 O (6c)
-0.248000000000000 -0.233000000000000 0.777006666666667 O (6c)
0.233000000000000 -0.015000000000000 0.443673333333333 O (6c)
-0.015000000000000 -0.248000000000000 0.110340000000000 O (6c)
0.248000000000000 0.233000000000000 0.777006666666667 O (6c)
-0.233000000000000 0.015000000000000 0.443673333333333 O (6c)
0.681000000000000 0.192000000000000 0.167330000000000 O (6c)
-0.192000000000000 0.489000000000000 0.833996666666667 O (6c)
-0.489000000000000 -0.681000000000000 0.500663333333333 O (6c)
-0.681000000000000 -0.192000000000000 0.167330000000000 O (6c)
0.192000000000000 -0.489000000000000 0.833996666666667 O (6c)
0.489000000000000 0.681000000000000 0.500663333333333 O (6c)
0.448000000000000 0.188000000000000 0.295330000000000 O (6c)
-0.188000000000000 0.260000000000000 0.961996666666667 O (6c)
-0.260000000000000 -0.448000000000000 0.628663333333333 O (6c)
-0.448000000000000 -0.188000000000000 0.295330000000000 O (6c)
0.188000000000000 -0.260000000000000 0.961996666666667 O (6c)
0.260000000000000 0.448000000000000 0.628663333333333 O (6c)
0.449000000000000 0.250000000000000 0.048000000000000 O (6c)
-0.250000000000000 0.199000000000000 0.714666666666667 O (6c)
-0.199000000000000 -0.449000000000000 0.381333333333333 O (6c)
-0.449000000000000 -0.250000000000000 0.048000000000000 O (6c)
0.250000000000000 -0.199000000000000 0.714666666666667 O (6c)
0.199000000000000 0.449000000000000 0.381333333333333 O (6c)
0.373000000000000 0.065000000000000 0.504670000000000 S (6c)
-0.065000000000000 0.308000000000000 1.171336666666667 S (6c)
-0.308000000000000 -0.373000000000000 0.838003333333333 S (6c)
-0.373000000000000 -0.065000000000000 0.504670000000000 S (6c)
0.065000000000000 -0.308000000000000 1.171336666666667 S (6c)
0.308000000000000 0.373000000000000 0.838003333333333 S (6c)
0.000000000000000 0.000000000000000 0.000000000000000 Sr (3a)
0.000000000000000 0.000000000000000 0.666666666666667 Sr (3a)
0.000000000000000 0.000000000000000 0.333333333333333 Sr (3a)

```

Sr[S<sub>2</sub>O<sub>6</sub>](H<sub>2</sub>O)<sub>4</sub>: A10B2C\_hP39\_172\_5c\_c\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Sr[S2O6][H2O]4'
_chemical_formula_sum 'O10 S2 Sr'

_aflow_title 'Sr[SS_2]SOS_6][HS_2]SO_4] Structure '
_aflow_proto 'A10B2C_hP39_172_5c_c_a'
_aflow_params 'a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7'
↳ 4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7'
_aflow_params_values '6.3199906634, 3.05221518986, 0.0, -0.004, 0.253,
↳ 0.76367, 0.015, 0.248, 0.88966, 0.681, 0.192, 0.83267, 0.448, 0.188,
↳ 0.70467, 0.449, 0.25, -0.048, 0.373, 0.065, 0.49533'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP39'

_cell_length_a 6.3199906634
_cell_length_b 6.3199906634
_cell_length_c 19.2899715026
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M 'P 64'
_symmetry_Int_Tables_number 172

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x-y, x, z+2/3
3 -y, x-y, z+1/3

```

```

4 -x, -y, z
5 -x+y, -x, z+2/3
6 y, -x+y, z+1/3

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Sr1 Sr 3 a 0.00000 0.00000 1.00000
O1 O 6 c -0.00400 0.25300 0.23633 1.00000
O2 O 6 c 0.01500 0.24800 0.11034 1.00000
O3 O 6 c 0.68100 0.19200 0.16733 1.00000
O4 O 6 c 0.44800 0.18800 0.29533 1.00000
O5 O 6 c 0.44900 0.25000 0.04800 1.00000
S1 S 6 c 0.37300 0.06500 0.50467 1.00000

```

Sr[S<sub>2</sub>O<sub>6</sub>](H<sub>2</sub>O)<sub>4</sub>: A10B2C\_hP39\_172\_5c\_c\_a - POSCAR

```

A10B2C_hP39_172_5c_c_a & a, c/a, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6
↳ , y6, z6, x7, y7, z7 --params=6.3199906634, 3.05221518986, 0.0, -0.004,
↳ 0.253, 0.76367, 0.015, 0.248, 0.88966, 0.681, 0.192, 0.83267, 0.448,
↳ 0.188, 0.70467, 0.449, 0.25, -0.048, 0.373, 0.065, 0.49533 & P6_4 C_
↳ {6}^5 #172 (ac^6) & hP39 & None & Sr[S2O6][H2O]4 & Sr[S2O6][
↳ H2O]4 &
1.000000000000000
3.15999533170000 -5.47327246618487 0.000000000000000
3.15999533170000 5.47327246618487 0.000000000000000
0.000000000000000 0.000000000000000 19.28997150260000
O S Sr
30 6 3
Direct
-0.004000000000000 0.253000000000000 0.763670000000000 O (6c)
-0.253000000000000 -0.257000000000000 1.097003333333333 O (6c)
0.257000000000000 0.004000000000000 0.889660000000000 O (6c)
0.004000000000000 -0.253000000000000 0.763670000000000 O (6c)
0.253000000000000 0.257000000000000 1.097003333333333 O (6c)
-0.257000000000000 -0.004000000000000 1.430336666666667 O (6c)
0.015000000000000 0.248000000000000 0.889660000000000 O (6c)
-0.248000000000000 -0.233000000000000 1.222993333333333 O (6c)
0.233000000000000 -0.015000000000000 1.556326666666667 O (6c)
-0.015000000000000 -0.248000000000000 0.889660000000000 O (6c)
0.248000000000000 0.233000000000000 1.222993333333333 O (6c)
-0.233000000000000 0.015000000000000 1.556326666666667 O (6c)
0.681000000000000 0.192000000000000 0.167330000000000 O (6c)
-0.192000000000000 0.489000000000000 0.832670000000000 O (6c)
-0.489000000000000 -0.681000000000000 1.166003333333333 O (6c)
-0.681000000000000 -0.192000000000000 0.832670000000000 O (6c)
0.192000000000000 -0.489000000000000 1.166003333333333 O (6c)
0.489000000000000 0.681000000000000 1.499336666666667 O (6c)
0.448000000000000 0.188000000000000 0.295330000000000 O (6c)
-0.188000000000000 0.260000000000000 1.038003333333333 O (6c)
-0.260000000000000 -0.448000000000000 1.371336666666667 O (6c)
-0.448000000000000 -0.188000000000000 0.704670000000000 O (6c)
0.188000000000000 -0.260000000000000 1.038003333333333 O (6c)
0.260000000000000 0.448000000000000 1.371336666666667 O (6c)
0.449000000000000 0.250000000000000 0.048000000000000 O (6c)
-0.250000000000000 0.199000000000000 1.038003333333333 O (6c)
-0.199000000000000 -0.449000000000000 1.371336666666667 O (6c)
-0.449000000000000 -0.250000000000000 0.048000000000000 O (6c)
0.250000000000000 -0.199000000000000 1.038003333333333 O (6c)
0.199000000000000 0.449000000000000 1.371336666666667 O (6c)
0.373000000000000 0.065000000000000 0.504670000000000 O (6c)
-0.065000000000000 0.308000000000000 1.161996666666667 O (6c)
-0.308000000000000 -0.373000000000000 0.828663333333333 S (6c)
-0.373000000000000 -0.065000000000000 0.504670000000000 O (6c)
0.065000000000000 -0.308000000000000 1.161996666666667 O (6c)
0.308000000000000 0.373000000000000 0.828663333333333 S (6c)
0.000000000000000 0.000000000000000 0.000000000000000 Sr (3a)
0.000000000000000 0.000000000000000 0.666666666666667 Sr (3a)
0.000000000000000 0.000000000000000 0.333333333333333 Sr (3a)

```

PI<sub>3</sub>: A3B\_hP8\_173\_c\_b - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'PI3'
_chemical_formula_sum 'I3 P'

loop_
_publ_author_name
'E. T. Lance'
'J. M. Haschke'
'D. R. Peacor'
_journal_name_full_name
;
Inorganic Chemistry
;
_journal_volume 15
_journal_year 1976
_journal_page_first 780
_journal_page_last 781
_publ_section_title
;
Crystal and molecular structure of phosphorus triiodide
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

```

```

_aflow_title 'PI3_{3}$ Structure'
_aflow_proto 'A3B_hP8_173_c_b'
_aflow_params 'a,c/a,z_{1},x_{2},y_{2},z_{2}'
_aflow_params_values '7.1329719992,1.03939436422,0.0,0.0337,0.3475,0.146
↪
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP8'

_cell_length_a 7.1329719992
_cell_length_b 7.1329719992
_cell_length_c 7.4139708961
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 63"
_symmetry_Int_Tables_number 173

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z+1/2
3 -y,x-y,z
4 -x,-y,z+1/2
5 -x+y,-x,z
6 y,-x+y,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
N1 N 2 b 0.33333 0.66667 0.00000 1.00000
N2 N 6 c 0.32840 0.03130 0.05000 1.00000
Si1 Si 6 c 0.23140 0.40630 0.01300 1.00000

```

PI<sub>3</sub>: A3B\_hP8\_173\_c\_b - POSCAR

```

A3B_hP8_173_c_b & a,c/a,z1,x2,y2,z2 --params=7.1329719992,1.03939436422,
↪ 0.0,0.0337,0.3475,0.146 & P6_{3} C_{6}^{6} #173 (bc) & hP8 &
↪ None & PI3 & E. T. Lance and J. M. Haschke and D. R. Peacor,
↪ Inorg. Chem. 15, 780-781 (1976)
1.0000000000000000
3.56648599960000 -6.17733495579027 0.0000000000000000
3.56648599960000 6.17733495579027 0.0000000000000000
0.00000000000000 0.00000000000000 7.41397089610000
1 P
6 2
Direct
0.03370000000000 0.34750000000000 0.14600000000000 I (6c)
-0.34750000000000 -0.31380000000000 0.14600000000000 I (6c)
0.31380000000000 -0.03370000000000 0.14600000000000 I (6c)
-0.03370000000000 -0.34750000000000 0.64600000000000 I (6c)
0.34750000000000 0.31380000000000 0.64600000000000 I (6c)
-0.31380000000000 0.03370000000000 0.64600000000000 I (6c)
0.33333333333333 0.66666666666667 0.00000000000000 P (2b)
0.66666666666667 0.33333333333333 0.50000000000000 P (2b)

```

β-Si<sub>3</sub>N<sub>4</sub>: A4B3\_hP14\_173\_bc\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'beta-Si3N4'
_chemical_formula_sum 'N4 Si3'

loop_
_publ_author_name
'W. D. Forgeng'
'B. F. Decker'
_journal_name_full_name
;
Transactions of the American Institute of Mining and Metallurgical
↪ Engineers
;
_journal_volume 212
_journal_year 1958
_journal_page_first 343
_journal_page_last 348
_publ_section_title
;
Nitrides of silicon
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title '$\beta$-Si3N4$ Structure'
_aflow_proto 'A4B3_hP14_173_bc_c'
_aflow_params 'a,c/a,z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3}'
_aflow_params_values '7.603038022,0.382612126795,0.0,0.3284,0.0313,0.05,
↪ 0.2314,0.4063,0.013'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP14'

_cell_length_a 7.6030380220
_cell_length_b 7.6030380220
_cell_length_c 2.9090145477
_cell_angle_alpha 90.0000000000

```

```

_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 63"
_symmetry_Int_Tables_number 173

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z+1/2
3 -y,x-y,z
4 -x,-y,z+1/2
5 -x+y,-x,z
6 y,-x+y,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
N1 N 2 b 0.33333 0.66667 0.00000 1.00000
N2 N 6 c 0.32840 0.03130 0.05000 1.00000
Si1 Si 6 c 0.23140 0.40630 0.01300 1.00000

```

β-Si<sub>3</sub>N<sub>4</sub>: A4B3\_hP14\_173\_bc\_c - POSCAR

```

A4B3_hP14_173_bc_c & a,c/a,z1,x2,y2,z2,x3,y3,z3 --params=7.603038022,
↪ 0.382612126795,0.0,0.3284,0.0313,0.05,0.2314,0.4063,0.013 & P6_
↪ {3} C_{6}^{6} #173 (bc^2) & hP14 & None & Si3N4 & beta & W. D.
↪ Forgeng and B. F. Decker, T. Am. I. Min. Met. Eng. 212, 343-348
↪ (1958)
1.0000000000000000
3.80151901100000 -6.58442407299099 0.0000000000000000
3.80151901100000 6.58442407299099 0.0000000000000000
0.00000000000000 0.00000000000000 2.90901454770000
N Si
8 6
Direct
0.33333333333333 0.66666666666667 0.00000000000000 N (2b)
0.66666666666667 0.33333333333333 0.50000000000000 N (2b)
0.32840000000000 0.03130000000000 0.05000000000000 N (6c)
-0.03130000000000 0.29710000000000 0.05000000000000 N (6c)
-0.29710000000000 -0.32840000000000 0.05000000000000 N (6c)
-0.32840000000000 -0.03130000000000 0.55000000000000 N (6c)
0.03130000000000 -0.29710000000000 0.55000000000000 N (6c)
0.29710000000000 0.32840000000000 0.55000000000000 N (6c)
0.23140000000000 0.40630000000000 0.01300000000000 Si (6c)
-0.40630000000000 -0.17490000000000 0.01300000000000 Si (6c)
0.17490000000000 -0.23140000000000 0.01300000000000 Si (6c)
-0.23140000000000 -0.40630000000000 0.51300000000000 Si (6c)
0.40630000000000 0.17490000000000 0.51300000000000 Si (6c)
-0.17490000000000 0.23140000000000 0.51300000000000 Si (6c)

```

Fe<sub>2</sub>Zr<sub>2</sub>P<sub>7</sub>: A12B7C2\_hP21\_174\_2j2k\_ajk\_cf - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Fe12Zr2P7'
_chemical_formula_sum 'Fe12 P7 Zr2'

loop_
_publ_author_name
'E. Ganglberger'
_journal_name_full_name
;
Monatshefte f{"u}r Chemie - Chemical Monthly
;
_journal_volume 99
_journal_year 1968
_journal_page_first 557
_journal_page_last 565
_publ_section_title
;
Die Kristallstruktur von FeS_{12}ZrS_{2}SPS_{7}$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'FeS_{12}ZrS_{2}SPS_{7}$ Structure'
_aflow_proto 'A12B7C2_hP21_174_2j2k_ajk_cf'
_aflow_params 'a,c/a,x_{4},y_{4},x_{5},y_{5},x_{6},y_{6},x_{7},y_{7},x_{
↪ 8},y_{8},x_{9},y_{9}'
_aflow_params_values '9.0004021308,0.399102242177,0.4309,0.3719,0.1189,
↪ 0.2772,0.4163,0.1204,0.0495,0.4359,0.2232,0.124,0.2889,0.4096'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP21'

_cell_length_a 9.0004021308
_cell_length_b 9.0004021308
_cell_length_c 3.5920806709
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P -6"
_symmetry_Int_Tables_number 174

```

```

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 -x+y,-x,-z
5 x,y,-z
6 -y,x-y,-z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
P1 P 1 a 0.00000 0.00000 0.00000 1.00000
Zr1 Zr 1 c 0.33333 0.66667 0.00000 1.00000
Zr2 Zr 1 f 0.66667 0.33333 0.50000 1.00000
Fe1 Fe 3 j 0.43090 0.37190 0.00000 1.00000
Fe2 Fe 3 j 0.11890 0.27720 0.00000 1.00000
P2 P 3 j 0.41630 0.12040 0.00000 1.00000
Fe3 Fe 3 k 0.04950 0.43590 0.50000 1.00000
Fe4 Fe 3 k 0.22320 0.12400 0.50000 1.00000
P3 P 3 k 0.28890 0.40960 0.50000 1.00000

```

Fe<sub>12</sub>Zr<sub>2</sub>P<sub>7</sub>: A12B7C2\_hP21\_174\_2j2k\_ajk\_cf - POSCAR

```

A12B7C2_hP21_174_2j2k_ajk_cf & a,c/a,x4,y4,x5,y5,x6,y6,x7,y7,x8,y8,x9,y9
--params=9.0004021308,0.399102242177,0.4309,0.3719,0.1189,
0.2772,0.4163,0.1204,0.0495,0.4359,0.2232,0.124,0.2889,0.4096 &
P-6 C_{3h}^{1} #174 (acfj^3k^3) & hP21 & None & Fe12Zr2P7 & &
E. Ganglberger, Monatsh. Chem. 99, 557-565 (1968)
1.0000000000000000
4.50020106540000 -7.79457688954839 0.0000000000000000
4.50020106540000 7.79457688954839 0.0000000000000000
0.0000000000000000 0.0000000000000000 3.59208067090000
Fe P Zr
12 7 2
Direct
0.4309000000000000 0.3719000000000000 0.0000000000000000 Fe (3j)
-0.3719000000000000 0.0590000000000000 0.0000000000000000 Fe (3j)
-0.0590000000000000 -0.4309000000000000 0.0000000000000000 Fe (3j)
0.1189000000000000 0.2772000000000000 0.0000000000000000 Fe (3j)
-0.2772000000000000 -0.1583000000000000 0.0000000000000000 Fe (3j)
0.1583000000000000 -0.1189000000000000 0.0000000000000000 Fe (3j)
0.0495000000000000 0.4359000000000000 0.5000000000000000 Fe (3k)
-0.4359000000000000 -0.3864000000000000 0.5000000000000000 Fe (3k)
0.3864000000000000 -0.0495000000000000 0.5000000000000000 Fe (3k)
0.2232000000000000 0.1240000000000000 0.5000000000000000 Fe (3k)
-0.1240000000000000 0.0992000000000000 0.5000000000000000 Fe (3k)
-0.0992000000000000 -0.2232000000000000 0.5000000000000000 Fe (3k)
0.0000000000000000 0.0000000000000000 0.0000000000000000 P (1a)
0.4163000000000000 0.1204000000000000 0.0000000000000000 P (3j)
-0.1204000000000000 0.2959000000000000 0.0000000000000000 P (3j)
-0.2959000000000000 -0.4163000000000000 0.0000000000000000 P (3j)
0.2889000000000000 0.4096000000000000 0.5000000000000000 P (3k)
-0.4096000000000000 -0.1207000000000000 0.5000000000000000 P (3k)
0.1207000000000000 -0.2889000000000000 0.5000000000000000 P (3k)
0.3333333333333333 0.6666666666666667 0.0000000000000000 Zr (1c)
0.6666666666666667 0.3333333333333333 0.5000000000000000 Zr (1f)

```

GdSI: ABC\_hP12\_174\_cj\_fk\_aj - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'GdSI'
_chemical_formula_sum 'Gd I S'

loop_
  _publ_author_name
  'C. Dagron'
  'F. Thevet'
  _journal_name_full_name
  ;
Comptes Rendus Hebdomadaires des S{\'e}ances de l'Acad{\'e}mie des
  ↪ Sciences S{\'e}rie C - Sciences chimiques
;
_journal_volume 268
_journal_year 1969
_journal_page_first 1867
_journal_page_last 1869
_publ_section_title
;
R{\'e}partition des types cristallins dans la s{\'e}rie des
  ↪ iodures et fluorures des {\'e}l{\'e}ments des
  ↪ terres rares et d'yttrium
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'GdSI Structure'
_aflow_proto 'ABC_hP12_174_cj_fk_aj'
_aflow_params 'a,c/a,x_{4},y_{4},x_{5},y_{5},x_{6},y_{6}'
_aflow_params_values '10.7303215747,0.395153774459,0.30167,0.15433,
  ↪ 0.03467,0.51733,0.14967,0.31433'
_aflow_Structurbericht 'None'
_aflow_Pearson 'hP12'

```

```

_cell_length_a 10.7303215747
_cell_length_b 10.7303215747
_cell_length_c 4.2401270714
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P -6"
_symmetry_Int_Tables_number 174

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 -x+y,-x,-z
5 x,y,-z
6 -y,x-y,-z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
S1 S 1 a 0.00000 0.00000 0.00000 1.00000
Gd1 Gd 1 c 0.33333 0.66667 0.00000 1.00000
I1 I 1 f 0.66667 0.33333 0.50000 1.00000
Gd2 Gd 3 j 0.30167 0.15433 0.00000 1.00000
S2 S 3 j 0.03467 0.51733 0.00000 1.00000
I2 I 3 k 0.14967 0.31433 0.50000 1.00000

```

GdSI: ABC\_hP12\_174\_cj\_fk\_aj - POSCAR

```

ABC_hP12_174_cj_fk_aj & a,c/a,x4,y4,x5,y5,x6,y6 --params=10.7303215747,
  ↪ 0.395153774459,0.30167,0.15433,0.03467,0.51733,0.14967,0.31433
  ↪ & P-6 C_{3h}^{1} #174 (acfj^2k) & hP12 & None & GdSI & C.
  ↪ Dagron and F. Thevet, {C. R. Hebd. S{\'e}ances Acad. Sci. C 268,
  ↪ 1867-1869 (1969)
1.0000000000000000
5.36516078735000 -9.29273107446644 0.0000000000000000
5.36516078735000 9.29273107446644 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.24012707140000
Gd I S
4 4 4
Direct
0.3333333333333333 0.6666666666666667 0.0000000000000000 Gd (1c)
0.3016700000000000 0.1543300000000000 0.0000000000000000 Gd (3j)
-0.1543300000000000 0.1473400000000000 0.0000000000000000 Gd (3j)
-0.1473400000000000 -0.3016700000000000 0.0000000000000000 Gd (3j)
0.6666666666666667 0.3333333333333333 0.5000000000000000 I (1f)
0.1496700000000000 0.3143300000000000 0.5000000000000000 I (3k)
-0.3143300000000000 -0.1646600000000000 0.5000000000000000 I (3k)
0.1646600000000000 -0.1496700000000000 0.5000000000000000 I (3k)
0.0000000000000000 0.0000000000000000 0.0000000000000000 S (1a)
0.0346700000000000 0.5173300000000000 0.0000000000000000 S (3j)
-0.5173300000000000 -0.4826600000000000 0.0000000000000000 S (3j)
0.4826600000000000 -0.0346700000000000 0.0000000000000000 S (3j)

```

Nb<sub>7</sub>Ru<sub>6</sub>B<sub>8</sub>: A8B7C6\_hP21\_175\_ck\_aj\_k - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Nb7Ru6B8'
_chemical_formula_sum 'B8 Nb7 Ru6'

loop_
  _publ_author_name
  'Q. Zheng'
  'M. Kohout'
  'R. Gumenuik'
  'N. Abramchuk'
  'H. Borrmann'
  'Y. Prots'
  'U. Burkhardt'
  'W. Schnelle'
  'L. Akselrud'
  'H. Gu'
  'A. {Leithe-Jasper}'
  'Y. Grin'
  _journal_name_full_name
  ;
Inorganic Chemistry
;
_journal_volume 51
_journal_year 2012
_journal_page_first 7472
_journal_page_last 7483
_publ_section_title
;
TMS_{7} TM_{6} SBS_{8} (TM = Ta, Nb; TM' = Ru, Rh, Ir): New
  ↪ Compounds with [B_{6}] Ring Polyaniions
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'Nb_{7}Ru_{6}SBS_{8} Structure'
_aflow_proto 'A8B7C6_hP21_175_ck_aj_k'

```

```

_aflow_params 'a,c/a,x_{3},y_{3},x_{4},y_{4},x_{5},y_{5}'
_aflow_params_values '9.5057625379,0.329093950194,0.36335,0.08627,0.0661
↪ ,0.221,0.15405,0.51373'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP21'

_cell_length_a 9.5057625379
_cell_length_b 9.5057625379
_cell_length_c 3.1282889432
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 6/m"
_symmetry_Int_Tables_number 175

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z
3 -y,x-y,z
4 -x,-y,z
5 -x+y,-x,z
6 y,-x+y,z
7 -x,-y,-z
8 -x+y,-x,-z
9 y,-x+y,-z
10 x,y,-z
11 x-y,x,-z
12 -y,x-y,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Nb1 Nb 1 a 0.00000 0.00000 1.00000
B1 B 2 c 0.33333 0.66667 0.00000 1.00000
Nb2 Nb 6 j 0.36335 0.08627 0.00000 1.00000
B2 B 6 k 0.06610 0.22100 0.50000 1.00000
Ru1 Ru 6 k 0.15405 0.51373 0.50000 1.00000

```

Nb<sub>7</sub>Ru<sub>6</sub>B<sub>8</sub>: A8B7C6\_hP21\_175\_ck\_aj\_k - POSCAR

```

A8B7C6_hP21_175_ck_aj_k & a,c/a,x3,y3,x4,y4,x5,y5 --params=9.5057625379,
↪ 0.329093950194,0.36335,0.08627,0.0661,0.221,0.15405,0.51373 &
↪ P6/m C_{6h}^{1} #175 (acjk^2) & hP21 & None & Nb7Ru6B8 & C & Q.
↪ Zheng et al., Inorg. Chem. 51, 7472-7483 (2012)
1.0000000000000000
4.75288126895000 -8.23223184016384 0.0000000000000000
4.75288126895000 8.23223184016384 0.0000000000000000
0.00000000000000 0.00000000000000 3.12828894320000
B Nb Ru
8 7 6
Direct
0.33333333333333 0.66666666666667 0.00000000000000 B (2c)
0.66666666666667 0.33333333333333 0.00000000000000 B (2c)
0.06610000000000 0.22100000000000 0.50000000000000 B (6k)
-0.22100000000000 -0.15490000000000 0.50000000000000 B (6k)
0.15490000000000 -0.06610000000000 0.50000000000000 B (6k)
-0.06610000000000 -0.22100000000000 0.50000000000000 B (6k)
0.22100000000000 0.15490000000000 0.50000000000000 B (6k)
-0.15490000000000 0.06610000000000 0.50000000000000 B (6k)
0.00000000000000 0.00000000000000 0.00000000000000 Nb (1a)
0.36335000000000 0.08627000000000 0.00000000000000 Nb (6j)
-0.08627000000000 0.27708000000000 0.00000000000000 Nb (6j)
-0.27708000000000 -0.36335000000000 0.00000000000000 Nb (6j)
-0.36335000000000 -0.08627000000000 0.00000000000000 Nb (6j)
0.08627000000000 -0.27708000000000 0.00000000000000 Nb (6j)
0.27708000000000 0.36335000000000 0.00000000000000 Nb (6j)
0.15405000000000 0.51373000000000 0.50000000000000 Ru (6k)
-0.51373000000000 -0.35968000000000 0.50000000000000 Ru (6k)
0.35968000000000 -0.15405000000000 0.50000000000000 Ru (6k)
-0.15405000000000 -0.51373000000000 0.50000000000000 Ru (6k)
0.51373000000000 0.35968000000000 0.50000000000000 Ru (6k)
-0.35968000000000 0.15405000000000 0.50000000000000 Ru (6k)

```

Mg[NH]: ABC\_hP36\_175\_jk\_jk\_jk - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Mg[NH]'
_chemical_formula_sum 'H Mg N'

loop_
_publ_author_name
'F. Dolci'
'E. Napolitano'
'E. Weidner'
'S. Enzo'
'P. Moretto'
'M. Brunelli'
'T. Hansen'
'M. Fichtner'
'W. Lohstroh'
_journal_name_full_name
;
Inorganic Chemistry

```

```

;
_journal_volume 50
_journal_year 2010
_journal_page_first 1116
_journal_page_last 1122
_publ_Section_title
;
Magnesium imide: synthesis and structure determination of an
↪ unconventional alkaline earth imide from decomposition of
↪ magnesium amide
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'Mg[NH] Structure'
_aflow_proto 'ABC_hP36_175_jk_jk_jk'
_aflow_params 'a,c/a,x_{1},y_{1},x_{2},y_{2},x_{3},y_{3},x_{4},y_{4},x_{
↪ 5},y_{5},x_{6},y_{6}'
_aflow_params_values '11.5799622371,0.317895264089,0.255,0.0598,0.1323,
↪ 0.416,0.3483,0.0762,0.2334,0.5727,0.4279,0.0715,0.1367,0.5046'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP36'

_cell_length_a 11.5799622371
_cell_length_b 11.5799622371
_cell_length_c 3.6812151535
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 6/m"
_symmetry_Int_Tables_number 175

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z
3 -y,x-y,z
4 -x,-y,z
5 -x+y,-x,z
6 y,-x+y,z
7 -x,-y,-z
8 -x+y,-x,-z
9 y,-x+y,-z
10 x,y,-z
11 x-y,x,-z
12 -y,x-y,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 6 j 0.25500 0.05980 0.00000 1.00000
Mg1 Mg 6 j 0.13230 0.41600 0.00000 1.00000
N1 N 6 j 0.34830 0.07620 0.00000 1.00000
H2 H 6 k 0.23340 0.57270 0.50000 1.00000
Mg2 Mg 6 k 0.42790 0.07150 0.50000 1.00000
N2 N 6 k 0.13670 0.50460 0.50000 1.00000

```

Mg[NH]: ABC\_hP36\_175\_jk\_jk\_jk - POSCAR

```

ABC_hP36_175_jk_jk_jk & a,c/a,x1,y1,x2,y2,x3,y3,x4,y4,x5,y5,x6,y6 --
↪ params=11.5799622371,0.317895264089,0.255,0.0598,0.1323,0.416,
↪ 0.3483,0.0762,0.2334,0.5727,0.4279,0.0715,0.1367,0.5046 & P6/m
↪ C_{6h}^{1} #175 (j^3k^3) & hP36 & None & Mg[NH] & F & F. Dolci
↪ et al., Inorg. Chem. 50, 1116-1122 (2010)
1.0000000000000000
5.78998111855000 -10.02854147219310 0.00000000000000
5.78998111855000 10.02854147219310 0.00000000000000
0.00000000000000 0.00000000000000 3.68121515350000
H Mg N
12 12 12
Direct
0.25500000000000 0.05980000000000 0.00000000000000 H (6j)
-0.05980000000000 0.19520000000000 0.00000000000000 H (6j)
-0.19520000000000 -0.25500000000000 0.00000000000000 H (6j)
-0.25500000000000 -0.05980000000000 0.00000000000000 H (6j)
0.05980000000000 -0.19520000000000 0.00000000000000 H (6j)
0.19520000000000 0.25500000000000 0.00000000000000 H (6j)
0.23340000000000 0.57270000000000 0.50000000000000 H (6k)
-0.57270000000000 -0.33930000000000 0.50000000000000 H (6k)
0.33930000000000 -0.23340000000000 0.50000000000000 H (6k)
-0.23340000000000 -0.57270000000000 0.50000000000000 H (6k)
0.57270000000000 0.33930000000000 0.50000000000000 H (6k)
-0.33930000000000 0.23340000000000 0.50000000000000 H (6k)
0.13230000000000 0.41600000000000 0.00000000000000 Mg (6j)
-0.41600000000000 -0.28370000000000 0.00000000000000 Mg (6j)
0.28370000000000 -0.13230000000000 0.00000000000000 Mg (6j)
-0.13230000000000 -0.41600000000000 0.00000000000000 Mg (6j)
0.41600000000000 0.28370000000000 0.00000000000000 Mg (6j)
-0.28370000000000 0.13230000000000 0.00000000000000 Mg (6j)
0.42790000000000 0.07150000000000 0.50000000000000 Mg (6k)
-0.07150000000000 0.35640000000000 0.50000000000000 Mg (6k)
-0.35640000000000 -0.42790000000000 0.50000000000000 Mg (6k)
-0.42790000000000 -0.07150000000000 0.50000000000000 Mg (6k)
0.07150000000000 -0.35640000000000 0.50000000000000 Mg (6k)
0.35640000000000 0.42790000000000 0.50000000000000 Mg (6k)
0.34830000000000 0.07620000000000 0.00000000000000 N (6j)

```



-0.07620000000000	0.27210000000000	0.00000000000000	N	(6j)
-0.27210000000000	-0.34830000000000	0.00000000000000	N	(6j)
-0.34830000000000	-0.07620000000000	0.00000000000000	N	(6j)
0.07620000000000	-0.27210000000000	0.00000000000000	N	(6j)
0.27210000000000	0.34830000000000	0.00000000000000	N	(6j)
0.13670000000000	0.50460000000000	0.50000000000000	N	(6k)
-0.50460000000000	-0.36790000000000	0.50000000000000	N	(6k)
0.36790000000000	-0.13670000000000	0.50000000000000	N	(6k)
-0.13670000000000	-0.50460000000000	0.50000000000000	N	(6k)
0.50460000000000	0.36790000000000	0.50000000000000	N	(6k)
-0.36790000000000	0.13670000000000	0.50000000000000	N	(6k)

Er<sub>3</sub>Ru<sub>2</sub>: A3B2\_hP10\_176\_h\_bd - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Er3Ru2'
_chemical_formula_sum 'Er3 Ru2'

loop_
_publ_author_name
'A. Palenzona'
_journal_name_full_name
;
Journal of the Less-Common Metals
;
_journal_volume 159
_journal_year 1990
_journal_page_first L21
_journal_page_last L23
_publ_section_title
;
The phase diagram of the Er-Ru system
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'Er$_{3}$Ru$_{2}$ Structure'
_aflow_proto 'A3B2_hP10_176_h_bd'
_aflow_params 'a,c/a,x_{3},y_{3}'
_aflow_params_values '7.8700439404,0.50025412961,0.0915,0.7068'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP10'

_cell_length_a 7.8700439404
_cell_length_b 7.8700439404
_cell_length_c 3.9370219814
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 63/m"
_symmetry_Int_Tables_number 176

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z+1/2
3 -y,x-y,z
4 -x,-y,z+1/2
5 -x+y,-x,z
6 y,-x+y,z+1/2
7 -x,-y,-z
8 -x+y,-x,-z+1/2
9 y,-x+y,-z
10 x,y,-z+1/2
11 x-y,x,-z
12 -y,x-y,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ru1 Ru 2 b 0.00000 0.00000 0.00000 1.00000
Ru2 Ru 2 d 0.66667 0.33333 0.25000 1.00000
Er1 Er 6 h 0.09150 0.70680 0.25000 1.00000
```

Er<sub>3</sub>Ru<sub>2</sub>: A3B2\_hP10\_176\_h\_bd - POSCAR

```
A3B2_hP10_176_h_bd & a,c/a,x3,y3 --params=7.8700439404,0.50025412961,
↳ 0.0915,0.7068 & P6_{3}/m C_{6h}^{2} #176 (bdh) & hP10 & None &
↳ Er3Ru2 & A. Palenzona, J. Less-Common Met. 159, L21-L23 (
↳ 1990)
1.00000000000000
3.93502197020000 -6.81565798128618 0.00000000000000
3.93502197020000 6.81565798128618 0.00000000000000
0.00000000000000 0.00000000000000 3.93702198140000
Er Ru
6 4
Direct
0.09150000000000 0.70680000000000 0.25000000000000 Er (6h)
-0.70680000000000 -0.61530000000000 0.25000000000000 Er (6h)
0.61530000000000 -0.09150000000000 0.25000000000000 Er (6h)
-0.09150000000000 -0.70680000000000 0.75000000000000 Er (6h)
0.70680000000000 0.61530000000000 0.75000000000000 Er (6h)
-0.61530000000000 0.09150000000000 0.75000000000000 Er (6h)
```

0.00000000000000	0.00000000000000	0.00000000000000	Ru	(2b)
0.00000000000000	0.00000000000000	0.50000000000000	Ru	(2b)
0.66666666666667	0.33333333333333	0.25000000000000	Ru	(2d)
0.33333333333333	0.66666666666667	0.75000000000000	Ru	(2d)

Fe<sub>3</sub>Te<sub>3</sub>Tl: A3B3C\_hP14\_176\_h\_h\_d - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Fe3Te3Tl'
_chemical_formula_sum 'Fe3 Te3 Tl'

loop_
_publ_author_name
'K. Klepp'
'H. Boller'
_journal_name_full_name
;
Acta Crystallographica Section A: Foundations and Advances
;
_journal_volume 34
_journal_year 1978
_journal_page_first S160
_journal_page_last S161
_publ_section_title
;
Crystal Structures of Thallium-Iron Chalcogenides
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'Fe$_{3}$Te$_{3}$Tl Structure'
_aflow_proto 'A3B3C_hP14_176_h_h_d'
_aflow_params 'a,c/a,x_{2},y_{2},x_{3},y_{3}'
_aflow_params_values '9.3500327107,0.451336898402,0.1701,0.0208,0.0462,
↳ 0.6892'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP14'

_cell_length_a 9.3500327107
_cell_length_b 9.3500327107
_cell_length_c 4.2200147636
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 63/m"
_symmetry_Int_Tables_number 176

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z+1/2
3 -y,x-y,z
4 -x,-y,z+1/2
5 -x+y,-x,z
6 y,-x+y,z+1/2
7 -x,-y,-z
8 -x+y,-x,-z+1/2
9 y,-x+y,-z
10 x,y,-z+1/2
11 x-y,x,-z
12 -y,x-y,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Tl1 Tl 2 d 0.66667 0.33333 0.25000 1.00000
Fe1 Fe 6 h 0.17010 0.02080 0.25000 1.00000
Te1 Te 6 h 0.04620 0.68920 0.25000 1.00000
```

Fe<sub>3</sub>Te<sub>3</sub>Tl: A3B3C\_hP14\_176\_h\_h\_d - POSCAR

```
A3B3C_hP14_176_h_h_d & a,c/a,x2,y2,x3,y3 --params=9.3500327107,
↳ 0.451336898402,0.1701,0.0208,0.0462,0.6892 & P6_{3}/m C_{6h}^{2} #176 (dh^2) & hP14 & None & Fe3Te3Tl & K. Klepp and H.
↳ Boller, Acta Crystallogr. Sect. A 34, S160-S161 (1978)
1.00000000000000
4.67501635535000 -8.09736585368168 0.00000000000000
4.67501635535000 8.09736585368168 0.00000000000000
0.00000000000000 0.00000000000000 4.22001476360000
Fe Te Tl
6 6 2
Direct
0.17010000000000 0.02080000000000 0.25000000000000 Fe (6h)
-0.02080000000000 -0.14930000000000 0.25000000000000 Fe (6h)
-0.14930000000000 -0.17010000000000 0.25000000000000 Fe (6h)
-0.17010000000000 -0.02080000000000 0.75000000000000 Fe (6h)
0.02080000000000 -0.14930000000000 0.75000000000000 Fe (6h)
0.14930000000000 0.17010000000000 0.75000000000000 Fe (6h)
0.04620000000000 0.68920000000000 0.25000000000000 Te (6h)
-0.68920000000000 -0.64300000000000 0.25000000000000 Te (6h)
0.64300000000000 -0.04620000000000 0.25000000000000 Te (6h)
-0.04620000000000 -0.68920000000000 0.75000000000000 Te (6h)
0.68920000000000 0.64300000000000 0.75000000000000 Te (6h)
```

```
-0.64300000000000 0.04620000000000 0.75000000000000 Te (6h)
0.66666666666667 0.33333333333333 0.25000000000000 Tl (2d)
0.33333333333333 0.66666666666667 0.75000000000000 Tl (2d)
```

UCl<sub>3</sub>: A3B\_hP8\_176\_h\_d - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'UCl3'
_chemical_formula_sum 'Cl3 U'

loop_
  _publ_author_name
  'W. H. Zachariassen'
  _journal_name_full_name
  ;
Acta Crystallographica
;
_journal_volume 1
_journal_year 1948
_journal_page_first 265
_journal_page_last 268
_publ_section_title
;
Crystal chemical studies of the 5f-series of elements. I. New structure
↪ types
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_flow_title 'UCI3_{3}$ Structure'
_flow_proto 'A3B_hP8_176_h_d'
_flow_params 'a,c/a,x_{1},x_{2},y_{2}'
_flow_params_values '7.4429335392,0.580545478976,0.083,0.708'
_flow_Structurbericht 'None'
_flow_Pearson 'hP8'

_cell_length_a 7.4429335392
_cell_length_b 7.4429335392
_cell_length_c 4.3209614165
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 63/m"
_symmetry_Int_Tables_number 176

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z+1/2
3 -y,x-y,z
4 -x,-y,z+1/2
5 -x+y,-x,z
6 y,-x+y,z+1/2
7 -x,-y,-z
8 -x+y,-x,-z+1/2
9 y,-x+y,-z
10 x,y,-z+1/2
11 x-y,x,-z
12 -y,x-y,-z+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
U1 U 2 d 0.66667 0.33333 0.25000 1.00000
Cl1 Cl 6 h 0.08300 0.70800 0.25000 1.00000
```

UCl<sub>3</sub>: A3B\_hP8\_176\_h\_d - POSCAR

```
A3B_hP8_176_h_d & a,c/a,x2,y2 --params=7.4429335392,0.580545478976,0.083
↪ 0.708 & P6_{3}/m C_{6h}^{2} #176 (dh) & hP8 & None & UCl3 & &
↪ W. H. Zachariassen, Acta Cryst. 1, 265-268 (1948)
1.00000000000000
3.72146676960000 -6.44576952362642 0.00000000000000
3.72146676960000 6.44576952362642 0.00000000000000
0.00000000000000 0.00000000000000 4.32096141650000
Cl U
6 2
Direct
0.08300000000000 0.70800000000000 0.25000000000000 Cl (6h)
-0.70800000000000 -0.62500000000000 0.25000000000000 Cl (6h)
0.62500000000000 -0.08300000000000 0.25000000000000 Cl (6h)
-0.08300000000000 -0.70800000000000 0.75000000000000 Cl (6h)
0.70800000000000 0.62500000000000 0.75000000000000 Cl (6h)
-0.62500000000000 0.08300000000000 0.75000000000000 Cl (6h)
0.66666666666667 0.33333333333333 0.25000000000000 U (2d)
0.33333333333333 0.66666666666667 0.75000000000000 U (2d)
```

SiO<sub>2</sub>: A2B\_hP36\_177\_j2lm\_n - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
```

```
_chemical_name_mineral 'SiO2'
_chemical_formula_sum 'O2 Si'

_flow_title 'SiOS_{2}$ Structure'
_flow_proto 'A2B_hP36_177_j2lm_n'
_flow_params 'a,c/a,x_{1},x_{2},x_{3},x_{4},x_{5},y_{5},z_{5}'
_flow_params_values '12.7835,0.291064262526,0.61855,0.39242,0.79257,
↪ 0.44445,0.52169,0.86952,0.16458'
_flow_Structurbericht 'None'
_flow_Pearson 'hP36'

_cell_length_a 12.7835000000
_cell_length_b 12.7835000000
_cell_length_c 3.7208200000
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 6 2 2"
_symmetry_Int_Tables_number 177

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z
3 -y,x-y,z
4 -x,-y,z
5 -x+y,-x,z
6 y,-x+y,z
7 x-y,-y,-z
8 x,x-y,-z
9 y,x,-z
10 -x+y,y,-z
11 -x,-x+y,-z
12 -y,-x,-z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
O1 O 6 j 0.61855 0.00000 0.00000 1.00000
O2 O 6 l 0.39242 0.60758 0.00000 1.00000
O3 O 6 l 0.79257 0.20743 0.00000 1.00000
O4 O 6 m 0.44445 0.55555 0.50000 1.00000
Si1 Si 12 n 0.52169 0.86952 0.16458 1.00000
```

SiO<sub>2</sub>: A2B\_hP36\_177\_j2lm\_n - POSCAR

```
A2B_hP36_177_j2lm_n & a,c/a,x1,x2,x3,x4,x5,y5,z5 --params=12.7835,
↪ 0.291064262526,0.61855,0.39242,0.79257,0.44445,0.52169,0.86952,
↪ 0.16458 & P622 D_{6}^{1} #177 (j1^2mm) & hP36 & None & SiO2 &
↪ &
1.00000000000000
6.39175000000000 -11.07083574927840 0.00000000000000
6.39175000000000 11.07083574927840 0.00000000000000
0.00000000000000 0.00000000000000 3.72082000000000
O Si
24 12
Direct
0.61855000000000 0.00000000000000 0.00000000000000 O (6j)
0.00000000000000 0.61855000000000 0.00000000000000 O (6j)
-0.61855000000000 -0.61855000000000 0.00000000000000 O (6j)
-0.61855000000000 0.00000000000000 0.00000000000000 O (6j)
0.00000000000000 -0.61855000000000 0.00000000000000 O (6j)
0.61855000000000 0.61855000000000 0.00000000000000 O (6j)
0.39242000000000 -0.39242000000000 0.00000000000000 O (6l)
0.39242000000000 0.78484000000000 0.00000000000000 O (6l)
-0.78484000000000 -0.39242000000000 0.00000000000000 O (6l)
-0.39242000000000 0.39242000000000 0.00000000000000 O (6l)
-0.39242000000000 -0.78484000000000 0.00000000000000 O (6l)
0.78484000000000 0.39242000000000 0.00000000000000 O (6l)
0.78484000000000 -0.79257000000000 0.00000000000000 O (6l)
0.79257000000000 1.58514000000000 0.00000000000000 O (6l)
-1.58514000000000 -0.79257000000000 0.00000000000000 O (6l)
-0.79257000000000 0.79257000000000 0.00000000000000 O (6l)
-0.79257000000000 -1.58514000000000 0.00000000000000 O (6l)
1.58514000000000 0.79257000000000 0.00000000000000 O (6l)
0.44445000000000 -0.44445000000000 0.50000000000000 O (6m)
0.44445000000000 0.88890000000000 0.50000000000000 O (6m)
-0.88890000000000 -0.44445000000000 0.50000000000000 O (6m)
-0.44445000000000 0.44445000000000 0.50000000000000 O (6m)
-0.44445000000000 -0.88890000000000 0.50000000000000 O (6m)
0.88890000000000 0.44445000000000 0.50000000000000 O (6m)
0.52169000000000 0.86952000000000 0.16458000000000 Si (12n)
-0.86952000000000 -0.34783000000000 0.16458000000000 Si (12n)
0.34783000000000 -0.52169000000000 0.16458000000000 Si (12n)
-0.52169000000000 -0.86952000000000 0.16458000000000 Si (12n)
0.86952000000000 0.34783000000000 0.16458000000000 Si (12n)
-0.34783000000000 0.52169000000000 0.16458000000000 Si (12n)
0.86952000000000 0.52169000000000 -0.16458000000000 Si (12n)
-0.34783000000000 -0.86952000000000 0.16458000000000 Si (12n)
-0.52169000000000 0.34783000000000 -0.16458000000000 Si (12n)
-0.86952000000000 -0.52169000000000 0.16458000000000 Si (12n)
0.34783000000000 0.86952000000000 -0.16458000000000 Si (12n)
0.52169000000000 -0.34783000000000 0.16458000000000 Si (12n)
```

AuF<sub>3</sub>: AB<sub>3</sub>hP24\_178\_b\_ac - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'AuF3'
_chemical_formula_sum 'Au F3'

loop_
  _publ_author_name
  'L. B. Asprey'
  'F. H. Kruse'
  'K. H. Jack'
  'R. Maitland'
  _journal_name_full_name
  ;
  Inorganic Chemistry
  ;
  _journal_volume 3
  _journal_year 1964
  _journal_page_first 602
  _journal_page_last 604
  _publ_section_title
  ;
  Preparation and properties of crystalline gold trifluoride
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title 'AuF3_{3}$ Structure'
_aflow_proto 'AB3_hP24_178_b_ac'
_aflow_params 'a,c/a,x_{1},x_{2},x_{3},y_{3},z_{3}'
_aflow_params_values '5.14898393,3.15789473684,0.8361,0.7601,0.5338,
  ↳ 0.3099,-0.0053'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP24'

_cell_length_a 5.1489839300
_cell_length_b 5.1489839300
_cell_length_c 16.2599492526
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 61 2 2"
_symmetry_Int_Tables_number 178

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x-y,x,z+1/6
  3 -y,x-y,z+1/3
  4 -x,-y,z+1/2
  5 -x+y,-x,z+2/3
  6 y,-x+y,z+5/6
  7 x-y,-y,-z
  8 x,x-y,-z+1/6
  9 y,x,-z+1/3
  10 -x+y,y,-z+1/2
  11 -x,-x+y,-z+2/3
  12 -y,-x,-z+5/6

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  F1 F 6 a 0.83610 0.00000 0.00000 1.00000
  Au1 Au 6 b 0.76010 0.52020 0.25000 1.00000
  F2 F 12 c 0.53380 0.30990 -0.00530 1.00000
```

AuF<sub>3</sub>: AB<sub>3</sub>hP24\_178\_b\_ac - POSCAR

```
AB3_hP24_178_b_ac & a,c/a,x1,x2,x3,y3,z3 --params=5.14898393,
  ↳ 3.15789473684,0.8361,0.7601,0.5338,0.3099,-0.0053 & P6_{1}22 D_
  ↳ {6}^{2} #178 (abc) & hP24 & None & AuF3 & L. B. Asprey et
  ↳ al., Inorg. Chem. 3, 602-604 (1964)
1.00000000000000
2.57449196500000 -4.45915088705784 0.00000000000000
2.57449196500000 4.45915088705784 0.00000000000000
0.00000000000000 0.00000000000000 16.25994925260000
Au F
6 18
Direct
0.76010000000000 1.52020000000000 0.25000000000000 Au (6b)
-1.52020000000000 -0.76010000000000 0.58333333333333 Au (6b)
0.76010000000000 -0.76010000000000 0.91666666666667 Au (6b)
-0.76010000000000 -1.52020000000000 0.75000000000000 Au (6b)
1.52020000000000 0.76010000000000 0.08333333333333 Au (6b)
-0.76010000000000 0.76010000000000 0.41666666666667 Au (6b)
0.83610000000000 0.00000000000000 0.00000000000000 F (6a)
0.00000000000000 0.83610000000000 0.33333333333333 F (6a)
-0.83610000000000 -0.83610000000000 0.66666666666667 F (6a)
-0.83610000000000 0.00000000000000 0.50000000000000 F (6a)
0.00000000000000 -0.83610000000000 0.83333333333333 F (6a)
0.83610000000000 0.83610000000000 0.16666666666667 F (6a)
0.53380000000000 0.30990000000000 -0.00530000000000 F (12c)
-0.30990000000000 0.22390000000000 0.22390000000000 F (12c)
-0.22390000000000 -0.53380000000000 0.66136666666667 F (12c)
-0.53380000000000 -0.30990000000000 0.49470000000000 F (12c)
```

```
0.30990000000000 -0.22390000000000 0.82803333333333 F (12c)
0.22390000000000 0.53380000000000 0.16136666666667 F (12c)
0.30990000000000 0.53380000000000 0.33863333333333 F (12c)
0.22390000000000 -0.30990000000000 0.00530000000000 F (12c)
-0.53380000000000 -0.22390000000000 0.67196666666667 F (12c)
-0.30990000000000 -0.53380000000000 0.83863333333333 F (12c)
-0.22390000000000 0.30990000000000 0.50530000000000 F (12c)
0.53380000000000 0.22390000000000 0.17196666666667 F (12c)
```

Sc-V (High-pressure): A\_hP6\_178\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Sc V'
_chemical_formula_sum 'Sc'

loop_
  _publ_author_name
  'Y. Akahama'
  'H. Fujihisa'
  'H. Kawamura'
  _journal_name_full_name
  ;
  Physical Review Letters
  ;
  _journal_volume 94
  _journal_year 2005
  _journal_page_first 195503
  _journal_page_last 195503
  _publ_section_title
  ;
  New Helical Chain Structure for Scandium at 240 GPa
  ;

_aflow_title 'Sc-V (High-pressure) Structure'
_aflow_proto 'A_hP6_178_a'
_aflow_params 'a,c/a,x_{1}'
_aflow_params_values '2.355,4.43566878981,0.461'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP6'

_symmetry_space_group_name_H-M "P 61 2 2"
_symmetry_Int_Tables_number 178

_cell_length_a 2.35500
_cell_length_b 2.35500
_cell_length_c 10.44600
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x-y,x,z+1/6
  3 -y,x-y,z+1/3
  4 -x,-y,z+1/2
  5 -x+y,-x,z+2/3
  6 y,-x+y,z+5/6
  7 x-y,-y,-z
  8 x,x-y,-z+1/6
  9 y,x,-z+1/3
  10 -x+y,y,-z+1/2
  11 -x,-x+y,-z+2/3
  12 -y,-x,-z+5/6

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Sc1 Sc 6 a 0.46100 0.00000 0.00000 1.00000
```

Sc-V (High-pressure): A\_hP6\_178\_a - POSCAR

```
A_hP6_178_a & a,c/a,x1 --params=2.355,4.43566878981,0.461 & P6_{1}22 D_{
  ↳ 6}^{2} #178 (a) & hP6 & None & Sc & Sc V & Y. Akahama and H.
  ↳ Fujihisa and H. Kawamura, Phys. Rev. Lett. 94, 195503 (2005)
1.00000000000000
1.17750000000000 -2.03948982591235 0.00000000000000
1.17750000000000 2.03948982591235 0.00000000000000
0.00000000000000 0.00000000000000 10.44600000000000
Sc
6
Direct
0.46100000000000 0.00000000000000 0.00000000000000 Sc (6a)
0.00000000000000 0.46100000000000 0.33333333333333 Sc (6a)
-0.46100000000000 -0.46100000000000 0.66666666666667 Sc (6a)
-0.46100000000000 0.00000000000000 0.50000000000000 Sc (6a)
0.00000000000000 -0.46100000000000 0.83333333333333 Sc (6a)
0.46100000000000 0.46100000000000 0.16666666666667 Sc (6a)
```

AuF<sub>3</sub>: AB<sub>3</sub>hP24\_179\_b\_ac - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
```

```

_chemical_name_mineral 'AuF3'
_chemical_formula_sum 'Au F3'

_aflow_title 'AuFS_{3}$ Structure'
_aflow_proto 'AB3_hP24_179_b_ac'
_aflow_params 'a,c/a,x_{1},x_{2},x_{3},y_{3},z_{3}'
_aflow_params_values '5.14898393,3.15789473684,0.8361,0.7601,0.5338,
↪ 0.3099,0.0053'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP24'

_cell_length_a 5.1489839300
_cell_length_b 5.1489839300
_cell_length_c 16.2599492526
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 65 2 2"
_symmetry_Int_Tables_number 179

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z+5/6
3 -y,x-y,z+2/3
4 -x,-y,z+1/2
5 -x+y,-x,z+1/3
6 y,-x+y,z+1/6
7 x-y,-y,-z
8 x,x-y,-z+5/6
9 y,x,-z+2/3
10 -x+y,y,-z+1/2
11 -x,-x+y,-z+1/3
12 -y,-x,-z+1/6

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
F1 F 6 a 0.83610 0.00000 0.00000 1.00000
Au1 Au 6 b 0.76010 0.52020 0.75000 1.00000
F2 F 12 c 0.53380 0.30990 0.00530 1.00000

```

AuF<sub>3</sub>: AB<sub>3</sub>\_hP24\_179\_b\_ac - POSCAR

```

AB3_hP24_179_b_ac & a,c/a,x1,x2,x3,y3,z3 --params=5.14898393,
↪ 3.15789473684,0.8361,0.7601,0.5338,0.3099,0.0053 & P6_{5}22 D_{
↪ 6}^{3} #179 (abc) & hP24 & None & AuF3 & AuF3 &
1.0000000000000000
2.5744919650000000 -4.45915088705784 0.0000000000000000
2.5744919650000000 4.45915088705784 0.0000000000000000
0.0000000000000000 0.0000000000000000 16.2599492526000000
Au F
6 18
Direct
0.7601000000000000 1.5202000000000000 0.7500000000000000 Au (6b)
-1.5202000000000000 -0.7601000000000000 0.4166666666666667 Au (6b)
0.7601000000000000 -0.7601000000000000 0.0833333333333333 Au (6b)
-0.7601000000000000 -1.5202000000000000 0.2500000000000000 Au (6b)
1.5202000000000000 0.7601000000000000 0.9166666666666667 Au (6b)
-0.7601000000000000 0.7601000000000000 0.5833333333333333 Au (6b)
0.8361000000000000 0.0000000000000000 0.0000000000000000 F (6a)
0.0000000000000000 0.8361000000000000 0.6666666666666667 F (6a)
-0.8361000000000000 -0.8361000000000000 0.3333333333333333 F (6a)
-0.8361000000000000 0.0000000000000000 0.5000000000000000 F (6a)
0.0000000000000000 -0.8361000000000000 0.1666666666666667 F (6a)
0.8361000000000000 0.8361000000000000 0.8333333333333333 F (6a)
0.5338000000000000 0.3099000000000000 0.0053000000000000 F (12c)
-0.3099000000000000 0.2239000000000000 0.6719666666666667 F (12c)
-0.2239000000000000 -0.5338000000000000 0.3386333333333333 F (12c)
-0.5338000000000000 -0.3099000000000000 0.5053000000000000 F (12c)
0.3099000000000000 -0.2239000000000000 0.1719666666666667 F (12c)
0.2239000000000000 0.5338000000000000 0.8386333333333333 F (12c)
0.3099000000000000 0.5338000000000000 0.6613666666666667 F (12c)
0.2239000000000000 -0.3099000000000000 -0.0053000000000000 F (12c)
-0.5338000000000000 -0.2239000000000000 0.3280333333333333 F (12c)
-0.3099000000000000 -0.5338000000000000 0.1613666666666667 F (12c)
-0.2239000000000000 0.3099000000000000 0.4947000000000000 F (12c)
0.5338000000000000 0.2239000000000000 0.8280333333333333 F (12c)

```

β-SiO<sub>2</sub>: A2B\_hP9\_181\_j\_c - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'beta-SiO2'
_chemical_formula_sum 'O2 Si'

_aflow_title '$\beta$SiO_{2}$ Structure'
_aflow_proto 'A2B_hP9_181_j_c'
_aflow_params 'a,c/a,x_{2}'
_aflow_params_values '4.9977,1.09252256038,0.2072'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP9'

_cell_length_a 4.9977000000

```

```

_cell_length_b 4.9977000000
_cell_length_c 5.4601000000
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 64 2 2"
_symmetry_Int_Tables_number 181

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z+2/3
3 -y,x-y,z+1/3
4 -x,-y,z
5 -x+y,-x,z+2/3
6 y,-x+y,z+1/3
7 x-y,-y,-z
8 x,x-y,-z+2/3
9 y,x,-z+1/3
10 -x+y,y,-z
11 -x,-x+y,-z+2/3
12 -y,-x,-z+1/3

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Si1 Si 3 c 0.50000 0.00000 0.00000 1.00000
O1 O 6 j 0.20720 0.41440 0.50000 1.00000

```

β-SiO<sub>2</sub>: A2B\_hP9\_181\_j\_c - POSCAR

```

A2B_hP9_181_j_c & a,c/a,x2 --params=4.9977,1.09252256038,0.2072 & P6_{4}22 D_{
↪ 22} D_{6}^{5} #181 (cj) & hP9 & None & SiO2 & beta &
1.0000000000000000
2.4988500000000000 -4.32813516049349 0.0000000000000000
2.4988500000000000 4.32813516049349 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.4601000000000000
O Si
6 3
Direct
0.2072000000000000 0.4144000000000000 0.5000000000000000 O (6j)
-0.4144000000000000 -0.2072000000000000 0.8333333333333333 O (6j)
0.2072000000000000 -0.2072000000000000 0.1666666666666667 O (6j)
-0.2072000000000000 -0.4144000000000000 0.5000000000000000 O (6j)
0.4144000000000000 0.2072000000000000 0.8333333333333333 O (6j)
-0.2072000000000000 0.2072000000000000 0.1666666666666667 O (6j)
0.5000000000000000 0.0000000000000000 0.0000000000000000 Si (3c)
0.0000000000000000 0.5000000000000000 0.3333333333333333 Si (3c)
0.5000000000000000 0.5000000000000000 0.6666666666666667 Si (3c)

```

AuCN: ABC\_hP3\_183\_a\_a\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'AuCN'
_chemical_formula_sum 'Au C N'

loop_
_publ_author_name
'S. J. Hibble'
'A. C. Hannon'
'S. M. Cheyne'
_journal_name_full_name
;
Inorganic Chemistry
;
_journal_volume 42
_journal_year 2003
_journal_page_first 4724
_journal_page_last 4730
_publ_section_title
;
Structure of AuCN determined from total neutron diffraction
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'AuCN Structure'
_aflow_proto 'ABC_hP3_183_a_a_a'
_aflow_params 'a,c/a,z_{1},z_{2},z_{3}'
_aflow_params_values '3.3908401495,1.49568037743,0.608,0.0,0.226'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP3'

_cell_length_a 3.3908401495
_cell_length_b 3.3908401495
_cell_length_c 5.0716130746
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 6 m m"
_symmetry_Int_Tables_number 183

```

```

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z
3 -y,x-y,z
4 -x,-y,z
5 -x+y,-x,z
6 y,-x+y,z
7 -x+y,y,z
8 -x,-x+y,z
9 -y,-x,z
10 x-y,-y,z
11 x,x-y,z
12 y,x,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Au1 Au 1 a 0.00000 0.00000 0.60800 1.00000
Cl C 1 a 0.00000 0.00000 0.00000 1.00000
Ni N 1 a 0.00000 0.00000 0.22600 1.00000

```

AuCN: ABC\_hp3\_183\_a\_a - POSCAR

```

ABC_hp3_183_a_a_a & a,c/a,z1,z2,z3 --params=3.3908401495,1.49568037743,
  ↪ 0.608,0.0,0.226 & P6mm C_{6v}^{1} #183 (a^3) & hP3 & None &
  ↪ AuCN & S. J. Hibble and A. C. Hannon and S. M. Cheyne,
  ↪ Inorg. Chem. 42, 4724-4730 (2003)
1.0000000000000000
1.69542007475000 -2.93655370963922 0.0000000000000000
1.69542007475000 2.93655370963922 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.0716130746000000
  Au C N
  1 1 1
Direct
0.0000000000000000 0.0000000000000000 0.6080000000000000 Au (1a)
0.0000000000000000 0.0000000000000000 0.0000000000000000 C (1a)
0.0000000000000000 0.0000000000000000 0.2260000000000000 N (1a)

```

CrFe<sub>3</sub>NiSn<sub>5</sub>: AB\_hp6\_183\_c\_ab - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'CrFe3NiSn5'
_chemical_formula_sum 'M Sn'

loop_
  _publ_author_name
  'J. Huang'
  'L. Zeng'
  'Z. Sun'
  _journal_name_full_name
  ;
Powder Diffraction
;
_journal_volume 19
_journal_year 2004
_journal_page_first 372
_journal_page_last 374
_publ_section_title
;
X-ray powder diffraction data and Rietveld refinement of CrFe3
  ↪ NiSn5
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'CrFe3NiSn5 Structure'
_aflow_proto 'AB_hp6_183_c_ab'
_aflow_params 'a,c/a,z_{1},z_{2},z_{3}'
_aflow_params_values '5.3175214551,0.83247442072,0.0,0.513,0.01'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP6'

_cell_length_a 5.3175214551
_cell_length_b 5.3175214551
_cell_length_c 4.4267005930
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 6 m m"
_symmetry_Int_Tables_number 183

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z
3 -y,x-y,z
4 -x,-y,z
5 -x+y,-x,z
6 y,-x+y,z
7 -x+y,y,z+1/2
8 -x,-x+y,z+1/2
9 -y,-x,z+1/2
10 x-y,-y,z+1/2
11 x,x-y,z+1/2
12 y,x,z+1/2

```

```

9 -y,-x,z
10 x-y,-y,z
11 x,x-y,z
12 y,x,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Sn1 Sn 1 a 0.00000 0.00000 0.00000 1.00000
Sn2 Sn 2 b 0.33333 0.66667 0.51300 1.00000
Ml M 3 c 0.50000 0.00000 0.01000 1.00000

```

CrFe<sub>3</sub>NiSn<sub>5</sub>: AB\_hp6\_183\_c\_ab - POSCAR

```

AB_hp6_183_c_ab & a,c/a,z1,z2,z3 --params=5.3175214551,0.83247442072,0.0
  ↪ ,0.513,0.01 & P6mm C_{6v}^{1} #183 (abc) & hP6 & None &
  ↪ CrFe3NiSn5 & J. Huang and L. Zeng and Z. Sun, Powder
  ↪ Diffraction 19, 372-374 (2004)
1.0000000000000000
2.65876072755000 -4.60510866528539 0.0000000000000000
2.65876072755000 4.60510866528539 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.4267005930000000
  M Sn
  3 3
Direct
0.5000000000000000 0.0000000000000000 0.0100000000000000 M (3c)
0.0000000000000000 0.5000000000000000 0.0100000000000000 M (3c)
0.5000000000000000 0.5000000000000000 0.0100000000000000 M (3c)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Sn (1a)
0.3333333333333333 0.6666666666666667 0.5130000000000000 Sn (2b)
0.6666666666666667 0.3333333333333333 0.5130000000000000 Sn (2b)

```

Al[PO<sub>4</sub>] (Framework type AFI): AB4C\_hp72\_184\_d\_4d\_d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Al[PO4]'
_chemical_formula_sum 'Al O4 P'

loop_
  _publ_author_name
  'G. J. Klap'
  'H. {van Koningsveld}'
  'H. Graafsma'
  'A. M. M. Schreurs'
  _journal_name_full_name
  ;
Microporous and Mesoporous Materials
;
_journal_volume 38
_journal_year 2000
_journal_page_first 403
_journal_page_last 412
_publ_section_title
;
Absolute configuration and domain structure of AlPO4 studied by
  ↪ single crystal X-ray diffraction
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'Al[PO4] (Framework type AFI) Structure'
_aflow_proto 'AB4C_hp72_184_d_4d_d'
_aflow_params 'a,c/a,x_{1},y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3},
  ↪ x_{4},y_{4},z_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6}'
_aflow_params_values '13.7178848276,0.616168537688,0.45652,0.12053,0.0,
  ↪ 0.42,0.2069,0.071,0.1224,0.4519,0.2982,0.3629,0.0019,0.0649,
  ↪ 0.1538,0.5737,0.0602,0.12298,0.4525,0.12746'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP72'

_cell_length_a 13.7178848276
_cell_length_b 13.7178848276
_cell_length_c 8.4525290344
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 6 c c"
_symmetry_Int_Tables_number 184

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z
3 -y,x-y,z
4 -x,-y,z
5 -x+y,-x,z
6 y,-x+y,z
7 -x+y,y,z+1/2
8 -x,-x+y,z+1/2
9 -y,-x,z+1/2
10 x-y,-y,z+1/2
11 x,x-y,z+1/2
12 y,x,z+1/2

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 12 d 0.45652 0.12053 0.00000 1.00000
O1 O 12 d 0.42000 0.20690 0.07100 1.00000
O2 O 12 d 0.12240 0.45190 0.29820 1.00000
O3 O 12 d 0.36290 0.00190 0.06490 1.00000
O4 O 12 d 0.15380 0.57370 0.06020 1.00000
P1 P 12 d 0.12298 0.45250 0.12746 1.00000

```

Al[PO<sub>4</sub>] (Framework type AFI): AB4C\_hP72\_184\_d\_4d\_d - POSCAR

```

AB4C_hP72_184_d_4d_d & a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5,
  ↪ z5, x6, y6, z6 --params=13.7178848276, 0.616168537688, 0.45652,
  ↪ 0.12053, 0.0, 0.42, 0.2069, 0.071, 0.1224, 0.4519, 0.2982, 0.3629,
  ↪ 0.0019, 0.0649, 0.1538, 0.5737, 0.0602, 0.12298, 0.4525, 0.12746 &
  ↪ P6cc C_{6v}^{2} #184 (d^6) & hP72 & None & Al[PO4] & & G. J.
  ↪ Klap et al., Microporous Mesoporous Mater. 38, 403-412 (2000)
1.000000000000000
6.85894241380000 -11.88003674689070 0.000000000000000
6.85894241380000 11.88003674689070 0.000000000000000
0.000000000000000 0.000000000000000 8.452529034400000
Al O P
12 48 12
Direct
0.456520000000000 0.120530000000000 0.000000000000000 Al (12d)
-0.120530000000000 -0.335990000000000 0.000000000000000 Al (12d)
-0.335990000000000 -0.456520000000000 0.000000000000000 Al (12d)
-0.456520000000000 -0.120530000000000 0.000000000000000 Al (12d)
0.120530000000000 -0.335990000000000 0.000000000000000 Al (12d)
0.335990000000000 0.456520000000000 0.000000000000000 Al (12d)
-0.120530000000000 -0.456520000000000 0.500000000000000 Al (12d)
-0.335990000000000 0.120530000000000 0.500000000000000 Al (12d)
0.456520000000000 0.335990000000000 0.500000000000000 Al (12d)
0.120530000000000 0.456520000000000 0.500000000000000 Al (12d)
-0.120530000000000 -0.120530000000000 0.500000000000000 Al (12d)
-0.456520000000000 -0.335990000000000 0.500000000000000 Al (12d)
0.420000000000000 0.206900000000000 0.071000000000000 O (12d)
-0.206900000000000 0.213100000000000 0.071000000000000 O (12d)
-0.213100000000000 -0.420000000000000 0.071000000000000 O (12d)
-0.420000000000000 -0.206900000000000 0.071000000000000 O (12d)
0.206900000000000 -0.213100000000000 0.071000000000000 O (12d)
0.213100000000000 0.420000000000000 0.071000000000000 O (12d)
-0.206900000000000 -0.420000000000000 0.571000000000000 O (12d)
-0.213100000000000 0.206900000000000 0.571000000000000 O (12d)
0.420000000000000 0.213100000000000 0.571000000000000 O (12d)
0.206900000000000 0.420000000000000 0.571000000000000 O (12d)
0.213100000000000 -0.206900000000000 0.571000000000000 O (12d)
-0.420000000000000 -0.213100000000000 0.571000000000000 O (12d)
0.122400000000000 0.451900000000000 0.298200000000000 O (12d)
-0.451900000000000 -0.329500000000000 0.298200000000000 O (12d)
0.329500000000000 -0.122400000000000 0.298200000000000 O (12d)
-0.122400000000000 -0.451900000000000 0.298200000000000 O (12d)
0.451900000000000 0.329500000000000 0.298200000000000 O (12d)
-0.329500000000000 0.122400000000000 0.298200000000000 O (12d)
-0.451900000000000 -0.122400000000000 0.798200000000000 O (12d)
0.329500000000000 0.451900000000000 0.798200000000000 O (12d)
0.122400000000000 -0.329500000000000 0.798200000000000 O (12d)
0.451900000000000 0.122400000000000 0.798200000000000 O (12d)
-0.329500000000000 -0.451900000000000 0.798200000000000 O (12d)
-0.122400000000000 0.329500000000000 0.798200000000000 O (12d)
0.362900000000000 0.001900000000000 0.064900000000000 O (12d)
-0.001900000000000 0.361000000000000 0.064900000000000 O (12d)
-0.361000000000000 -0.362900000000000 0.064900000000000 O (12d)
0.001900000000000 -0.001900000000000 0.064900000000000 O (12d)
0.361000000000000 0.362900000000000 0.064900000000000 O (12d)
-0.001900000000000 -0.362900000000000 0.564900000000000 O (12d)
-0.361000000000000 0.001900000000000 0.564900000000000 O (12d)
0.362900000000000 0.361000000000000 0.564900000000000 O (12d)
0.001900000000000 0.362900000000000 0.564900000000000 O (12d)
-0.362900000000000 -0.361000000000000 0.564900000000000 O (12d)
0.153800000000000 0.573700000000000 0.060200000000000 O (12d)
-0.573700000000000 -0.419900000000000 0.060200000000000 O (12d)
0.419900000000000 -0.153800000000000 0.060200000000000 O (12d)
-0.153800000000000 -0.573700000000000 0.060200000000000 O (12d)
0.573700000000000 0.419900000000000 0.060200000000000 O (12d)
-0.419900000000000 0.153800000000000 0.060200000000000 O (12d)
-0.573700000000000 -0.153800000000000 0.560200000000000 O (12d)
0.419900000000000 0.573700000000000 0.560200000000000 O (12d)
0.153800000000000 -0.419900000000000 0.560200000000000 O (12d)
0.573700000000000 0.153800000000000 0.560200000000000 O (12d)
-0.419900000000000 -0.573700000000000 0.560200000000000 O (12d)
-0.153800000000000 0.419900000000000 0.560200000000000 O (12d)
0.122980000000000 0.452500000000000 0.127460000000000 P (12d)
-0.452500000000000 -0.329520000000000 0.127460000000000 P (12d)
0.329520000000000 -0.122980000000000 0.127460000000000 P (12d)
-0.122980000000000 -0.452500000000000 0.127460000000000 P (12d)
0.452500000000000 0.329520000000000 0.127460000000000 P (12d)
-0.329520000000000 -0.122980000000000 0.627460000000000 P (12d)
-0.452500000000000 0.122980000000000 0.627460000000000 P (12d)
0.122980000000000 -0.452500000000000 0.627460000000000 P (12d)
0.452500000000000 0.122980000000000 0.627460000000000 P (12d)
-0.329520000000000 -0.452500000000000 0.627460000000000 P (12d)
-0.122980000000000 0.329520000000000 0.627460000000000 P (12d)

```

KNiCl<sub>3</sub> (Room-temperature): A3BC\_hP30\_185\_cd\_c\_ab - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'KNiCl3'
_chemical_formula_sum 'Cl3 K Ni'

loop_
_publ_author_name
'D. Visser'
'G. C. Verschoor'
'D. J. W. {IJdo}'
_journal_name_full_name
;
Acta Crystallographica Section B: Structural Science
;
_journal_volume 36
_journal_year 1980
_journal_page_first 28
_journal_page_last 34
_publ_section_title
;
The structure of KNiCl3_{3}$ at room temperature
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'KNiCl3_{3}$ (Room-temperature) Structure'
_aflow_proto 'A3BC_hP30_185_cd_c_ab'
_aflow_params 'a, c/a, z_{1}, z_{2}, x_{3}, z_{3}, x_{4}, z_{4}, x_{5}, y_{5}, z_{5}'
_aflow_params_values '11.795090915, 0.502416278086, 0.0, 0.377, 0.1598,
  ↪ 0.2396, 0.6647, 0.1706, 0.1732, 0.5056, 0.1148'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP30'

_cell_length_a 11.7950909150
_cell_length_b 11.7950909150
_cell_length_c 5.9260456772
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 63 c m"
_symmetry_Int_Tables_number 185

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -x, -y, z+1/2
3 -y, -x, z
4 -x, -y, z+1/2
5 -x+y, -x, z
6 y, -x+y, z+1/2
7 -x+y, y, z+1/2
8 -x, -x+y, z
9 -y, -x, z+1/2
10 x-y, -y, z
11 x, x-y, z+1/2
12 y, x, z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ni1 Ni 2 a 0.00000 0.00000 0.00000 1.00000
Ni2 Ni 4 b 0.33333 0.66667 0.37700 1.00000
Cl1 Cl 6 c 0.15980 0.00000 0.23960 1.00000
K1 K 6 c 0.66470 0.00000 0.17060 1.00000
Cl2 Cl 12 d 0.17320 0.50560 0.11480 1.00000

```

KNiCl<sub>3</sub> (Room-temperature): A3BC\_hP30\_185\_cd\_c\_ab - POSCAR

```

A3BC_hP30_185_cd_c_ab & a, c/a, z1, z2, x3, z3, x4, z4, x5, y5, z5 --params=
  ↪ 11.795090915, 0.502416278086, 0.0, 0.377, 0.1598, 0.2396, 0.6647,
  ↪ 0.1706, 0.1732, 0.5056, 0.1148 & P6_{3}cm C_{6v}^{3} #185 (abc^2d)
  ↪ & hP30 & None & KNiCl3 & & D. Visser and G. C. Verschoor and
  ↪ D. J. W. {IJdo}, Acta Crystallogr. Sect. B Struct. Sci. 36,
  ↪ 28-34 (1980)
1.000000000000000
5.89754545750000 -10.21484837233700 0.000000000000000
5.89754545750000 10.21484837233700 0.000000000000000
0.000000000000000 0.000000000000000 5.92604567720000
Cl K Ni
18 6 6
Direct
0.159800000000000 0.000000000000000 0.239600000000000 Cl (6c)
0.000000000000000 0.159800000000000 0.239600000000000 Cl (6c)
-0.159800000000000 -0.159800000000000 0.239600000000000 Cl (6c)
-0.159800000000000 0.000000000000000 0.739600000000000 Cl (6c)
0.000000000000000 -0.159800000000000 0.739600000000000 Cl (6c)
0.159800000000000 0.159800000000000 0.739600000000000 Cl (6c)
0.173200000000000 0.505600000000000 0.114800000000000 Cl (12d)
-0.505600000000000 -0.332400000000000 0.114800000000000 Cl (12d)
0.332400000000000 -0.173200000000000 0.114800000000000 Cl (12d)
-0.173200000000000 -0.505600000000000 0.614800000000000 Cl (12d)

```

0.50560000000000	0.33240000000000	0.61480000000000	Cl (12d)
-0.33240000000000	0.17320000000000	0.61480000000000	Cl (12d)
-0.50560000000000	-0.17320000000000	0.61480000000000	Cl (12d)
0.33240000000000	0.50560000000000	0.61480000000000	Cl (12d)
0.17320000000000	-0.33240000000000	0.61480000000000	Cl (12d)
0.50560000000000	0.17320000000000	0.11480000000000	Cl (12d)
-0.33240000000000	-0.50560000000000	0.11480000000000	Cl (12d)
-0.17320000000000	0.33240000000000	0.11480000000000	Cl (12d)
0.66470000000000	0.00000000000000	0.17060000000000	K (6c)
0.00000000000000	0.66470000000000	0.17060000000000	K (6c)
-0.66470000000000	-0.66470000000000	0.17060000000000	K (6c)
-0.66470000000000	0.00000000000000	0.67060000000000	K (6c)
0.00000000000000	-0.66470000000000	0.67060000000000	K (6c)
0.66470000000000	0.66470000000000	0.67060000000000	K (6c)
0.00000000000000	0.00000000000000	0.00000000000000	Ni (2a)
0.00000000000000	0.00000000000000	0.50000000000000	Ni (2a)
0.33333333333333	0.66666666666667	0.37700000000000	Ni (4b)
0.66666666666667	0.33333333333333	0.87700000000000	Ni (4b)
0.33333333333333	0.66666666666667	0.87700000000000	Ni (4b)
0.66666666666667	0.33333333333333	0.37700000000000	Ni (4b)

Cu<sub>3</sub>P: A3B\_hP24\_185\_ab2c\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Cu3 P'

loop_
  _publ_author_name
  'O. Olofsson'
  _journal_name_full_name
  ;
  Acta Chemica Scandinavica
  ;
  _journal_volume 26
  _journal_year 1972
  _journal_page_first 2777
  _journal_page_last 2787
  _publ_section_title
  ;
  The Crystal Structure of Cu3{3}SP
  ;
  _aflow_title 'Cu3{3}SP Structure'
  _aflow_proto 'A3B_hP24_185_ab2c_c'
  _aflow_params 'a,c/a,z_{1},z_{2},x_{3},z_{3},x_{4},z_{4},x_{5},z_{5}'
  _aflow_params_values '6.9593,1.02639633296,0.3213,0.1998,0.2806,0.0765,
  ↪ 0.3761,0.4246,0.3322,0.75'
  _aflow_strukturbericht 'None'
  _aflow_pearson 'hP24'

_symmetry_space_group_name_H-M "P 63 c m"
_symmetry_Int_Tables_number 185

_cell_length_a 6.95930
_cell_length_b 6.95930
_cell_length_c 7.14300
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x-y,x,z+1/2
  3 -y,x-y,z
  4 -x,-y,z+1/2
  5 -x+y,-x,z
  6 y,-x+y,z+1/2
  7 -x+y,y,z+1/2
  8 -x,-x+y,z
  9 -y,-x,z+1/2
  10 x-y,-y,z
  11 x,x-y,z+1/2
  12 y,x,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Cu1 Cu 2 a 0.00000 0.00000 0.32130 1.00000
  Cu2 Cu 4 b 0.33333 0.66667 0.19980 1.00000
  Cu3 Cu 6 c 0.28060 0.00000 0.07650 1.00000
  Cu4 Cu 6 c 0.37610 0.00000 0.42460 1.00000
  P1 P 6 c 0.33220 0.00000 0.75000 1.00000
```

Cu<sub>3</sub>P: A3B\_hP24\_185\_ab2c\_c - POSCAR

```
A3B_hP24_185_ab2c_c & a,c/a,z1,z2,x3,z3,x4,z4,x5,z5 --params=6.9593,
  ↪ 1.02639633296,0.3213,0.1998,0.2806,0.0765,0.3761,0.4246,0.3322,
  ↪ 0.75 & P6_{3}cm C_{6v}^{3} #185 (abc^3) & hP24 & None & Cu3P &
  ↪ & O. Olofsson, Acta Chem. Scand. 26, 2777-2787 (1972)
  1.00000000000000
  3.47965000000000 -6.02693059255704 0.00000000000000
  3.47965000000000 6.02693059255704 0.00000000000000
  0.00000000000000 0.00000000000000 7.14300000000000
```

Cu	P		
18	6		
Direct			
0.00000000000000	0.00000000000000	0.32130000000000	Cu (2a)
0.00000000000000	0.00000000000000	0.82130000000000	Cu (2a)
0.33333333333333	0.66666666666667	0.19980000000000	Cu (4b)
0.66666666666667	0.33333333333333	0.69980000000000	Cu (4b)
0.33333333333333	0.66666666666667	0.69980000000000	Cu (4b)
0.66666666666667	0.33333333333333	0.19980000000000	Cu (4b)
0.28060000000000	0.00000000000000	0.07650000000000	Cu (6c)
0.00000000000000	0.28060000000000	0.07650000000000	Cu (6c)
-0.28060000000000	-0.28060000000000	0.07650000000000	Cu (6c)
-0.28060000000000	0.00000000000000	0.57650000000000	Cu (6c)
0.00000000000000	-0.28060000000000	0.57650000000000	Cu (6c)
0.28060000000000	0.28060000000000	0.57650000000000	Cu (6c)
0.37610000000000	0.00000000000000	0.42460000000000	Cu (6c)
0.00000000000000	0.37610000000000	0.42460000000000	Cu (6c)
-0.37610000000000	-0.37610000000000	0.42460000000000	Cu (6c)
-0.37610000000000	0.00000000000000	0.92460000000000	Cu (6c)
0.00000000000000	-0.37610000000000	0.92460000000000	Cu (6c)
0.37610000000000	0.37610000000000	0.92460000000000	Cu (6c)
0.33220000000000	0.00000000000000	0.75000000000000	P (6c)
0.00000000000000	0.33220000000000	0.75000000000000	P (6c)
-0.33220000000000	-0.33220000000000	0.75000000000000	P (6c)
-0.33220000000000	0.00000000000000	1.25000000000000	P (6c)
0.00000000000000	-0.33220000000000	1.25000000000000	P (6c)
0.33220000000000	0.33220000000000	1.25000000000000	P (6c)

β-RuCl<sub>3</sub>: A3B\_hP8\_185\_c\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'beta-RuCl3'
_chemical_formula_sum 'Cl3 Ru'

loop_
  _publ_author_name
  'J. M. Fletcher'
  'W. E. Gardner'
  'A. C. Fox'
  'G. Topping'
  _journal_name_full_name
  ;
  Journal of the Chemical Society A
  ;
  _journal_volume ~
  _journal_year 1967
  _journal_page_first 1038
  _journal_page_last 1045
  _publ_section_title
  ;
  X-Ray, infrared, and magnetic studies of $\alpha$- and $\beta$-ruthenium
  ↪ trichloride

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title '$\beta$-RuCl3{3} Structure'
_aflow_proto 'A3B_hP8_185_c_a'
_aflow_params 'a,c/a,z_{1},x_{2},z_{2}'
_aflow_params_values '6.1197165237,0.924509803925,0.0,0.305,0.245'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP8'

_cell_length_a 6.1197165237
_cell_length_b 6.1197165237
_cell_length_c 5.6577379234
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 63 c m"
_symmetry_Int_Tables_number 185

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x-y,x,z+1/2
  3 -y,x-y,z
  4 -x,-y,z+1/2
  5 -x+y,-x,z
  6 y,-x+y,z+1/2
  7 -x+y,y,z+1/2
  8 -x,-x+y,z
  9 -y,-x,z+1/2
  10 x-y,-y,z
  11 x,x-y,z+1/2
  12 y,x,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Ru1 Ru 2 a 0.00000 0.00000 1.00000
  Cl1 Cl 6 c 0.30500 0.00000 0.24500 1.00000
```

$\beta$ -RuCl<sub>3</sub>: A3B\_hP8\_185\_c\_a - POSCAR

```
A3B_hP8_185_c_a & a, c/a, z1, x2, z2 --params=6.1197165237, 0.924509803925,
↪ 0.0, 0.305, 0.245 & P6_{3}cm C_{6v}^{3} #185 (ac) & hP8 & None &
↪ RuCl3 & beta & J. M. Fletcher et al., J. Chem. Soc. A,
↪ 1038-1045 (1967)
1.0000000000000000
3.05985826185000 -5.29982997348359 0.0000000000000000
3.05985826185000 5.29982997348359 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.65773792340000
Cl Ru
6 2
Direct
0.305000000000000 0.000000000000000 0.245000000000000 Cl (6c)
0.000000000000000 0.305000000000000 0.245000000000000 Cl (6c)
-0.305000000000000 -0.305000000000000 0.245000000000000 Cl (6c)
-0.305000000000000 0.000000000000000 0.745000000000000 Cl (6c)
0.000000000000000 -0.305000000000000 0.745000000000000 Cl (6c)
0.305000000000000 0.305000000000000 0.745000000000000 Cl (6c)
0.000000000000000 0.000000000000000 0.000000000000000 Ru (2a)
0.000000000000000 0.000000000000000 0.500000000000000 Ru (2a)
```

Na<sub>3</sub>As: AB3\_hP24\_185\_c\_ab2c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Na3As'
_chemical_formula_sum 'As Na3'
loop_
_publ_author_name
'P. Hafner'
'K.-J. Range'
_journal_name_full_name
'Journal of Alloys and Compounds'
_journal_volume 216
_journal_year 1994
_journal_page_first 7
_journal_page_last 10
_publ_section_title
'NaS_{3}SAs revisited: high-pressure synthesis of single crystals and
↪ structure refinement'
_aflow_title 'NaS_{3}SAs Structure'
_aflow_proto 'AB3_hP24_185_c_ab2c'
_aflow_params 'a, c/a, z_{1}, z_{2}, x_{3}, z_{3}, x_{4}, z_{4}, x_{5}, z_{5}'
_aflow_params_values '8.7838, 1.02449964708, 0.2684, 0.2311, 0.3321, 0.25,
↪ 0.3153, 0.5863, 0.3518, -0.0769'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP24'
_symmetry_space_group_name_H-M 'P 63 c m'
_symmetry_Int_Tables_number 185
_cell_length_a 8.78380
_cell_length_b 8.78380
_cell_length_c 8.99900
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x-y, x, z+1/2
3 -y, x-y, z
4 -x, -y, z+1/2
5 -x+y, -x, z
6 y, -x+y, z+1/2
7 -x+y, y, z+1/2
8 -x, -x+y, z
9 -y, -x, z+1/2
10 x-y, -y, z
11 x, x-y, z+1/2
12 y, x, z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Na1 Na 2 a 0.00000 0.00000 0.26840 1.00000
Na2 Na 4 b 0.33333 0.66667 0.23110 1.00000
As1 As 6 c 0.33210 0.00000 0.25000 1.00000
Na3 Na 6 c 0.31530 0.00000 0.58630 1.00000
Na4 Na 6 c 0.35180 0.00000 -0.07690 1.00000
```

Na<sub>3</sub>As: AB3\_hP24\_185\_c\_ab2c - POSCAR

```
AB3_hP24_185_c_ab2c & a, c/a, z1, z2, x3, z3, x4, z4, x5, z5 --params=8.7838,
↪ 1.02449964708, 0.2684, 0.2311, 0.3321, 0.25, 0.3153, 0.5863, 0.3518, -
↪ 0.0769 & P6_{3}cm C_{6v}^{3} #185 (abc^3) & hP24 & None & Na3As
↪ & Na3As & P. Hafner and K.-J. Range, J. Alloys Compd. 216,
↪ 7-10 (1994)
```

```
1.0000000000000000
4.3919000000000000 -7.60699394176175 0.0000000000000000
4.3919000000000000 7.60699394176175 0.0000000000000000
0.0000000000000000 0.0000000000000000 8.9990000000000000
As Na
6 18
Direct
0.332100000000000 0.000000000000000 0.250000000000000 As (6c)
0.000000000000000 0.332100000000000 0.250000000000000 As (6c)
-0.332100000000000 -0.332100000000000 0.250000000000000 As (6c)
-0.332100000000000 0.000000000000000 0.750000000000000 As (6c)
0.000000000000000 -0.332100000000000 0.750000000000000 As (6c)
0.332100000000000 0.332100000000000 0.750000000000000 As (6c)
0.000000000000000 0.000000000000000 0.268400000000000 Na (2a)
0.000000000000000 0.000000000000000 0.768400000000000 Na (2a)
0.333333333333333 0.666666666666667 0.231100000000000 Na (4b)
0.666666666666667 0.333333333333333 0.731100000000000 Na (4b)
0.333333333333333 0.666666666666667 0.731100000000000 Na (4b)
0.666666666666667 0.333333333333333 0.231100000000000 Na (4b)
0.315300000000000 0.000000000000000 0.586300000000000 Na (6c)
0.000000000000000 0.315300000000000 0.586300000000000 Na (6c)
-0.315300000000000 -0.315300000000000 0.586300000000000 Na (6c)
-0.315300000000000 0.000000000000000 1.086300000000000 Na (6c)
0.000000000000000 -0.315300000000000 1.086300000000000 Na (6c)
0.315300000000000 0.315300000000000 1.086300000000000 Na (6c)
0.351800000000000 0.000000000000000 -0.076900000000000 Na (6c)
0.000000000000000 0.351800000000000 -0.076900000000000 Na (6c)
-0.351800000000000 -0.351800000000000 0.423100000000000 Na (6c)
-0.351800000000000 0.000000000000000 0.423100000000000 Na (6c)
0.000000000000000 -0.351800000000000 0.423100000000000 Na (6c)
0.351800000000000 0.351800000000000 0.423100000000000 Na (6c)
```

Fe<sub>3</sub>Th<sub>7</sub> (D10<sub>2</sub>): A3B7\_hP20\_186\_c\_b2c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral ''
_chemical_formula_sum 'Fe3 Th7'
loop_
_publ_author_name
'J. V. Florio'
'N. C. Baenziger'
'R. E. Rundle'
_journal_name_full_name
'Acta Crystallographica'
_journal_volume 9
_journal_year 1956
_journal_page_first 367
_journal_page_last 372
_publ_section_title
'Compounds of thorium with transition metals. II. Systems with iron,
↪ cobalt and nickel'
# Found in Inorganic Crystal Structure Database, {ID 401657},
_aflow_title 'FeS_{3}Th_{7}S (SD10_{2}S) Structure'
_aflow_proto 'A3B7_hP20_186_c_b2c'
_aflow_params 'a, c/a, z_{1}, x_{2}, z_{2}, x_{3}, z_{3}, x_{4}, z_{4}'
_aflow_params_values '9.85, 0.624365482234, 0.06, 0.815, 0.31, 0.126, 0.25,
↪ 0.544, 0.31'
_aflow_Strukturbericht 'SD10_{2}S'
_aflow_Pearson 'hP20'
_symmetry_space_group_name_H-M 'P 63 m c'
_symmetry_Int_Tables_number 186
_cell_length_a 9.85000
_cell_length_b 9.85000
_cell_length_c 6.15000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x-y, x, z+1/2
3 -y, x-y, z
4 -x, -y, z+1/2
5 -x+y, -x, z
6 y, -x+y, z+1/2
7 -x+y, y, z
8 -x, -x+y, z+1/2
9 -y, -x, z
10 x-y, -y, z+1/2
11 x, x-y, z
12 y, x, z+1/2
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
```



```

Th1 Th 2 b 0.33333 0.66667 0.06000 1.00000
Fe1 Fe 6 c 0.81500 0.18500 0.31000 1.00000
Th2 Th 6 c 0.12600 0.87400 0.25000 1.00000
Th3 Th 6 c 0.54400 0.45600 0.31000 1.00000

```

Fe<sub>3</sub>Th<sub>7</sub> (D10<sub>2</sub>): A3B7\_hP20\_186\_c\_b2c - POSCAR

```

A3B7_hP20_186_c_b2c & a, c/a, z1, z2, z3, z4 --params=9.85,
↳ 0.624365482234, 0.06, 0.815, 0.31, 0.126, 0.25, 0.544, 0.31 & P6_3}mc
↳ C_{6v}^{4} #186 (bc^3) & hP20 & SD10_{2}$ & Fe3Th7 & J. V.
↳ Florio and N. C. Baenziger and R. E. Rundle, Acta Cryst. 9,
↳ 367-372 (1956)
1.0000000000000000
4.9250000000000000 -8.53035022727672 0.0000000000000000
4.9250000000000000 8.53035022727672 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.1500000000000000
Fe Th
6 14
Direct
0.8150000000000000 -0.8150000000000000 0.3100000000000000 Fe (6c)
0.8150000000000000 1.6300000000000000 0.3100000000000000 Fe (6c)
-1.6300000000000000 -0.8150000000000000 0.3100000000000000 Fe (6c)
-0.8150000000000000 0.8150000000000000 0.8100000000000000 Fe (6c)
-0.8150000000000000 -1.6300000000000000 0.8100000000000000 Fe (6c)
1.6300000000000000 0.8150000000000000 0.8100000000000000 Fe (6c)
0.3333333333333333 0.6666666666666667 0.0600000000000000 Th (2b)
0.6666666666666667 0.3333333333333333 0.5600000000000000 Th (2b)
0.1260000000000000 -0.1260000000000000 0.2500000000000000 Th (6c)
0.1260000000000000 0.2520000000000000 0.2500000000000000 Th (6c)
-0.2520000000000000 -0.1260000000000000 0.2500000000000000 Th (6c)
-0.1260000000000000 0.1260000000000000 0.7500000000000000 Th (6c)
-0.1260000000000000 -0.2520000000000000 0.7500000000000000 Th (6c)
0.2520000000000000 0.1260000000000000 0.7500000000000000 Th (6c)
0.5440000000000000 -0.5440000000000000 0.3100000000000000 Th (6c)
0.5440000000000000 1.0880000000000000 0.3100000000000000 Th (6c)
-1.0880000000000000 -0.5440000000000000 0.3100000000000000 Th (6c)
-0.5440000000000000 0.5440000000000000 0.8100000000000000 Th (6c)
-0.5440000000000000 -1.0880000000000000 0.8100000000000000 Th (6c)
1.0880000000000000 0.5440000000000000 0.8100000000000000 Th (6c)

```

Re<sub>3</sub>N: AB3\_hP4\_187\_e\_fh - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Re3N'
_chemical_formula_sum 'N Re3'

loop_
_publ_author_name
'A. Friedrich'
'B. Winkler'
'L. Bayarjargal'
'W. Morgenroth'
'E. A. Juarez-Arellano'
'V. Milman'
'K. Refson'
'M. Kunz'
'K. Chen'
_journal_name_full_name
;
Physical Review Letters
;
_journal_volume 105
_journal_year 2010
_journal_page_first 085504
_journal_page_last 085504
_publ_section_title
;
Novel Rhenium Nitrides
;
_aflow_title 'ReS_{3}N Structure'
_aflow_proto 'AB3_hP4_187_e_fh'
_aflow_params 'a, c/a, z_{3}'
_aflow_params_values '2.8065, 2.53411722786, 0.198'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP4'

_symmetry_space_group_name_H-M "P -6 m 2"
_symmetry_Int_Tables_number 187

_cell_length_a 2.80650
_cell_length_b 2.80650
_cell_length_c 7.11200
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 x, x-y, -z
5 -x+y, y, -z
6 -y, -x, -z
7 -x+y, -x, -z
8 x, y, -z
9 -y, x-y, -z
10 -x+y, y, z+1/2
11 -y, -x, z+1/2
12 x, x-y, z+1/2

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
N1 N 1 e 0.66667 0.33333 0.00000 1.00000
Re1 Re 1 f 0.66667 0.33333 0.50000 1.00000
Re2 Re 2 h 0.33333 0.66667 0.19800 1.00000

```

Re<sub>3</sub>N: AB3\_hP4\_187\_e\_fh - POSCAR

```

AB3_hP4_187_e_fh & a, c/a, z3 --params=2.8065, 2.53411722786, 0.198 & P-6m2
↳ D_{3h}^{1} #187 (efh) & hP4 & None & Re3N & Re3N & A. Friedrich
↳ et al., Phys. Rev. Lett. 105, 085504(2010)
1.0000000000000000
1.4032500000000000 -2.43050029572103 0.0000000000000000
1.4032500000000000 2.43050029572103 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.1120000000000000
N Re
1 3
Direct
0.6666666666666667 0.3333333333333333 0.0000000000000000 N (1e)
0.6666666666666667 0.3333333333333333 0.5000000000000000 Re (1f)
0.3333333333333333 0.6666666666666667 0.1980000000000000 Re (2h)
0.3333333333333333 0.6666666666666667 -0.1980000000000000 Re (2h)

```

LiScI<sub>3</sub>: A3BC\_hP10\_188\_k\_a\_e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'LiScI3'
_chemical_formula_sum 'I3 Li Sc'

loop_
_publ_author_name
'A. Lachgar'
'D. S. Dudis'
'P. K. Dorhout'
'J. D. Corbett'
_journal_name_full_name
;
Inorganic Chemistry
;
_journal_volume 30
_journal_year 1991
_journal_page_first 3321
_journal_page_last 3326
_publ_section_title
;
Synthesis and properties of two novel line phases that contain linear
↳ scandium chains, lithium scandium iodide (LiScI_{3}) and
↳ sodium scandium iodide (NaS_{0.5}ScI_{3})
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'LiScI_{3} Structure'
_aflow_proto 'A3BC_hP10_188_k_a_e'
_aflow_params 'a, c/a, x_{3}, y_{3}'
_aflow_params_values '7.2864263258, 0.928891999832, 0.67077, 0.01058'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP10'

_cell_length_a 7.2864263258
_cell_length_b 7.2864263258
_cell_length_c 6.7683031214
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P -6 c 2"
_symmetry_Int_Tables_number 188

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 x, x-y, -z
5 -x+y, y, -z
6 -y, -x, -z
7 -x+y, -x, -z+1/2
8 x, y, -z+1/2
9 -y, x-y, -z+1/2
10 -x+y, y, z+1/2
11 -y, -x, z+1/2
12 x, x-y, z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

```

```
_atom_site_occupancy
Li1 Li 2 a 0.00000 0.00000 0.00000 1.00000
Sc1 Sc 2 e 0.66667 0.33333 0.00000 1.00000
I1 I 6 k 0.67077 0.01058 0.25000 1.00000
```

LiSc<sub>3</sub>: A3BC\_hP10\_188\_k\_a\_e - POSCAR

```
A3BC_hP10_188_k_a_e & a, c/a, x3, y3 --params=7.2864263258, 0.928891999832,
↳ 0.67077, 0.01058 & P-6c2 D_{3h}^{(2)} #188 (aek) & hP10 & None &
↳ LiSc13 & A. Lachgar et al., Inorg. Chem. 30, 3321-3326 (1991)
↳ )
1.0000000000000000
3.64321316290000 -6.31023030094651 0.0000000000000000
3.64321316290000 6.31023030094651 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.76830312140000
I Li Sc
6 2 2
Direct
0.670770000000000 0.010580000000000 0.250000000000000 I (6k)
-0.010580000000000 0.660190000000000 0.250000000000000 I (6k)
-0.660190000000000 -0.670770000000000 0.250000000000000 I (6k)
-0.010580000000000 -0.670770000000000 0.750000000000000 I (6k)
-0.660190000000000 0.010580000000000 0.750000000000000 I (6k)
0.670770000000000 0.660190000000000 0.750000000000000 I (6k)
0.000000000000000 0.000000000000000 0.000000000000000 Li (2a)
0.000000000000000 0.000000000000000 0.500000000000000 Li (2a)
0.666666666666667 0.333333333333333 0.000000000000000 Sc (2e)
0.666666666666667 0.333333333333333 0.500000000000000 Sc (2e)
```

BaSi<sub>4</sub>O<sub>9</sub>: AB9C4\_hp28\_188\_e\_kl\_ak - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'BaSi4O9'
_chemical_formula_sum 'Ba O9 Si4'
loop_
_publ_author_name
'L. W. Finger'
'R. M. Hazen'
'B. A. Fursenko'
_journal_name_full_name
;
Journal of Physics and Chemistry of Solids
;
_journal_volume 56
_journal_year 1995
_journal_page_first 1389
_journal_page_last 1393
_publ_section_title
;
Refinement of the crystal structure of BaSi_{4}O_{9} in the
↳ benitoite form
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013
_aflow_title 'BaSi_{4}O_{9} Structure'
_aflow_proto 'AB9C4_hp28_188_e_kl_ak'
_aflow_params 'a, c/a, x_{3}, y_{3}, x_{4}, y_{4}, x_{5}, y_{5}, z_{5}'
_aflow_params_values '6.4953629976, 1.43896355826, 0.07103, 0.48306, 0.12023'
↳ , 0.75436, 0.22923, 0.00127, 0.6032'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP28'
_cell_length_a 6.4953629976
_cell_length_b 6.4953629976
_cell_length_c 9.3465906512
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000
_symmetry_space_group_name_H-M "P -6 c 2"
_symmetry_Int_Tables_number 188
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 x, x-y, -z
5 -x+y, y, -z
6 -y, -x, -z
7 -x+y, -x, -z+1/2
8 x, y, -z+1/2
9 -y, x-y, -z+1/2
10 -x+y, y, z+1/2
11 -y, -x, z+1/2
12 x, x-y, z+1/2
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Si1 Si 2 a 0.00000 0.00000 0.00000 1.00000
Ba1 Ba 2 e 0.66667 0.33333 0.00000 1.00000
```

```
O1 O 6 k 0.07103 0.48306 0.25000 1.00000
Si2 Si 6 k 0.12023 0.75436 0.25000 1.00000
O2 O 12 l 0.22923 0.00127 0.60320 1.00000
```

BaSi<sub>4</sub>O<sub>9</sub>: AB9C4\_hp28\_188\_e\_kl\_ak - POSCAR

```
AB9C4_hp28_188_e_kl_ak & a, c/a, x3, y3, x4, y4, x5, y5, z5 --params=
↳ 6.4953629976, 1.43896355826, 0.07103, 0.48306, 0.12023, 0.75436,
↳ 0.22923, 0.00127, 0.6032 & P-6c2 D_{3h}^{(2)} #188 (aek^21) & hP28
↳ & None & BaSi4O9 & L. W. Finger and R. M. Hazen and B. A.
↳ Fursenko, J. Phys. Chem. Solids 56, 1389-1393 (1995)
1.0000000000000000
3.24768149880000 -5.62514936272304 0.0000000000000000
3.24768149880000 5.62514936272304 0.0000000000000000
0.0000000000000000 0.0000000000000000 9.34659065120000
Ba O Si
2 18 8
Direct
0.666666666666667 0.333333333333333 0.000000000000000 Ba (2e)
0.666666666666667 0.333333333333333 0.500000000000000 Ba (2e)
0.071030000000000 0.483060000000000 0.250000000000000 O (6k)
-0.483060000000000 -0.412030000000000 0.250000000000000 O (6k)
0.412030000000000 -0.071030000000000 0.250000000000000 O (6k)
-0.483060000000000 -0.071030000000000 0.750000000000000 O (6k)
0.412030000000000 0.483060000000000 0.750000000000000 O (6k)
0.071030000000000 -0.412030000000000 0.750000000000000 O (6k)
0.229230000000000 0.001270000000000 0.603200000000000 O (12l)
-0.001270000000000 0.227960000000000 0.603200000000000 O (12l)
-0.227960000000000 -0.229230000000000 0.603200000000000 O (12l)
0.229230000000000 0.001270000000000 -0.103200000000000 O (12l)
-0.001270000000000 0.227960000000000 -0.103200000000000 O (12l)
-0.227960000000000 -0.229230000000000 -0.103200000000000 O (12l)
-0.001270000000000 -0.229230000000000 1.103200000000000 O (12l)
-0.227960000000000 0.001270000000000 1.103200000000000 O (12l)
0.229230000000000 0.227960000000000 1.103200000000000 O (12l)
-0.001270000000000 -0.229230000000000 -0.603200000000000 O (12l)
-0.227960000000000 0.001270000000000 -0.603200000000000 O (12l)
0.229230000000000 0.227960000000000 -0.603200000000000 O (12l)
0.000000000000000 0.000000000000000 0.000000000000000 Si (2a)
0.000000000000000 0.000000000000000 0.500000000000000 Si (2a)
0.120230000000000 0.754360000000000 0.250000000000000 Si (6k)
-0.754360000000000 -0.634130000000000 0.250000000000000 Si (6k)
0.634130000000000 -0.120230000000000 0.250000000000000 Si (6k)
-0.754360000000000 -0.120230000000000 0.750000000000000 Si (6k)
0.634130000000000 0.754360000000000 0.750000000000000 Si (6k)
0.120230000000000 -0.634130000000000 0.750000000000000 Si (6k)
```

π-FeMg<sub>3</sub>Al<sub>8</sub>Si<sub>6</sub> (E<sub>9</sub>): A8BC3D6\_hp18\_189\_bfh\_a\_g\_i - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral '$\pi$FeMg_{3}Al_{8}Si_{6}$'
_chemical_formula_sum 'Al8 Fe Mg3 Si6'
loop_
_publ_author_name
'H. Perltz'
'A. Westgren'
_journal_name_full_name
;
Arkiv f{\"}r Kemi, Mineralogi och Geologi
;
_journal_volume 15B
_journal_year 1942
_journal_page_first 1
_journal_page_last 8
_publ_section_title
;
The Crystal Structure of Al_{8}Si_{6}Mg_{3}Fe
;
# Found in Determination of the crystal structure of the $\pi$-AlFeMgSi
↳ phase using symmetry- and site-sensitive electron microscope
↳ techniques, 2003
_aflow_title '$\pi$FeMg_{3}Al_{8}Si_{6}$ (SE9_{b}) Structure'
_aflow_proto 'A8BC3D6_hp18_189_bfh_a_g_i'
_aflow_params 'a, c/a, x_{3}, x_{4}, z_{5}, x_{6}, z_{6}'
_aflow_params_values '6.62, 1.20241691843, 0.403, 0.444, 0.231, 0.75, 0.222'
_aflow_Strukturbericht 'SE9_{b}'
_aflow_Pearson 'hP18'
_symmetry_space_group_name_H-M "P -6 2 m"
_symmetry_Int_Tables_number 189
_cell_length_a 6.62000
_cell_length_b 6.62000
_cell_length_c 7.96000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 -y, x-y, z
3 -x+y, -x, z
4 x-y, -y, -z
5 y, x, -z
6 -x, -x+y, -z
7 -x+y, -x, -z
8 x, y, -z
```

```

9 -y,x-y,-z
10 -x,-x+y,z
11 x-y,-y,z
12 y,x,z

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Fe1 Fe 1 a 0.00000 0.00000 0.00000 1.00000
Al1 Al 1 b 0.00000 0.00000 0.50000 1.00000
Al2 Al 3 f 0.40300 0.00000 0.00000 1.00000
Mg1 Mg 3 g 0.44400 0.00000 0.50000 1.00000
Al3 Al 4 h 0.33333 0.66667 0.23100 1.00000
Si1 Si 6 i 0.75000 0.00000 0.22200 1.00000

```

$\pi$ -FeMg<sub>3</sub>Al<sub>8</sub>Si<sub>6</sub> (E<sub>9</sub>): A8BC3D6\_hP18\_189\_bfh\_a\_g\_i - POSCAR

```

A8BC3D6_hP18_189_bfh_a_g_i & a,c/a,x3,x4,z5,x6,z6 --params=6.62,
↪ 1.20241691843,0.403,0.444,0.231,0.75,0.222 & P-62m D_{3h}^{3} #
↪ 189 (abfghi) & hP18 & SE9_{b} & FeMg3Al8Si6 & \pi S-FeMgS_{3}
↪ SAIS_{8}SiS_{6} & H. Perltz and A. Westgren, {Ark. Kem.
↪ Mineral. Geol. 15B, 1-8 (1942)
1.0000000000000000
3.3100000000000000 -5.73308817305298 0.0000000000000000
3.3100000000000000 5.73308817305298 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.9600000000000000
Al Fe Mg Si
8 1 3 6
Direct
0.0000000000000000 0.0000000000000000 0.5000000000000000 Al (1b)
0.4030000000000000 0.0000000000000000 0.0000000000000000 Al (3f)
0.0000000000000000 0.4030000000000000 0.0000000000000000 Al (3f)
-0.4030000000000000 -0.4030000000000000 0.0000000000000000 Al (3f)
0.3333333333333333 0.6666666666666667 0.2310000000000000 Al (4h)
0.3333333333333333 0.6666666666666667 -0.2310000000000000 Al (4h)
0.6666666666666667 0.3333333333333333 -0.2310000000000000 Al (4h)
0.6666666666666667 0.3333333333333333 0.2310000000000000 Al (4h)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Fe (1a)
0.4440000000000000 0.0000000000000000 0.5000000000000000 Mg (3g)
0.0000000000000000 0.4440000000000000 0.5000000000000000 Mg (3g)
-0.4440000000000000 -0.4440000000000000 0.5000000000000000 Mg (3g)
0.7500000000000000 0.0000000000000000 0.2220000000000000 Si (6i)
0.0000000000000000 0.7500000000000000 0.2220000000000000 Si (6i)
-0.7500000000000000 -0.7500000000000000 0.2220000000000000 Si (6i)
0.7500000000000000 0.0000000000000000 -0.2220000000000000 Si (6i)
0.0000000000000000 0.7500000000000000 -0.2220000000000000 Si (6i)
-0.7500000000000000 -0.7500000000000000 -0.2220000000000000 Si (6i)

```

$\pi$ -FeMg<sub>3</sub>Al<sub>9</sub>Si<sub>5</sub>: A9BC3D5\_hP18\_189\_fi\_a\_g\_bh - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '\pi S-FeMgS_{3}SAIS_{9}SiS_{5}S'
_chemical_formula_sum 'Al9 Fe Mg3 Si5'

loop_
  _publ_author_name
  'S. Foss'
  'A. Olsen'
  'C. J. Simensen'
  'J. Taft{\o}'
  _journal_name_full_name
  ;
  Acta Crystallographica Section B: Structural Science
  ;
  _journal_volume 59
  _journal_year 2003
  _journal_page_first 36
  _journal_page_last 42
  _publ_Section_title
  ;
  Determination of the crystal structure of the \pi S-AlFeMgSi phase
  ↪ using symmetry- and site-sensitive electron microscope
  ↪ techniques
  ;
# Found in The Materials Project, MgS_{3}SAIS_{9}FeSiS_{5}S, {ID
↪ mp-7062},

_aflow_title '\pi S-FeMgS_{3}SAIS_{9}SiS_{5}S Structure'
_aflow_proto 'A9BC3D5_hP18_189_fi_a_g_bh'
_aflow_params 'a,c/a,x_{3},x_{4},z_{5},x_{6},z_{6}'
_aflow_params_values '6.6,1.19696969697,0.378,0.43,0.266,0.755,0.236'
_aflow_Structurbericht 'None'
_aflow_Pearson 'hP18'

_symmetry_space_group_name_H-M "P -6 2 m"
_symmetry_Int_Tables_number 189

_cell_length_a 6.60000
_cell_length_b 6.60000
_cell_length_c 7.90000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_

```

```

_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,-z
3 -x+y,-x,z
4 x-y,-y,-z
5 y,x,-z
6 -x,-x+y,-z
7 -x+y,-x,-z
8 x,y,-z
9 -y,x-y,-z
10 -x,-x+y,z
11 x-y,-y,z
12 y,x,z

```

```

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Fe1 Fe 1 a 0.00000 0.00000 0.00000 1.00000
Si1 Si 1 b 0.00000 0.00000 0.00000 1.00000
Al1 Al 3 f 0.37800 0.00000 0.00000 1.00000
Mg1 Mg 3 g 0.43000 0.00000 0.50000 1.00000
Si2 Si 4 h 0.33333 0.66667 0.26600 1.00000
Al2 Al 6 i 0.75500 0.00000 0.23600 1.00000

```

$\pi$ -FeMg<sub>3</sub>Al<sub>9</sub>Si<sub>5</sub>: A9BC3D5\_hP18\_189\_fi\_a\_g\_bh - POSCAR

```

A9BC3D5_hP18_189_fi_a_g_bh & a,c/a,x3,x4,z5,x6,z6 --params=6.6,
↪ 1.19696969697,0.378,0.43,0.266,0.755,0.236 & P-62m D_{3h}^{3} #
↪ 189 (abfghi) & hP18 & None & FeMg3Al9Si5 & \pi S-FeMgS_{3}SAIS_{9}
↪ [9]SiS_{5}S & S. Foss et al., Acta Crystallogr. Sect. B
↪ Struct. Sci. 59, 36-42 (2003)
1.0000000000000000
3.3000000000000000 -5.71576766497729 0.0000000000000000
3.3000000000000000 5.71576766497729 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.9000000000000000
Al Fe Mg Si
9 1 3 5
Direct
0.3780000000000000 0.0000000000000000 0.0000000000000000 Al (3f)
0.0000000000000000 0.3780000000000000 0.0000000000000000 Al (3f)
-0.3780000000000000 -0.3780000000000000 0.0000000000000000 Al (3f)
0.7500000000000000 0.0000000000000000 0.2360000000000000 Al (6i)
0.0000000000000000 0.7500000000000000 0.2360000000000000 Al (6i)
-0.7500000000000000 -0.7500000000000000 0.2360000000000000 Al (6i)
0.7500000000000000 0.0000000000000000 -0.2360000000000000 Al (6i)
0.0000000000000000 0.7500000000000000 -0.2360000000000000 Al (6i)
-0.7500000000000000 -0.7500000000000000 -0.2360000000000000 Al (6i)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Fe (1a)
0.4300000000000000 0.0000000000000000 0.5000000000000000 Mg (3g)
0.0000000000000000 0.4300000000000000 0.5000000000000000 Mg (3g)
-0.4300000000000000 -0.4300000000000000 0.5000000000000000 Mg (3g)
0.0000000000000000 0.0000000000000000 0.5000000000000000 Si (1b)
0.3333333333333333 0.6666666666666667 0.2660000000000000 Si (4h)
0.3333333333333333 0.6666666666666667 -0.2660000000000000 Si (4h)
0.6666666666666667 0.3333333333333333 -0.2660000000000000 Si (4h)
0.6666666666666667 0.3333333333333333 0.2660000000000000 Si (4h)

```

Li<sub>2</sub>Sb: A2B\_hP18\_190\_gh\_bf - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Li2 Sb'

loop_
  _publ_author_name
  'Wiking M{\u}ller'
  _journal_name_full_name
  ;
  Zeitschrift f{\u}r Naturforschung B
  ;
  _journal_volume 32
  _journal_year 1977
  _journal_page_first 357
  _journal_page_last 359
  _publ_Section_title
  ;
  Darstellung und Struktur der Phase LiS_{2}SSb
  ;
_aflow_title 'LiS_{2}SSb Structure'
_aflow_proto 'A2B_hP18_190_gh_bf'
_aflow_params 'a,c/a,z_{2},x_{3},x_{4},y_{4}'
_aflow_params_values '7.946,0.789076264787,0.0225,0.294,0.612,0.01'
_aflow_Structurbericht 'None'
_aflow_Pearson 'hP18'

_symmetry_space_group_name_H-M "P -6 2 c"
_symmetry_Int_Tables_number 190

_cell_length_a 7.94600
_cell_length_b 7.94600
_cell_length_c 6.27000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

```

```

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 x-y,-y,-z
5 y,x,-z
6 -x,-x+y,-z
7 -x+y,-x,-z+1/2
8 x,y,-z+1/2
9 -y,x-y,-z+1/2
10 -x,-x+y,z+1/2
11 x-y,-y,z+1/2
12 y,x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Sb1 Sb 2 b 0.00000 0.00000 0.25000 1.00000
Sb2 Sb 4 f 0.33333 0.66667 0.02250 1.00000
Li1 Li 6 g 0.29400 0.00000 0.00000 1.00000
Li2 Li 6 h 0.61200 0.01000 0.25000 1.00000

```

Li<sub>2</sub>Sb: A2B\_hP18\_190\_gh\_bf - POSCAR

```

A2B_hP18_190_gh_bf & a,c/a,z2,x3,x4,y4 --params=7.946,0.789076264787,
↪ 0.0225,0.294,0.612,0.01 & P-62c D_{3h}^{4} #190 (bfgH) & hP18 &
↪ None & Li2Sb & & Wiking M^{u}lller, Z. Naturforsch. B 32,
↪ 357-359 (1977)
1.0000000000000000
3.9730000000000000 -6.88143785847115 0.0000000000000000
3.9730000000000000 6.88143785847115 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.2700000000000000
Li Sb
12 6
Direct
0.2940000000000000 0.0000000000000000 0.0000000000000000 Li (6g)
0.0000000000000000 0.2940000000000000 0.0000000000000000 Li (6g)
-0.2940000000000000 -0.2940000000000000 0.0000000000000000 Li (6g)
0.2940000000000000 0.0000000000000000 0.5000000000000000 Li (6g)
0.0000000000000000 0.2940000000000000 0.5000000000000000 Li (6g)
-0.2940000000000000 -0.2940000000000000 0.5000000000000000 Li (6g)
0.6120000000000000 0.0100000000000000 0.2500000000000000 Li (6h)
-0.0100000000000000 0.6020000000000000 0.2500000000000000 Li (6h)
-0.6020000000000000 -0.6120000000000000 0.2500000000000000 Li (6h)
0.0100000000000000 0.6120000000000000 0.7500000000000000 Li (6h)
0.6020000000000000 -0.0100000000000000 0.7500000000000000 Li (6h)
-0.6120000000000000 -0.6020000000000000 0.7500000000000000 Li (6h)
0.0000000000000000 0.0000000000000000 0.2500000000000000 Sb (2b)
0.0000000000000000 0.0000000000000000 0.7500000000000000 Sb (2b)
0.3333333333333333 0.6666666666666667 0.0225000000000000 Sb (4f)
0.3333333333333333 0.6666666666666667 0.4775000000000000 Sb (4f)
0.6666666666666667 0.3333333333333333 -0.0225000000000000 Sb (4f)
0.6666666666666667 0.3333333333333333 0.5225000000000000 Sb (4f)

```

α-Sm<sub>3</sub>Ge<sub>5</sub> (High-temperature): A5B3\_hP16\_190\_bd\_h\_g - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'alpha-Sm3Ge5'
_chemical_formula_sum 'Ge5 Sm3'

loop_
_publ_author_name
'P. H. Tobash'
'D. Lins'
'S. Bobev'
'N. Hur'
'J. D. Thompson'
'J. L. Sarrao'
_journal_name_full_name
;
Inorganic Chemistry
;
_journal_volume 45
_journal_year 2006
_journal_page_first 7286
_journal_page_last 7294
_publ_section_title
;
Vacancy ordering in SmGe_{2-x}S and GdGe_{2-x}S ($x$ = 0.33):
↪ Structure and properties of two SmS_{3}GeS_{5} polymorphs
↪ and of GdS_{3}GeS_{5}
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title '$\alpha$-Sm_{3}Ge_{5} (High-temperature) Structure'
_aflow_proto 'A5B3_hP16_190_bd_h_g'
_aflow_params 'a,c/a,x_{3},x_{4},y_{4}'
_aflow_params_values '6.9236970109,1.22634969237,0.3313,0.0628,0.6682'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP16'

```

```

_cell_length_a 6.9236970109
_cell_length_b 6.9236970109
_cell_length_c 8.4908736994
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P -6 2 c"
_symmetry_Int_Tables_number 190

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 x-y,-y,-z
5 y,x,-z
6 -x,-x+y,-z
7 -x+y,-x,-z+1/2
8 x,y,-z+1/2
9 -y,x-y,-z+1/2
10 -x,-x+y,z+1/2
11 x-y,-y,z+1/2
12 y,x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ge1 Ge 2 b 0.00000 0.00000 0.00000 0.25000 1.00000
Ge2 Ge 2 d 0.66667 0.33333 0.25000 1.00000
Sm1 Sm 6 g 0.33130 0.00000 0.00000 1.00000
Ge3 Ge 6 h 0.06280 0.66820 0.25000 1.00000

```

α-Sm<sub>3</sub>Ge<sub>5</sub> (High-temperature): A5B3\_hP16\_190\_bd\_h\_g - POSCAR

```

A5B3_hP16_190_bd_h_g & a,c/a,x3,x4,y4 --params=6.9236970109,1.22634969237
↪ ,0.3313,0.0628,0.6682 & P-62c D_{3h}^{4} #190 (bdgh) & hP16 &
↪ None & Sm3Ge5 & alpha & P. H. Tobash et al., Inorg. Chem. 45,
↪ 7286-7294 (2006)
1.0000000000000000
3.46184850545000 -5.99609749954578 0.0000000000000000
3.46184850545000 5.99609749954578 0.0000000000000000
0.0000000000000000 0.0000000000000000 8.49087369940000
Ge Sm
10 6
Direct
0.0000000000000000 0.0000000000000000 0.2500000000000000 Ge (2b)
0.0000000000000000 0.0000000000000000 0.7500000000000000 Ge (2b)
0.6666666666666667 0.3333333333333333 0.2500000000000000 Ge (2d)
0.3333333333333333 0.6666666666666667 0.7500000000000000 Ge (2d)
0.0628000000000000 0.6682000000000000 0.2500000000000000 Ge (6h)
-0.6682000000000000 -0.6054000000000000 0.2500000000000000 Ge (6h)
0.6054000000000000 -0.0628000000000000 0.2500000000000000 Ge (6h)
0.6682000000000000 0.0628000000000000 0.7500000000000000 Ge (6h)
-0.6054000000000000 -0.6682000000000000 0.7500000000000000 Ge (6h)
-0.0628000000000000 0.6054000000000000 0.7500000000000000 Ge (6h)
0.3313000000000000 0.0000000000000000 0.0000000000000000 Sm (6g)
0.0000000000000000 0.3313000000000000 0.0000000000000000 Sm (6g)
-0.3313000000000000 -0.3313000000000000 0.0000000000000000 Sm (6g)
0.3313000000000000 0.0000000000000000 0.5000000000000000 Sm (6g)
0.0000000000000000 0.3313000000000000 0.5000000000000000 Sm (6g)
-0.3313000000000000 -0.3313000000000000 0.5000000000000000 Sm (6g)

```

Troilite (FeS): AB\_hp24\_190\_i\_ah - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'FeS'
_chemical_formula_sum 'Fe S'

loop_
_publ_author_name
'N. Morimoto'
'H. Nakazawa'
'K. Nishigucmi'
'M. Tokonami'
_journal_name_full_name
;
Science
;
_journal_volume 168
_journal_year 1970
_journal_page_first 964
_journal_page_last 966
_publ_section_title
;
Pyrrhotites: Stoichiometric Compounds with Composition FeS_{n-1}SS_{n}
↪ $ ($n \ge 8$)
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'Troilite (FeS) Structure'
_aflow_proto 'AB_hp24_190_i_ah'
_aflow_params 'a,c/a,z_{2},x_{3},y_{3},x_{4},y_{4},z_{4}'

```

```

_aflow_params_values '5.9699820408 , 1.96984924623 , 0.52 , 0.6683 , 0.6653 ,
↳ 0.3786 , 0.3233 , 0.623 '
_aflow_Strukturbericht 'None'
_aflow_Pearson 'hP24'

_cell_length_a 5.9699820408
_cell_length_b 5.9699820408
_cell_length_c 11.7599646231
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P -6 2 c"
_symmetry_Int_Tables_number 190

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -y,-x,-z
3 -x+y,-x,z
4 x-y,-y,-z
5 y,x,-z
6 -x,-x+y,-z
7 -x+y,-x,-z+1/2
8 x,y,-z+1/2
9 -y,x-y,-z+1/2
10 -x,-x+y,z+1/2
11 x-y,-y,z+1/2
12 y,x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
S1 S 2 a 0.00000 0.00000 0.00000 1.00000
S2 S 4 f 0.33333 0.66667 0.52000 1.00000
S3 S 6 h 0.66830 0.66530 0.25000 1.00000
Fe1 Fe 12 i 0.37860 0.32330 0.62300 1.00000

```

Troilite (FeS): AB\_hP24\_190\_i\_afh - POSCAR

```

AB_hP24_190_i_afh & a,c/a,z2,x3,y3,x4,y4,z4 --params=5.9699820408 ,
↳ 1.96984924623 , 0.52 , 0.6683 , 0.6653 , 0.3786 , 0.3233 , 0.623 & P-62c D_
↳ [3h]^4 #190 (afhi) & hP24 & None & FeS & N. Morimoto et
↳ al., Science 168, 964-966 (1970)
1.0000000000000000
2.98499102040000 -5.17015610746967 0.0000000000000000
2.98499102040000 5.17015610746967 0.0000000000000000
0.0000000000000000 0.0000000000000000 11.75996462310000
Fe S
12 12
Direct
0.378600000000000 0.323300000000000 0.623000000000000 Fe (12i)
-0.323300000000000 0.055300000000000 0.623000000000000 Fe (12i)
-0.055300000000000 -0.378600000000000 0.623000000000000 Fe (12i)
0.378600000000000 -0.323300000000000 -0.123000000000000 Fe (12i)
-0.323300000000000 0.055300000000000 -0.123000000000000 Fe (12i)
-0.055300000000000 -0.378600000000000 -0.123000000000000 Fe (12i)
0.323300000000000 -0.378600000000000 -0.623000000000000 Fe (12i)
-0.378600000000000 -0.055300000000000 -0.623000000000000 Fe (12i)
0.323300000000000 0.378600000000000 1.123000000000000 Fe (12i)
0.055300000000000 -0.323300000000000 1.123000000000000 Fe (12i)
-0.378600000000000 -0.055300000000000 1.123000000000000 Fe (12i)
0.000000000000000 0.000000000000000 0.000000000000000 S (2a)
0.000000000000000 0.000000000000000 0.500000000000000 S (2a)
0.333333333333333 0.666666666666667 0.520000000000000 S (4f)
0.333333333333333 0.666666666666667 -0.020000000000000 S (4f)
0.666666666666667 0.333333333333333 -0.520000000000000 S (4f)
0.666666666666667 0.333333333333333 1.020000000000000 S (4f)
0.668300000000000 0.665300000000000 0.250000000000000 S (6h)
-0.665300000000000 0.003000000000000 0.250000000000000 S (6h)
-0.003000000000000 -0.668300000000000 0.250000000000000 S (6h)
0.665300000000000 0.668300000000000 0.750000000000000 S (6h)
0.003000000000000 -0.665300000000000 0.750000000000000 S (6h)
-0.668300000000000 -0.003000000000000 0.750000000000000 S (6h)

```

Beryl (Be<sub>3</sub>Al<sub>2</sub>Si<sub>6</sub>O<sub>18</sub>, G<sub>31</sub>): A2B3C18D6\_hP58\_192\_c\_f\_lm\_1 - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Beryl'
_chemical_formula_sum 'Al2 Be3 O18 Si6'

loop_
_publ_author_name
'R. M. Hazen'
'A. Y. Au'
'L. W. Finger'
_journal_name_full_name
;
American Mineralogist
;
_journal_volume 71
_journal_year 1986
_journal_page_first 977
_journal_page_last 984

```

```

_publ_section_title
;
High-pressure crystal chemistry of beryl (Be$_{3}$Al$_{2}$Si$_{6}$O$_{18}$) and euclase (BeAlSiO$_{5}$OH)
;

# Found in The American Mineralogist Crystal Structure Database, 2003

_aflow_title 'Beryl (Be$_{3}$Al$_{2}$Si$_{6}$O$_{18}$), SG3_1}$)
↳ Structure'
_aflow_proto 'A2B3C18D6_hP58_192_c_f_lm_1'
_aflow_params 'a,c/a,x_{3},y_{3},x_{4},y_{4},x_{5},y_{5},z_{5}'
_aflow_params_values '9.214 , 0.997829390059 , 0.3103 , 0.2369 , 0.3876 , 0.1159 ,
↳ 0.4985 , 0.1456 , 0.1453 '
_aflow_Strukturbericht '$G3_1}$'
_aflow_Pearson 'hP58'

_symmetry_space_group_name_H-M "P 6/m 2/c 2/c"
_symmetry_Int_Tables_number 192

_cell_length_a 9.21400
_cell_length_b 9.21400
_cell_length_c 9.19400
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z
3 -y,-x-y,z
4 -x,-y,z
5 -x+y,-x,z
6 y,-x+y,z
7 x-y,-y,-z+1/2
8 x,x-y,-z+1/2
9 y,x,-z+1/2
10 -x+y,-y,-z+1/2
11 -x,-x+y,-z+1/2
12 -y,-x,-z+1/2
13 -x,-y,-z
14 -x+y,-x,-z
15 y,-x+y,-z
16 x,y,-z
17 x-y,x,-z
18 -y,x-y,-z
19 -x+y,y,z+1/2
20 -x,-x+y,z+1/2
21 -y,-x,z+1/2
22 x-y,-y,z+1/2
23 x,x-y,z+1/2
24 y,x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
All Al 4 c 0.33333 0.66667 0.25000 1.00000
Be1 Be 6 f 0.50000 0.00000 0.25000 1.00000
O1 O 12 l 0.31030 0.23690 0.00000 1.00000
Si1 Si 12 l 0.38760 0.11590 0.00000 1.00000
O2 O 24 m 0.49850 0.14560 0.14530 1.00000

```

Beryl (Be<sub>3</sub>Al<sub>2</sub>Si<sub>6</sub>O<sub>18</sub>, G<sub>31</sub>): A2B3C18D6\_hP58\_192\_c\_f\_lm\_1 - POSCAR

```

A2B3C18D6_hP58_192_c_f_lm_1 & a,c/a,x3,y3,x4,y4,x5,y5,z5 --params=9.214 ,
↳ 0.997829390059 , 0.3103 , 0.2369 , 0.3876 , 0.1159 , 0.4985 , 0.1456 , 0.1453
↳ & P6/mcc D_{6h}^{2} #192 (cfl^2m) & hP58 & $G3_1}$ &
↳ Be3Al2Si6O18 & Beryl & R. M. Hazen and A. Y. Au and L. W.
↳ Finger, Am. Mineral. 71, 977-984 (1986)
1.0000000000000000
4.607000000000000 -7.97955807046982 0.0000000000000000
4.607000000000000 7.97955807046982 0.0000000000000000
0.000000000000000 0.000000000000000 9.1940000000000000
Al Be O Si
4 6 36 12
Direct
0.333333333333333 0.666666666666667 0.250000000000000 Al (4c)
0.666666666666667 0.333333333333333 0.250000000000000 Al (4c)
0.666666666666667 0.333333333333333 0.750000000000000 Al (4c)
0.333333333333333 0.666666666666667 0.750000000000000 Al (4c)
0.500000000000000 0.000000000000000 0.250000000000000 Be (6f)
0.000000000000000 0.500000000000000 0.250000000000000 Be (6f)
0.500000000000000 0.500000000000000 0.250000000000000 Be (6f)
0.500000000000000 0.000000000000000 0.750000000000000 Be (6f)
0.000000000000000 0.500000000000000 0.750000000000000 Be (6f)
0.500000000000000 0.500000000000000 0.750000000000000 Be (6f)
0.310300000000000 0.236900000000000 0.000000000000000 O (12i)
-0.236900000000000 0.073400000000000 0.000000000000000 O (12i)
-0.073400000000000 -0.310300000000000 0.000000000000000 O (12i)
-0.310300000000000 -0.236900000000000 0.000000000000000 O (12i)
0.236900000000000 -0.073400000000000 0.000000000000000 O (12i)
0.073400000000000 0.310300000000000 0.000000000000000 O (12i)
0.236900000000000 0.310300000000000 0.500000000000000 O (12i)
0.073400000000000 -0.236900000000000 0.500000000000000 O (12i)
-0.310300000000000 -0.073400000000000 0.500000000000000 O (12i)
-0.236900000000000 -0.310300000000000 0.500000000000000 O (12i)
-0.073400000000000 0.236900000000000 0.500000000000000 O (12i)

```



0.54450000000000	0.66880000000000	0.50000000000000	O (121)
0.12430000000000	-0.54450000000000	0.50000000000000	O (121)
-0.66880000000000	-0.12430000000000	0.50000000000000	O (121)
-0.54450000000000	-0.66880000000000	0.50000000000000	O (121)
-0.12430000000000	0.54450000000000	0.50000000000000	O (121)
0.66880000000000	0.12430000000000	0.50000000000000	O (121)

Mavlyanovite (Mn<sub>5</sub>Si<sub>3</sub>): A5B3\_hP16\_193\_dg - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Mn5Si3'
_chemical_formula_sum 'Mn5 Si3'

loop_
_publ_author_name
'B. Aronsson'
_journal_name_full_name
;
Acta Chemica Scandinavica
;
_journal_volume 14
_journal_year 1960
_journal_page_first 1414
_journal_page_last 1418
_publ_section_title
;
A note on the compositions and crystal structures of Mn5{2}$, Mn5{3}
↪ $Si, Mn5{5}$Si3{3}$, and FeSi2{2}$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'Mavlyanovite (Mn5{5}$Si3{3}$) Structure'
_aflow_proto 'A5B3_hP16_193_dg_g'
_aflow_params 'a, c/a, x2{2}, x3{3}'
_aflow_params_values '6.9104160691, 0.696671490596, 0.2358, 0.5992'
_aflow_strukturbericht 'None'
_aflow_pearson 'hP16'

_cell_length_a 6.9104160691
_cell_length_b 6.9104160691
_cell_length_c 4.8142898635
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 120.0000000000

_symmetry_space_group_name_H-M "P 63/m 2/c 2/m"
_symmetry_int_tables_number 193

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x-y, x, z+1/2
3 -y, x-y, z
4 -x, -y, z+1/2
5 -x+y, -x, z
6 y, -x+y, z+1/2
7 x-y, -y, -z+1/2
8 x, x-y, -z
9 y, x, -z+1/2
10 -x+y, y, -z
11 -x, -x+y, -z+1/2
12 -y, -x, -z
13 -x, -y, -z
14 -x+y, -x, -z+1/2
15 y, -x+y, -z
16 x, y, -z+1/2
17 x-y, x, -z
18 -y, x-y, -z+1/2
19 -x+y, y, z+1/2
20 -x, -x+y, z
21 -y, -x, z+1/2
22 x-y, -y, z
23 x, x-y, z+1/2
24 y, x, z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mn1 Mn 4 d 0.33333 0.66667 0.00000 1.00000
Mn2 Mn 6 g 0.23580 0.00000 0.25000 1.00000
Si1 Si 6 g 0.59920 0.00000 0.25000 1.00000
```

Mavlyanovite (Mn<sub>5</sub>Si<sub>3</sub>): A5B3\_hP16\_193\_dg - POSCAR

```
A5B3_hP16_193_dg_g & a, c/a, x2, x3 --params=6.9104160691, 0.696671490596,
↪ 0.2358, 0.5992 & P63/mcm D6h3 #193 (dg^2) & hP16 & None
↪ & Mn5Si3 & B. Aronsson, Acta Chem. Scand. 14, 1414-1418 (
↪ 1960)
1.000000000000000
3.45520803455000 -5.98459586656080 0.00000000000000
3.45520803455000 5.98459586656080 0.00000000000000
0.00000000000000 0.00000000000000 4.81428986350000
Mn Si
```

10	6				
Direct	0.33333333333333	0.66666666666667	0.00000000000000	Mn (4d)	
	0.66666666666667	0.33333333333333	0.50000000000000	Mn (4d)	
	0.66666666666667	0.33333333333333	0.00000000000000	Mn (4d)	
	0.33333333333333	0.66666666666667	0.50000000000000	Mn (4d)	
	0.23580000000000	0.00000000000000	0.25000000000000	Mn (6g)	
	0.00000000000000	0.23580000000000	0.25000000000000	Mn (6g)	
	-0.23580000000000	-0.23580000000000	0.25000000000000	Mn (6g)	
	-0.23580000000000	0.00000000000000	0.75000000000000	Mn (6g)	
	0.00000000000000	-0.23580000000000	0.75000000000000	Mn (6g)	
	0.23580000000000	0.23580000000000	0.75000000000000	Mn (6g)	
	0.59920000000000	0.00000000000000	0.25000000000000	Si (6g)	
	0.00000000000000	0.59920000000000	0.25000000000000	Si (6g)	
	-0.59920000000000	-0.59920000000000	0.25000000000000	Si (6g)	
	-0.59920000000000	0.00000000000000	0.75000000000000	Si (6g)	
	0.00000000000000	-0.59920000000000	0.75000000000000	Si (6g)	
	0.59920000000000	0.59920000000000	0.75000000000000	Si (6g)	

Ni<sub>3</sub>Ti (D0<sub>24</sub>): A3B\_hP16\_194\_gh\_ac - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Ni3 Ti'

loop_
_publ_author_name
'F. Laves'
'H. J. Wallbaum'
_journal_name_full_name
;
Zeitschrift f{"u}r Kristallographiya
;
_journal_volume 101
_journal_year 1939
_journal_page_first 78
_journal_page_last 93
_publ_section_title
;
Die Kristallstruktur von Ni3STi und Si2STi (Zwei neue Typen.)
;

_aflow_title 'Ni3STi (SD024) Structure'
_aflow_proto 'A3B_hP16_194_gh_ac'
_aflow_params 'a, c/a, x4{4}'
_aflow_params_values '5.096, 1.6295133438, -0.16667'
_aflow_strukturbericht 'SD024'
_aflow_pearson 'hP16'

_symmetry_space_group_name_H-M "P 63/m 2/m 2/c"
_symmetry_int_tables_number 194

_cell_length_a 5.09600
_cell_length_b 5.09600
_cell_length_c 8.30400
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x-y, x, z+1/2
3 -y, x-y, z
4 -x, -y, z+1/2
5 -x+y, -x, z
6 y, -x+y, z+1/2
7 x-y, -y, -z
8 x, x-y, -z+1/2
9 y, x, -z
10 -x+y, y, -z+1/2
11 -x, -x+y, -z
12 -y, -x, -z+1/2
13 -x, -y, -z
14 -x+y, -x, -z+1/2
15 y, -x+y, -z
16 x, y, -z+1/2
17 x-y, x, -z
18 -y, x-y, -z+1/2
19 -x+y, y, z
20 -x, -x+y, z+1/2
21 -y, -x, z
22 x-y, -y, z+1/2
23 x, x-y, z
24 y, x, z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ti1 Ti 2 a 0.00000 0.00000 0.00000 1.00000
Ti2 Ti 2 c 0.33333 0.66667 0.25000 1.00000
Ni1 Ni 6 g 0.50000 0.00000 0.00000 1.00000
Ni2 Ni 6 h -0.16667 -0.33333 0.25000 1.00000
```

Ni<sub>3</sub>Ti (D0<sub>24</sub>): A3B\_hP16\_194\_gh\_ac - POSCAR

```

A3B_hP16_194_gh_ac & a,c/a,x4 --params=5.096,1.6295133438,-0.16667 & P6_
↪ {3}/mmc D_{6h}^{4} #194 (acgh) & hP16 & SD0_{24}$ & Ni3Ti & &
↪ F. Laves and H. J. Wallbaum, Z. Kristallogr. 101, 78-93 (1939)
1.00000000000000
2.54800000000000 -4.41326545768550 0.00000000000000
2.54800000000000 4.41326545768550 0.00000000000000
0.00000000000000 0.00000000000000 8.30400000000000
Ni Ti
12 4
Direct
0.50000000000000 0.00000000000000 0.00000000000000 Ni (6g)
0.00000000000000 0.50000000000000 0.00000000000000 Ni (6g)
0.50000000000000 0.50000000000000 0.00000000000000 Ni (6g)
0.50000000000000 0.00000000000000 0.50000000000000 Ni (6g)
0.00000000000000 0.50000000000000 0.50000000000000 Ni (6g)
0.50000000000000 0.50000000000000 0.50000000000000 Ni (6g)
-0.16667000000000 -0.33334000000000 0.25000000000000 Ni (6h)
0.33334000000000 0.16667000000000 0.25000000000000 Ni (6h)
-0.16667000000000 0.16667000000000 0.25000000000000 Ni (6h)
0.16667000000000 0.33334000000000 0.75000000000000 Ni (6h)
-0.33334000000000 -0.16667000000000 0.75000000000000 Ni (6h)
0.16667000000000 -0.16667000000000 0.75000000000000 Ni (6h)
0.00000000000000 0.00000000000000 0.00000000000000 Ti (2a)
0.00000000000000 0.00000000000000 0.50000000000000 Ti (2a)
0.33333333333333 0.66666666666667 0.25000000000000 Ti (2c)
0.66666666666667 0.33333333333333 0.75000000000000 Ti (2c)

```

Co2Al5 (D811): A5B2\_hP28\_194\_ahk\_ch - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Co2Al5'
_chemical_formula_sum 'Al5 Co2'

loop_
_publ_author_name
'J. B. Newkirk'
'P. J. Black'
'A. Damjanovic'
_journal_name_full_name
;
Acta Crystallographica
;
_journal_volume 14
_journal_year 1961
_journal_page_first 532
_journal_page_last 533
_publ_section_title
;
The refinement of the Co_{2}Al_{5} structures
;

# Found in A Palladium-Magnesium Alloy Phase of Co_{2}Al_{5} Type,
↪ 1968

_aflow_title 'Co_{2}Al_{5} ($D8_{11}$) Structure'
_aflow_proto 'A5B2_hP28_194_ahk_ch'
_aflow_params 'a,c/a,x_{3},x_{4},x_{5},z_{5}'
_aflow_params_values '7.656,0.991771159875,0.533,0.872,0.196,0.439'
_aflow_Strukturbericht '$D8_{11}$'
_aflow_Pearson 'hP28'

_symmetry_space_group_name_H-M "P 63/m 2/m 2/c"
_symmetry_Int_Tables_number 194

_cell_length_a 7.65600
_cell_length_b 7.65600
_cell_length_c 7.59300
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z+1/2
3 -y,x-y,z
4 -x,-y,z+1/2
5 -x+y,-x,z
6 y,-x+y,z+1/2
7 x-y,-y,-z
8 x,x-y,-z+1/2
9 y,x,-z
10 -x+y,-y,-z+1/2
11 -x,-x+y,-z
12 -y,-x,-z+1/2
13 -x,-y,-z
14 -x+y,-x,-z+1/2
15 y,-x+y,-z
16 x,y,-z+1/2
17 x-y,x,-z
18 -y,x-y,-z+1/2
19 -x+y,y,z
20 -x,-x+y,z+1/2
21 -y,-x,z
22 x-y,-y,z+1/2
23 x,x-y,z
24 y,x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol

```

```

_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 2 a 0.00000 0.00000 0.00000 1.00000
Co1 Co 2 c 0.33333 0.66667 0.25000 1.00000
Al2 Al 6 h 0.53300 0.06600 0.25000 1.00000
Co2 Co 6 h 0.87200 0.74400 0.25000 1.00000
Al3 Al 12 k 0.19600 0.39200 0.43900 1.00000

```

Co2Al5 (D811): A5B2\_hP28\_194\_ahk\_ch - POSCAR

```

A5B2_hP28_194_ahk_ch & a,c/a,x3,x4,x5,z5 --params=7.656,0.991771159875,
↪ 0.533,0.872,0.196,0.439 & P6_{3}/mmc D_{6h}^{4} #194 (ach^2k) &
↪ hP28 & SD8_{11}$ & Co2Al5 & Co2Al5 & J. B. Newkirk and P. J.
↪ Black and A. Damjanovic, Acta Cryst. 14, 532-533 (1961)
1.00000000000000
3.82800000000000 -6.63029049137366 0.00000000000000
3.82800000000000 6.63029049137366 0.00000000000000
0.00000000000000 0.00000000000000 7.59300000000000
Al Co
20 8
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Al (2a)
0.00000000000000 0.00000000000000 0.50000000000000 Al (2a)
0.53300000000000 1.06600000000000 0.25000000000000 Al (6h)
-1.06600000000000 -0.53300000000000 0.25000000000000 Al (6h)
0.53300000000000 -0.53300000000000 0.25000000000000 Al (6h)
-0.53300000000000 -1.06600000000000 0.25000000000000 Al (6h)
1.06600000000000 0.53300000000000 0.75000000000000 Al (6h)
-0.53300000000000 0.53300000000000 0.75000000000000 Al (6h)
0.19600000000000 0.39200000000000 0.39200000000000 Al (12k)
-0.39200000000000 -0.19600000000000 0.43900000000000 Al (12k)
0.19600000000000 -0.19600000000000 0.43900000000000 Al (12k)
-0.19600000000000 -0.39200000000000 0.93900000000000 Al (12k)
0.39200000000000 0.19600000000000 0.93900000000000 Al (12k)
-0.19600000000000 0.19600000000000 0.93900000000000 Al (12k)
0.39200000000000 0.19600000000000 -0.43900000000000 Al (12k)
-0.19600000000000 -0.39200000000000 -0.43900000000000 Al (12k)
-0.39200000000000 -0.19600000000000 0.06100000000000 Al (12k)
0.19600000000000 0.39200000000000 0.06100000000000 Al (12k)
0.19600000000000 -0.19600000000000 0.06100000000000 Al (12k)
0.33333333333333 0.66666666666667 0.25000000000000 Co (2c)
0.66666666666667 0.33333333333333 0.75000000000000 Co (2c)
0.87200000000000 1.74400000000000 0.25000000000000 Co (6h)
-1.74400000000000 -0.87200000000000 0.25000000000000 Co (6h)
0.87200000000000 -0.87200000000000 0.25000000000000 Co (6h)
-0.87200000000000 -1.74400000000000 0.75000000000000 Co (6h)
1.74400000000000 0.87200000000000 0.75000000000000 Co (6h)
-0.87200000000000 0.87200000000000 0.75000000000000 Co (6h)

```

Al9Mn3Si (E9c): A9B3C\_hP26\_194\_hk\_h\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Al9Mn3Si'
_chemical_formula_sum 'Al9 Mn3 Si'

loop_
_publ_author_name
'K. Robinson'
_journal_name_full_name
;
Philosophical Magazine
;
_journal_volume 43
_journal_year 1952
_journal_page_first 775
_journal_page_last 782
_publ_section_title
;
LXXIII. The unit cell and Brillouin Zones of Ni_{4}Mn_{11}Al_{60}$
↪ and belated compounds
;

# Found in A Handbook of Lattice Spacings and Structures of Metals and
↪ Alloys, 1958

_aflow_title 'Al_{9}Mn_{3}Si ($E9_{c}$) Structure'
_aflow_proto 'A9B3C_hP26_194_hk_h_a'
_aflow_params 'a,c/a,x_{2},x_{3},x_{4},z_{4}'
_aflow_params_values '7.513,1.03087980833,0.458,0.12,0.201,-0.067'
_aflow_Strukturbericht '$E9_{c}$'
_aflow_Pearson 'hP26'

_symmetry_space_group_name_H-M "P 63/m 2/m 2/c"
_symmetry_Int_Tables_number 194

_cell_length_a 7.51300
_cell_length_b 7.51300
_cell_length_c 7.74500
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 120.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z+1/2

```



```

3 -y,x-y,z
4 -x,-y,z+1/2
5 -x+y,-x,z
6 y,-x+y,z+1/2
7 x-y,-y,-z
8 x,x-y,-z+1/2
9 y,x,-z
10 -x+y,y,-z+1/2
11 -x,-x+y,-z
12 -y,-x,-z+1/2
13 -x,-y,-z
14 -x+y,-x,-z+1/2
15 y,-x+y,-z
16 x,y,-z+1/2
17 x-y,x,-z
18 -y,x-y,-z+1/2
19 -x+y,y,z
20 -x,-x+y,z+1/2
21 -y,-x,z
22 x-y,-y,z+1/2
23 x,x-y,z
24 y,x,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Si1 Si 2 a 0.00000 0.00000 0.00000 1.00000
Al1 Al 6 h 0.45800 0.91600 0.25000 1.00000
Mn1 Mn 6 h 0.12000 0.24000 0.25000 1.00000
Al2 Al 12 k 0.20100 0.40200 -0.06700 1.00000

```

Al<sub>9</sub>Mn<sub>3</sub>Si (E<sub>9</sub>): A9B3C\_hP26\_194\_hk\_h\_a - POSCAR

```

A9B3C_hP26_194_hk_h_a & a,c/a,x2,x3,x4,z4 --params=7.513,1.03087980833,
↳ 0.458,0.12,0.201,-0.067 & P6_{3}/mmc D_{6h}^{4} #194 (ah^2k) &
↳ hP26 & $E9_{c}$ & Al9Mn3Si & Al9Mn3Si & K. Robinson, Philos.
↳ Mag. 43, 775-782 (1952)
1.0000000000000000
3.7565000000000000 -6.50644885863249 0.0000000000000000
3.7565000000000000 6.50644885863249 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.7450000000000000
Al Mn Si
18 6 2
Direct
0.4580000000000000 0.9160000000000000 0.2500000000000000 Al (6h)
-0.9160000000000000 -0.4580000000000000 0.2500000000000000 Al (6h)
0.4580000000000000 -0.4580000000000000 0.2500000000000000 Al (6h)
-0.4580000000000000 -0.9160000000000000 0.7500000000000000 Al (6h)
0.9160000000000000 0.4580000000000000 0.7500000000000000 Al (6h)
-0.4580000000000000 0.4580000000000000 0.7500000000000000 Al (6h)
0.2010000000000000 0.4020000000000000 -0.0670000000000000 Al (12k)
-0.4020000000000000 -0.2010000000000000 -0.0670000000000000 Al (12k)
0.2010000000000000 -0.2010000000000000 -0.0670000000000000 Al (12k)
-0.2010000000000000 -0.4020000000000000 0.4330000000000000 Al (12k)
0.4020000000000000 0.2010000000000000 0.4330000000000000 Al (12k)
-0.2010000000000000 0.2010000000000000 0.4330000000000000 Al (12k)
0.4020000000000000 0.2010000000000000 0.0670000000000000 Al (12k)
-0.2010000000000000 -0.4020000000000000 0.0670000000000000 Al (12k)
-0.4020000000000000 -0.2010000000000000 0.5670000000000000 Al (12k)
0.2010000000000000 -0.2010000000000000 0.5670000000000000 Al (12k)
0.1200000000000000 0.2400000000000000 0.2500000000000000 Mn (6h)
-0.2400000000000000 -0.1200000000000000 0.2500000000000000 Mn (6h)
0.1200000000000000 -0.1200000000000000 0.2500000000000000 Mn (6h)
-0.1200000000000000 -0.2400000000000000 0.7500000000000000 Mn (6h)
0.2400000000000000 0.1200000000000000 0.7500000000000000 Mn (6h)
-0.1200000000000000 0.1200000000000000 0.7500000000000000 Mn (6h)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Si (2a)
0.0000000000000000 0.0000000000000000 0.5000000000000000 Si (2a)

```

PrRu<sub>4</sub>P<sub>12</sub>: A12BC4\_cP34\_195\_2j\_ab\_2e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'PrRu4P12'
_chemical_formula_sum 'P12 Pr Ru4'

loop_
_publ_author_name
'C. H. Lee'
'H. Matsuhata'
'H. Yamaguchi'
'C. Sekine'
'K. Kihou'
'I. Shirotnani'
_journal_name_full_name
;
Journal of Magnetism and Magnetic Materials
;
_journal_volume 272
_journal_year 2004
_journal_page_first 426
_journal_page_last 427
_publ_section_title
;

```

```

A study of the crystal structure at low temperature in the
↳ metal--insulator transition compound PrRu_{4}$SPS_{12}$
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'PrRu_{4}$SPS_{12}$ Structure'
_aflow_proto 'A12BC4_cP34_195_2j_ab_2e'
_aflow_params 'a,x_{3},x_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6}'
_aflow_params_values '8.0357772599,0.2493,0.7507,0.14225,0.5,0.35579,
↳ 0.0002,0.14286,0.35831'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cP34'

_cell_length_a 8.0357772599
_cell_length_b 8.0357772599
_cell_length_c 8.0357772599
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2 3"
_symmetry_Int_Tables_number 195

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Pr1 Pr 1 a 0.00000 0.00000 0.00000 1.00000
Pr2 Pr 1 b 0.50000 0.50000 0.50000 1.00000
Ru1 Ru 4 e 0.24930 0.24930 0.24930 1.00000
Ru2 Ru 4 e 0.75070 0.75070 0.75070 1.00000
P1 P 12 j 0.14225 0.50000 0.35579 1.00000
P2 P 12 j 0.00020 0.14286 0.35831 1.00000

```

PrRu<sub>4</sub>P<sub>12</sub>: A12BC4\_cP34\_195\_2j\_ab\_2e - POSCAR

```

A12BC4_cP34_195_2j_ab_2e & a,x3,x4,x5,y5,z5,x6,y6,z6 --params=
↳ 8.0357772599,0.2493,0.7507,0.14225,0.5,0.35579,0.0002,0.14286,
↳ 0.35831 & P23 T^{1} #195 (abe^2j^2) & cP34 & None & PrRu4P12 &
↳ & C. H. Lee et al., J. Magn. Magn. Mater. 272, 426-427 (2004)
1.0000000000000000
8.03577725990000 0.00000000000000 0.0000000000000000
0.0000000000000000 8.03577725990000 0.0000000000000000
0.0000000000000000 0.0000000000000000 8.03577725990000
P Pr Ru
24 2 8
Direct
0.1422500000000000 0.5000000000000000 0.3557900000000000 P (12j)
-0.1422500000000000 -0.5000000000000000 0.3557900000000000 P (12j)
-0.1422500000000000 0.5000000000000000 -0.3557900000000000 P (12j)
0.1422500000000000 -0.5000000000000000 -0.3557900000000000 P (12j)
0.3557900000000000 0.1422500000000000 0.5000000000000000 P (12j)
0.3557900000000000 -0.1422500000000000 -0.5000000000000000 P (12j)
-0.3557900000000000 -0.1422500000000000 0.5000000000000000 P (12j)
-0.3557900000000000 0.1422500000000000 -0.5000000000000000 P (12j)
0.5000000000000000 0.3557900000000000 0.1422500000000000 P (12j)
-0.5000000000000000 0.3557900000000000 -0.1422500000000000 P (12j)
0.5000000000000000 -0.3557900000000000 -0.1422500000000000 P (12j)
-0.5000000000000000 -0.3557900000000000 0.1422500000000000 P (12j)
0.0002000000000000 0.1428600000000000 0.3583100000000000 P (12j)
-0.0002000000000000 -0.1428600000000000 0.3583100000000000 P (12j)
-0.0002000000000000 0.1428600000000000 -0.3583100000000000 P (12j)
0.0002000000000000 -0.1428600000000000 -0.3583100000000000 P (12j)
0.3583100000000000 0.0002000000000000 0.1428600000000000 P (12j)
0.3583100000000000 -0.0002000000000000 -0.1428600000000000 P (12j)
-0.3583100000000000 -0.0002000000000000 0.1428600000000000 P (12j)
-0.3583100000000000 0.0002000000000000 -0.1428600000000000 P (12j)
0.1428600000000000 0.3583100000000000 0.0002000000000000 P (12j)
-0.1428600000000000 0.3583100000000000 -0.0002000000000000 P (12j)
0.1428600000000000 -0.3583100000000000 -0.0002000000000000 P (12j)
-0.1428600000000000 -0.3583100000000000 0.0002000000000000 P (12j)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Pr (1a)
0.5000000000000000 0.5000000000000000 0.5000000000000000 Pr (1b)
0.2493000000000000 0.2493000000000000 0.2493000000000000 Ru (4e)
-0.2493000000000000 -0.2493000000000000 0.2493000000000000 Ru (4e)
-0.2493000000000000 0.2493000000000000 -0.2493000000000000 Ru (4e)
0.2493000000000000 -0.2493000000000000 -0.2493000000000000 Ru (4e)
0.7507000000000000 0.7507000000000000 0.7507000000000000 Ru (4e)
-0.7507000000000000 -0.7507000000000000 0.7507000000000000 Ru (4e)
-0.7507000000000000 0.7507000000000000 -0.7507000000000000 Ru (4e)
0.7507000000000000 -0.7507000000000000 -0.7507000000000000 Ru (4e)

```

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Cu2Fe[CN]6'
_chemical_formula_sum 'C12 Cu2 Fe'

loop_
  _publ_author_name
    'R. Rigamonti'
  _journal_name_full_name
    :
    Gazzetta Chimica Italiana
  :
  _journal_volume 67
  _journal_year 1937
  _journal_page_first 137
  _journal_page_last 146
  _publ_section_title
    :
    Structure of Cupriferrrocyanides I. Copper Ferrocyanide and Potassium
    ↪ Copper Ferrocyanide
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'Cu$[2]$Fe[CN]$_{6}$ Structure'
_aflow_proto 'A12B2C_cF60_196_h_bc_a'
_aflow_params 'a,x_{4},y_{4},z_{4}'
_aflow_params_values '9.9799933334,0.0,0.0625,0.25'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cF60'

_cell_length_a 9.9799933334
_cell_length_b 9.9799933334
_cell_length_c 9.9799933334
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "F 2 3"
_symmetry_Int_Tables_number 196

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x,-y,-z
  3 -x,y,-z
  4 -x,-y,z
  5 y,z,x
  6 y,-z,-x
  7 -y,z,-x
  8 -y,-z,x
  9 z,x,y
  10 z,-x,-y
  11 -z,x,-y
  12 -z,-x,y
  13 x,y+1/2,z+1/2
  14 x,-y+1/2,-z+1/2
  15 -x,y+1/2,-z+1/2
  16 -x,-y+1/2,z+1/2
  17 y,z+1/2,x+1/2
  18 y,-z+1/2,-x+1/2
  19 -y,z+1/2,-x+1/2
  20 -y,-z+1/2,x+1/2
  21 z,x+1/2,y+1/2
  22 z,-x+1/2,-y+1/2
  23 -z,x+1/2,-y+1/2
  24 -z,-x+1/2,y+1/2
  25 x+1/2,y,z+1/2
  26 x+1/2,-y,-z+1/2
  27 -x+1/2,y,-z+1/2
  28 -x+1/2,-y,z+1/2
  29 y+1/2,z,x+1/2
  30 y+1/2,-z,-x+1/2
  31 -y+1/2,z,-x+1/2
  32 -y+1/2,-z,x+1/2
  33 z+1/2,x,y+1/2
  34 z+1/2,-x,-y+1/2
  35 -z+1/2,x,-y+1/2
  36 -z+1/2,-x,y+1/2
  37 x+1/2,y+1/2,z
  38 x+1/2,-y+1/2,-z
  39 -x+1/2,y+1/2,-z
  40 -x+1/2,-y+1/2,z
  41 y+1/2,z+1/2,x
  42 y+1/2,-z+1/2,-x
  43 -y+1/2,z+1/2,-x
  44 -y+1/2,-z+1/2,x
  45 z+1/2,x+1/2,y
  46 z+1/2,-x+1/2,-y
  47 -z+1/2,x+1/2,-y
  48 -z+1/2,-x+1/2,y

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
```

```
_atom_site_occupancy
Fe1 Fe 4 a 0.00000 0.00000 1.00000
Cu1 Cu 4 b 0.50000 0.50000 0.50000 1.00000
Cu2 Cu 4 c 0.25000 0.25000 0.25000 1.00000
C1 C 48 h 0.00000 0.06250 0.25000 1.00000
```

Cu<sub>2</sub>Fe[CN]<sub>6</sub>: A12B2C\_cF60\_196\_h\_bc\_a - POSCAR

```
A12B2C_cF60_196_h_bc_a & a,x4,y4,z4 --params=9.9799933334,0.0,0.0625,
↪ 0.25 & F23 T^2 #196 (abch) & cF60 & None & Cu2Fe[CN]6 & R.
↪ Rigamonti, Gazz. Chim. Ital. 67, 137-146 (1937)
1.0000000000000000
0.0000000000000000 4.98999666670000 4.98999666670000
4.98999666670000 0.0000000000000000 4.98999666670000
4.98999666670000 4.98999666670000 0.0000000000000000
C Cu Fe
12 2 1
Direct
0.312500000000000 0.187500000000000 -0.187500000000000 C (48h)
0.187500000000000 0.312500000000000 -0.312500000000000 C (48h)
-0.187500000000000 -0.312500000000000 0.312500000000000 C (48h)
-0.312500000000000 -0.187500000000000 0.187500000000000 C (48h)
-0.187500000000000 0.312500000000000 0.187500000000000 C (48h)
-0.312500000000000 0.187500000000000 0.312500000000000 C (48h)
0.312500000000000 -0.187500000000000 -0.312500000000000 C (48h)
0.187500000000000 -0.312500000000000 -0.187500000000000 C (48h)
0.187500000000000 -0.187500000000000 0.312500000000000 C (48h)
0.312500000000000 -0.312500000000000 0.187500000000000 C (48h)
-0.312500000000000 0.312500000000000 -0.187500000000000 C (48h)
-0.187500000000000 0.187500000000000 -0.312500000000000 C (48h)
0.500000000000000 0.500000000000000 0.500000000000000 Cu (4b)
0.250000000000000 0.250000000000000 0.250000000000000 Cu (4c)
0.000000000000000 0.000000000000000 0.000000000000000 Fe (4a)
```

MgB<sub>12</sub>H<sub>12</sub>[H<sub>2</sub>O]<sub>12</sub>: A12B36CD12\_cF488\_196\_2h\_6h\_ac\_fgh - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'MgB12H12[H2O]12'
_chemical_formula_sum 'B12 H36 Mg O12'

loop_
  _publ_author_name
    'I. Tiritiris'
  _journal_year 2004
  _publ_section_title
    :
    Synthesis, Crystal Structure, and Thermal Decomposition of Mg(HS_{2})SO
    ↪ $[6]$_{12}$HS_{12}$$_{12}$SO
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'MgB$_{12}$HS$_{12}$$_{12}$SO$_{12}$ Structure'
_aflow_proto 'A12B36CD12_cF488_196_2h_6h_ac_fgh'
_aflow_params 'a,x_{3},x_{4},x_{5},y_{5},z_{5},x_{6},y_{6},z_{6},x_{7},
↪ y_{7},z_{7},x_{8},y_{8},z_{8},x_{9},y_{9},z_{9},x_{10},y_{10},
↪ z_{10},x_{11},y_{11},z_{11},x_{12},y_{12},z_{12},x_{13},y_{13},
↪ z_{13}'
_aflow_params_values '16.4321054599,0.12536,0.37536,0.55423,0.08845,
↪ 0.00025,0.83845,0.30423,0.24975,0.0008,0.09,0.3557,0.84,0.2508,
↪ 0.3943,0.0123,0.0411,0.1708,0.2911,0.2623,0.0792,0.0347,0.2125,
↪ 0.0888,0.4625,0.2847,0.1612,0.125,0.01382,0.23628'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cF488'

_cell_length_a 16.4321054599
_cell_length_b 16.4321054599
_cell_length_c 16.4321054599
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "F 2 3"
_symmetry_Int_Tables_number 196

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x,-y,-z
  3 -x,y,-z
  4 -x,-y,z
  5 y,z,x
  6 y,-z,-x
  7 -y,z,-x
  8 -y,-z,x
  9 z,x,y
  10 z,-x,-y
  11 -z,x,-y
  12 -z,-x,y
  13 x,y+1/2,z+1/2
  14 x,-y+1/2,-z+1/2
  15 -x,y+1/2,-z+1/2
  16 -x,-y+1/2,z+1/2
  17 y,z+1/2,x+1/2
  18 y,-z+1/2,-x+1/2
  19 -y,z+1/2,-x+1/2
  20 -y,-z+1/2,x+1/2
  21 z,x+1/2,y+1/2
  22 z,-x+1/2,-y+1/2
```



```

_journal_page_last 675
_publ_section_title
;
The absolute configuration of sodium chlorate
;
# Found in Acentric cubic NaClO3--a new crystal for Raman lasers ,
↪ 1998

_aflow_title 'Sodium Chlorate (NaClO3, G3) Structure'
_aflow_proto 'ABC3_cP20_198_a_a_b'
_aflow_params 'a,x_{1},x_{2},x_{3},y_{3},z_{3}'
_aflow_params_values '6.57,0.417,0.064,0.303,0.592,0.5'
_aflow_Strukturbericht 'G3$'
_aflow_Pearson 'cP20'

_symmetry_space_group_name_H-M "P 21 3"
_symmetry_Int_Tables_number 198

_cell_length_a 6.57000
_cell_length_b 6.57000
_cell_length_c 6.57000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y+1/2,-z
3 -x,y+1/2,-z+1/2
4 -x+1/2,-y,z+1/2
5 y,z,x
6 y+1/2,-z+1/2,-x
7 -y,z+1/2,-x+1/2
8 -y+1/2,-z,x+1/2
9 z,x,y
10 z+1/2,-x+1/2,-y
11 -z,x+1/2,-y+1/2
12 -z+1/2,-x,y+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cl1 Cl 4 a 0.41700 0.41700 0.41700 1.00000
Na1 Na 4 a 0.06400 0.06400 0.06400 1.00000
O1 O 12 b 0.30300 0.59200 0.50000 1.00000

```

Sodium Chlorate (NaClO<sub>3</sub>, G3): ABC3\_cP20\_198\_a\_a\_b - POSCAR

```

ABC3_cP20_198_a_a_b & a,x1,x2,x3,y3,z3 --params=6.57,0.417,0.064,0.303,
↪ 0.592,0.5 & P2_1{3} T^4 #198 (a^2b) & cP20 & G3$ & NaClO3 &
↪ Sodium chlorate & G. N. Ramachandran and K. S. Chandrasekaran &
↪ Acta Cryst. 10, 671-675 (1957)
1.0000000000000000
6.5700000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 6.5700000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.5700000000000000
Cl Na O
4 4 12
Direct
0.4170000000000000 0.4170000000000000 0.4170000000000000 Cl (4a)
0.0830000000000000 -0.4170000000000000 0.9170000000000000 Cl (4a)
-0.4170000000000000 0.9170000000000000 0.0830000000000000 Cl (4a)
0.9170000000000000 0.0830000000000000 -0.4170000000000000 Cl (4a)
0.0640000000000000 0.0640000000000000 0.0640000000000000 Na (4a)
0.4360000000000000 -0.0640000000000000 0.5640000000000000 Na (4a)
-0.0640000000000000 0.5640000000000000 0.4360000000000000 Na (4a)
0.5640000000000000 0.4360000000000000 -0.0640000000000000 Na (4a)
0.3030000000000000 0.5920000000000000 0.5000000000000000 O (12b)
0.1970000000000000 -0.5920000000000000 1.0000000000000000 O (12b)
-0.3030000000000000 1.0920000000000000 0.0000000000000000 O (12b)
0.8030000000000000 -0.0920000000000000 -0.5000000000000000 O (12b)
0.5000000000000000 0.3030000000000000 0.5920000000000000 O (12b)
1.0000000000000000 0.1970000000000000 -0.5920000000000000 O (12b)
0.0000000000000000 -0.3030000000000000 1.0920000000000000 O (12b)
-0.5000000000000000 0.8030000000000000 -0.0920000000000000 O (12b)
0.5920000000000000 0.5000000000000000 0.3030000000000000 O (12b)
-0.5920000000000000 1.0000000000000000 0.1970000000000000 O (12b)
1.0920000000000000 0.0000000000000000 -0.3030000000000000 O (12b)
-0.0920000000000000 -0.5000000000000000 0.8030000000000000 O (12b)

```

Mg<sub>2</sub>Zn<sub>11</sub>: A2B11\_cP39\_200\_f\_aghij - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Mg2Zn11'
_chemical_formula_sum 'Mg2 Zn11'

loop_
_publ_author_name
'S. Samson'
_journal_name_full_name
;
Acta Chemica Scandinavica
;

```

```

_journal_volume 3
_journal_year 1949
_journal_page_first 835
_journal_page_last 843
_publ_section_title
;
Die Kristallstruktur von MgS_{2}ZnS_{11} Isomorphie zwischen MgS_{2}
↪ ZnS_{11} und MgS_{2}CuS_{6}AlS_{5}
;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'MgS_{2}ZnS_{11} Structure'
_aflow_proto 'A2B11_cP39_200_f_aghij'
_aflow_params 'a,x_{2},x_{3},x_{4},x_{5},y_{6},z_{6}'
_aflow_params_values '8.5520223662,0.18,0.34,0.265,0.157,0.257'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cP39'

_cell_length_a 8.5520223662
_cell_length_b 8.5520223662
_cell_length_c 8.5520223662
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2/m -3"
_symmetry_Int_Tables_number 200

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 -x,-y,-z
14 -x,y,z
15 x,-y,z
16 x,y,-z
17 -y,-z,-x
18 -y,z,x
19 y,-z,x
20 y,z,-x
21 -z,-x,-y
22 -z,x,y
23 z,-x,y
24 z,x,-y

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Zn1 Zn 1 a 0.00000 0.00000 0.00000 1.00000
Mg1 Mg 6 f 0.18000 0.00000 0.50000 1.00000
Zn2 Zn 6 g 0.34000 0.50000 0.00000 1.00000
Zn3 Zn 6 h 0.26500 0.50000 0.50000 1.00000
Zn4 Zn 8 i 0.27800 0.27800 0.27800 1.00000
Zn5 Zn 12 j 0.00000 0.15700 0.25700 1.00000

```

Mg<sub>2</sub>Zn<sub>11</sub>: A2B11\_cP39\_200\_f\_aghij - POSCAR

```

A2B11_cP39_200_f_aghij & a,x2,x3,x4,x5,y6,z6 --params=8.5520223662,0.18,
↪ 0.34,0.265,0.278,0.157,0.257 & Pm-3 T_{h}^{1} #200 (afghij) &
↪ cP39 & None & Mg2Zn11 & S. Samson, Acta Chem. Scand. 3,
↪ 835-843 (1949)
1.0000000000000000
8.55202236620000 0.00000000000000 0.0000000000000000
0.0000000000000000 8.55202236620000 0.0000000000000000
0.0000000000000000 0.0000000000000000 8.55202236620000
Mg Zn
6 33
Direct
0.1800000000000000 0.0000000000000000 0.5000000000000000 Mg (6f)
-0.1800000000000000 0.0000000000000000 0.5000000000000000 Mg (6f)
0.5000000000000000 0.1800000000000000 0.0000000000000000 Mg (6f)
0.5000000000000000 -0.1800000000000000 0.0000000000000000 Mg (6f)
0.0000000000000000 0.5000000000000000 0.1800000000000000 Mg (6f)
0.0000000000000000 0.5000000000000000 -0.1800000000000000 Mg (6f)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Zn (1a)
-0.3400000000000000 0.5000000000000000 0.0000000000000000 Zn (6g)
0.3400000000000000 0.5000000000000000 0.0000000000000000 Zn (6g)
0.0000000000000000 0.3400000000000000 0.5000000000000000 Zn (6g)
0.0000000000000000 -0.3400000000000000 0.5000000000000000 Zn (6g)
0.5000000000000000 0.0000000000000000 0.3400000000000000 Zn (6g)
0.5000000000000000 0.0000000000000000 -0.3400000000000000 Zn (6g)
0.2650000000000000 0.5000000000000000 0.5000000000000000 Zn (6h)
-0.2650000000000000 0.5000000000000000 0.5000000000000000 Zn (6h)
0.5000000000000000 0.2650000000000000 0.5000000000000000 Zn (6h)
0.5000000000000000 -0.2650000000000000 0.5000000000000000 Zn (6h)
0.5000000000000000 0.5000000000000000 0.2650000000000000 Zn (6h)

```

```
0.50000000000000 0.50000000000000 -0.26500000000000 Zn (6h)
0.27800000000000 0.27800000000000 0.27800000000000 Zn (8i)
-0.27800000000000 -0.27800000000000 0.27800000000000 Zn (8i)
-0.27800000000000 -0.27800000000000 -0.27800000000000 Zn (8i)
0.27800000000000 -0.27800000000000 -0.27800000000000 Zn (8i)
-0.27800000000000 0.27800000000000 -0.27800000000000 Zn (8i)
0.00000000000000 0.15700000000000 0.25700000000000 Zn (12j)
0.00000000000000 -0.15700000000000 0.25700000000000 Zn (12j)
0.00000000000000 0.15700000000000 -0.25700000000000 Zn (12j)
0.00000000000000 -0.15700000000000 -0.25700000000000 Zn (12j)
0.25700000000000 0.00000000000000 0.15700000000000 Zn (12j)
0.25700000000000 0.00000000000000 -0.15700000000000 Zn (12j)
-0.25700000000000 0.00000000000000 0.15700000000000 Zn (12j)
-0.25700000000000 0.00000000000000 -0.15700000000000 Zn (12j)
0.15700000000000 0.25700000000000 0.00000000000000 Zn (12j)
-0.15700000000000 0.25700000000000 0.00000000000000 Zn (12j)
0.15700000000000 -0.25700000000000 0.00000000000000 Zn (12j)
-0.15700000000000 -0.25700000000000 0.00000000000000 Zn (12j)
```

KSbO<sub>3</sub> (High-temperature): AB3C\_cP60\_201\_ce\_fh\_g - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'KSbO3'
_chemical_formula_sum 'K O3 Sb'

loop_
  _publ_author_name
    'P. Spiegelberg'
  _journal_name_full_name
    ;
    Arkiv f[\"o)r Kemi, Mineralogi och Geologi
  ;
  _journal_volume 14A
  _journal_year 1940
  _journal_page_first 1
  _journal_page_last 12
  _publ_section_title
    ;
  X-ray studies on potassium antimonates
  ;
# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013
_aflow_title 'KSbO3_{3}$ (High-temperature) Structure '
_aflow_proto 'AB3C_cP60_201_ce_fh_g'
_aflow_params 'a,x_{2},x_{3},x_{4},x_{5},y_{5},z_{5}'
_aflow_params_values '9.5599167841,0.8889,0.8889,0.4028,0.5389,0.5972,
  ↪ 0.25'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cP60'

_cell_length_a 9.5599167841
_cell_length_b 9.5599167841
_cell_length_c 9.5599167841
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 2/n -3 (origin choice 2)"
_symmetry_Int_Tables_number 201

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x,-y+1/2,-z+1/2
3 -x+1/2,y,-z+1/2
4 -x+1/2,-y+1/2,z
5 y,z,x
6 y,-z+1/2,-x+1/2
7 -y+1/2,z,-x+1/2
8 -y+1/2,-z+1/2,x
9 z,x,y
10 z,-x+1/2,-y+1/2
11 -z+1/2,x,-y+1/2
12 -z+1/2,-x+1/2,y
13 -x,-y,-z
14 -x,y+1/2,z+1/2
15 x+1/2,-y,z+1/2
16 x+1/2,y+1/2,-z
17 -y,-z,-x
18 -y,z+1/2,x+1/2
19 y+1/2,-z,x+1/2
20 y+1/2,z+1/2,-x
21 -z,-x,-y
22 -z,x+1/2,y+1/2
23 z+1/2,-x,y+1/2
24 z+1/2,x+1/2,-y

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
```

```
K1 K 4 c 0.50000 0.50000 0.50000 1.00000
K2 K 8 e 0.88890 0.88890 0.88890 1.00000
O1 O 12 f 0.88890 0.25000 0.25000 1.00000
Sb1 Sb 12 g 0.40280 0.75000 0.25000 1.00000
O2 O 24 h 0.53890 0.59720 0.25000 1.00000
```

KSbO<sub>3</sub> (High-temperature): AB3C\_cP60\_201\_ce\_fh\_g - POSCAR

```
AB3C_cP60_201_ce_fh_g & a,x2,x3,x4,x5,y5,z5 --params=9.5599167841,0.8889
  ↪ ,0.8889,0.4028,0.5389,0.5972,0.25 & Pn-3 T_{h}^{2} #201 (cefhg)
  ↪ & cP60 & None & KSbO3 & & P. Spiegelberg, {Ark. Kem. Mineral.
  ↪ Geol. 14A, 1-12 (1940)
1.00000000000000
9.55991678410000 0.00000000000000 0.00000000000000
0.00000000000000 9.55991678410000 0.00000000000000
0.00000000000000 0.00000000000000 9.55991678410000
K O Sb
12 36 12
Direct
0.50000000000000 0.50000000000000 0.50000000000000 K (4c)
0.00000000000000 0.00000000000000 0.50000000000000 K (4c)
0.00000000000000 0.50000000000000 0.00000000000000 K (4c)
0.50000000000000 0.00000000000000 0.00000000000000 K (4c)
0.88890000000000 0.88890000000000 0.88890000000000 K (8e)
-0.88890000000000 -0.88890000000000 0.88890000000000 K (8e)
-0.88890000000000 0.88890000000000 -0.88890000000000 K (8e)
0.88890000000000 -0.88890000000000 -0.88890000000000 K (8e)
1.38890000000000 1.38890000000000 -0.88890000000000 K (8e)
1.38890000000000 -0.88890000000000 1.38890000000000 K (8e)
-0.88890000000000 1.38890000000000 1.38890000000000 K (8e)
0.88890000000000 0.25000000000000 0.25000000000000 O (12f)
-0.88890000000000 0.25000000000000 0.25000000000000 O (12f)
0.25000000000000 0.88890000000000 0.25000000000000 O (12f)
0.25000000000000 -0.88890000000000 0.25000000000000 O (12f)
0.25000000000000 0.25000000000000 0.88890000000000 O (12f)
0.25000000000000 0.25000000000000 -0.88890000000000 O (12f)
-0.88890000000000 0.75000000000000 0.75000000000000 O (12f)
1.38890000000000 0.75000000000000 0.75000000000000 O (12f)
0.75000000000000 -0.88890000000000 0.75000000000000 O (12f)
0.75000000000000 1.38890000000000 0.75000000000000 O (12f)
0.75000000000000 0.75000000000000 -0.88890000000000 O (12f)
0.75000000000000 0.75000000000000 1.38890000000000 O (12f)
0.53890000000000 0.59720000000000 0.25000000000000 O (24h)
-0.03890000000000 -0.09720000000000 0.25000000000000 O (24h)
-0.03890000000000 0.59720000000000 0.25000000000000 O (24h)
0.53890000000000 -0.09720000000000 0.25000000000000 O (24h)
0.25000000000000 0.53890000000000 0.53890000000000 O (24h)
0.25000000000000 -0.03890000000000 -0.09720000000000 O (24h)
0.25000000000000 -0.03890000000000 0.59720000000000 O (24h)
0.25000000000000 0.53890000000000 -0.09720000000000 O (24h)
0.59720000000000 0.25000000000000 0.53890000000000 O (24h)
-0.09720000000000 0.25000000000000 0.25000000000000 O (24h)
0.59720000000000 0.25000000000000 -0.03890000000000 O (24h)
-0.09720000000000 0.25000000000000 0.53890000000000 O (24h)
-0.53890000000000 -0.59720000000000 -0.25000000000000 O (24h)
1.03890000000000 1.09720000000000 -0.25000000000000 O (24h)
-0.53890000000000 -0.59720000000000 0.75000000000000 O (24h)
-0.25000000000000 -0.53890000000000 -0.59720000000000 O (24h)
-0.25000000000000 1.03890000000000 -0.59720000000000 O (24h)
0.75000000000000 1.03890000000000 -0.59720000000000 O (24h)
0.75000000000000 -0.53890000000000 1.09720000000000 O (24h)
-0.59720000000000 -0.25000000000000 -0.53890000000000 O (24h)
1.09720000000000 -0.25000000000000 1.03890000000000 O (24h)
-0.59720000000000 0.75000000000000 1.03890000000000 O (24h)
1.09720000000000 0.75000000000000 -0.53890000000000 O (24h)
0.40280000000000 0.75000000000000 0.25000000000000 Sb (12g)
0.09720000000000 0.75000000000000 0.25000000000000 Sb (12g)
0.25000000000000 0.40280000000000 0.75000000000000 Sb (12g)
0.25000000000000 0.09720000000000 0.75000000000000 Sb (12g)
-0.40280000000000 0.25000000000000 0.75000000000000 Sb (12g)
0.90280000000000 0.25000000000000 0.75000000000000 Sb (12g)
0.75000000000000 -0.40280000000000 0.25000000000000 Sb (12g)
0.75000000000000 0.90280000000000 0.25000000000000 Sb (12g)
0.25000000000000 0.75000000000000 -0.40280000000000 Sb (12g)
0.25000000000000 0.75000000000000 0.90280000000000 Sb (12g)
```

KB<sub>6</sub>H<sub>6</sub>: A6B6\_cF104\_202\_h\_h\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'KB6H6'
_chemical_formula_sum 'B6 H6 K'

loop_
  _publ_author_name
    'J. A. Wunderlich'
    'W. N. Lipscomb'
  _journal_name_full_name
    ;
    Journal of the American Chem Society
  ;
  _journal_volume 82
  _journal_year 1960
  _journal_page_first 4427
  _journal_page_last 4428
  _publ_section_title
    ;
    Structure of B_{12}SH_{12}^{-2}$ Ion
  ;
```

# Found in Pearson's Crystal Data - Crystal Structure Database for  
↳ Inorganic Compounds, 2013

```
_aflow_title 'KBS_{6}SHS_{6}S Structure'  
_aflow_proto 'A6B6C_cF104_202_h_h_c'  
_aflow_params 'a,y_{2},z_{2},y_{3},z_{3}'  
_aflow_params_values '10.6100296668,0.5827,0.6359,0.638,0.72'  
_aflow_Strukturbericht 'None'  
_aflow_Pearson 'cF104'
```

```
_cell_length_a 10.6100296668  
_cell_length_b 10.6100296668  
_cell_length_c 10.6100296668  
_cell_angle_alpha 90.0000000000  
_cell_angle_beta 90.0000000000  
_cell_angle_gamma 90.0000000000
```

```
_symmetry_space_group_name_H-M "F 2/m -3"  
_symmetry_Int_Tables_number 202
```

```
loop_  
_space_group_symop_id  
_space_group_symop_operation_xyz
```

```
1 x,y,z  
2 x,-y,-z  
3 -x,y,-z  
4 -x,-y,z  
5 y,z,x  
6 y,-z,-x  
7 -y,z,-x  
8 -y,-z,x  
9 z,x,y  
10 z,-x,-y  
11 -z,x,-y  
12 -z,-x,y  
13 -x,-y,-z  
14 -x,y,z  
15 x,-y,z  
16 x,y,-z  
17 -y,-z,-x  
18 -y,z,x  
19 y,-z,x  
20 y,z,-x  
21 -z,-x,-y  
22 -z,x,y  
23 z,-x,y  
24 z,x,-y  
25 x,y+1/2,z+1/2  
26 x,-y+1/2,-z+1/2  
27 -x,y+1/2,-z+1/2  
28 -x,-y+1/2,z+1/2  
29 y,z+1/2,x+1/2  
30 y,-z+1/2,-x+1/2  
31 -y,z+1/2,-x+1/2  
32 -y,-z+1/2,x+1/2  
33 z,x+1/2,y+1/2  
34 z,-x+1/2,-y+1/2  
35 -z,x+1/2,-y+1/2  
36 -z,-x+1/2,y+1/2  
37 -x,-y+1/2,-z+1/2  
38 -x,y+1/2,z+1/2  
39 x,-y+1/2,z+1/2  
40 x,y+1/2,-z+1/2  
41 -y,-z+1/2,-x+1/2  
42 -y,z+1/2,x+1/2  
43 y,-z+1/2,x+1/2  
44 y,z+1/2,-x+1/2  
45 -z,-x+1/2,-y+1/2  
46 -z,x+1/2,y+1/2  
47 z,-x+1/2,y+1/2  
48 z,x+1/2,-y+1/2  
49 x+1/2,y,z+1/2  
50 x+1/2,-y,-z+1/2  
51 -x+1/2,y,-z+1/2  
52 -x+1/2,-y,z+1/2  
53 y+1/2,z,x+1/2  
54 y+1/2,-z,-x+1/2  
55 -y+1/2,z,-x+1/2  
56 -y+1/2,-z,x+1/2  
57 z+1/2,x,y+1/2  
58 z+1/2,-x,-y+1/2  
59 -z+1/2,x,-y+1/2  
60 -z+1/2,-x,y+1/2  
61 -x+1/2,-y,-z+1/2  
62 -x+1/2,y,z+1/2  
63 x+1/2,-y,z+1/2  
64 x+1/2,y,-z+1/2  
65 -y+1/2,-z,-x+1/2  
66 -y+1/2,z,x+1/2  
67 y+1/2,-z,x+1/2  
68 y+1/2,z,-x+1/2  
69 -z+1/2,-x,-y+1/2  
70 -z+1/2,x,y+1/2  
71 z+1/2,-x,y+1/2  
72 z+1/2,x,-y+1/2  
73 x+1/2,y+1/2,z  
74 x+1/2,-y+1/2,-z  
75 -x+1/2,y+1/2,-z  
76 -x+1/2,-y+1/2,z  
77 y+1/2,z+1/2,x  
78 y+1/2,-z+1/2,-x  
79 -y+1/2,z+1/2,-x  
80 -y+1/2,-z+1/2,x  
81 z+1/2,x+1/2,y
```

```
82 z+1/2,-x+1/2,-y  
83 -z+1/2,x+1/2,-y  
84 -z+1/2,-x+1/2,y  
85 -x+1/2,-y+1/2,-z  
86 -x+1/2,y+1/2,z  
87 x+1/2,-y+1/2,z  
88 x+1/2,y+1/2,-z  
89 -y+1/2,-z+1/2,-x  
90 -y+1/2,z+1/2,x  
91 y+1/2,-z+1/2,x  
92 y+1/2,z+1/2,-x  
93 -z+1/2,-x+1/2,-y  
94 -z+1/2,x+1/2,y  
95 z+1/2,-x+1/2,y  
96 z+1/2,x+1/2,-y
```

```
loop_  
_atom_site_label  
_atom_site_type_symbol  
_atom_site_symmetry_multiplicity  
_atom_site_Wyckoff_label  
_atom_site_fract_x  
_atom_site_fract_y  
_atom_site_fract_z  
_atom_site_occupancy  
K1 K 8 c 0.25000 0.25000 1.00000  
B1 B 48 h 0.00000 0.58270 0.63590 1.00000  
H1 H 48 h 0.00000 0.63800 0.72000 1.00000
```

KB<sub>6</sub>H<sub>6</sub>: A6B6C\_cF104\_202\_h\_h\_c - POSCAR

```
A6B6C_cF104_202_h_h_c & a,y2,z2,y3,z3 --params=10.6100296668,0.5827,  
↳ 0.6359,0.638,0.72 & Fm-3 T_{h}^{3} #202 (ch^2) & cF104 & None &  
↳ KB6H6 & J. A. Wunderlich and W. N. Lipscomb, J. Am. Ceram.  
↳ Soc. 82, 4427-4428 (1960)  
1.0000000000000000  
0.0000000000000000 5.30501483340000 5.30501483340000  
5.30501483340000 0.0000000000000000 5.30501483340000  
5.30501483340000 5.30501483340000 0.0000000000000000  
B H K  
12 12 2  
Direct  
1.2186000000000000 0.0532000000000000 -0.0532000000000000 B (48h)  
0.0532000000000000 1.2186000000000000 -1.2186000000000000 B (48h)  
-0.0532000000000000 -1.2186000000000000 1.2186000000000000 B (48h)  
-1.2186000000000000 -0.0532000000000000 0.0532000000000000 B (48h)  
-0.0532000000000000 1.2186000000000000 0.0532000000000000 B (48h)  
-1.2186000000000000 0.0532000000000000 1.2186000000000000 B (48h)  
1.2186000000000000 -0.0532000000000000 -1.2186000000000000 B (48h)  
0.0532000000000000 -1.2186000000000000 -0.0532000000000000 B (48h)  
-0.0532000000000000 1.2186000000000000 0.0532000000000000 B (48h)  
-1.2186000000000000 1.2186000000000000 -0.0532000000000000 B (48h)  
-0.0532000000000000 0.0532000000000000 -1.2186000000000000 B (48h)  
1.3580000000000000 0.0820000000000000 -0.0820000000000000 H (48h)  
0.0820000000000000 1.3580000000000000 -1.3580000000000000 H (48h)  
-0.0820000000000000 -1.3580000000000000 1.3580000000000000 H (48h)  
-1.3580000000000000 0.0820000000000000 0.0820000000000000 H (48h)  
0.0820000000000000 -1.3580000000000000 0.0820000000000000 H (48h)  
-1.3580000000000000 0.0820000000000000 -1.3580000000000000 H (48h)  
0.0820000000000000 -0.0820000000000000 1.3580000000000000 H (48h)  
1.3580000000000000 -1.3580000000000000 0.0820000000000000 H (48h)  
-1.3580000000000000 1.3580000000000000 -0.0820000000000000 H (48h)  
-0.0820000000000000 0.0820000000000000 -1.3580000000000000 H (48h)  
0.2500000000000000 0.2500000000000000 0.2500000000000000 K (8c)  
0.7500000000000000 0.7500000000000000 0.7500000000000000 K (8c)
```

FCC C<sub>60</sub> Buckminsterfullerene: A\_cF240\_202\_h2i - CIF

```
# CIF file  
data_findsym-output  
_audit_creation_method FINDSYM  
  
_chemical_name_mineral 'Buckminsterfullerene'  
_chemical_formula_sum 'C'  
  
loop_  
_publ_author_name  
'D. L. Dorset'  
'M. P. McCourt'  
_journal_name_full_name  
; Acta Crystallographica Section A: Foundations and Advances  
; _journal_volume 50  
_journal_year 1994  
_journal_page_first 344  
_journal_page_last 351  
_publ_section_title  
; Disorder and the molecular packing of CS_{60}S  
buckminsterfullerene: a direct  
electron-crystallographic analysis  
;  
  
_aflow_title 'FCC CS_{60}S Buckminsterfullerene Structure'  
_aflow_proto 'A_cF240_202_h2i'  
_aflow_params 'a,y_{1},z_{1},x_{2},y_{2},z_{2},x_{3},y_{3},z_{3}'  
_aflow_params_values '14.26,0.249,0.052,0.105,0.085,0.22,0.185,0.052,  
↳ 0.165'  
_aflow_Strukturbericht 'None'  
_aflow_Pearson 'cF240'
```

```

_symmetry_space_group_name_H-M "F 2/m -3"
_symmetry_Int_Tables_number 202

_cell_length_a 14.26000
_cell_length_b 14.26000
_cell_length_c 14.26000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 -x,-y,-z
14 -x,y,z
15 x,-y,z
16 x,y,-z
17 -y,-z,-x
18 -y,z,x
19 y,-z,x
20 y,z,-x
21 -z,-x,-y
22 -z,x,y
23 z,-x,y
24 z,x,-y
25 x,y+1/2,z+1/2
26 x,-y+1/2,-z+1/2
27 -x,y+1/2,-z+1/2
28 -x,-y+1/2,z+1/2
29 y,z+1/2,x+1/2
30 y,-z+1/2,-x+1/2
31 -y,z+1/2,-x+1/2
32 -y,-z+1/2,x+1/2
33 z,x+1/2,y+1/2
34 z,-x+1/2,-y+1/2
35 -z,x+1/2,-y+1/2
36 -z,-x+1/2,y+1/2
37 -x,-y+1/2,-z+1/2
38 -x,y+1/2,z+1/2
39 x,-y+1/2,z+1/2
40 x,y+1/2,-z+1/2
41 -y,-z+1/2,-x+1/2
42 -y,z+1/2,x+1/2
43 y,-z+1/2,x+1/2
44 y,z+1/2,-x+1/2
45 -z,-x+1/2,-y+1/2
46 -z,x+1/2,y+1/2
47 z,-x+1/2,y+1/2
48 z,x+1/2,-y+1/2
49 x+1/2,y,z+1/2
50 x+1/2,-y,-z+1/2
51 -x+1/2,y,-z+1/2
52 -x+1/2,-y,z+1/2
53 y+1/2,z,x+1/2
54 y+1/2,-z,-x+1/2
55 -y+1/2,z,-x+1/2
56 -y+1/2,-z,x+1/2
57 z+1/2,x,y+1/2
58 z+1/2,-x,-y+1/2
59 -z+1/2,x,-y+1/2
60 -z+1/2,-x,y+1/2
61 -x+1/2,-y,-z+1/2
62 -x+1/2,y,z+1/2
63 x+1/2,-y,z+1/2
64 x+1/2,y,-z+1/2
65 -y+1/2,-z,-x+1/2
66 -y+1/2,z,x+1/2
67 y+1/2,-z,x+1/2
68 y+1/2,z,-x+1/2
69 -z+1/2,-x,-y+1/2
70 -z+1/2,x,y+1/2
71 z+1/2,-x,y+1/2
72 z+1/2,x,-y+1/2
73 x+1/2,y+1/2,z
74 x+1/2,-y+1/2,-z
75 -x+1/2,y+1/2,-z
76 -x+1/2,-y+1/2,z
77 y+1/2,z+1/2,x
78 y+1/2,-z+1/2,-x
79 -y+1/2,z+1/2,-x
80 -y+1/2,-z+1/2,x
81 z+1/2,x+1/2,y
82 z+1/2,-x+1/2,-y
83 -z+1/2,x+1/2,-y
84 -z+1/2,-x+1/2,y
85 -x+1/2,-y+1/2,-z
86 -x+1/2,y+1/2,z
87 x+1/2,-y+1/2,z
88 x+1/2,y+1/2,-z
89 -y+1/2,-z+1/2,-x
90 -y+1/2,z+1/2,x
91 y+1/2,-z+1/2,x
92 y+1/2,z+1/2,-x

```

```

93 -z+1/2,-x+1/2,-y
94 -z+1/2,x+1/2,y
95 z+1/2,-x+1/2,y
96 z+1/2,x+1/2,-y

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
C1 C 48 h 0.00000 0.24900 0.05200 1.00000
C2 C 96 i 0.10500 0.08500 0.22000 1.00000
C3 C 96 i 0.18500 0.05200 0.16500 1.00000

```

FCC C<sub>60</sub> Buckminsterfullerene: A\_cF240\_202\_h2i - POSCAR

```

A_cF240_202_h2i & a,y1,z1,x2,y2,z2,x3,y3,z3 --params=14.26,0.249,0.052,
↳ 0.105,0.085,0.22,0.185,0.052,0.165 & Fm-3 T_{h}^{3} #202 (hi^2)
↳ & cF240 & None & C & Buckminsterfullerene & D. L. Dorset and
↳ M. P. McCourt, Acta Crystallogr. Sect. A 50, 344-351 (1994)
1.0000000000000000
0.0000000000000000 7.130000000000000 7.130000000000000
7.130000000000000 0.000000000000000 7.130000000000000
7.130000000000000 7.130000000000000 0.000000000000000
C
60
Direct
0.301000000000000 -0.197000000000000 0.197000000000000 C (48h)
-0.197000000000000 0.301000000000000 -0.301000000000000 C (48h)
0.197000000000000 -0.301000000000000 0.301000000000000 C (48h)
-0.301000000000000 0.197000000000000 -0.197000000000000 C (48h)
0.197000000000000 0.301000000000000 -0.197000000000000 C (48h)
-0.301000000000000 -0.197000000000000 0.301000000000000 C (48h)
0.301000000000000 0.197000000000000 -0.301000000000000 C (48h)
-0.197000000000000 -0.301000000000000 0.197000000000000 C (48h)
0.197000000000000 -0.197000000000000 -0.301000000000000 C (48h)
0.200000000000000 0.240000000000000 -0.030000000000000 C (96i)
0.240000000000000 0.200000000000000 -0.410000000000000 C (96i)
-0.030000000000000 -0.410000000000000 0.200000000000000 C (96i)
-0.410000000000000 -0.030000000000000 0.240000000000000 C (96i)
0.200000000000000 0.240000000000000 0.200000000000000 C (96i)
-0.030000000000000 0.200000000000000 0.240000000000000 C (96i)
-0.240000000000000 0.200000000000000 -0.030000000000000 C (96i)
0.200000000000000 -0.030000000000000 -0.410000000000000 C (96i)
0.240000000000000 -0.410000000000000 -0.030000000000000 C (96i)
0.240000000000000 -0.030000000000000 0.200000000000000 C (96i)
0.200000000000000 -0.410000000000000 0.240000000000000 C (96i)
-0.410000000000000 0.200000000000000 -0.030000000000000 C (96i)
-0.030000000000000 0.240000000000000 -0.410000000000000 C (96i)
-0.200000000000000 -0.240000000000000 0.030000000000000 C (96i)
-0.240000000000000 -0.200000000000000 0.410000000000000 C (96i)
0.030000000000000 0.410000000000000 -0.200000000000000 C (96i)
0.410000000000000 0.030000000000000 -0.240000000000000 C (96i)
0.030000000000000 -0.200000000000000 -0.240000000000000 C (96i)
0.410000000000000 -0.240000000000000 -0.200000000000000 C (96i)
-0.200000000000000 0.030000000000000 0.410000000000000 C (96i)
-0.240000000000000 0.410000000000000 0.030000000000000 C (96i)
-0.240000000000000 0.030000000000000 -0.200000000000000 C (96i)
-0.200000000000000 0.410000000000000 -0.240000000000000 C (96i)
0.410000000000000 -0.200000000000000 0.030000000000000 C (96i)
0.030000000000000 -0.240000000000000 0.410000000000000 C (96i)
0.032000000000000 0.298000000000000 0.072000000000000 C (96i)
0.298000000000000 0.032000000000000 -0.402000000000000 C (96i)
0.072000000000000 -0.402000000000000 0.032000000000000 C (96i)
-0.402000000000000 0.072000000000000 0.298000000000000 C (96i)
0.032000000000000 0.072000000000000 -0.402000000000000 C (96i)
0.298000000000000 -0.402000000000000 0.072000000000000 C (96i)
0.072000000000000 -0.402000000000000 0.032000000000000 C (96i)
0.032000000000000 -0.402000000000000 0.298000000000000 C (96i)
-0.402000000000000 0.032000000000000 0.072000000000000 C (96i)
0.072000000000000 0.298000000000000 -0.402000000000000 C (96i)
-0.032000000000000 -0.298000000000000 -0.072000000000000 C (96i)
-0.298000000000000 -0.032000000000000 0.402000000000000 C (96i)
-0.072000000000000 0.402000000000000 -0.032000000000000 C (96i)
0.402000000000000 -0.072000000000000 -0.298000000000000 C (96i)
-0.072000000000000 -0.032000000000000 -0.298000000000000 C (96i)
0.402000000000000 -0.298000000000000 0.072000000000000 C (96i)
-0.072000000000000 -0.298000000000000 0.402000000000000 C (96i)

```

Pyrochlore (Na<sub>3</sub>Co(CO<sub>3</sub>)<sub>2</sub>Cl): A2BCD3E6\_cF208\_203\_e\_c\_d\_f\_g - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Na3Co(CO3)2Cl'
_chemical_formula_sum 'C2 Cl Co Na3 O6'

loop_
_publ_author_name
'Z. Fu'
'Y. Zheng'

```

```

'Y. Xiao'
'S. Bedanta'
'A. Senyshyn'
'G. G. Simeoni'
'Y. Su'
'U. R\'{u}ckler'
'P. K\'{o}gerler'
'Thomas Br\'{u}ckel'
_journal_name_full_name
;
Physical Review B
;
_journal_volume 87
_journal_year 2013
_journal_page_first 214406
_journal_page_last 214406
_publ_section_title
;
Coexistence of magnetic order and spin-glass-like phase in the
  ↪ pyrochlore antiferromagnet Na3Co(CO3)2Cl
;
_aflow_title 'Pyrochlore (Na3Co(CO3)2Cl) Structure'
_aflow_proto 'A2BCD3E6_cF208_203_e_c_d_f_g'
_aflow_params 'a,x_{3},x_{4},x_{5},y_{5},z_{5}'
_aflow_params_values '13.9898,0.2826,-0.099,0.2257,0.2665,0.3531'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cF208'

_symmetry_space_group_name_H-M "F 2/d -3 (origin choice 2)"
_symmetry_Int_Tables_number 203

_cell_length_a 13.98980
_cell_length_b 13.98980
_cell_length_c 13.98980
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y+3/4,-z+3/4
3 -x+3/4,y,-z+3/4
4 -x+3/4,-y+3/4,z
5 y,z,x
6 y,-z+3/4,-x+3/4
7 -y+3/4,z,-x+3/4
8 -y+3/4,-z+3/4,x
9 z,x,y
10 z,-x+3/4,-y+3/4
11 -z+3/4,x,-y+3/4
12 -z+3/4,-x+3/4,y
13 -x,-y,-z
14 -x,y+1/4,z+1/4
15 x+1/4,-y,z+1/4
16 x+1/4,y+1/4,-z
17 -y,-z,-x
18 -y,z+1/4,x+1/4
19 y+1/4,-z,x+1/4
20 y+1/4,z+1/4,-x
21 -z,-x,-y
22 -z,x+1/4,y+1/4
23 z+1/4,-x,y+1/4
24 z+1/4,x+1/4,-y
25 x,y+1/2,z+1/2
26 x,-y+1/4,-z+1/4
27 -x+3/4,y+1/2,-z+1/4
28 -x+3/4,-y+1/4,z+1/2
29 y,z+1/2,x+1/2
30 y,-z+1/4,-x+1/4
31 -y+3/4,z+1/2,-x+1/4
32 -y+3/4,-z+1/4,x+1/2
33 z,x+1/2,y+1/2
34 z,-x+1/4,-y+1/4
35 -z+3/4,x+1/2,-y+1/4
36 -z+3/4,-x+1/4,y+1/2
37 -x,-y+1/2,-z+1/2
38 -x,y+3/4,z+3/4
39 x+1/4,-y+1/2,z+3/4
40 x+1/4,y+3/4,-z+1/2
41 -y,-z+1/2,-x+1/2
42 -y,z+3/4,x+3/4
43 y+1/4,-z+1/2,x+3/4
44 y+1/4,z+3/4,-x+1/2
45 -z,-x+1/2,-y+1/2
46 -z,x+3/4,y+3/4
47 z+1/4,-x+1/2,y+3/4
48 z+1/4,x+3/4,-y+1/2
49 x+1/2,y,z+1/2
50 x+1/2,-y+3/4,-z+1/4
51 -x+1/4,y,-z+1/4
52 -x+1/4,-y+3/4,z+1/2
53 y+1/2,z,x+1/2
54 y+1/2,-z+3/4,-x+1/4
55 -y+1/4,z,-x+1/4
56 -y+1/4,-z+3/4,x+1/2
57 z+1/2,x,y+1/2
58 z+1/2,-x+3/4,-y+1/4
59 -z+1/4,x,-y+1/4
60 -z+1/4,-x+3/4,y+1/2
61 -x+1/2,-y,-z+1/2
62 -x+1/2,y+1/4,z+3/4
63 x+3/4,-y,z+3/4

```

```

64 x+3/4,y+1/4,-z+1/2
65 -y+1/2,-z,-x+1/2
66 -y+1/2,z+1/4,x+3/4
67 y+3/4,-z,x+3/4
68 y+3/4,z+1/4,-x+1/2
69 -z+1/2,-x,-y+1/2
70 -z+1/2,x+1/4,y+3/4
71 z+3/4,-x,y+3/4
72 z+3/4,x+1/4,-y+1/2
73 x+1/2,y+1/2,z
74 x+1/2,-y+1/4,-z+3/4
75 -x+1/4,y+1/2,-z+3/4
76 -x+1/4,-y+1/4,z
77 y+1/2,z+1/2,x
78 y+1/2,-z+1/4,-x+3/4
79 -y+1/4,z+1/2,-x+3/4
80 -y+1/4,-z+1/4,x
81 z+1/2,x+1/2,y
82 z+1/2,-x+1/4,-y+3/4
83 -z+1/4,x+1/2,-y+3/4
84 -z+1/4,-x+1/4,y
85 -x+1/2,-y+1/2,-z
86 -x+1/2,y+3/4,z+1/4
87 x+3/4,-y+1/2,z+1/4
88 x+3/4,y+3/4,-z
89 -y+1/2,-z+1/2,-x
90 -y+1/2,z+3/4,x+1/4
91 y+3/4,-z+1/2,x+1/4
92 y+3/4,z+3/4,-x
93 -z+1/2,-x+1/2,-y
94 -z+1/2,x+3/4,y+1/4
95 z+3/4,-x+1/2,y+1/4
96 z+3/4,x+3/4,-y

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Cl1 Cl 16 c 0.00000 0.00000 1.00000
Co1 Co 16 d 0.50000 0.50000 1.00000
Cl C 32 e 0.28260 0.28260 0.28260 1.00000
Na1 Na 48 f -0.09900 0.12500 0.12500 1.00000
O1 O 96 g 0.22570 0.26650 0.35310 1.00000

```

Pyrochlore (Na<sub>3</sub>Co(CO<sub>3</sub>)<sub>2</sub>Cl): A2BCD3E6\_cF208\_203\_e\_c\_d\_f\_g - POSCAR

```

A2BCD3E6_cF208_203_e_c_d_f_g & a,x3,x4,x5,y5,z5 --params=13.9898,0.2826
  ↪ -0.099,0.2257,0.2665,0.3531 & Fd-3 T_{h}^{4} #203 (cdfg) &
  ↪ cF208 & None & Na3Co(CO3)2Cl & Na3Co(CO3)2Cl & Z. Fu et al.,
  ↪ Phys. Rev. B 87, 214406(2013)
1.0000000000000000
0.0000000000000000 6.994900000000000 6.994900000000000
6.994900000000000 0.000000000000000 6.994900000000000
6.994900000000000 6.994900000000000 0.000000000000000
C Cl Co Na O
8 4 4 12 24
Direct
0.282600000000000 0.282600000000000 0.282600000000000 C (32e)
0.282600000000000 0.282600000000000 -0.347800000000000 C (32e)
0.282600000000000 -0.347800000000000 0.282600000000000 C (32e)
-0.347800000000000 0.282600000000000 0.282600000000000 C (32e)
-0.282600000000000 -0.282600000000000 -0.282600000000000 C (32e)
-0.282600000000000 -0.282600000000000 1.347800000000000 C (32e)
-0.282600000000000 1.347800000000000 -0.282600000000000 C (32e)
1.347800000000000 -0.282600000000000 -0.282600000000000 C (32e)
0.000000000000000 0.000000000000000 0.000000000000000 Cl (16c)
0.000000000000000 0.000000000000000 0.500000000000000 Cl (16c)
0.000000000000000 0.500000000000000 0.000000000000000 Cl (16c)
0.500000000000000 0.000000000000000 0.000000000000000 Cl (16c)
0.500000000000000 0.500000000000000 0.500000000000000 Co (16d)
0.500000000000000 0.500000000000000 0.000000000000000 Co (16d)
0.500000000000000 0.000000000000000 0.500000000000000 Co (16d)
0.000000000000000 0.500000000000000 0.500000000000000 Co (16d)
0.349000000000000 -0.099000000000000 -0.099000000000000 Na (48f)
-0.099000000000000 0.349000000000000 0.349000000000000 Na (48f)
-0.099000000000000 0.349000000000000 -0.099000000000000 Na (48f)
0.349000000000000 -0.099000000000000 0.349000000000000 Na (48f)
-0.099000000000000 -0.099000000000000 0.349000000000000 Na (48f)
0.349000000000000 0.349000000000000 -0.099000000000000 Na (48f)
0.651000000000000 0.099000000000000 0.099000000000000 Na (48f)
0.099000000000000 0.651000000000000 0.651000000000000 Na (48f)
0.099000000000000 0.651000000000000 0.099000000000000 Na (48f)
0.651000000000000 0.099000000000000 0.651000000000000 Na (48f)
0.099000000000000 0.099000000000000 0.651000000000000 Na (48f)
0.651000000000000 0.312300000000000 0.139100000000000 O (96g)
0.312300000000000 0.393900000000000 -0.345300000000000 O (96g)
0.139100000000000 -0.345300000000000 0.393900000000000 O (96g)
-0.345300000000000 0.139100000000000 0.312300000000000 O (96g)
0.139100000000000 0.393900000000000 0.312300000000000 O (96g)
-0.345300000000000 0.312300000000000 0.393900000000000 O (96g)
0.393900000000000 0.312300000000000 -0.345300000000000 O (96g)
0.312300000000000 -0.345300000000000 0.139100000000000 O (96g)
0.312300000000000 0.139100000000000 0.393900000000000 O (96g)
0.393900000000000 -0.345300000000000 0.312300000000000 O (96g)
-0.345300000000000 0.393900000000000 0.139100000000000 O (96g)
0.139100000000000 0.312300000000000 -0.345300000000000 O (96g)
-0.393900000000000 -0.312300000000000 -0.139100000000000 O (96g)
-0.312300000000000 -0.393900000000000 1.345300000000000 O (96g)
-0.139100000000000 1.345300000000000 -0.393900000000000 O (96g)

```



1.34530000000000	-0.13910000000000	-0.31230000000000	O (96g)
-0.13910000000000	-0.39390000000000	-0.31230000000000	O (96g)
1.34530000000000	-0.31230000000000	-0.39390000000000	O (96g)
-0.39390000000000	-0.13910000000000	1.34530000000000	O (96g)
-0.31230000000000	1.34530000000000	-0.13910000000000	O (96g)
-0.31230000000000	-0.13910000000000	-0.39390000000000	O (96g)
-0.39390000000000	1.34530000000000	-0.31230000000000	O (96g)
1.34530000000000	-0.39390000000000	-0.13910000000000	O (96g)
-0.13910000000000	-0.31230000000000	1.34530000000000	O (96g)

Tychite (Na<sub>6</sub>Mg<sub>2</sub>(SO<sub>4</sub>)(CO<sub>3</sub>)<sub>4</sub>): A4B2C6D16E\_cF232\_203\_e\_d\_f\_eg\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Tychite'
_chemical_formula_sum 'C4 Mg2 Na6 O16 S'

loop_
  _publ_author_name
    'G. R. Schmidt'
    'R. Jacqueline'
    'H. Yang'
    'R. T. Downs'
  _journal_name_full_name
;
Acta Crystallographica Section E: Crystallographic Communications
;
_journal_volume 62
_journal_year 2006
_journal_page_first i207
_journal_page_last i209
_publ_section_title
;
Tychite, Na6{6}SMg2{2}(SO4{4})(CO3{3})4: Structure analysis
↪ and Raman spectroscopic data
;

# Found in The American Mineralogist Crystal Structure Database, 2003
_aflow_title 'Tychite (Na6{6}SMg2{2}(SO4{4})(CO3{3})4)
↪ Structure'
_aflow_proto 'A4B2C6D16E_cF232_203_e_d_f_eg_a'
_aflow_params 'a, x_{3}, x_{4}, x_{5}, x_{6}, y_{6}, z_{6}'
_aflow_params_values '13.9038 , 0.28207 , 0.06362 , 0.34379 , 0.26626 , 0.22529 ,
↪ 0.35333'
_aflow_strukturbericht 'None'
_aflow_pearson 'cF232'

_symmetry_space_group_name_H-M "F 2/d -3 (origin choice 2)"
_symmetry_Int_Tables_number 203

_cell_length_a 13.90380
_cell_length_b 13.90380
_cell_length_c 13.90380
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x, y, z
2 x, -y+3/4, -z+3/4
3 -x+3/4, y, -z+3/4
4 -x+3/4, -y+3/4, z
5 y, z, x
6 y, -z+3/4, -x+3/4
7 -y+3/4, z, -x+3/4
8 -y+3/4, -z+3/4, x
9 z, x, y
10 z, -x+3/4, -y+3/4
11 -z+3/4, x, -y+3/4
12 -z+3/4, -x+3/4, y
13 -x, -y, -z
14 -x, y+1/4, z+1/4
15 x+1/4, -y, z+1/4
16 x+1/4, y+1/4, -z
17 -y, -z, -x
18 -y, z+1/4, x+1/4
19 y+1/4, -z, x+1/4
20 y+1/4, z+1/4, -x
21 -z, -x, -y
22 -z, x+1/4, y+1/4
23 z+1/4, -x, y+1/4
24 z+1/4, x+1/4, -y
25 x, y+1/2, z+1/2
26 x, -y+1/4, -z+1/4
27 -x+3/4, y+1/2, -z+1/4
28 -x+3/4, -y+1/4, z+1/2
29 y, z+1/2, x+1/2
30 y, -z+1/4, -x+1/4
31 -y+3/4, z+1/2, -x+1/4
32 -y+3/4, -z+1/4, x+1/2
33 z, x+1/2, y+1/2
34 z, -x+1/4, -y+1/4
35 -z+3/4, x+1/2, -y+1/4
36 -z+3/4, -x+1/4, y+1/2
37 -x, -y+1/2, -z+1/2
38 -x, y+3/4, z+3/4
39 x+1/4, -y+1/2, z+3/4
40 x+1/4, y+3/4, -z+1/2
41 -y, -z+1/2, -x+1/2
42 -y, z+3/4, x+3/4
```

43	y+1/4, -z+1/2, x+3/4
44	y+1/4, z+3/4, -x+1/2
45	-z, -x+1/2, -y+1/2
46	-z, x+3/4, y+3/4
47	z+1/4, -x+1/2, y+3/4
48	z+1/4, x+3/4, -y+1/2
49	x+1/2, y, z+1/2
50	x+1/2, -y+3/4, -z+1/4
51	-x+1/4, y, -z+1/4
52	-x+1/4, -y+3/4, z+1/2
53	y+1/2, z, x+1/2
54	y+1/2, -z+3/4, -x+1/4
55	-y+1/4, z, -x+1/4
56	-y+1/4, -z+3/4, x+1/2
57	z+1/2, x, y+1/2
58	z+1/2, -x+3/4, -y+1/4
59	-z+1/4, x, -y+1/4
60	-z+1/4, -x+3/4, y+1/2
61	-x+1/2, -y, -z+1/2
62	-x+1/2, y+1/4, z+3/4
63	x+3/4, -y, z+3/4
64	x+3/4, y+1/4, -z+1/2
65	-y+1/2, -z, -x+1/2
66	-y+1/2, z+1/4, x+3/4
67	y+3/4, -z, x+3/4
68	y+3/4, z+1/4, -x+1/2
69	-z+1/2, -x, -y+1/2
70	-z+1/2, x+1/4, y+3/4
71	z+3/4, -x, y+3/4
72	z+3/4, x+1/4, -y+1/2
73	x+1/2, y+1/2, z
74	x+1/2, -y+1/4, -z+3/4
75	-x+1/4, y+1/2, -z+3/4
76	-x+1/4, -y+1/4, z
77	y+1/2, z+1/2, x
78	y+1/2, -z+1/4, -x+3/4
79	-y+1/4, z+1/2, -x+3/4
80	-y+1/4, -z+1/4, x
81	z+1/2, x+1/2, y
82	z+1/2, -x+1/4, -y+3/4
83	-z+1/4, x+1/2, -y+3/4
84	-z+1/4, -x+1/4, y
85	-x+1/2, -y+1/2, -z
86	-x+1/2, y+3/4, z+1/4
87	x+3/4, -y+1/2, z+1/4
88	x+3/4, y+3/4, -z
89	-y+1/2, -z+1/2, -x
90	-y+1/2, z+3/4, x+1/4
91	y+3/4, -z+1/2, x+1/4
92	y+3/4, z+3/4, -x
93	-z+1/2, -x+1/2, -y
94	-z+1/2, x+3/4, y+1/4
95	z+3/4, -x+1/2, y+1/4
96	z+3/4, x+3/4, -y

Tychite (Na<sub>6</sub>Mg<sub>2</sub>(SO<sub>4</sub>)(CO<sub>3</sub>)<sub>4</sub>): A4B2C6D16E\_cF232\_203\_e\_d\_f\_eg\_a - POSCAR

```
A4B2C6D16E_cF232_203_e_d_f_eg_a & a, x3, x4, x5, x6, y6, z6 --params=13.9038 .
↪ 0.28207 , 0.06362 , 0.34379 , 0.26626 , 0.22529 , 0.35333 & Fd-3 T[h]^4
↪ } #203 (ade^2fg) & cF232 & None & Na6Mg2(SO4)(CO3)4 & Tychite &
↪ G. R. Schmidt et al., Acta Crystallogr. E 62, i207-i209 (2006)

1.00000000000000
0.00000000000000 6.95190000000000 6.95190000000000
6.95190000000000 0.00000000000000 6.95190000000000
6.95190000000000 6.95190000000000 0.00000000000000
C Mg Na O S
8 4 12 32 2

Direct
0.28207000000000 0.28207000000000 0.28207000000000 C (32e)
0.28207000000000 0.28207000000000 -0.34621000000000 C (32e)
0.28207000000000 -0.34621000000000 0.28207000000000 C (32e)
-0.34621000000000 0.28207000000000 0.28207000000000 C (32e)
-0.28207000000000 -0.28207000000000 -0.28207000000000 C (32e)
-0.28207000000000 -0.28207000000000 1.34621000000000 C (32e)
-0.28207000000000 1.34621000000000 -0.28207000000000 C (32e)
1.34621000000000 -0.28207000000000 -0.28207000000000 C (32e)
0.50000000000000 0.50000000000000 0.50000000000000 Mg (16d)
0.50000000000000 0.50000000000000 0.00000000000000 Mg (16d)
0.50000000000000 0.00000000000000 0.50000000000000 Mg (16d)
0.00000000000000 0.50000000000000 0.50000000000000 Mg (16d)
-0.09379000000000 0.34379000000000 0.34379000000000 Na (48f)
0.34379000000000 -0.09379000000000 -0.09379000000000 Na (48f)
0.34379000000000 -0.09379000000000 0.34379000000000 Na (48f)
-0.09379000000000 0.34379000000000 -0.09379000000000 Na (48f)
0.34379000000000 0.34379000000000 -0.09379000000000 Na (48f)
-0.09379000000000 -0.09379000000000 0.34379000000000 Na (48f)
1.09379000000000 -0.34379000000000 -0.34379000000000 Na (48f)
-0.34379000000000 1.09379000000000 1.09379000000000 Na (48f)
-0.34379000000000 1.09379000000000 -0.34379000000000 Na (48f)
```

1.09379000000000	-0.34379000000000	1.09379000000000	Na (48f)
-0.34379000000000	-0.34379000000000	1.09379000000000	Na (48f)
1.09379000000000	1.09379000000000	-0.34379000000000	Na (48f)
0.06362000000000	0.06362000000000	0.06362000000000	O (32e)
0.06362000000000	0.06362000000000	0.30914000000000	O (32e)
0.06362000000000	0.30914000000000	0.06362000000000	O (32e)
0.30914000000000	0.06362000000000	0.06362000000000	O (32e)
-0.06362000000000	-0.06362000000000	-0.06362000000000	O (32e)
-0.06362000000000	-0.06362000000000	0.69086000000000	O (32e)
-0.06362000000000	0.69086000000000	-0.06362000000000	O (32e)
0.69086000000000	-0.06362000000000	-0.06362000000000	O (32e)
0.31236000000000	0.39430000000000	0.13822000000000	O (96g)
0.39430000000000	0.31236000000000	-0.34488000000000	O (96g)
0.13822000000000	-0.34488000000000	0.31236000000000	O (96g)
-0.34488000000000	0.13822000000000	0.39430000000000	O (96g)
0.13822000000000	0.31236000000000	0.39430000000000	O (96g)
-0.34488000000000	0.39430000000000	0.31236000000000	O (96g)
0.31236000000000	0.13822000000000	-0.34488000000000	O (96g)
0.39430000000000	-0.34488000000000	0.13822000000000	O (96g)
0.39430000000000	0.13822000000000	0.31236000000000	O (96g)
0.31236000000000	-0.34488000000000	0.39430000000000	O (96g)
-0.34488000000000	0.31236000000000	0.13822000000000	O (96g)
0.13822000000000	0.39430000000000	-0.34488000000000	O (96g)
-0.31236000000000	-0.39430000000000	-0.13822000000000	O (96g)
-0.39430000000000	-0.31236000000000	1.34488000000000	O (96g)
-0.13822000000000	1.34488000000000	-0.31236000000000	O (96g)
1.34488000000000	-0.13822000000000	-0.39430000000000	O (96g)
-0.13822000000000	-0.31236000000000	-0.39430000000000	O (96g)
1.34488000000000	-0.39430000000000	-0.31236000000000	O (96g)
-0.31236000000000	-0.13822000000000	1.34488000000000	O (96g)
-0.39430000000000	-0.13822000000000	1.34488000000000	O (96g)
-0.13822000000000	-0.39430000000000	1.34488000000000	O (96g)
0.12500000000000	0.12500000000000	0.12500000000000	S (8a)
0.87500000000000	0.87500000000000	0.87500000000000	S (8a)

Rb<sub>3</sub>AsSe<sub>16</sub>: AB3C16\_cF160\_203\_b\_ad\_eg - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Rb3AsSe16'
_chemical_formula_sum 'As Rb3 Se16'

loop_
  _publ_author_name
    'M. Wachhold'
    'W. S. Sheldrick'
  _journal_name_full_name
    ;
  Zeitschrift f{"u"}r Naturforschung B
  ;
  _journal_volume 52
  _journal_year 1997
  _journal_page_first 169
  _journal_page_last 175
  _publ_section_title
    ;
  Methanolthermale Synthese von RbS_{3}AsSeS_{4}S{\textperiodcentered}
    ↪ 2SeS_{6}S und CsS_{3}AsSeS_{4}S{\textperiodcentered} 2CsS_{2}
    ↪ }AsS_{2}SSeS_{4}S{\textperiodcentered} 6TeS_{4}SSeS_{2}S,
    ↪ zwei Selenidoarsenate mit sechsgliedrigen Chalkogenringen/
    ↪ Methanolthermal Synthesis of RbS_{3}AsSeS_{4}S{\
    ↪ textperiodcentered} 2SeS_{6}S and CsS_{3}AsSeS_{4}S{\
    ↪ textperiodcentered} 2CsS_{2}AsS_{2}SSeS_{4}S{\
    ↪ textperiodcentered} 6TeS_{4}SSeS_{2}S. Two Selenidoarsenates
    ↪ with Six-Membered Chalkogen Rings
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↪ Inorganic Compounds, 2013

_aflow_title 'RbS_{3}AsSeS_{16}S Structure'
_aflow_proto 'AB3C16_cF160_203_b_ad_eg'
_aflow_params 'a,x_{4},x_{5},y_{5},z_{5}'
_aflow_params_values '16.6600284675,0.70516,0.51201,0.111,0.42978'
_aflow_strukturbericht 'None'
_aflow_pearson 'cF160'

_cell_length_a 16.6600284675
_cell_length_b 16.6600284675
_cell_length_c 16.6600284675
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "F 2/d -3 (origin choice 2)"
_symmetry_Int_Tables_number 203

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x,-y+3/4,-z+3/4
  3 -x+3/4,y,-z+3/4
  4 -x+3/4,-y+3/4,z
  5 y,z,x
  6 y,-z+3/4,-x+3/4
  7 -y+3/4,z,-x+3/4
  8 -y+3/4,-z+3/4,x
  9 z,x,y
  10 z,-x+3/4,-y+3/4
```

11	-z+3/4,x,-y+3/4
12	-z+3/4,-x+3/4,y
13	-x,-y,-z
14	-x,y+1/4,z+1/4
15	x+1/4,-y,z+1/4
16	x+1/4,y+1/4,-z
17	-y,-z,-x
18	-y,z+1/4,x+1/4
19	y+1/4,-z,x+1/4
20	y+1/4,z+1/4,-x
21	-z,-x,-y
22	-z,x+1/4,y+1/4
23	z+1/4,-x,y+1/4
24	z+1/4,x+1/4,-y
25	x,y+1/2,z+1/2
26	x,-y+1/4,-z+1/4
27	-x+3/4,y+1/2,-z+1/4
28	-x+3/4,-y+1/4,z+1/2
29	y,z+1/2,x+1/2
30	y,-z+1/4,-x+1/4
31	-y+3/4,z+1/2,-x+1/4
32	-y+3/4,-z+1/4,x+1/2
33	z,x+1/2,y+1/2
34	z,-x+1/4,-y+1/4
35	-z+3/4,x+1/2,-y+1/4
36	-z+3/4,-x+1/4,y+1/2
37	-x,-y+1/2,-z+1/2
38	-x,y+3/4,z+3/4
39	x+1/4,-y+1/2,z+3/4
40	x+1/4,y+3/4,-z+1/2
41	-y,-z+1/2,-x+1/2
42	-y,z+3/4,x+3/4
43	y+1/4,-z+1/2,x+3/4
44	y+1/4,z+3/4,-x+1/2
45	-z,-x+1/2,-y+1/2
46	-z,x+3/4,y+3/4
47	z+1/4,-x+1/2,y+3/4
48	z+1/4,x+3/4,-y+1/2
49	x+1/2,y,z+1/2
50	x+1/2,-y+3/4,-z+1/4
51	-x+1/4,y,-z+1/4
52	-x+1/4,-y+3/4,z+1/2
53	y+1/2,z,x+1/2
54	y+1/2,-z+3/4,-x+1/4
55	-y+1/4,z,-x+1/4
56	-y+1/4,-z+3/4,x+1/2
57	z+1/2,x,y+1/2
58	z+1/2,-x+3/4,-y+1/4
59	-z+1/4,x,-y+1/4
60	-z+1/4,-x+3/4,y+1/2
61	-x+1/2,-y,-z+1/2
62	-x+1/2,y+1/4,z+3/4
63	x+3/4,-y,z+3/4
64	x+3/4,y+1/4,-z+1/2
65	-y+1/2,-z,-x+1/2
66	-y+1/2,z+1/4,x+3/4
67	y+3/4,-z,x+3/4
68	y+3/4,z+1/4,-x+1/2
69	-z+1/2,-x,-y+1/2
70	-z+1/2,x+1/4,y+3/4
71	z+3/4,-x,y+3/4
72	z+3/4,x+1/4,-y+1/2
73	x+1/2,y+1/2,z
74	x+1/2,-y+1/4,-z+3/4
75	-x+1/4,y+1/2,-z+3/4
76	-x+1/4,-y+1/4,z
77	y+1/2,z+1/2,x
78	y+1/2,-z+1/4,-x+3/4
79	-y+1/4,z+1/2,-x+3/4
80	-y+1/4,-z+1/4,x
81	z+1/2,x+1/2,y
82	z+1/2,-x+1/4,-y+3/4
83	-z+1/4,x+1/2,-y+3/4
84	-z+1/4,-x+1/4,y
85	-x+1/2,-y+1/2,-z
86	-x+1/2,y+3/4,z+1/4
87	x+3/4,-y+1/2,z+1/4
88	x+3/4,y+3/4,-z
89	-y+1/2,-z+1/2,-x
90	-y+1/2,z+3/4,x+1/4
91	y+3/4,-z+1/2,x+1/4
92	y+3/4,z+3/4,-x
93	-z+1/2,-x+1/2,-y
94	-z+1/2,x+3/4,y+1/4
95	z+3/4,-x+1/2,y+1/4
96	z+3/4,x+3/4,-y

```
loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  Rb1 Rb 8 a 0.12500 0.12500 1.00000
  As1 As 8 b 0.62500 0.62500 0.62500 1.00000
  Rb2 Rb 16 d 0.50000 0.50000 0.50000 1.00000
  Se1 Se 32 e 0.70516 0.70516 0.70516 1.00000
  Se2 Se 96 g 0.51201 0.11100 0.42978 1.00000
```

Rb<sub>3</sub>AsSe<sub>16</sub>: AB3C16\_cF160\_203\_b\_ad\_eg - POSCAR

AB3C16\_cF160\_203\_b\_ad\_eg & a,x4,x5,y5,z5 --params=16.6600284675,0.70516,

↪ 0.51201, 0.111, 0.42978 & Fd-3 T<sub>[h]</sub><sup>4</sup> #203 (abdeg) & cF160 &  
 ↪ None & Rb3AsSe16 & M. Wachhold and W. S. Sheldrick, Z.  
 ↪ Naturforsch. B 52, 169-175 (1997)

1.00000000000000	8.33001423375000	8.33001423375000	
0.00000000000000	0.00000000000000	0.00000000000000	
8.33001423375000	8.33001423375000	8.33001423375000	
8.33001423375000	8.33001423375000	0.00000000000000	

As Rb Se  
 2 6 32

Direct

0.62500000000000	0.62500000000000	0.62500000000000	As (8b)
0.37500000000000	0.37500000000000	0.37500000000000	As (8b)
0.12500000000000	0.12500000000000	0.12500000000000	Rb (8a)
0.87500000000000	0.87500000000000	0.87500000000000	Rb (8a)
0.50000000000000	0.50000000000000	0.50000000000000	Rb (16d)
0.50000000000000	0.50000000000000	0.00000000000000	Rb (16d)
0.50000000000000	0.00000000000000	0.50000000000000	Rb (16d)
0.00000000000000	0.50000000000000	0.50000000000000	Rb (16d)
0.70516000000000	0.70516000000000	0.70516000000000	Se (32e)
0.70516000000000	0.70516000000000	-1.61548000000000	Se (32e)
0.70516000000000	-1.61548000000000	0.70516000000000	Se (32e)
-1.61548000000000	0.70516000000000	0.70516000000000	Se (32e)
-0.70516000000000	-0.70516000000000	-0.70516000000000	Se (32e)
-0.70516000000000	-0.70516000000000	2.61548000000000	Se (32e)
-0.70516000000000	2.61548000000000	-0.70516000000000	Se (32e)
2.61548000000000	-0.70516000000000	-0.70516000000000	Se (32e)
0.02877000000000	0.83079000000000	0.19323000000000	Se (96g)
0.83079000000000	0.02877000000000	-0.55279000000000	Se (96g)
0.19323000000000	-0.55279000000000	0.02877000000000	Se (96g)
-0.55279000000000	0.19323000000000	0.83079000000000	Se (96g)
0.19323000000000	0.02877000000000	0.83079000000000	Se (96g)
-0.55279000000000	0.83079000000000	0.02877000000000	Se (96g)
0.02877000000000	0.19323000000000	-0.55279000000000	Se (96g)
-0.55279000000000	-0.55279000000000	0.19323000000000	Se (96g)
0.19323000000000	0.02877000000000	0.83079000000000	Se (96g)
-0.02877000000000	-0.83079000000000	-0.19323000000000	Se (96g)
-0.83079000000000	-0.02877000000000	1.55279000000000	Se (96g)
-0.19323000000000	1.55279000000000	-0.02877000000000	Se (96g)
-0.02877000000000	-0.19323000000000	-0.83079000000000	Se (96g)
-0.83079000000000	-0.02877000000000	1.55279000000000	Se (96g)
-0.19323000000000	1.55279000000000	-0.02877000000000	Se (96g)
-0.02877000000000	-0.83079000000000	-0.19323000000000	Se (96g)
1.55279000000000	-0.02877000000000	-0.19323000000000	Se (96g)
-0.19323000000000	-0.83079000000000	1.55279000000000	Se (96g)

Ca<sub>3</sub>Al<sub>2</sub>O<sub>6</sub>: A2B3C6\_cP264\_205\_2d\_ab2c2d\_6d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ca3Al2O6'
_chemical_formula_sum 'Al2 Ca3 O6'

loop_
  _publ_author_name
    'P. Mondal'
    'J. W. Jeffery'
  _journal_name_full_name
;
Acta Crystallographica Section B: Structural Science
;
_journal_volume 31
_journal_year 1975
_journal_page_first 689
_journal_page_last 697
_publ_section_title
;
The crystal structure of tricalcium aluminate, CaS_{3}AlS_{2}SO_{6}S
;
_aflow_title 'CaS_{3}AlS_{2}SO_{6}S Structure'
_aflow_proto 'A2B3C6_cP264_205_2d_ab2c2d_6d'
_aflow_params 'a_x_{3}, x_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}, x_{7},
  ↪ y_{7}, z_{7}, x_{8}, y_{8}, z_{8}, x_{9}, y_{9}, z_{9}, x_{10}, y_{10},
  ↪ z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13},
  ↪ z_{13}, x_{14}, y_{14}, z_{14}'
_aflow_params_values '15.263, 0.2561, 0.375, 0.2526, 0.0133, 0.0197, 0.2444,
  ↪ 0.2335, 0.0046, 0.1386, 0.3763, 0.1272, 0.38, 0.3838, 0.1209, 0.2777,
  ↪ 0.1241, 0.0103, 0.4835, 0.1315, 0.2536, 0.2664, 0.2841, 0.1049, 0.235,
  ↪ 0.4047, 0.2921, 0.3491, -0.0385, -0.1074, 0.1509, -0.0104, -0.0242'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cP264'

_symmetry_space_group_name_H-M 'P 21/a -3'
_symmetry_Int_Tables_number 205

_cell_length_a 15.26300
_cell_length_b 15.26300
_cell_length_c 15.26300
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x, y, z
  2 x+1/2, -y+1/2, -z
  
```

3	-x, y+1/2, -z+1/2
4	-x+1/2, -y, z+1/2
5	y, z, x
6	y+1/2, -z+1/2, -x
7	-y, z+1/2, -x+1/2
8	-y+1/2, -z, x+1/2
9	z, x, y
10	z+1/2, -x+1/2, -y
11	-z, x+1/2, -y+1/2
12	-z+1/2, -x, y+1/2
13	-x, -y, -z
14	-x+1/2, y+1/2, z
15	x, -y+1/2, z+1/2
16	x+1/2, y, -z+1/2
17	-y, -z, -x
18	-y+1/2, z+1/2, x
19	y, -z+1/2, x+1/2
20	y+1/2, z, -x+1/2
21	-z, -x, -y
22	-z+1/2, x+1/2, y
23	z, -x+1/2, y+1/2
24	z+1/2, x, -y+1/2

loop\_  
 \_atom\_site\_label  
 \_atom\_site\_type\_symbol  
 \_atom\_site\_symmetry\_multiplicity  
 \_atom\_site\_Wyckoff\_label  
 \_atom\_site\_fract\_x  
 \_atom\_site\_fract\_y  
 \_atom\_site\_fract\_z  
 \_atom\_site\_occupancy  
 Ca1 Ca 4 a 0.50000 0.50000 0.50000 1.00000  
 Ca2 Ca 4 b 0.00000 0.00000 0.00000 1.00000  
 Ca3 Ca 8 c 0.25610 0.25610 0.25610 1.00000  
 Ca4 Ca 8 c 0.37500 0.37500 0.37500 1.00000  
 Al1 Al 24 d 0.25260 0.01330 0.01970 1.00000  
 Al2 Al 24 d 0.24440 0.23350 0.00460 1.00000  
 Ca5 Ca 24 d 0.13860 0.37630 0.12720 1.00000  
 Ca6 Ca 24 d 0.38000 0.38380 0.12090 1.00000  
 O1 O 24 d 0.27770 0.12410 0.01030 1.00000  
 O2 O 24 d 0.48350 0.13150 0.25360 1.00000  
 O3 O 24 d 0.26640 0.28410 0.10490 1.00000  
 O4 O 24 d 0.23500 0.40470 0.29210 1.00000  
 O5 O 24 d 0.34910 -0.03850 -0.10740 1.00000  
 O6 O 24 d 0.15090 -0.01040 -0.02420 1.00000

Ca<sub>3</sub>Al<sub>2</sub>O<sub>6</sub>: A2B3C6\_cP264\_205\_2d\_ab2c2d\_6d - POSCAR

```

A2B3C6_cP264_205_2d_ab2c2d_6d & a, x3, x4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8
  ↪ z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13,
  ↪ x14, y14, z14 --params=15.263, 0.2561, 0.375, 0.2526, 0.0133, 0.0197,
  ↪ 0.2444, 0.2335, 0.0046, 0.1386, 0.3763, 0.1272, 0.38, 0.3838, 0.1209,
  ↪ 0.2777, 0.1241, 0.0103, 0.4835, 0.1315, 0.2536, 0.2664, 0.2841, 0.1049,
  ↪ 0.235, 0.4047, 0.2921, 0.3491, -0.0385, -0.1074, 0.1509, -0.0104, -
  ↪ 0.0242 & Pa-3 T_{h}^{6} #205 (abc^{2d}10) & cP264 & None &
  ↪ Ca3Al2O6 & Ca3Al2O6 & P. Mondal and J. W. Jeffery, Acta
  ↪ Crystallogr. Sect. B Struct. Sci. 31, 689-697 (1975)

1.00000000000000
15.26300000000000 0.00000000000000 0.00000000000000
0.00000000000000 15.26300000000000 0.00000000000000
0.00000000000000 0.00000000000000 15.26300000000000
Al Ca O
48 72 144
Direct
0.25260000000000 0.01330000000000 0.01970000000000 Al (24d)
0.24740000000000 -0.01330000000000 0.51970000000000 Al (24d)
-0.25260000000000 0.51330000000000 0.48030000000000 Al (24d)
0.75260000000000 0.48670000000000 -0.01970000000000 Al (24d)
0.01970000000000 0.25260000000000 0.01330000000000 Al (24d)
0.51970000000000 0.24740000000000 -0.01330000000000 Al (24d)
0.48030000000000 -0.25260000000000 0.51330000000000 Al (24d)
-0.01970000000000 0.75260000000000 0.48670000000000 Al (24d)
0.01330000000000 0.01970000000000 0.25260000000000 Al (24d)
-0.01330000000000 0.51970000000000 0.24740000000000 Al (24d)
0.51330000000000 0.48030000000000 -0.25260000000000 Al (24d)
0.48670000000000 -0.01970000000000 0.75260000000000 Al (24d)
-0.25260000000000 -0.01330000000000 -0.01970000000000 Al (24d)
0.75260000000000 0.01330000000000 0.48030000000000 Al (24d)
0.25260000000000 0.48670000000000 0.51970000000000 Al (24d)
0.24740000000000 0.51330000000000 0.01970000000000 Al (24d)
-0.01970000000000 -0.25260000000000 -0.01330000000000 Al (24d)
0.48030000000000 0.75260000000000 0.01330000000000 Al (24d)
0.51970000000000 0.25260000000000 0.48670000000000 Al (24d)
0.01970000000000 0.24740000000000 0.51330000000000 Al (24d)
-0.01330000000000 -0.01970000000000 -0.25260000000000 Al (24d)
0.01330000000000 0.48030000000000 0.75260000000000 Al (24d)
0.48670000000000 0.51970000000000 0.25260000000000 Al (24d)
0.51330000000000 0.01970000000000 0.24740000000000 Al (24d)
0.24440000000000 0.23350000000000 0.00460000000000 Al (24d)
0.25260000000000 -0.23350000000000 0.50460000000000 Al (24d)
-0.24440000000000 0.73350000000000 0.49540000000000 Al (24d)
0.74440000000000 0.26650000000000 -0.00460000000000 Al (24d)
0.00460000000000 0.24440000000000 0.23350000000000 Al (24d)
0.50460000000000 0.25600000000000 -0.23350000000000 Al (24d)
0.49540000000000 -0.24440000000000 0.73350000000000 Al (24d)
-0.00460000000000 0.74440000000000 0.26650000000000 Al (24d)
0.23350000000000 0.00460000000000 0.24440000000000 Al (24d)
-0.23350000000000 0.50460000000000 0.25600000000000 Al (24d)
0.73350000000000 0.49540000000000 -0.24440000000000 Al (24d)
0.26650000000000 -0.00460000000000 0.74440000000000 Al (24d)
-0.24440000000000 -0.23350000000000 -0.00460000000000 Al (24d)
0.74440000000000 0.23350000000000 0.49540000000000 Al (24d)
0.24440000000000 0.26650000000000 0.50460000000000 Al (24d)
0.25600000000000 0.73350000000000 0.00460000000000 Al (24d)
  
```

-0.00460000000000	-0.24440000000000	-0.23350000000000	Al (24d)	0.01650000000000	-0.13150000000000	0.75360000000000	O (24d)
0.49540000000000	0.74440000000000	0.23350000000000	Al (24d)	-0.48350000000000	0.63150000000000	0.26460000000000	O (24d)
0.50460000000000	0.24440000000000	0.26650000000000	Al (24d)	0.98350000000000	0.36850000000000	-0.25360000000000	O (24d)
0.00460000000000	0.25560000000000	0.73350000000000	Al (24d)	0.25360000000000	0.48350000000000	0.13150000000000	O (24d)
-0.23350000000000	-0.00460000000000	-0.24440000000000	Al (24d)	0.75360000000000	0.01650000000000	-0.13150000000000	O (24d)
0.23350000000000	0.49540000000000	0.74440000000000	Al (24d)	0.24640000000000	-0.48350000000000	0.63150000000000	O (24d)
0.26650000000000	0.50460000000000	0.24440000000000	Al (24d)	-0.25360000000000	0.98350000000000	0.36850000000000	O (24d)
0.73350000000000	0.00460000000000	0.25560000000000	Al (24d)	0.13150000000000	0.25360000000000	0.48350000000000	O (24d)
0.00000000000000	0.00000000000000	0.00000000000000	Ca (4a)	-0.13150000000000	0.75360000000000	0.01650000000000	O (24d)
0.50000000000000	0.00000000000000	0.50000000000000	Ca (4a)	0.63150000000000	0.24640000000000	-0.48350000000000	O (24d)
0.00000000000000	0.50000000000000	0.50000000000000	Ca (4a)	0.36850000000000	-0.25360000000000	0.98350000000000	O (24d)
0.50000000000000	0.50000000000000	0.00000000000000	Ca (4a)	-0.48350000000000	-0.13150000000000	-0.25360000000000	O (24d)
0.50000000000000	0.50000000000000	0.50000000000000	Ca (4b)	0.98350000000000	0.13150000000000	0.24640000000000	O (24d)
0.00000000000000	0.50000000000000	0.00000000000000	Ca (4b)	0.48350000000000	0.36850000000000	0.75360000000000	O (24d)
0.50000000000000	0.00000000000000	0.00000000000000	Ca (4b)	0.01650000000000	0.63150000000000	0.25360000000000	O (24d)
0.00000000000000	0.00000000000000	0.50000000000000	Ca (4b)	-0.25360000000000	-0.48350000000000	-0.13150000000000	O (24d)
0.25610000000000	0.25610000000000	0.25610000000000	Ca (8c)	0.24640000000000	0.98350000000000	0.13150000000000	O (24d)
0.24390000000000	-0.25610000000000	0.75610000000000	Ca (8c)	0.75360000000000	0.48350000000000	0.36850000000000	O (24d)
-0.25610000000000	0.75610000000000	0.24390000000000	Ca (8c)	0.25360000000000	0.01650000000000	0.63150000000000	O (24d)
0.75610000000000	0.24390000000000	-0.25610000000000	Ca (8c)	-0.13150000000000	-0.25360000000000	-0.48350000000000	O (24d)
-0.25610000000000	-0.25610000000000	-0.25610000000000	Ca (8c)	0.13150000000000	0.24640000000000	0.98350000000000	O (24d)
0.75610000000000	0.25610000000000	0.24390000000000	Ca (8c)	0.36850000000000	0.75360000000000	0.48350000000000	O (24d)
0.25610000000000	0.24390000000000	0.75610000000000	Ca (8c)	0.63150000000000	0.25360000000000	0.01650000000000	O (24d)
0.24390000000000	0.75610000000000	0.25610000000000	Ca (8c)	0.26640000000000	0.28410000000000	0.10490000000000	O (24d)
0.37500000000000	0.37500000000000	0.37500000000000	Ca (8c)	0.23360000000000	-0.28410000000000	0.60490000000000	O (24d)
0.12500000000000	-0.37500000000000	0.87500000000000	Ca (8c)	-0.26640000000000	0.78410000000000	0.39510000000000	O (24d)
-0.37500000000000	0.87500000000000	0.12500000000000	Ca (8c)	0.76640000000000	0.21590000000000	-0.10490000000000	O (24d)
0.87500000000000	0.12500000000000	-0.37500000000000	Ca (8c)	0.10490000000000	0.26640000000000	0.28410000000000	O (24d)
-0.37500000000000	-0.37500000000000	-0.37500000000000	Ca (8c)	0.60490000000000	0.23360000000000	-0.28410000000000	O (24d)
0.87500000000000	0.37500000000000	0.12500000000000	Ca (8c)	0.39510000000000	-0.26640000000000	0.78410000000000	O (24d)
0.37500000000000	0.12500000000000	0.87500000000000	Ca (8c)	-0.10490000000000	0.76640000000000	0.21590000000000	O (24d)
0.12500000000000	0.87500000000000	0.37500000000000	Ca (8c)	0.28410000000000	0.10490000000000	0.26640000000000	O (24d)
0.13860000000000	0.37630000000000	0.12720000000000	Ca (24d)	-0.28410000000000	0.60490000000000	0.23360000000000	O (24d)
0.36140000000000	-0.37630000000000	0.62720000000000	Ca (24d)	0.78410000000000	0.39510000000000	-0.26640000000000	O (24d)
-0.13860000000000	0.87630000000000	0.37280000000000	Ca (24d)	0.21590000000000	-0.10490000000000	0.76640000000000	O (24d)
0.63860000000000	0.12370000000000	-0.12720000000000	Ca (24d)	-0.26640000000000	-0.28410000000000	-0.10490000000000	O (24d)
0.12720000000000	0.13860000000000	0.37630000000000	Ca (24d)	0.76640000000000	0.28410000000000	0.39510000000000	O (24d)
0.62720000000000	0.36140000000000	-0.37630000000000	Ca (24d)	0.26640000000000	0.21590000000000	0.60490000000000	O (24d)
0.37280000000000	-0.13860000000000	0.87630000000000	Ca (24d)	0.23360000000000	0.78410000000000	0.10490000000000	O (24d)
-0.12720000000000	0.63860000000000	0.12370000000000	Ca (24d)	-0.10490000000000	-0.26640000000000	-0.28410000000000	O (24d)
0.37630000000000	0.12720000000000	0.13860000000000	Ca (24d)	0.39510000000000	0.76640000000000	0.28410000000000	O (24d)
-0.37630000000000	0.62720000000000	0.36140000000000	Ca (24d)	0.60490000000000	0.26640000000000	0.21590000000000	O (24d)
0.87630000000000	0.37280000000000	-0.13860000000000	Ca (24d)	0.10490000000000	0.23360000000000	0.78410000000000	O (24d)
0.12370000000000	-0.12720000000000	0.63860000000000	Ca (24d)	-0.28410000000000	-0.10490000000000	-0.26640000000000	O (24d)
-0.13860000000000	-0.37630000000000	-0.12720000000000	Ca (24d)	0.28410000000000	0.39510000000000	0.76640000000000	O (24d)
0.63860000000000	0.37630000000000	0.37280000000000	Ca (24d)	0.21590000000000	0.60490000000000	0.26640000000000	O (24d)
0.13860000000000	0.12370000000000	0.62720000000000	Ca (24d)	0.78410000000000	0.10490000000000	0.23360000000000	O (24d)
0.36140000000000	0.87630000000000	0.12720000000000	Ca (24d)	0.23500000000000	0.40470000000000	0.29210000000000	O (24d)
-0.12720000000000	-0.13860000000000	-0.37630000000000	Ca (24d)	0.26500000000000	-0.40470000000000	0.79210000000000	O (24d)
0.37280000000000	0.63860000000000	0.37630000000000	Ca (24d)	-0.23500000000000	0.90470000000000	0.20790000000000	O (24d)
0.62720000000000	0.13860000000000	0.12370000000000	Ca (24d)	0.73500000000000	0.09530000000000	-0.29210000000000	O (24d)
0.12720000000000	0.36140000000000	0.87630000000000	Ca (24d)	0.29210000000000	0.23500000000000	0.40470000000000	O (24d)
-0.37630000000000	-0.12720000000000	-0.13860000000000	Ca (24d)	0.79210000000000	0.26500000000000	-0.40470000000000	O (24d)
0.37630000000000	0.37280000000000	0.63860000000000	Ca (24d)	0.20790000000000	-0.23500000000000	0.90470000000000	O (24d)
0.12370000000000	0.62720000000000	0.13860000000000	Ca (24d)	-0.29210000000000	0.73500000000000	0.09530000000000	O (24d)
0.87630000000000	0.12720000000000	0.36140000000000	Ca (24d)	0.40470000000000	0.29210000000000	0.23500000000000	O (24d)
0.38000000000000	0.38380000000000	0.12090000000000	Ca (24d)	-0.40470000000000	0.79210000000000	0.26500000000000	O (24d)
0.12000000000000	-0.38380000000000	0.62090000000000	Ca (24d)	0.90470000000000	0.20790000000000	-0.23500000000000	O (24d)
-0.38000000000000	0.88380000000000	0.37910000000000	Ca (24d)	-0.29210000000000	-0.29210000000000	0.73500000000000	O (24d)
0.88000000000000	0.11620000000000	-0.12090000000000	Ca (24d)	-0.23500000000000	-0.40470000000000	-0.29210000000000	O (24d)
0.12090000000000	0.38000000000000	0.38380000000000	Ca (24d)	0.73500000000000	0.40470000000000	0.20790000000000	O (24d)
0.62090000000000	0.12000000000000	-0.38380000000000	Ca (24d)	0.23500000000000	0.09530000000000	0.79210000000000	O (24d)
0.37910000000000	-0.38000000000000	0.88380000000000	Ca (24d)	0.26500000000000	0.90470000000000	0.29210000000000	O (24d)
-0.12090000000000	0.88000000000000	0.11620000000000	Ca (24d)	-0.29210000000000	-0.23500000000000	-0.40470000000000	O (24d)
0.38380000000000	0.12090000000000	0.38000000000000	Ca (24d)	0.20790000000000	0.73500000000000	0.40470000000000	O (24d)
-0.38380000000000	0.62090000000000	0.12000000000000	Ca (24d)	0.79210000000000	0.23500000000000	0.09530000000000	O (24d)
0.88380000000000	0.37910000000000	-0.38000000000000	Ca (24d)	0.29210000000000	0.26500000000000	0.90470000000000	O (24d)
0.11620000000000	-0.12090000000000	0.88000000000000	Ca (24d)	-0.40470000000000	-0.29210000000000	-0.23500000000000	O (24d)
-0.38380000000000	-0.38380000000000	-0.12090000000000	Ca (24d)	0.40470000000000	0.20790000000000	0.73500000000000	O (24d)
0.88000000000000	0.38380000000000	0.37910000000000	Ca (24d)	0.09530000000000	0.79210000000000	0.23500000000000	O (24d)
0.38000000000000	0.11620000000000	0.62090000000000	Ca (24d)	0.90470000000000	0.29210000000000	0.26500000000000	O (24d)
0.12000000000000	0.88380000000000	0.12090000000000	Ca (24d)	0.34910000000000	-0.03850000000000	-0.10740000000000	O (24d)
-0.12090000000000	-0.38000000000000	-0.38380000000000	Ca (24d)	0.15090000000000	0.03850000000000	0.39260000000000	O (24d)
0.37910000000000	0.88000000000000	0.38380000000000	Ca (24d)	-0.34910000000000	0.46150000000000	0.60740000000000	O (24d)
0.62090000000000	0.38000000000000	0.11620000000000	Ca (24d)	0.84910000000000	0.53850000000000	0.10740000000000	O (24d)
0.12090000000000	0.12000000000000	0.88380000000000	Ca (24d)	-0.10740000000000	0.34910000000000	-0.03850000000000	O (24d)
-0.38380000000000	-0.12090000000000	-0.38000000000000	Ca (24d)	0.39260000000000	0.15090000000000	0.03850000000000	O (24d)
0.38380000000000	0.37910000000000	0.88000000000000	Ca (24d)	0.60740000000000	-0.34910000000000	0.46150000000000	O (24d)
0.11620000000000	0.62090000000000	0.38000000000000	Ca (24d)	0.10740000000000	0.84910000000000	0.53850000000000	O (24d)
0.88380000000000	0.12090000000000	0.12000000000000	Ca (24d)	-0.03850000000000	-0.10740000000000	0.34910000000000	O (24d)
0.27770000000000	0.12410000000000	0.01030000000000	O (24d)	0.03850000000000	0.39260000000000	0.15090000000000	O (24d)
0.22230000000000	-0.12410000000000	0.51030000000000	O (24d)	0.46150000000000	0.60740000000000	-0.34910000000000	O (24d)
-0.27770000000000	0.62410000000000	0.48970000000000	O (24d)</				

0.48960000000000	0.52420000000000	-0.15090000000000	O (24d)
0.51040000000000	0.02420000000000	0.65090000000000	O (24d)
-0.15090000000000	0.01040000000000	0.02420000000000	O (24d)
0.65090000000000	-0.01040000000000	0.52420000000000	O (24d)
0.15090000000000	0.51040000000000	0.47580000000000	O (24d)
0.34910000000000	0.48960000000000	-0.02420000000000	O (24d)
0.02420000000000	-0.15090000000000	0.01040000000000	O (24d)
0.52420000000000	0.65090000000000	-0.01040000000000	O (24d)
0.47580000000000	0.15090000000000	0.51040000000000	O (24d)
-0.02420000000000	0.34910000000000	0.48960000000000	O (24d)
0.01040000000000	0.02420000000000	-0.15090000000000	O (24d)
-0.01040000000000	0.52420000000000	0.65090000000000	O (24d)
0.51040000000000	0.47580000000000	0.15090000000000	O (24d)
0.48960000000000	-0.02420000000000	0.34910000000000	O (24d)

Simple Cubic C<sub>60</sub> Buckminsterfullerene: A\_cp240\_205\_10d - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Buckminsterfullerene'
_chemical_formula_sum 'C'

loop_
  _publ_author_name
    'W. I. F. David'
    'R. M. Ibberson'
    'J. C. Matthewman'
    'K. Prassides'
    'T. J. S. Dennis'
    'J. P. Hare'
    'H. W. Kroto'
    'R. Taylor'
    'D. R. M. Walton'
  _journal_name_full_name
    'Nature'
  _journal_volume 353
  _journal_year 1991
  _journal_page_first 147
  _journal_page_last 149
  _publ_section_title
    'Crystal structure and bonding of ordered CS_{60}S'

  _aflow_title 'Simple Cubic CS_{60}S Buckminsterfullerene Structure'
  _aflow_proto 'A_cp240_205_10d'
  _aflow_params 'a, x_{1}, y_{1}, z_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3},
    x_{4}, y_{4}, z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}, x_{7}, y_{7}, z_{7},
    x_{8}, y_{8}, z_{8}, x_{9}, y_{9}, z_{9}, x_{10}, y_{10}, z_{10}'
  _aflow_params_values '14.04078, 0.2294, -0.0325, 0.101, 0.2467, -0.054, 0.0061,
    0.2081, 0.0646, 0.1289, 0.2066, 0.8599, -0.036, 0.171, -0.0963, 0.159,
    0.2236, 0.1122, -0.0371, 0.2439, 0.0192, -0.0636, 0.2053, 0.1349,
    0.0616, 0.1503, 0.7983, 0.0202, 0.1323, 0.8207, 0.1186'
  _aflow_strukturbericht 'None'
  _aflow_pearson 'cP240'

_symmetry_space_group_name_H-M 'P 21/a -3'
_symmetry_Int_tables_number 205

_cell_length_a 14.04078
_cell_length_b 14.04078
_cell_length_c 14.04078
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
    1 x, y, z
    2 x+1/2, -y+1/2, -z
    3 -x, y+1/2, -z+1/2
    4 -x+1/2, -y, z+1/2
    5 y, z, x
    6 y+1/2, -z+1/2, -x
    7 -y, z+1/2, -x+1/2
    8 -y+1/2, -z, x+1/2
    9 z, x, y
    10 z+1/2, -x+1/2, -y
    11 -z, x+1/2, -y+1/2
    12 -z+1/2, -x, y+1/2
    13 -x, -y, -z
    14 -x+1/2, y+1/2, z
    15 x, -y+1/2, z+1/2
    16 x+1/2, y, -z+1/2
    17 -y, -z, -x
    18 -y+1/2, z+1/2, x
    19 y, -z+1/2, x+1/2
    20 y+1/2, z, -x+1/2
    21 -z, -x, -y
    22 -z+1/2, x+1/2, y
    23 z, -x+1/2, y+1/2
    24 z+1/2, x, -y+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
```

_atom_site_fract_y			
_atom_site_fract_z			
_atom_site_occupancy			
C1	C	24 d	0.22940 -0.03250 0.10100 1.00000
C2	C	24 d	0.24670 -0.05400 0.00610 1.00000
C3	C	24 d	0.20810 0.06460 0.12890 1.00000
C4	C	24 d	0.20660 0.85990 -0.03600 1.00000
C5	C	24 d	0.17100 -0.09630 0.15900 1.00000
C6	C	24 d	0.22360 0.11220 -0.03710 1.00000
C7	C	24 d	0.24390 0.01920 -0.06360 1.00000
C8	C	24 d	0.20530 0.13490 0.06160 1.00000
C9	C	24 d	0.15030 0.79830 0.02020 1.00000
C10	C	24 d	0.13230 0.82070 0.11860 1.00000

Simple Cubic C<sub>60</sub> Buckminsterfullerene: A\_cp240\_205\_10d - POSCAR

```
A_cp240_205_10d & a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6,
  z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10 --params=14.04078,
  0.2294, -0.0325, 0.101, 0.2467, -0.054, 0.0061, 0.2081, 0.0646, 0.1289,
  0.2066, 0.8599, -0.036, 0.171, -0.0963, 0.159, 0.2236, 0.1122, -0.0371,
  0.2439, 0.0192, -0.0636, 0.2053, 0.1349, 0.0616, 0.1503, 0.7983, 0.0202
  0.1323, 0.8207, 0.1186 & Pa-3 T_{h}^{6} #205 (d^{10}) & cP240 &
  None & C & Buckminsterfullerene & W. I. F. David et al., Nature
  353, 147-149 (1991)

1.00000000000000
14.04078000000000 0.00000000000000 0.00000000000000
0.00000000000000 14.04078000000000 0.00000000000000
0.00000000000000 0.00000000000000 14.04078000000000
C
240
Direct
0.22940000000000 -0.03250000000000 0.10100000000000 C (24d)
0.27060000000000 0.03250000000000 0.60100000000000 C (24d)
-0.22940000000000 0.46750000000000 0.39900000000000 C (24d)
0.72940000000000 0.53250000000000 -0.10100000000000 C (24d)
0.10100000000000 0.22940000000000 -0.03250000000000 C (24d)
0.60100000000000 0.27060000000000 0.03250000000000 C (24d)
0.39900000000000 -0.22940000000000 0.46750000000000 C (24d)
-0.10100000000000 0.72940000000000 0.53250000000000 C (24d)
-0.03250000000000 0.10100000000000 0.22940000000000 C (24d)
0.03250000000000 0.60100000000000 0.27060000000000 C (24d)
0.46750000000000 0.39900000000000 -0.22940000000000 C (24d)
0.53250000000000 -0.10100000000000 0.72940000000000 C (24d)
-0.22940000000000 0.03250000000000 -0.10100000000000 C (24d)
0.72940000000000 -0.03250000000000 0.39900000000000 C (24d)
0.22940000000000 0.53250000000000 0.60100000000000 C (24d)
0.27060000000000 0.46750000000000 0.10100000000000 C (24d)
-0.10100000000000 -0.22940000000000 0.03250000000000 C (24d)
0.39900000000000 0.72940000000000 -0.03250000000000 C (24d)
0.60100000000000 0.22940000000000 0.53250000000000 C (24d)
0.10100000000000 0.27060000000000 0.46750000000000 C (24d)
0.03250000000000 -0.10100000000000 -0.22940000000000 C (24d)
-0.03250000000000 0.39900000000000 0.72940000000000 C (24d)
0.53250000000000 0.60100000000000 0.22940000000000 C (24d)
0.46750000000000 0.10100000000000 0.27060000000000 C (24d)
0.24670000000000 -0.05400000000000 0.00610000000000 C (24d)
0.25330000000000 0.05400000000000 0.50610000000000 C (24d)
-0.24670000000000 0.44600000000000 0.49390000000000 C (24d)
0.74670000000000 0.55400000000000 -0.00610000000000 C (24d)
0.00610000000000 0.24670000000000 -0.05400000000000 C (24d)
0.50610000000000 0.25330000000000 0.05400000000000 C (24d)
0.49390000000000 -0.24670000000000 0.44600000000000 C (24d)
-0.00610000000000 0.74670000000000 0.55400000000000 C (24d)
-0.05400000000000 0.00610000000000 0.24670000000000 C (24d)
0.05400000000000 0.50610000000000 0.25330000000000 C (24d)
0.44600000000000 0.49390000000000 -0.24670000000000 C (24d)
0.55400000000000 -0.00610000000000 0.74670000000000 C (24d)
-0.24670000000000 0.05400000000000 -0.00610000000000 C (24d)
0.74670000000000 -0.05400000000000 0.49390000000000 C (24d)
0.24670000000000 0.55400000000000 0.50610000000000 C (24d)
0.25330000000000 0.44600000000000 0.00610000000000 C (24d)
-0.00610000000000 -0.24670000000000 0.05400000000000 C (24d)
0.49390000000000 0.74670000000000 -0.05400000000000 C (24d)
0.50610000000000 0.24670000000000 0.55400000000000 C (24d)
0.00610000000000 0.25330000000000 0.44600000000000 C (24d)
0.05400000000000 -0.00610000000000 -0.24670000000000 C (24d)
-0.05400000000000 0.49390000000000 0.74670000000000 C (24d)
0.55400000000000 0.50610000000000 0.24670000000000 C (24d)
0.44600000000000 0.00610000000000 0.25330000000000 C (24d)
0.20810000000000 0.06460000000000 0.12890000000000 C (24d)
0.29190000000000 -0.06460000000000 0.62890000000000 C (24d)
-0.20810000000000 0.56460000000000 0.37110000000000 C (24d)
0.70810000000000 0.43540000000000 -0.12890000000000 C (24d)
0.12890000000000 0.20810000000000 0.06460000000000 C (24d)
0.62890000000000 0.29190000000000 -0.06460000000000 C (24d)
0.37110000000000 -0.20810000000000 0.56460000000000 C (24d)
-0.12890000000000 0.70810000000000 0.43540000000000 C (24d)
0.06460000000000 0.12890000000000 0.20810000000000 C (24d)
-0.06460000000000 0.62890000000000 0.29190000000000 C (24d)
0.56460000000000 0.37110000000000 -0.20810000000000 C (24d)
0.43540000000000 -0.12890000000000 0.70810000000000 C (24d)
-0.20810000000000 -0.06460000000000 -0.12890000000000 C (24d)
0.70810000000000 0.06460000000000 0.37110000000000 C (24d)
0.29190000000000 0.56460000000000 0.12890000000000 C (24d)
-0.12890000000000 -0.20810000000000 -0.06460000000000 C (24d)
0.37110000000000 0.70810000000000 0.43540000000000 C (24d)
0.62890000000000 0.20810000000000 0.06460000000000 C (24d)
0.12890000000000 0.29190000000000 0.56460000000000 C (24d)
-0.06460000000000 -0.12890000000000 -0.20810000000000 C (24d)
0.06460000000000 0.37110000000000 0.70810000000000 C (24d)
0.43540000000000 0.62890000000000 0.20810000000000 C (24d)
0.56460000000000 0.12890000000000 0.29190000000000 C (24d)
0.20660000000000 0.85990000000000 -0.03600000000000 C (24d)
0.29340000000000 -0.85990000000000 0.46400000000000 C (24d)
```



```

_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z+1/2
3 -x+1/2, y, -z
4 -x, -y+1/2, z
5 y, z, x
6 y, -z, -x+1/2
7 -y+1/2, z, -x
8 -y, -z+1/2, x
9 z, x, y
10 z, -x, -y+1/2
11 -z+1/2, x, -y
12 -z, -x+1/2, y
13 -x, -y, -z
14 -x, y, z+1/2
15 x+1/2, -y, z
16 x, y+1/2, -z
17 -y, -z, -x
18 -y, z, x+1/2
19 y+1/2, -z, x
20 y, z+1/2, -x
21 -z, -x, -y
22 -z, x, y+1/2
23 z+1/2, -x, y
24 z, x+1/2, -y
25 x+1/2, y+1/2, z+1/2
26 x+1/2, -y+1/2, -z
27 -x, y+1/2, -z+1/2
28 -x+1/2, -y, z+1/2
29 y+1/2, z+1/2, x+1/2
30 y+1/2, -z+1/2, -x
31 -y, z+1/2, -x+1/2
32 -y+1/2, -z, x+1/2
33 z+1/2, x+1/2, y+1/2
34 z+1/2, -x+1/2, -y
35 -z, x+1/2, -y+1/2
36 -z+1/2, -x, y+1/2
37 -x+1/2, -y+1/2, -z+1/2
38 -x+1/2, y+1/2, z
39 x, -y+1/2, z+1/2
40 x+1/2, y, -z+1/2
41 -y+1/2, -z+1/2, -x+1/2
42 -y+1/2, z+1/2, x
43 y, -z+1/2, x+1/2
44 y+1/2, z, -x+1/2
45 -z+1/2, -x+1/2, -y+1/2
46 -z+1/2, x+1/2, y
47 z, -x+1/2, y+1/2
48 z+1/2, x, -y+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
N1 N 8 a 0.00000 0.00000 0.00000 1.00000
Al1 Al 16 c 0.11500 0.11500 0.11500 1.00000
N2 N 24 d 0.20500 0.00000 0.25000 1.00000
Li1 Li 48 e 0.16000 0.38200 0.11000 1.00000

```

Alli<sub>3</sub>N<sub>2</sub> (E<sub>9d</sub>): AB3C2\_c196\_206\_c\_e\_ad - POSCAR

```

AB3C2_c196_206_c_e_ad & a, x2, x3, x4, y4, z4 --params=9.46 , 0.115 , 0.205 , 0.16 ,
↪ 0.382, 0.11 & 1a-3 T_{h}^{(7)} #206 (acde) & c196 & $E9_{(d)}$ &
↪ ALi3N2 & & R. Jutta and F. Hund, (Z. Anorg. Allg. Chem. 257,
↪ 13-25 (1948))
1.0000000000000000
-4.7300000000000000 4.7300000000000000 4.7300000000000000
4.7300000000000000 -4.7300000000000000 4.7300000000000000
4.7300000000000000 4.7300000000000000 -4.7300000000000000
Al Li N
8 24 16
Direct
0.2300000000000000 0.2300000000000000 0.2300000000000000 Al (16c)
0.5000000000000000 0.0000000000000000 0.2700000000000000 Al (16c)
0.0000000000000000 0.2700000000000000 0.5000000000000000 Al (16c)
0.2700000000000000 0.5000000000000000 0.0000000000000000 Al (16c)
-0.2300000000000000 -0.2300000000000000 -0.2300000000000000 Al (16c)
0.5000000000000000 0.0000000000000000 0.7300000000000000 Al (16c)
0.0000000000000000 0.7300000000000000 0.5000000000000000 Al (16c)
0.7300000000000000 0.5000000000000000 0.0000000000000000 Al (16c)
0.4920000000000000 0.2700000000000000 0.5420000000000000 Li (48e)
0.2280000000000000 -0.0500000000000000 -0.0420000000000000 Li (48e)
0.2720000000000000 0.2300000000000000 0.7220000000000000 Li (48e)
0.0080000000000000 0.5500000000000000 -0.2220000000000000 Li (48e)
0.5420000000000000 0.4920000000000000 0.2700000000000000 Li (48e)
-0.0420000000000000 0.2280000000000000 -0.0500000000000000 Li (48e)
0.7220000000000000 0.2700000000000000 0.2300000000000000 Li (48e)
-0.2220000000000000 0.0080000000000000 0.5500000000000000 Li (48e)
0.2700000000000000 0.5420000000000000 0.4920000000000000 Li (48e)
-0.0500000000000000 -0.0420000000000000 0.2280000000000000 Li (48e)
0.2300000000000000 0.7220000000000000 0.2700000000000000 Li (48e)
0.5500000000000000 -0.2220000000000000 0.0080000000000000 Li (48e)
-0.4920000000000000 -0.2700000000000000 -0.5420000000000000 Li (48e)
0.7720000000000000 0.0500000000000000 1.0420000000000000 Li (48e)

```

```

-0.2720000000000000 0.7700000000000000 0.2780000000000000 Li (48e)
0.9920000000000000 0.4500000000000000 0.2220000000000000 Li (48e)
-0.5420000000000000 -0.4920000000000000 -0.2700000000000000 Li (48e)
1.0420000000000000 0.7720000000000000 0.0500000000000000 Li (48e)
0.2780000000000000 -0.2720000000000000 0.7700000000000000 Li (48e)
0.2220000000000000 0.9920000000000000 0.4500000000000000 Li (48e)
-0.2700000000000000 -0.5420000000000000 -0.4920000000000000 Li (48e)
0.0500000000000000 1.0420000000000000 0.7720000000000000 Li (48e)
0.7700000000000000 0.2780000000000000 -0.2720000000000000 Li (48e)
0.4500000000000000 0.2220000000000000 0.9920000000000000 Li (48e)
0.0000000000000000 0.0000000000000000 0.0000000000000000 N (8a)
0.5000000000000000 0.0000000000000000 0.5000000000000000 N (8a)
0.0000000000000000 0.5000000000000000 0.5000000000000000 N (8a)
0.5000000000000000 0.5000000000000000 0.5000000000000000 N (8a)
0.2500000000000000 0.4500000000000000 0.2050000000000000 N (24d)
0.7500000000000000 0.0450000000000000 0.2950000000000000 N (24d)
0.2500000000000000 0.2500000000000000 0.4550000000000000 N (24d)
0.2950000000000000 0.7500000000000000 0.0450000000000000 N (24d)
0.4550000000000000 0.2050000000000000 0.2500000000000000 N (24d)
0.0450000000000000 0.2950000000000000 0.7500000000000000 N (24d)
0.7500000000000000 0.5450000000000000 -0.2050000000000000 N (24d)
0.2500000000000000 0.9550000000000000 0.7050000000000000 N (24d)
-0.2050000000000000 0.7500000000000000 0.5450000000000000 N (24d)
0.7050000000000000 0.2500000000000000 0.9550000000000000 N (24d)
0.5450000000000000 -0.2050000000000000 0.7500000000000000 N (24d)
0.9550000000000000 0.7050000000000000 0.2500000000000000 N (24d)

```

Pd<sub>17</sub>Se<sub>15</sub>: A17B15\_cP64\_207\_acfk\_eij - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Pd17Se15'
_chemical_formula_sum 'Pd17 Se15'

loop_
_publ_author_name
'S. Geller'
_journal_name_full_name
;
Acta Crystallographica
;
_journal_volume 15
_journal_year 1962
_journal_page_first 713
_journal_page_last 721
_publ_section_title
;
The crystal structure of PdS_{17}SeS_{15}
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'PdS_{17}SeS_{15} Structure'
_aflow_proto 'A17B15_cP64_207_acfk_eij'
_aflow_params 'a, x_{3}, x_{4}, y_{5}, y_{6}, x_{7}, y_{7}, z_{7}'
_aflow_params_values '10.6058825779, 0.2422, 0.2622, 0.3319, 0.2701, 0.142,
↪ 0.1539, 0.3498'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cP64'

_cell_length_a 10.6058825779
_cell_length_b 10.6058825779
_cell_length_c 10.6058825779
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4 3 2"
_symmetry_Int_Tables_number 207

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y, -z
4 -x, -y, z
5 y, z, x
6 y, -z, -x
7 -y, z, -x
8 -y, -z, x
9 z, x, y
10 z, -x, -y
11 -z, x, -y
12 -z, -x, y
13 -y, -x, -z
14 -y, x, z
15 y, -x, z
16 y, x, -z
17 -x, -z, -y
18 -x, z, y
19 x, -z, y
20 x, z, -y
21 -z, -y, -x
22 -z, y, x
23 z, -y, x
24 z, y, -x

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity

```

```

_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Pd1 Pd 1 a 0.00000 0.00000 0.00000 1.00000
Pd2 Pd 3 c 0.00000 0.50000 0.50000 1.00000
Se1 Se 6 e 0.24220 0.00000 0.00000 1.00000
Pd3 Pd 6 f 0.26220 0.50000 0.50000 1.00000
Se2 Se 12 i 0.00000 0.33190 0.33190 1.00000
Se3 Se 12 j 0.50000 0.27010 0.27010 1.00000
Pd4 Pd 24 k 0.14200 0.15390 0.34980 1.00000

```

Pd<sub>7</sub>Se<sub>15</sub>: A17B15\_cP64\_207\_acfk\_eij - POSCAR

```

A17B15_cP64_207_acfk_eij & a, x3, x4, y5, y6, x7, y7, z7 --params=10.6058825779
↪ , 0.2422, 0.2622, 0.3319, 0.2701, 0.142, 0.1539, 0.3498 & P432 O^{1} #
↪ 207 (acefijk) & cP64 & None & Pd17Se15 & & S. Geller, Acta
↪ Cryst. 15, 713-721 (1962)
1.0000000000000000
10.60588257790000 0.00000000000000 0.00000000000000
0.00000000000000 10.60588257790000 0.00000000000000
0.00000000000000 0.00000000000000 10.60588257790000
Pd Se
34 30
Direct
0.00000000000000 0.00000000000000 0.00000000000000 Pd (1a)
0.00000000000000 0.50000000000000 0.50000000000000 Pd (3c)
0.50000000000000 0.00000000000000 0.50000000000000 Pd (3c)
0.50000000000000 0.50000000000000 0.00000000000000 Pd (3c)
0.26220000000000 0.50000000000000 0.50000000000000 Pd (6f)
-0.26220000000000 0.50000000000000 0.50000000000000 Pd (6f)
0.50000000000000 0.26220000000000 0.50000000000000 Pd (6f)
0.50000000000000 -0.26220000000000 0.50000000000000 Pd (6f)
0.50000000000000 0.50000000000000 0.26220000000000 Pd (6f)
0.50000000000000 0.50000000000000 -0.26220000000000 Pd (6f)
0.14200000000000 0.15390000000000 0.34980000000000 Pd (24k)
-0.14200000000000 -0.15390000000000 0.34980000000000 Pd (24k)
-0.14200000000000 0.15390000000000 -0.34980000000000 Pd (24k)
0.14200000000000 -0.15390000000000 -0.34980000000000 Pd (24k)
0.34980000000000 0.14200000000000 0.15390000000000 Pd (24k)
0.34980000000000 -0.14200000000000 -0.15390000000000 Pd (24k)
-0.34980000000000 -0.14200000000000 0.15390000000000 Pd (24k)
-0.34980000000000 0.14200000000000 -0.15390000000000 Pd (24k)
0.15390000000000 0.34980000000000 0.14200000000000 Pd (24k)
-0.15390000000000 0.34980000000000 -0.14200000000000 Pd (24k)
0.15390000000000 -0.34980000000000 -0.14200000000000 Pd (24k)
-0.15390000000000 -0.34980000000000 0.14200000000000 Pd (24k)
0.15390000000000 0.14200000000000 0.34980000000000 Pd (24k)
-0.15390000000000 0.14200000000000 -0.34980000000000 Pd (24k)
0.14200000000000 -0.34980000000000 -0.15390000000000 Pd (24k)
-0.14200000000000 -0.34980000000000 0.15390000000000 Pd (24k)
0.34980000000000 0.15390000000000 0.14200000000000 Pd (24k)
0.34980000000000 -0.15390000000000 -0.14200000000000 Pd (24k)
-0.34980000000000 -0.15390000000000 0.14200000000000 Pd (24k)
-0.34980000000000 0.15390000000000 -0.14200000000000 Pd (24k)
0.24220000000000 0.00000000000000 0.00000000000000 Se (6e)
-0.24220000000000 0.00000000000000 0.00000000000000 Se (6e)
0.00000000000000 -0.24220000000000 0.00000000000000 Se (6e)
0.00000000000000 0.00000000000000 0.24220000000000 Se (6e)
0.00000000000000 0.00000000000000 -0.24220000000000 Se (6e)
0.00000000000000 0.00000000000000 0.33190000000000 Se (12i)
0.00000000000000 -0.33190000000000 0.33190000000000 Se (12i)
0.00000000000000 0.00000000000000 -0.33190000000000 Se (12i)
0.00000000000000 -0.33190000000000 0.33190000000000 Se (12i)
0.33190000000000 0.00000000000000 0.33190000000000 Se (12i)
0.33190000000000 0.00000000000000 -0.33190000000000 Se (12i)
-0.33190000000000 0.00000000000000 0.33190000000000 Se (12i)
-0.33190000000000 0.00000000000000 -0.33190000000000 Se (12i)
0.33190000000000 0.33190000000000 0.00000000000000 Se (12i)
-0.33190000000000 0.33190000000000 0.00000000000000 Se (12i)
0.33190000000000 -0.33190000000000 0.00000000000000 Se (12i)
-0.33190000000000 -0.33190000000000 0.00000000000000 Se (12i)
0.50000000000000 0.27010000000000 0.27010000000000 Se (12j)
0.50000000000000 -0.27010000000000 0.27010000000000 Se (12j)
0.50000000000000 0.27010000000000 -0.27010000000000 Se (12j)
0.50000000000000 -0.27010000000000 -0.27010000000000 Se (12j)
0.27010000000000 0.50000000000000 0.27010000000000 Se (12j)
0.27010000000000 0.50000000000000 -0.27010000000000 Se (12j)
-0.27010000000000 0.50000000000000 0.27010000000000 Se (12j)
-0.27010000000000 0.50000000000000 -0.27010000000000 Se (12j)
0.27010000000000 0.27010000000000 0.50000000000000 Se (12j)
0.27010000000000 0.27010000000000 0.50000000000000 Se (12j)
-0.27010000000000 0.27010000000000 0.50000000000000 Se (12j)
-0.27010000000000 0.27010000000000 0.50000000000000 Se (12j)

```

PH<sub>3</sub>: A3B\_cP16\_208\_j\_b - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'PH3'
_chemical_formula_sum 'H3 P'
loop_
_publ_author_name
'G. Natta '
'E. Casazza '
_journal_name_full_name

```

```

;
Gazzetta Chimica Italiana
;
_journal_volume 60
_journal_year 1930
_journal_page_first 851
_journal_page_last 859
_publ_section_title
;
La struttura dell'idrogeno fosforato (PH3{3}$) e dell'idrogeno
↪ arsenicale (AsH3{3}$)
;
# Found in The American Mineralogist Crystal Structure Database, 2003
_aflow_title 'PH3{3}$ Structure '
_aflow_proto 'A3B_cP16_208_j_b'
_aflow_params 'a, x_{2}'
_aflow_params_values '6.31, 0.184'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cP16'
_symmetry_space_group_name_H-M "P 42 3 2"
_symmetry_Int_Tables_number 208
_cell_length_a 6.31000
_cell_length_b 6.31000
_cell_length_c 6.31000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y, -z
4 -x, -y, z
5 y, z, x
6 y, -z, -x
7 -y, z, -x
8 -y, -z, x
9 z, x, y
10 z, -x, -y
11 -z, x, -y
12 -z, -x, y
13 -y+1/2, -x+1/2, -z+1/2
14 -y+1/2, x+1/2, z+1/2
15 y+1/2, -x+1/2, z+1/2
16 y+1/2, x+1/2, -z+1/2
17 -x+1/2, -z+1/2, -y+1/2
18 -x+1/2, z+1/2, y+1/2
19 x+1/2, -z+1/2, y+1/2
20 x+1/2, z+1/2, -y+1/2
21 -z+1/2, -y+1/2, -x+1/2
22 -z+1/2, y+1/2, x+1/2
23 z+1/2, -y+1/2, x+1/2
24 z+1/2, y+1/2, -x+1/2
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
P1 P 4 b 0.25000 0.25000 0.25000 1.00000
H1 H 12 j 0.18400 0.50000 0.00000 1.00000

```

PH<sub>3</sub>: A3B\_cP16\_208\_j\_b - POSCAR

```

A3B_cP16_208_j_b & a, x2 --params=6.31, 0.184 & P4_{2}32 O^{2} #208 (bj) &
↪ cP16 & None & PH3 & PH3 & G. Natta and E. Casazza, Gazz. Chim.
↪ Ital. 60, 851-859 (1930)
1.00000000000000
6.31000000000000 0.00000000000000 0.00000000000000
0.00000000000000 6.31000000000000 0.00000000000000
0.00000000000000 0.00000000000000 6.31000000000000
H P
12 4
Direct
0.18400000000000 0.50000000000000 0.00000000000000 H (12j)
-0.18400000000000 0.50000000000000 0.00000000000000 H (12j)
0.00000000000000 0.18400000000000 0.50000000000000 H (12j)
0.00000000000000 -0.18400000000000 0.50000000000000 H (12j)
0.50000000000000 0.00000000000000 0.18400000000000 H (12j)
0.50000000000000 0.00000000000000 -0.18400000000000 H (12j)
0.00000000000000 0.68400000000000 0.50000000000000 H (12j)
0.00000000000000 0.31600000000000 0.50000000000000 H (12j)
0.68400000000000 0.50000000000000 0.00000000000000 H (12j)
0.31600000000000 0.50000000000000 0.00000000000000 H (12j)
0.50000000000000 0.00000000000000 0.31600000000000 H (12j)
0.50000000000000 0.00000000000000 0.68400000000000 H (12j)
0.25000000000000 0.25000000000000 0.25000000000000 P (4b)
0.75000000000000 0.75000000000000 0.25000000000000 P (4b)
0.75000000000000 0.25000000000000 0.75000000000000 P (4b)
0.25000000000000 0.75000000000000 0.75000000000000 P (4b)

```

Cs<sub>2</sub>ZnFe(CN)<sub>6</sub>: A6B2CD6E\_cP64\_208\_m\_ad\_b\_m\_c - CIF

```

# CIF file
data_findsym-output

```



```

_audit_creation_method FINDSYM
_chemical_name_mineral 'Cs2ZnFe[CN]6'
_chemical_formula_sum 'C6 Cs2 Fe N6 Zn'
loop_
  _publ_author_name
    'V. G. Kuznetsov'
    'Z. V. Popova'
    'G. B. Seifer'
  _journal_name_full_name
    ;
  Russian Journal of Inorganic Chemistry
  ;
  _journal_volume 15
  _journal_year 1970
  _journal_page_first 1084
  _journal_page_last 1088
  _publ_Section_title
  ;
  X-ray diffraction study of ferrocyanides of copper, cobalt, nickel,
  ↪ trivalent iron and mixed copper ferrocyanide with potassium
  ;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013
_aflow_title 'Cs$_{2}$ZnFe[CN]$_{6}$ Structure'
_aflow_proto 'A6B2CD6E_cP64_208_m_ad_b_m_c'
_aflow_params 'a,x_{5},y_{5},z_{5},x_{6},y_{6},z_{6}'
_aflow_params_values '10.3701312618,0.057,0.25,0.23,0.235,0.25,0.458'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cP64'
_cell_length_a 10.3701312618
_cell_length_b 10.3701312618
_cell_length_c 10.3701312618
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000
_symmetry_space_group_name_H-M "P 43 2 2"
_symmetry_Int_Tables_number 208
loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 -y+1/2,-x+1/2,-z+1/2
14 -y+1/2,x+1/2,z+1/2
15 y+1/2,-x+1/2,z+1/2
16 y+1/2,x+1/2,-z+1/2
17 -x+1/2,-z+1/2,-y+1/2
18 -x+1/2,z+1/2,y+1/2
19 x+1/2,-z+1/2,y+1/2
20 x+1/2,z+1/2,-y+1/2
21 -z+1/2,-y+1/2,-x+1/2
22 -z+1/2,y+1/2,x+1/2
23 z+1/2,-y+1/2,x+1/2
24 z+1/2,y+1/2,-x+1/2
loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Cs1 Cs 2 a 0.00000 0.00000 0.00000 1.00000
Fe1 Fe 4 b 0.25000 0.25000 0.25000 1.00000
Zn1 Zn 4 c 0.75000 0.75000 0.75000 1.00000
Cs2 Cs 6 d 0.00000 0.50000 0.50000 1.00000
Cl C 24 m 0.05700 0.25000 0.23000 1.00000
N1 N 24 m 0.23500 0.25000 0.45800 1.00000

```

Cs<sub>2</sub>ZnFe[CN]<sub>6</sub>: A6B2CD6E\_cP64\_208\_m\_ad\_b\_m\_c - POSCAR

```

A6B2CD6E_cP64_208_m_ad_b_m_c & a,x5,y5,z5,x6,y6,z6 --params=
↪ 10.3701312618,0.057,0.25,0.23,0.235,0.25,0.458 & P4_{2}32 O^{2}
↪ #208 (abcdm^2) & cP64 & None & Cs2ZnFe[CN]6 & V. G.
↪ Kuznetsov and Z. V. Popova and G. B. Seifer, Russ. J. Inorg.
↪ Chem. 15, 1084-1088 (1970)
1.0000000000000000
10.37013126180000 0.00000000000000 0.00000000000000
0.00000000000000 10.37013126180000 0.00000000000000
0.00000000000000 0.00000000000000 10.37013126180000
C Cs Fe N Zn
24 8 4 24 4
Direct
0.05700000000000 0.25000000000000 0.23000000000000 C (24m)
-0.05700000000000 -0.25000000000000 0.23000000000000 C (24m)
-0.05700000000000 0.25000000000000 -0.23000000000000 C (24m)

```

```

0.05700000000000 -0.25000000000000 -0.23000000000000 C (24m)
0.23000000000000 0.05700000000000 0.25000000000000 C (24m)
0.23000000000000 -0.05700000000000 -0.25000000000000 C (24m)
-0.23000000000000 -0.05700000000000 0.25000000000000 C (24m)
-0.23000000000000 0.05700000000000 -0.25000000000000 C (24m)
0.25000000000000 0.23000000000000 0.05700000000000 C (24m)
-0.25000000000000 0.23000000000000 -0.05700000000000 C (24m)
0.25000000000000 -0.23000000000000 -0.05700000000000 C (24m)
-0.25000000000000 -0.23000000000000 0.05700000000000 C (24m)
0.75000000000000 0.55700000000000 0.27000000000000 C (24m)
0.25000000000000 0.44300000000000 0.27000000000000 C (24m)
0.75000000000000 0.44300000000000 0.73000000000000 C (24m)
0.25000000000000 0.55700000000000 0.73000000000000 C (24m)
0.55700000000000 0.73000000000000 0.25000000000000 C (24m)
0.44300000000000 0.73000000000000 0.75000000000000 C (24m)
0.44300000000000 0.27000000000000 0.25000000000000 C (24m)
0.55700000000000 0.27000000000000 0.75000000000000 C (24m)
0.73000000000000 0.75000000000000 0.44300000000000 C (24m)
0.73000000000000 0.25000000000000 0.55700000000000 C (24m)
0.27000000000000 0.75000000000000 0.55700000000000 C (24m)
0.27000000000000 0.25000000000000 0.44300000000000 C (24m)
0.00000000000000 0.00000000000000 0.00000000000000 Cs (2a)
0.50000000000000 0.50000000000000 0.50000000000000 Cs (2a)
0.00000000000000 0.50000000000000 0.50000000000000 Cs (6d)
0.50000000000000 0.00000000000000 0.50000000000000 Cs (6d)
0.50000000000000 0.50000000000000 0.00000000000000 Cs (6d)
0.00000000000000 0.50000000000000 0.00000000000000 Cs (6d)
0.50000000000000 0.00000000000000 0.00000000000000 Cs (6d)
0.00000000000000 0.00000000000000 0.50000000000000 Cs (6d)
0.25000000000000 0.25000000000000 0.25000000000000 Fe (4b)
0.75000000000000 0.75000000000000 0.25000000000000 Fe (4b)
0.75000000000000 0.25000000000000 0.75000000000000 Fe (4b)
0.25000000000000 0.75000000000000 0.75000000000000 Fe (4b)
0.23500000000000 0.25000000000000 0.45800000000000 N (24m)
-0.23500000000000 -0.25000000000000 0.45800000000000 N (24m)
-0.23500000000000 0.25000000000000 -0.45800000000000 N (24m)
0.23500000000000 -0.25000000000000 -0.45800000000000 N (24m)
0.45800000000000 0.23500000000000 0.25000000000000 N (24m)
0.45800000000000 -0.23500000000000 -0.25000000000000 N (24m)
-0.45800000000000 -0.23500000000000 0.25000000000000 N (24m)
-0.45800000000000 0.23500000000000 -0.25000000000000 N (24m)
0.25000000000000 0.45800000000000 0.23500000000000 N (24m)
-0.25000000000000 0.45800000000000 -0.23500000000000 N (24m)
0.25000000000000 -0.45800000000000 -0.23500000000000 N (24m)
-0.25000000000000 -0.45800000000000 0.23500000000000 N (24m)
0.75000000000000 0.73500000000000 0.04200000000000 N (24m)
0.25000000000000 0.26500000000000 0.04200000000000 N (24m)
0.75000000000000 0.26500000000000 0.95800000000000 N (24m)
0.25000000000000 0.73500000000000 0.95800000000000 N (24m)
0.73500000000000 0.95800000000000 0.25000000000000 N (24m)
0.26500000000000 0.95800000000000 0.75000000000000 N (24m)
0.26500000000000 0.04200000000000 0.25000000000000 N (24m)
0.73500000000000 0.04200000000000 0.75000000000000 N (24m)
0.95800000000000 0.75000000000000 0.26500000000000 N (24m)
0.95800000000000 0.25000000000000 0.73500000000000 N (24m)
0.04200000000000 0.75000000000000 0.73500000000000 N (24m)
0.04200000000000 0.25000000000000 0.26500000000000 N (24m)
0.75000000000000 0.75000000000000 0.75000000000000 Zn (4c)
0.25000000000000 0.25000000000000 0.75000000000000 Zn (4c)
0.25000000000000 0.75000000000000 0.25000000000000 Zn (4c)
0.75000000000000 0.25000000000000 0.25000000000000 Zn (4c)

```

F<sub>6</sub>KP: A24BC\_cF104\_209\_j\_a\_b - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'F6KP'
_chemical_formula_sum 'F24 K P'
loop_
  _publ_author_name
    'Y. P. Mascarenhas'
    'S. H. Pulcinelli'
  _journal_name_full_name
    ;
  Acta Crystallographica Section A: Foundations and Advances
  ;
  _journal_volume 37
  _journal_year 1981
  _journal_page_first C175
  _journal_page_last C175
  _publ_Section_title
  ;
  A redetermination of the structure of  $\alpha$ -potassium
  ↪ fluorophosphate
  ;
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013
_aflow_title 'FS_{6}SKP Structure'
_aflow_proto 'A24BC_cF104_209_j_a_b'
_aflow_params 'a,x_{3},y_{3},z_{3}'
_aflow_params_values '7.7099775082,0.043,0.109,0.165'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cF104'
_cell_length_a 7.7099775082
_cell_length_b 7.7099775082
_cell_length_c 7.7099775082
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

```

```

_symmetry_space_group_name_H-M "F 4 3 2"
_symmetry_Int_Tables_number 209

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y, -z
4 -x, -y, z
5 y, z, x
6 y, -z, -x
7 -y, z, -x
8 -y, -z, x
9 z, x, y
10 z, -x, -y
11 -z, x, -y
12 -z, -x, y
13 -y, -x, -z
14 -y, x, z
15 y, -x, z
16 y, x, -z
17 -x, -z, -y
18 -x, z, y
19 x, -z, y
20 x, z, -y
21 -z, -y, -x
22 -z, y, x
23 z, -y, x
24 z, y, -x
25 x, y+1/2, z+1/2
26 x, -y+1/2, -z+1/2
27 -x, y+1/2, -z+1/2
28 -x, -y+1/2, z+1/2
29 y, z+1/2, x+1/2
30 y, -z+1/2, -x+1/2
31 -y, z+1/2, -x+1/2
32 -y, -z+1/2, x+1/2
33 z, x+1/2, y+1/2
34 z, -x+1/2, -y+1/2
35 -z, x+1/2, -y+1/2
36 -z, -x+1/2, y+1/2
37 -y, -x+1/2, -z+1/2
38 -y, x+1/2, z+1/2
39 y, -x+1/2, z+1/2
40 y, x+1/2, -z+1/2
41 -x, -z+1/2, -y+1/2
42 -x, z+1/2, y+1/2
43 x, -z+1/2, y+1/2
44 x, z+1/2, -y+1/2
45 -z, -y+1/2, -x+1/2
46 -z, y+1/2, x+1/2
47 z, -y+1/2, x+1/2
48 z, y+1/2, -x+1/2
49 x+1/2, y, z+1/2
50 x+1/2, -y, -z+1/2
51 -x+1/2, y, -z+1/2
52 -x+1/2, -y, z+1/2
53 y+1/2, z, x+1/2
54 y+1/2, -z, -x+1/2
55 -y+1/2, z, -x+1/2
56 -y+1/2, -z, x+1/2
57 z+1/2, x, y+1/2
58 z+1/2, -x, -y+1/2
59 -z+1/2, x, -y+1/2
60 -z+1/2, -x, y+1/2
61 -y+1/2, -x, -z+1/2
62 -y+1/2, x, z+1/2
63 y+1/2, -x, z+1/2
64 y+1/2, x, -z+1/2
65 -x+1/2, -z, -y+1/2
66 -x+1/2, z, y+1/2
67 x+1/2, -z, y+1/2
68 x+1/2, z, -y+1/2
69 -z+1/2, -y, -x+1/2
70 -z+1/2, y, x+1/2
71 z+1/2, -y, x+1/2
72 z+1/2, y, -x+1/2
73 x+1/2, y+1/2, z
74 x+1/2, -y+1/2, -z
75 -x+1/2, y+1/2, -z
76 -x+1/2, -y+1/2, z
77 y+1/2, z+1/2, x
78 y+1/2, -z+1/2, -x
79 -y+1/2, z+1/2, -x
80 -y+1/2, -z+1/2, x
81 z+1/2, x+1/2, y
82 z+1/2, -x+1/2, -y
83 -z+1/2, x+1/2, -y
84 -z+1/2, -x+1/2, y
85 -y+1/2, -x+1/2, -z
86 -y+1/2, x+1/2, z
87 y+1/2, -x+1/2, z
88 y+1/2, x+1/2, -z
89 -x+1/2, -z+1/2, -y
90 -x+1/2, z+1/2, y
91 x+1/2, -z+1/2, y
92 x+1/2, z+1/2, -y
93 -z+1/2, -y+1/2, -x
94 -z+1/2, y+1/2, x
95 z+1/2, -y+1/2, x
96 z+1/2, y+1/2, -x

loop_

```

```

_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
K1 K 4 a 0.00000 0.00000 0.00000 1.00000
P1 P 4 b 0.50000 0.50000 0.50000 1.00000
F1 F 96 j 0.04300 0.10900 0.16500 1.00000

```

F<sub>6</sub>KP: A24BC\_cF104\_209\_j\_a\_b - POSCAR

```

A24BC_cF104_209_j_a_b & a, x3, y3, z3 --params=7.7099775082, 0.043, 0.109,
↳ 0.165 & F432 O^{3} #209 (abj) & cF104 & None & F6KP & & Y. P.
↳ Mascarenhas and S. H. Pulcinelli, Acta Crystallogr. Sect. A 37,
↳ C175(1981)
1.0000000000000000
0.0000000000000000 3.85498875410000 3.85498875410000
3.85498875410000 0.0000000000000000 3.85498875410000
3.85498875410000 3.85498875410000 0.0000000000000000
F K P
24 1 1
Direct
0.2310000000000000 0.0990000000000000 -0.0130000000000000 F (96j)
0.0990000000000000 0.2310000000000000 -0.3170000000000000 F (96j)
-0.0130000000000000 -0.3170000000000000 0.2310000000000000 F (96j)
-0.3170000000000000 -0.0130000000000000 0.0990000000000000 F (96j)
-0.0130000000000000 0.2310000000000000 0.0990000000000000 F (96j)
-0.3170000000000000 0.0990000000000000 0.2310000000000000 F (96j)
0.2310000000000000 -0.0130000000000000 -0.3170000000000000 F (96j)
0.0990000000000000 -0.3170000000000000 -0.0130000000000000 F (96j)
0.0990000000000000 -0.0130000000000000 0.2310000000000000 F (96j)
0.2310000000000000 -0.3170000000000000 0.0990000000000000 F (96j)
-0.3170000000000000 0.2310000000000000 0.0990000000000000 F (96j)
-0.0130000000000000 0.0990000000000000 -0.3170000000000000 F (96j)
-0.2310000000000000 -0.0990000000000000 0.3170000000000000 F (96j)
-0.0990000000000000 -0.2310000000000000 0.0130000000000000 F (96j)
0.0130000000000000 0.3170000000000000 -0.0990000000000000 F (96j)
0.3170000000000000 0.0130000000000000 -0.2310000000000000 F (96j)
0.0130000000000000 -0.2310000000000000 0.3170000000000000 F (96j)
0.3170000000000000 -0.0990000000000000 0.0130000000000000 F (96j)
-0.2310000000000000 0.0130000000000000 -0.0990000000000000 F (96j)
-0.0990000000000000 0.3170000000000000 -0.2310000000000000 F (96j)
-0.0990000000000000 0.0130000000000000 0.3170000000000000 F (96j)
-0.2310000000000000 0.3170000000000000 0.0130000000000000 F (96j)
0.3170000000000000 -0.2310000000000000 -0.0990000000000000 F (96j)
0.0130000000000000 -0.0990000000000000 -0.2310000000000000 F (96j)
0.0000000000000000 0.0000000000000000 0.0000000000000000 K (4a)
0.5000000000000000 0.5000000000000000 0.5000000000000000 P (4b)

```

Te[OH]<sub>6</sub>: A12B6C\_cF608\_210\_4h\_2h\_e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Te[OH]6'
_chemical_formula_sum 'H12 O6 Te'

loop_
_publ_author_name
'D. F. Mullica'
'J. D. Korp'
'W. O. Milligan'
'G. W. Beall'
'I. Bernal'
_journal_name_full_name
;
Acta Crystallographica Section B: Structural Science
;
_journal_volume 36
_journal_year 1980
_journal_page_first 2565
_journal_page_last 2570
_publ_section_title
;
Neutron structural refinement of cubic orthotelluric acid
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↳ Inorganic Compounds, 2013

_aflow_title 'Te[OH]$_{6}$ Structure'
_aflow_proto 'A12B6C_cF608_210_4h_2h_e'
_aflow_params 'a, x_{1}, x_{2}, y_{2}, z_{2}, x_{3}, y_{3}, z_{3}, x_{4}, y_{4},
↳ z_{4}, x_{5}, y_{5}, z_{5}, x_{6}, y_{6}, z_{6}, x_{7}, y_{7}, z_{7}'
_aflow_params_values '16.4321054599, 0.3771, 0.0157, 0.2009, 0.1224, 0.5287,
↳ 0.1425, 0.0068, 0.0949, 0.2596, 0.2225, 0.6117, 0.1785, 0.0224, 0.0928,
↳ 0.2607, 0.1616, 0.0194, 0.0793, 0.3503'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cF608'

_cell_length_a 16.4321054599
_cell_length_b 16.4321054599
_cell_length_c 16.4321054599
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "F 41 3 2"
_symmetry_Int_Tables_number 210

loop_

```

```

_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 -y+1/4,-x+1/4,-z+1/4
14 -y+1/4,x+1/4,z+1/4
15 y+1/4,-x+1/4,z+1/4
16 y+1/4,x+1/4,-z+1/4
17 -x+1/4,-z+1/4,-y+1/4
18 -x+1/4,z+1/4,y+1/4
19 x+1/4,-z+1/4,y+1/4
20 x+1/4,z+1/4,-y+1/4
21 -z+1/4,-y+1/4,-x+1/4
22 -z+1/4,y+1/4,x+1/4
23 z+1/4,-y+1/4,x+1/4
24 z+1/4,y+1/4,-x+1/4
25 x,y+1/2,z+1/2
26 x,-y+1/2,-z+1/2
27 -x,y+1/2,-z+1/2
28 -x,-y+1/2,z+1/2
29 y,z+1/2,x+1/2
30 y,-z+1/2,-x+1/2
31 -y,z+1/2,-x+1/2
32 -y,-z+1/2,x+1/2
33 z,x+1/2,y+1/2
34 z,-x+1/2,-y+1/2
35 -z,x+1/2,-y+1/2
36 -z,-x+1/2,y+1/2
37 -y+1/4,-x+3/4,-z+3/4
38 -y+1/4,x+3/4,z+3/4
39 y+1/4,-x+3/4,z+3/4
40 y+1/4,x+3/4,-z+3/4
41 -x+1/4,-z+3/4,-y+3/4
42 -x+1/4,z+3/4,y+3/4
43 x+1/4,-z+3/4,y+3/4
44 x+1/4,z+3/4,-y+3/4
45 -z+1/4,-y+3/4,-x+3/4
46 -z+1/4,y+3/4,x+3/4
47 z+1/4,-y+3/4,x+3/4
48 z+1/4,y+3/4,-x+3/4
49 x+1/2,y,z+1/2
50 x+1/2,-y,-z+1/2
51 -x+1/2,y,-z+1/2
52 -x+1/2,-y,z+1/2
53 y+1/2,z,x+1/2
54 y+1/2,-z,-x+1/2
55 -y+1/2,z,-x+1/2
56 -y+1/2,-z,x+1/2
57 z+1/2,x,y+1/2
58 z+1/2,-x,-y+1/2
59 -z+1/2,x,-y+1/2
60 -z+1/2,-x,y+1/2
61 -y+3/4,-x+1/4,-z+3/4
62 -y+3/4,x+1/4,z+3/4
63 y+3/4,-x+1/4,z+3/4
64 y+3/4,x+1/4,-z+3/4
65 -x+3/4,-z+1/4,-y+3/4
66 -x+3/4,z+1/4,y+3/4
67 x+3/4,-z+1/4,y+3/4
68 x+3/4,z+1/4,-y+3/4
69 -z+3/4,-y+1/4,-x+3/4
70 -z+3/4,y+1/4,x+3/4
71 z+3/4,-y+1/4,x+3/4
72 z+3/4,y+1/4,-x+3/4
73 x+1/2,y+1/2,z
74 x+1/2,-y+1/2,-z
75 -x+1/2,y+1/2,-z
76 -x+1/2,-y+1/2,z
77 y+1/2,z+1/2,x
78 y+1/2,-z+1/2,-x
79 -y+1/2,z+1/2,-x
80 -y+1/2,-z+1/2,x
81 z+1/2,x+1/2,y
82 z+1/2,-x+1/2,-y
83 -z+1/2,x+1/2,-y
84 -z+1/2,-x+1/2,y
85 -y+3/4,-x+3/4,-z+1/4
86 -y+3/4,x+3/4,z+1/4
87 y+3/4,-x+3/4,z+1/4
88 y+3/4,x+3/4,-z+1/4
89 -x+3/4,-z+3/4,-y+1/4
90 -x+3/4,z+3/4,y+1/4
91 x+3/4,-z+3/4,y+1/4
92 x+3/4,z+3/4,-y+1/4
93 -z+3/4,-y+3/4,-x+1/4
94 -z+3/4,y+3/4,x+1/4
95 z+3/4,-y+3/4,x+1/4
96 z+3/4,y+3/4,-x+1/4

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x

```

```

_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Te1 Te 32 e 0.37710 0.37710 1.00000
H1 H 96 h 0.01570 0.20090 0.12240 1.00000
H2 H 96 h 0.52870 0.14250 0.00680 1.00000
H3 H 96 h 0.09490 0.25960 0.22250 1.00000
H4 H 96 h 0.61170 0.17850 0.02240 1.00000
O1 O 96 h 0.09280 0.26070 0.16160 1.00000
O2 O 96 h 0.01940 0.07930 0.35030 1.00000

```

Te[OH]<sub>6</sub>: A12B6C\_cF608\_210\_4h\_2h\_e - POSCAR

```

A12B6C_cF608_210_4h_2h_e & a,x1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,
↳ y6,z6,x7,y7,z7 --params=16.4321054599,0.3771,0.0157,0.2009,
↳ 0.1224,0.5287,0.1425,0.0068,0.0949,0.2596,0.2225,0.6117,0.1785,
↳ 0.0224,0.0928,0.2607,0.1616,0.0194,0.0793,0.3503 & F4_{1}32 O^{\
↳ 4} #210 (ch^6) & cF608 & None & Te[OH]6 & & D. F. Mullica et
↳ al., Acta Crystallogr. Sect. B Struct. Sci. 36, 2565-2570 (1980
↳ )
1.0000000000000000
0.0000000000000000 8.21605272995000 8.21605272995000
8.21605272995000 0.0000000000000000 8.21605272995000
8.21605272995000 8.21605272995000 0.0000000000000000
H O Te
96 48 8
Direct
0.3076000000000000 -0.0628000000000000 0.0942000000000000 H (96h)
-0.0628000000000000 -0.3076000000000000 -0.3390000000000000 H (96h)
0.0942000000000000 -0.3390000000000000 0.3076000000000000 H (96h)
-0.3390000000000000 0.0942000000000000 -0.0628000000000000 H (96h)
0.0942000000000000 0.3076000000000000 -0.0628000000000000 H (96h)
-0.3390000000000000 -0.0628000000000000 0.3076000000000000 H (96h)
0.3076000000000000 0.0942000000000000 -0.3390000000000000 H (96h)
-0.0628000000000000 -0.3390000000000000 0.0942000000000000 H (96h)
-0.0628000000000000 0.0942000000000000 0.3076000000000000 H (96h)
0.3076000000000000 -0.3390000000000000 -0.0628000000000000 H (96h)
-0.3390000000000000 0.3076000000000000 0.0942000000000000 H (96h)
0.0942000000000000 -0.0628000000000000 -0.3390000000000000 H (96h)
-0.0628000000000000 0.3128000000000000 0.5890000000000000 H (96h)
-0.0576000000000000 -0.0576000000000000 0.1558000000000000 H (96h)
0.1558000000000000 0.5890000000000000 0.3128000000000000 H (96h)
0.5890000000000000 0.1558000000000000 -0.0576000000000000 H (96h)
0.1558000000000000 -0.0576000000000000 0.5890000000000000 H (96h)
0.5890000000000000 0.3128000000000000 0.1558000000000000 H (96h)
-0.0576000000000000 0.1558000000000000 0.3128000000000000 H (96h)
0.3128000000000000 0.5890000000000000 -0.0576000000000000 H (96h)
0.3128000000000000 0.1558000000000000 0.5890000000000000 H (96h)
-0.0576000000000000 0.5890000000000000 0.1558000000000000 H (96h)
0.5890000000000000 -0.0576000000000000 0.3128000000000000 H (96h)
0.1558000000000000 0.3128000000000000 -0.0576000000000000 H (96h)
-0.3794000000000000 0.3930000000000000 0.6644000000000000 H (96h)
0.3930000000000000 -0.3794000000000000 -0.6780000000000000 H (96h)
0.6644000000000000 -0.6780000000000000 -0.3794000000000000 H (96h)
-0.6780000000000000 0.6644000000000000 0.3930000000000000 H (96h)
0.6644000000000000 -0.3794000000000000 0.3930000000000000 H (96h)
-0.6780000000000000 0.6644000000000000 -0.3794000000000000 H (96h)
0.3930000000000000 -0.6780000000000000 0.6644000000000000 H (96h)
0.3930000000000000 0.6644000000000000 -0.3794000000000000 H (96h)
-0.3794000000000000 -0.6780000000000000 0.3930000000000000 H (96h)
-0.6780000000000000 -0.3794000000000000 0.6644000000000000 H (96h)
0.6644000000000000 0.3930000000000000 -0.6780000000000000 H (96h)
0.6294000000000000 -0.1430000000000000 0.9280000000000000 H (96h)
-0.1430000000000000 0.6294000000000000 -0.4144000000000000 H (96h)
-0.4144000000000000 0.9280000000000000 -0.1430000000000000 H (96h)
0.9280000000000000 -0.4144000000000000 0.6294000000000000 H (96h)
-0.4144000000000000 0.6294000000000000 0.9280000000000000 H (96h)
0.9280000000000000 -0.1430000000000000 -0.4144000000000000 H (96h)
0.6294000000000000 -0.4144000000000000 -0.1430000000000000 H (96h)
-0.1430000000000000 0.9280000000000000 0.6294000000000000 H (96h)
-0.4144000000000000 -0.1430000000000000 0.9280000000000000 H (96h)
0.9280000000000000 0.6294000000000000 -0.4144000000000000 H (96h)
0.6294000000000000 0.9280000000000000 -0.1430000000000000 H (96h)
-0.1430000000000000 -0.4144000000000000 0.9280000000000000 H (96h)
0.0578000000000000 0.3872000000000000 -0.5770000000000000 H (96h)
0.1320000000000000 -0.5770000000000000 0.3872000000000000 H (96h)
-0.5770000000000000 0.1320000000000000 0.3872000000000000 H (96h)
0.1320000000000000 0.3872000000000000 0.0578000000000000 H (96h)
-0.5770000000000000 0.0578000000000000 0.3872000000000000 H (96h)
0.3872000000000000 0.1320000000000000 -0.5770000000000000 H (96h)
0.0578000000000000 0.1320000000000000 0.3872000000000000 H (96h)
-0.5770000000000000 0.3872000000000000 0.0578000000000000 H (96h)
0.1320000000000000 0.0578000000000000 -0.5770000000000000 H (96h)
0.1922000000000000 -0.1372000000000000 0.8270000000000000 H (96h)
0.1180000000000000 0.8270000000000000 0.1922000000000000 H (96h)
0.8270000000000000 0.1180000000000000 -0.1372000000000000 H (96h)
0.1180000000000000 -0.1372000000000000 0.8270000000000000 H (96h)
0.8270000000000000 0.1922000000000000 0.1180000000000000 H (96h)
-0.1372000000000000 0.1180000000000000 0.1922000000000000 H (96h)
0.1922000000000000 0.8270000000000000 -0.1372000000000000 H (96h)
0.1922000000000000 0.1180000000000000 0.8270000000000000 H (96h)
-0.1372000000000000 0.8270000000000000 0.1180000000000000 H (96h)
0.8270000000000000 0.1922000000000000 -0.1372000000000000 H (96h)
0.1180000000000000 0.1922000000000000 -0.1372000000000000 H (96h)
-0.4108000000000000 0.4556000000000000 0.7678000000000000 H (96h)
0.4556000000000000 -0.4108000000000000 -0.8126000000000000 H (96h)
0.7678000000000000 -0.8126000000000000 -0.4108000000000000 H (96h)
-0.8126000000000000 0.7678000000000000 0.4556000000000000 H (96h)
0.7678000000000000 -0.4108000000000000 0.4556000000000000 H (96h)
-0.8126000000000000 0.4556000000000000 -0.4108000000000000 H (96h)

```



-0.13235000000000	0.36765000000000	-0.26470000000000	Si (24i)
0.63235000000000	1.13235000000000	1.26470000000000	Si (24i)
1.13235000000000	-0.13235000000000	0.50000000000000	Si (24i)

SrSi<sub>2</sub>: A2B\_cP12\_212\_c\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'SrSi2'
_chemical_formula_sum 'Si2 Sr'

_aflow_title 'SrSi2$ Structure'
_aflow_proto 'A2B_cP12_212_c_a'
_aflow_params 'a,x_{2}'
_aflow_params_values '6.54, 0.428'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cP12'

_cell_length_a 6.5400000000
_cell_length_b 6.5400000000
_cell_length_c 6.5400000000
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 43 3 2"
_symmetry_Int_Tables_number 212

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x+1/2, -y+1/2, -z
3 -x, y+1/2, -z+1/2
4 -x+1/2, -y, z+1/2
5 y, z, x
6 y+1/2, -z+1/2, -x
7 -y, z+1/2, -x+1/2
8 -y+1/2, -z, x+1/2
9 z, x, y
10 z+1/2, -x+1/2, -y
11 -z, x+1/2, -y+1/2
12 -z+1/2, -x, y+1/2
13 -y+1/4, -x+1/4, -z+1/4
14 -y+3/4, x+1/4, z+3/4
15 y+3/4, -x+3/4, z+1/4
16 y+1/4, x+3/4, -z+3/4
17 -x+1/4, -z+1/4, -y+1/4
18 -x+3/4, z+1/4, y+3/4
19 x+3/4, -z+3/4, y+1/4
20 x+1/4, z+3/4, -y+3/4
21 -z+1/4, -y+1/4, -x+1/4
22 -z+3/4, y+1/4, x+3/4
23 z+3/4, -y+3/4, x+1/4
24 z+1/4, y+3/4, -x+3/4

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Sr1 Sr 4 a 0.12500 0.12500 0.12500 1.00000
Si1 Si 8 c 0.42800 0.42800 0.42800 1.00000
```

SrSi<sub>2</sub>: A2B\_cP12\_212\_c\_a - POSCAR

```
A2B_cP12_212_c_a & a, x2 --params=6.54, 0.428 & P4_{3}32 O^{6} #212 (ac) &
↪ cP12 & None & SrSi2 & &
1.0000000000000000
6.5400000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 6.5400000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 6.5400000000000000
Si Sr
8 4
Direct
0.4280000000000000 0.4280000000000000 0.4280000000000000 Si (8c)
0.0720000000000000 -0.4280000000000000 0.9280000000000000 Si (8c)
-0.4280000000000000 0.9280000000000000 0.0720000000000000 Si (8c)
0.9280000000000000 0.0720000000000000 -0.4280000000000000 Si (8c)
0.6780000000000000 1.1780000000000000 0.3220000000000000 Si (8c)
-0.1780000000000000 -0.1780000000000000 -0.1780000000000000 Si (8c)
1.1780000000000000 0.3220000000000000 0.6780000000000000 Si (8c)
0.3220000000000000 0.6780000000000000 1.1780000000000000 Si (8c)
0.1250000000000000 0.1250000000000000 0.1250000000000000 Sr (4a)
0.3750000000000000 0.8750000000000000 0.6250000000000000 Sr (4a)
0.8750000000000000 0.6250000000000000 0.3750000000000000 Sr (4a)
0.6250000000000000 0.3750000000000000 0.8750000000000000 Sr (4a)
```

Ca<sub>3</sub>PI<sub>3</sub>: A3B3C\_cl56\_214\_g\_h\_a - CIF

```
# CIF file# This file was generated by FINDSYM
# Harold T. Stokes, Branton J. Campbell, Dorian M. Hatch
# Brigham Young University, Provo, Utah, USA

data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ca3PI3'
```

```
_chemical_formula_sum 'Ca3 I3 P'

loop_
_publ_author_name
'C. Hamon'
'R. Marchand'
'Y. Laurent'
'J. Lang'
_journal_name_full_name
;
Bulletin of Research Laboratory of Precision Machinery and Electronics
;
_journal_volume 97
_journal_year 1974
_journal_page_first 6
_journal_page_last 12
_publ_section_title
;
Etude d\`halogenopictures. m. Structures de Ca$_{2}$SPI et Ca$_{3}$SPIS_{
↪ 3}$$. Sur structures de type NaCl
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'Ca$_{3}$SPIS_{3}$ Structure'
_aflow_proto 'A3B3C_cl56_214_g_h_a'
_aflow_params 'a,y_{2},y_{3}'
_aflow_params_values '12.31504, 0.108, 0.384'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cI56'

_symmetry_space_group_name_H-M "I 41 3 2"
_symmetry_Int_Tables_number 214

_cell_length_a 12.31504
_cell_length_b 12.31504
_cell_length_c 12.31504
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z+1/2
3 -x+1/2, y, -z
4 -x, -y+1/2, z
5 y, z, x
6 y, -z, -x+1/2
7 -y+1/2, z, -x
8 -y, -z+1/2, x
9 z, x, y
10 z, -x, -y+1/2
11 -z+1/2, x, -y
12 -z, -x+1/2, y
13 -y+1/4, -x+1/4, -z+1/4
14 -y+1/4, x+3/4, z+1/4
15 y+1/4, -x+1/4, z+3/4
16 y+3/4, x+1/4, -z+1/4
17 -x+1/4, -z+1/4, -y+1/4
18 -x+1/4, z+3/4, y+1/4
19 x+1/4, -z+1/4, y+3/4
20 x+3/4, z+1/4, -y+1/4
21 -z+1/4, -y+1/4, -x+1/4
22 -z+1/4, y+3/4, x+1/4
23 z+1/4, -y+1/4, x+3/4
24 z+3/4, y+1/4, -x+1/4
25 x+1/2, y+1/2, z+1/2
26 x+1/2, -y+1/2, -z
27 -x, y+1/2, -z+1/2
28 -x+1/2, -y, z+1/2
29 y+1/2, z+1/2, x+1/2
30 y+1/2, -z+1/2, -x
31 -y, z+1/2, -x+1/2
32 -y+1/2, -z, x+1/2
33 z+1/2, x+1/2, y+1/2
34 z+1/2, -x+1/2, -y
35 -z, x+1/2, -y+1/2
36 -z+1/2, -x, y+1/2
37 -y+3/4, -x+3/4, -z+3/4
38 -y+3/4, x+1/4, z+3/4
39 y+3/4, -x+3/4, z+1/4
40 y+1/4, x+3/4, -z+3/4
41 -x+3/4, -z+3/4, -y+3/4
42 -x+3/4, z+1/4, y+3/4
43 x+3/4, -z+3/4, y+1/4
44 x+1/4, z+3/4, -y+3/4
45 -z+3/4, -y+3/4, -x+3/4
46 -z+3/4, y+1/4, x+3/4
47 z+3/4, -y+3/4, x+1/4
48 z+1/4, y+3/4, -x+3/4

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
P1 P 8 a 0.12500 0.12500 1.00000
Ca1 Ca 24 g 0.12500 0.10800 0.35800 1.00000
```

11 I 24 h 0.12500 0.38400 0.86600 1.00000

Ca<sub>3</sub>PI<sub>3</sub>: A3B3C\_c156\_214\_g\_h\_a - POSCAR

```
A3B3C_c156_214_g_h_a & a,y2,y3 --params=12.31504,0.108,0.384 & I4_{1}32
↪ O{8} #214 (agh) & c156 & None & Ca3PI3 & C. Hamon et al.,
↪ Bull. Soc. fr. Min'eral. Crystallogr. 97, 6-12 (1974)
1.0000000000000000
-6.157520000000000 6.157520000000000 6.157520000000000
6.157520000000000 -6.157520000000000 6.157520000000000
6.157520000000000 6.157520000000000 -6.157520000000000
Ca I P
12 12 4
Direct
0.466000000000000 0.483000000000000 0.233000000000000 Ca (24g)
0.750000000000000 0.233000000000000 0.267000000000000 Ca (24g)
0.750000000000000 0.017000000000000 0.483000000000000 Ca (24g)
0.034000000000000 0.267000000000000 0.017000000000000 Ca (24g)
0.233000000000000 0.466000000000000 0.483000000000000 Ca (24g)
0.267000000000000 0.750000000000000 0.233000000000000 Ca (24g)
0.483000000000000 0.750000000000000 0.017000000000000 Ca (24g)
0.017000000000000 0.034000000000000 0.267000000000000 Ca (24g)
0.483000000000000 0.233000000000000 0.466000000000000 Ca (24g)
0.233000000000000 0.267000000000000 0.750000000000000 Ca (24g)
0.017000000000000 0.483000000000000 0.750000000000000 Ca (24g)
0.267000000000000 0.017000000000000 0.034000000000000 Ca (24g)
0.250000000000000 -0.009000000000000 0.509000000000000 I (24h)
-0.018000000000000 -0.259000000000000 -0.009000000000000 I (24h)
1.518000000000000 0.509000000000000 0.759000000000000 I (24h)
0.250000000000000 0.759000000000000 -0.259000000000000 I (24h)
0.509000000000000 0.250000000000000 -0.009000000000000 I (24h)
-0.009000000000000 -0.018000000000000 -0.259000000000000 I (24h)
0.759000000000000 1.518000000000000 0.509000000000000 I (24h)
-0.259000000000000 0.250000000000000 0.759000000000000 I (24h)
-0.009000000000000 0.509000000000000 0.250000000000000 I (24h)
-0.259000000000000 -0.009000000000000 -0.018000000000000 I (24h)
0.509000000000000 0.759000000000000 1.518000000000000 I (24h)
0.759000000000000 -0.259000000000000 0.250000000000000 I (24h)
0.250000000000000 0.250000000000000 0.250000000000000 P (8a)
0.500000000000000 0.000000000000000 0.250000000000000 P (8a)
0.000000000000000 0.250000000000000 0.500000000000000 P (8a)
0.250000000000000 0.500000000000000 0.000000000000000 P (8a)
```

Petzite (Ag<sub>3</sub>AuTe<sub>2</sub>): A3BC2\_c148\_214\_f\_a\_e - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Petzite'
_chemical_formula_sum 'Ag3 Au Te2'

loop_
_publ_author_name
'A. J. {Frueh, Jr.}'
_journal_name_full_name
;
American Mineralogist
;
_journal_volume 44
_journal_year 1959
_journal_page_first 693
_journal_page_last 701
_publ_section_title
;
Crystallography of petzite, Ag3{3}AuTe2{2}$
;

# Found in The American Mineralogist Crystal Structure Database, 2003

_aflow_title 'Petzite (Ag3{3}AuTe2{2}$) Structure'
_aflow_proto 'A3BC2_c148_214_f_a_e'
_aflow_params 'a,x_{2},x_{3}'
_aflow_params_values '10.38,0.266,0.365'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'c148'

_symmetry_space_group_name_H-M "I 41 3 2"
_symmetry_Int_Tables_number 214

_cell_length_a 10.38000
_cell_length_b 10.38000
_cell_length_c 10.38000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z+1/2
3 -x+1/2,y,-z
4 -x,-y+1/2,z
5 y,z,x
6 y,-z,-x+1/2
7 -y+1/2,z,-x
8 -y,-z+1/2,x
9 z,x,y
10 z,-x,-y+1/2
11 -z+1/2,x,-y
12 -z,-x+1/2,y
13 -y+1/4,-x+1/4,-z+1/4
14 -y+1/4,x+3/4,z+1/4
15 y+1/4,-x+1/4,z+3/4
```

```
16 y+3/4,x+1/4,-z+1/4
17 -x+1/4,-z+1/4,-y+1/4
18 -x+1/4,z+3/4,y+1/4
19 x+1/4,-z+1/4,y+3/4
20 x+3/4,z+1/4,-y+1/4
21 -z+1/4,-y+1/4,-x+1/4
22 -z+1/4,y+3/4,x+1/4
23 z+1/4,-y+1/4,x+3/4
24 z+3/4,y+1/4,-x+1/4
25 x+1/2,y+1/2,z+1/2
26 x+1/2,-y+1/2,-z
27 -x,y+1/2,-z+1/2
28 -x+1/2,-y,z+1/2
29 y+1/2,z+1/2,x+1/2
30 y+1/2,-z+1/2,-x
31 -y,z+1/2,-x+1/2
32 -y+1/2,-z,x+1/2
33 z+1/2,x+1/2,y+1/2
34 z+1/2,-x+1/2,-y
35 -z,x+1/2,-y+1/2
36 -z+1/2,-x,y+1/2
37 -y+3/4,-x+3/4,-z+3/4
38 -y+3/4,x+1/4,z+3/4
39 y+3/4,-x+3/4,z+1/4
40 y+1/4,x+3/4,-z+3/4
41 -x+3/4,-z+3/4,-y+3/4
42 -x+3/4,z+1/4,y+3/4
43 x+3/4,-z+3/4,y+1/4
44 x+1/4,z+3/4,-y+3/4
45 -z+3/4,-y+3/4,-x+3/4
46 -z+3/4,y+1/4,x+3/4
47 z+3/4,-y+3/4,x+1/4
48 z+1/4,y+3/4,-x+3/4
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Au1 Au 8 a 0.12500 0.12500 0.12500 1.00000
Te1 Te 16 e 0.26600 0.26600 0.26600 1.00000
Ag1 Ag 24 f 0.36500 0.00000 0.25000 1.00000
```

Petzite (Ag<sub>3</sub>AuTe<sub>2</sub>): A3BC2\_c148\_214\_f\_a\_e - POSCAR

```
A3BC2_c148_214_f_a_e & a,x2,x3 --params=10.38,0.266,0.365 & I4_{1}32 O{8}
↪ 8} #214 (aef) & c148 & None & Ag3AuTe2 & Petzite & A. J. {Frueh
↪ , Jr.}, Am. Mineral. 44, 693-701 (1959)
1.0000000000000000
-5.190000000000000 5.190000000000000 5.190000000000000
5.190000000000000 -5.190000000000000 5.190000000000000
5.190000000000000 5.190000000000000 -5.190000000000000
Ag Au Te
12 4 8
Direct
0.250000000000000 0.615000000000000 0.365000000000000 Ag (24f)
0.750000000000000 -0.115000000000000 0.135000000000000 Ag (24f)
0.365000000000000 0.250000000000000 0.615000000000000 Ag (24f)
0.135000000000000 0.750000000000000 -0.115000000000000 Ag (24f)
0.615000000000000 0.365000000000000 0.250000000000000 Ag (24f)
-0.115000000000000 0.135000000000000 0.750000000000000 Ag (24f)
0.615000000000000 0.750000000000000 0.365000000000000 Ag (24f)
-0.115000000000000 0.250000000000000 0.135000000000000 Ag (24f)
0.750000000000000 0.365000000000000 0.615000000000000 Ag (24f)
0.250000000000000 0.135000000000000 -0.115000000000000 Ag (24f)
0.135000000000000 -0.115000000000000 0.250000000000000 Ag (24f)
0.365000000000000 0.615000000000000 0.750000000000000 Ag (24f)
0.250000000000000 0.250000000000000 0.250000000000000 Au (8a)
0.500000000000000 0.000000000000000 0.250000000000000 Au (8a)
0.000000000000000 0.250000000000000 0.500000000000000 Au (8a)
0.250000000000000 0.500000000000000 0.000000000000000 Au (8a)
0.532000000000000 0.532000000000000 0.532000000000000 Te (16e)
0.500000000000000 0.000000000000000 -0.032000000000000 Te (16e)
0.000000000000000 -0.032000000000000 0.500000000000000 Te (16e)
-0.032000000000000 0.500000000000000 0.000000000000000 Te (16e)
0.500000000000000 0.000000000000000 0.532000000000000 Te (16e)
-0.032000000000000 -0.032000000000000 -0.032000000000000 Te (16e)
0.000000000000000 0.532000000000000 0.500000000000000 Te (16e)
0.532000000000000 0.500000000000000 0.000000000000000 Te (16e)
```

γ-brass (Cu<sub>9</sub>Al<sub>4</sub>, D<sub>8h</sub>): A4B9\_cp52\_215\_ei\_3efgi - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '$\gamma$-brass Cu9{9}Al4{4}$'
_chemical_formula_sum 'A14 Cu9'

loop_
_publ_author_name
'L. Arnborg'
'S. Westman'
_journal_name_full_name
;
Acta Crystallographica Section A: Foundations and Advances
;
_journal_volume 34
_journal_year 1978
_journal_page_first 399
_journal_page_last 404
```

```

_publ_section_title
:
Crystal perfection in a noncentrosymmetric alloy. Refinement and test
of twinning of the  $\gamma$ -Cu9Al5 structure
;
# Found in Structure Types, 2005

_aflow_title '$\gamma$-brass (Cu9Al5) Structure'
_aflow_proto 'A4B9_cP52_215_ei_3efgi'
_aflow_params 'a,x_{1},x_{2},x_{3},x_{4},x_{5},x_{6},x_{7},z_{7},x_{8},
z_{8}'
_aflow_params_values '8.7068,0.1157,0.8296,0.3253,0.6066,0.3534,0.8549,
0.8113,0.5332,0.3153,0.0322'
_aflow_Strukturbericht '$D8_{3}$'
_aflow_Pearson 'cP52'

_symmetry_space_group_name_H-M "P -4 3 m"
_symmetry_Int_Tables_number 215

_cell_length_a 8.70680
_cell_length_b 8.70680
_cell_length_c 8.70680
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 y,x,z
14 y,-x,-z
15 -y,x,-z
16 -y,-x,z
17 x,z,y
18 x,-z,-y
19 -x,z,-y
20 -x,-z,y
21 z,y,x
22 z,-y,-x
23 -z,y,-x
24 -z,-y,x

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 4 e 0.11570 0.11570 0.11570 1.00000
Cu1 Cu 4 e 0.82960 0.82960 0.82960 1.00000
Cu2 Cu 4 e 0.32530 0.32530 0.32530 1.00000
Cu3 Cu 4 e 0.60660 0.60660 0.60660 1.00000
Cu4 Cu 6 f 0.35340 0.00000 0.00000 1.00000
Cu5 Cu 6 g 0.85490 0.50000 0.50000 1.00000
Al2 Al 12 i 0.81130 0.81130 0.53320 1.00000
Cu6 Cu 12 i 0.31530 0.31530 0.03220 1.00000

```

$\gamma$ -brass (Cu<sub>9</sub>Al<sub>4</sub>, D<sub>83</sub>): A4B9\_cP52\_215\_ei\_3efgi - POSCAR

```

A4B9_cP52_215_ei_3efgi & a,x1,x2,x3,x4,x5,x6,x7,z7,x8,z8 --params=8.7068
↪ 0.1157,0.8296,0.3253,0.6066,0.3534,0.8549,0.8113,0.5332,0.3153
↪ 0.0322 & P-43m Td[1] #215 (e4fgi2) & cP52 & SD8_{3}$ &
↪ Cu9Al4 & $\gamma$-brass Cu9Al5 & L. Arnberg and S.
↪ Westman, Acta Crystallogr. Sect. A 34, 399-404 (1978)
1.0000000000000000
8.7068000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.7068000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 8.7068000000000000
Al Cu
16 36
Direct
0.1157000000000000 0.1157000000000000 0.1157000000000000 Al (4e)
-0.1157000000000000 -0.1157000000000000 0.1157000000000000 Al (4e)
-0.1157000000000000 0.1157000000000000 -0.1157000000000000 Al (4e)
0.1157000000000000 -0.1157000000000000 -0.1157000000000000 Al (4e)
0.8113000000000000 0.8113000000000000 0.5332000000000000 Al (12i)
-0.8113000000000000 -0.8113000000000000 0.5332000000000000 Al (12i)
-0.8113000000000000 0.8113000000000000 -0.5332000000000000 Al (12i)
0.8113000000000000 -0.8113000000000000 -0.5332000000000000 Al (12i)
0.5332000000000000 0.8113000000000000 0.8113000000000000 Al (12i)
0.5332000000000000 -0.8113000000000000 -0.8113000000000000 Al (12i)
-0.5332000000000000 -0.8113000000000000 0.8113000000000000 Al (12i)
-0.5332000000000000 0.8113000000000000 -0.8113000000000000 Al (12i)
0.8113000000000000 0.5332000000000000 0.8113000000000000 Al (12i)
-0.8113000000000000 0.5332000000000000 -0.8113000000000000 Al (12i)
0.8113000000000000 -0.5332000000000000 -0.8113000000000000 Al (12i)
-0.8113000000000000 -0.5332000000000000 0.8113000000000000 Al (12i)
0.8296000000000000 0.8296000000000000 0.8296000000000000 Cu (4e)
-0.8296000000000000 -0.8296000000000000 0.8296000000000000 Cu (4e)

```

```

-0.8296000000000000 0.8296000000000000 -0.8296000000000000 Cu (4e)
0.8296000000000000 -0.8296000000000000 -0.8296000000000000 Cu (4e)
0.3253000000000000 0.3253000000000000 0.3253000000000000 Cu (4e)
-0.3253000000000000 -0.3253000000000000 0.3253000000000000 Cu (4e)
-0.3253000000000000 0.3253000000000000 -0.3253000000000000 Cu (4e)
0.3253000000000000 -0.3253000000000000 -0.3253000000000000 Cu (4e)
0.6066000000000000 0.6066000000000000 0.6066000000000000 Cu (4e)
-0.6066000000000000 -0.6066000000000000 0.6066000000000000 Cu (4e)
0.6066000000000000 -0.6066000000000000 -0.6066000000000000 Cu (4e)
0.3534000000000000 0.0000000000000000 0.0000000000000000 Cu (6f)
-0.3534000000000000 0.0000000000000000 0.0000000000000000 Cu (6f)
0.0000000000000000 0.3534000000000000 0.0000000000000000 Cu (6f)
0.0000000000000000 -0.3534000000000000 0.0000000000000000 Cu (6f)
0.0000000000000000 0.0000000000000000 0.3534000000000000 Cu (6f)
0.0000000000000000 0.0000000000000000 -0.3534000000000000 Cu (6f)
0.8549000000000000 0.5000000000000000 0.5000000000000000 Cu (6g)
-0.8549000000000000 0.5000000000000000 0.5000000000000000 Cu (6g)
0.5000000000000000 0.8549000000000000 0.8549000000000000 Cu (6g)
0.5000000000000000 -0.8549000000000000 0.5000000000000000 Cu (6g)
0.5000000000000000 0.5000000000000000 0.8549000000000000 Cu (6g)
0.5000000000000000 0.5000000000000000 -0.8549000000000000 Cu (6g)
0.3153000000000000 0.3153000000000000 0.0322000000000000 Cu (12i)
-0.3153000000000000 -0.3153000000000000 0.0322000000000000 Cu (12i)
-0.3153000000000000 0.3153000000000000 -0.0322000000000000 Cu (12i)
0.3153000000000000 -0.3153000000000000 -0.0322000000000000 Cu (12i)
0.0322000000000000 0.3153000000000000 0.3153000000000000 Cu (12i)
0.0322000000000000 -0.3153000000000000 -0.3153000000000000 Cu (12i)
-0.0322000000000000 -0.3153000000000000 0.3153000000000000 Cu (12i)
-0.0322000000000000 0.3153000000000000 -0.3153000000000000 Cu (12i)
0.3153000000000000 0.0322000000000000 0.3153000000000000 Cu (12i)
-0.3153000000000000 0.0322000000000000 -0.3153000000000000 Cu (12i)
0.3153000000000000 -0.0322000000000000 -0.3153000000000000 Cu (12i)
-0.3153000000000000 -0.0322000000000000 0.3153000000000000 Cu (12i)

```

Quaternary Heusler (LiMgAuSn): ABCD\_cF16\_216\_c\_d\_b\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Quaternary Heusler'
_chemical_formula_sum 'Au Li Mg Sn'

loop_
_publ_author_name
'U. Eberz'
'W. Seelentag'
'H.-U. Schuster'
_journal_name_full_name
;
Zeitschrift f{"u}r Naturforschung B
;
_journal_volume 35
_journal_year 1980
_journal_page_first 1341
_journal_page_last 1343
_publ_section_title
;
Zur Kenntnis farbiger tern{"a}rer und quatern{"a}rer Zintl-Phasen /
↪ Coloured Ternary and Quaternary Zintl-Phases
;
# Found in PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (
↪ online database), 2016

_aflow_title 'Quaternary Heusler (LiMgAuSn) Structure'
_aflow_proto 'ABCD_cF16_216_c_d_b_a'
_aflow_params 'a'
_aflow_params_values '6.465'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cF16'

_symmetry_space_group_name_H-M "F -4 3 m"
_symmetry_Int_Tables_number 216

_cell_length_a 6.46500
_cell_length_b 6.46500
_cell_length_c 6.46500
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 y,x,z
14 y,-x,-z
15 -y,x,-z
16 -y,-x,z
17 x,z,y
18 x,-z,-y
19 -x,z,-y

```

```

20 -x,-z,y
21 z,y,x
22 z,-y,-x
23 -z,y,-x
24 -z,-y,x
25 x,y+1/2,z+1/2
26 x,-y+1/2,-z+1/2
27 -x,y+1/2,-z+1/2
28 -x,-y+1/2,z+1/2
29 y,z+1/2,x+1/2
30 y,-z+1/2,-x+1/2
31 -y,z+1/2,-x+1/2
32 -y,-z+1/2,x+1/2
33 z,x+1/2,y+1/2
34 z,-x+1/2,-y+1/2
35 -z,x+1/2,-y+1/2
36 -z,-x+1/2,y+1/2
37 y,x+1/2,z+1/2
38 y,-x+1/2,-z+1/2
39 -y,x+1/2,-z+1/2
40 -y,-x+1/2,z+1/2
41 x,z+1/2,y+1/2
42 x,-z+1/2,-y+1/2
43 -x,z+1/2,-y+1/2
44 -x,-z+1/2,y+1/2
45 z,y+1/2,x+1/2
46 z,-y+1/2,-x+1/2
47 -z,y+1/2,-x+1/2
48 -z,-y+1/2,x+1/2
49 x+1/2,y,z+1/2
50 x+1/2,-y,-z+1/2
51 -x+1/2,y,-z+1/2
52 -x+1/2,-y,z+1/2
53 y+1/2,z,x+1/2
54 y+1/2,-z,-x+1/2
55 -y+1/2,z,-x+1/2
56 -y+1/2,-z,x+1/2
57 z+1/2,x,y+1/2
58 z+1/2,-x,-y+1/2
59 -z+1/2,x,-y+1/2
60 -z+1/2,-x,y+1/2
61 y+1/2,x,z+1/2
62 y+1/2,-x,-z+1/2
63 -y+1/2,x,-z+1/2
64 -y+1/2,-x,z+1/2
65 x+1/2,z,y+1/2
66 x+1/2,-z,-y+1/2
67 -x+1/2,z,-y+1/2
68 -x+1/2,-z,y+1/2
69 z+1/2,y,x+1/2
70 z+1/2,-y,-x+1/2
71 -z+1/2,y,-x+1/2
72 -z+1/2,-y,x+1/2
73 x+1/2,y+1/2,z
74 x+1/2,-y+1/2,-z
75 -x+1/2,y+1/2,-z
76 -x+1/2,-y+1/2,z
77 y+1/2,z+1/2,x
78 y+1/2,-z+1/2,-x
79 -y+1/2,z+1/2,-x
80 -y+1/2,-z+1/2,x
81 z+1/2,x+1/2,y
82 z+1/2,-x+1/2,-y
83 -z+1/2,x+1/2,-y
84 -z+1/2,-x+1/2,y
85 y+1/2,x+1/2,z
86 y+1/2,-x+1/2,-z
87 -y+1/2,x+1/2,-z
88 -y+1/2,-x+1/2,z
89 x+1/2,z+1/2,y
90 x+1/2,-z+1/2,-y
91 -x+1/2,z+1/2,-y
92 -x+1/2,-z+1/2,y
93 z+1/2,y+1/2,x
94 z+1/2,-y+1/2,-x
95 -z+1/2,y+1/2,-x
96 -z+1/2,-y+1/2,x

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Sn1 Sn 4 a 0.00000 0.00000 0.00000 1.00000
Mg1 Mg 4 b 0.50000 0.50000 0.50000 1.00000
Au1 Au 4 c 0.25000 0.25000 0.25000 1.00000
Li1 Li 4 d 0.75000 0.75000 0.75000 1.00000

```

Quaternary Heusler (LiMgAuSn): ABCD\_cF16\_216\_c\_d\_b\_a - POSCAR

```

ABCD_cF16_216_c_d_b_a & a --params=6.465 & F-43m T_{d}^{2} #216 (abcd) &
↪ cF16 & None & LiMgAuSn & Quaternary Heusler & U. Eberz and W.
↪ Seelentag and H.-U. Schuster, Z. Naturforsch. B 35, 1341-1343 (
↪ 1980)
1.0000000000000000
0.0000000000000000 3.232500000000000 3.232500000000000
3.232500000000000 0.000000000000000 3.232500000000000
3.232500000000000 3.232500000000000 0.000000000000000
Au Li Mg Sn
1 1 1 1
Direct

```

```

0.250000000000000 0.250000000000000 0.250000000000000 Au (4c)
0.750000000000000 0.750000000000000 0.750000000000000 Li (4d)
0.500000000000000 0.500000000000000 0.500000000000000 Mg (4b)
0.000000000000000 0.000000000000000 0.000000000000000 Sn (4a)

```

Ag<sub>3</sub>[PO<sub>4</sub>]: A3B4C\_cP16\_218\_c\_e\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ag3[PO4]'
_chemical_formula_sum 'Ag3 O4 P'

loop_
_publ_author_name
'R. Masse'
'I. Tordjman'
'A. Durif'
_journal_name_full_name
;
Zeitschrift f{"u}r Kristallographie - Crystalline Materials
;
_journal_volume 144
_journal_year 1976
_journal_page_first 76
_journal_page_last 81
_publ_section_title
;
Affinement de la structure cristalline du monophosphate d'argent Ag3_{
↪ 3}SPO_{4}$. Existence d'une forme haute temperature
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'Ag3_{3}S[PO_{4}]$ Structure'
_aflow_proto 'A3B4C_cP16_218_c_e_a'
_aflow_params 'a,x_{3}'
_aflow_params_values '6.0258147002,0.6486'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cP16'

_cell_length_a 6.0258147002
_cell_length_b 6.0258147002
_cell_length_c 6.0258147002
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P -4 3 n"
_symmetry_Int_Tables_number 218

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 y+1/2,x+1/2,z+1/2
14 y+1/2,-x+1/2,-z+1/2
15 -y+1/2,x+1/2,-z+1/2
16 -y+1/2,-x+1/2,z+1/2
17 x+1/2,z+1/2,y+1/2
18 x+1/2,-z+1/2,-y+1/2
19 -x+1/2,z+1/2,-y+1/2
20 -x+1/2,-z+1/2,y+1/2
21 z+1/2,y+1/2,x+1/2
22 z+1/2,-y+1/2,-x+1/2
23 -z+1/2,y+1/2,-x+1/2
24 -z+1/2,-y+1/2,x+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
P1 P 2 a 0.00000 0.00000 0.00000 1.00000
Ag1 Ag 6 c 0.25000 0.50000 0.00000 1.00000
O1 O 8 e 0.64860 0.64860 0.64860 1.00000

```

Ag<sub>3</sub>[PO<sub>4</sub>]: A3B4C\_cP16\_218\_c\_e\_a - POSCAR

```

A3B4C_cP16_218_c_e_a & a,x3 --params=6.0258147002,0.6486 & P-43n T_{d}^{2}
↪ 4} #218 (ace) & cP16 & None & Ag3[PO4] & R. Masse and I.
↪ Tordjman and A. Durif, Zeitschrift f{"u}r Kristallographie -
↪ Crystalline Materials 144, 76-81 (1976)
1.0000000000000000
6.02581470020000 0.00000000000000 0.000000000000000
0.000000000000000 6.02581470020000 0.000000000000000
0.000000000000000 0.000000000000000 6.02581470020000
Ag O P

```



6	8	2		
Direct				
0.2500000000000000	0.5000000000000000	0.0000000000000000	Ag	(6c)
0.7500000000000000	0.5000000000000000	0.0000000000000000	Ag	(6c)
0.0000000000000000	0.2500000000000000	0.5000000000000000	Ag	(6c)
0.0000000000000000	0.7500000000000000	0.5000000000000000	Ag	(6c)
0.5000000000000000	0.0000000000000000	0.2500000000000000	Ag	(6c)
0.5000000000000000	0.0000000000000000	0.7500000000000000	Ag	(6c)
0.6486000000000000	0.6486000000000000	0.6486000000000000	O	(8e)
-0.6486000000000000	-0.6486000000000000	0.6486000000000000	O	(8e)
-0.6486000000000000	0.6486000000000000	-0.6486000000000000	O	(8e)
0.6486000000000000	-0.6486000000000000	-0.6486000000000000	O	(8e)
1.1486000000000000	1.1486000000000000	1.1486000000000000	O	(8e)
-0.1486000000000000	-0.1486000000000000	1.1486000000000000	O	(8e)
1.1486000000000000	-0.1486000000000000	-0.1486000000000000	O	(8e)
-0.1486000000000000	1.1486000000000000	-0.1486000000000000	O	(8e)
0.0000000000000000	0.0000000000000000	0.0000000000000000	P	(2a)
0.5000000000000000	0.5000000000000000	0.5000000000000000	P	(2a)

Boracite (Mg<sub>3</sub>B<sub>7</sub>ClO<sub>13</sub>): A7BC3D13\_cF192\_219\_de\_b\_c\_ah - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Boracite'
_chemical_formula_sum 'B7 Cl Mg3 O13'

loop_
  _publ_author_name
  'S. Sueng'
  'J. R. Clark'
  'J. J. Papike'
  'J. A. Konnert'
  _journal_name_full_name
  :
  American Mineralogist
  ;
  _journal_volume 58
  _journal_year 1973
  _journal_page_first 691
  _journal_page_last 697
  _publ_section_title
  ;
  Crystal-Structure Refinement of Cubic Boracite
  ;

_aflow_title 'Boracite (Mg$_{3}$B$_{7}$ClO$_{13}$) Structure'
_aflow_proto 'A7BC3D13_cF192_219_de_b_c_ah'
_aflow_params 'a,x_{5},x_{6},y_{6},z_{6}'
_aflow_params_values '12.0986,0.0808,0.0987,0.0214,0.1821'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cF192'

_symmetry_space_group_name_H-M "F -4 3 c"
_symmetry_Int_Tables_number 219

_cell_length_a 12.09860
_cell_length_b 12.09860
_cell_length_c 12.09860
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x,y,z
  2 x,-y,-z
  3 -x,y,-z
  4 -x,-y,z
  5 y,z,x
  6 y,-z,-x
  7 -y,z,-x
  8 -y,-z,x
  9 z,x,y
  10 z,-x,-y
  11 -z,x,-y
  12 -z,-x,y
  13 y+1/2,x+1/2,z+1/2
  14 y+1/2,-x+1/2,-z+1/2
  15 -y+1/2,x+1/2,-z+1/2
  16 -y+1/2,-x+1/2,z+1/2
  17 x+1/2,z+1/2,y+1/2
  18 x+1/2,-z+1/2,-y+1/2
  19 -x+1/2,z+1/2,-y+1/2
  20 -x+1/2,-z+1/2,y+1/2
  21 z+1/2,y+1/2,x+1/2
  22 z+1/2,-y+1/2,-x+1/2
  23 -z+1/2,y+1/2,-x+1/2
  24 -z+1/2,-y+1/2,x+1/2
  25 x,y+1/2,z+1/2
  26 x,-y+1/2,-z+1/2
  27 -x,y+1/2,-z+1/2
  28 -x,-y+1/2,z+1/2
  29 y,z+1/2,x+1/2
  30 y,-z+1/2,-x+1/2
  31 -y,z+1/2,-x+1/2
  32 -y,-z+1/2,x+1/2
  33 z,x+1/2,y+1/2
  34 z,-x+1/2,-y+1/2
  35 -z,x+1/2,-y+1/2
  36 -z,-x+1/2,y+1/2
  37 y+1/2,x,z
  38 y+1/2,-x,-z
```

39	-y+1/2,x,-z
40	-y+1/2,-x,z
41	x+1/2,z,y
42	x+1/2,-z,-y
43	-x+1/2,z,-y
44	-x+1/2,-z,y
45	z+1/2,y,x
46	z+1/2,-y,-x
47	-z+1/2,y,-x
48	-z+1/2,-y,x
49	x+1/2,y,z+1/2
50	x+1/2,-y,-z+1/2
51	-x+1/2,y,-z+1/2
52	-x+1/2,-y,z+1/2
53	y+1/2,z,x+1/2
54	y+1/2,-z,-x+1/2
55	-y+1/2,z,-x+1/2
56	-y+1/2,-z,x+1/2
57	z+1/2,x,y+1/2
58	z+1/2,-x,-y+1/2
59	-z+1/2,x,-y+1/2
60	-z+1/2,-x,y+1/2
61	y,x+1/2,z
62	y,-x+1/2,-z
63	-y,x+1/2,-z
64	-y,-x+1/2,z
65	x,z+1/2,y
66	x,-z+1/2,-y
67	-x,z+1/2,-y
68	-x,-z+1/2,y
69	z,y+1/2,x
70	z,-y+1/2,-x
71	-z,y+1/2,-x
72	-z,-y+1/2,x
73	x+1/2,y+1/2,z
74	x+1/2,-y+1/2,-z
75	-x+1/2,y+1/2,-z
76	-x+1/2,-y+1/2,z
77	y+1/2,z+1/2,x
78	y+1/2,-z+1/2,-x
79	-y+1/2,z+1/2,-x
80	-y+1/2,-z+1/2,x
81	z+1/2,x+1/2,y
82	z+1/2,-x+1/2,-y
83	-z+1/2,x+1/2,-y
84	-z+1/2,-x+1/2,y
85	y,x,z+1/2
86	y,-x,-z+1/2
87	-y,x,-z+1/2
88	-y,-x,z+1/2
89	x,z,y+1/2
90	x,-z,-y+1/2
91	-x,z,-y+1/2
92	-x,-z,y+1/2
93	z,y,x+1/2
94	z,-y,-x+1/2
95	-z,y,-x+1/2
96	-z,-y,x+1/2

loop_	_atom_site_label	_atom_site_type_symbol	_atom_site_symmetry_multiplicity	_atom_site_Wyckoff_label	_atom_site_fract_x	_atom_site_fract_y	_atom_site_fract_z	_atom_site_occupancy
O1	O	8 a	0.00000	0.00000	1.00000			
Cl1	Cl	8 b	0.25000	0.25000	0.25000	1.00000		
Mg1	Mg	24 c	0.00000	0.25000	0.25000	1.00000		
B1	B	24 d	0.25000	0.00000	0.00000	1.00000		
B2	B	32 e	0.08080	0.08080	0.08080	1.00000		
O2	O	96 h	0.09870	0.02140	0.18210	1.00000		

Boracite (Mg<sub>3</sub>B<sub>7</sub>ClO<sub>13</sub>): A7BC3D13\_cF192\_219\_de\_b\_c\_ah - POSCAR

```
A7BC3D13_cF192_219_de_b_c_ah & a,x5,x6,y6,z6 --params=12.0986,0.0808,
  0.0987,0.0214,0.1821 & F-43c T_{d}^{h5} #219 (abcdeh) & cF192 &
  None & Mg3B7ClO13 & Boracite & S. Sueng et al., Am. Mineral. 58
  691-697 (1973)

1.0000000000000000
0.0000000000000000 6.049300000000000 6.049300000000000
6.049300000000000 0.000000000000000 6.049300000000000
6.049300000000000 6.049300000000000 0.000000000000000
  B Cl Mg O
  14 2 6 26

Direct
0.7500000000000000 0.2500000000000000 0.2500000000000000 B (24d)
0.2500000000000000 0.7500000000000000 0.7500000000000000 B (24d)
0.2500000000000000 0.7500000000000000 0.2500000000000000 B (24d)
0.7500000000000000 0.2500000000000000 0.7500000000000000 B (24d)
0.2500000000000000 0.2500000000000000 0.7500000000000000 B (24d)
0.7500000000000000 0.7500000000000000 0.2500000000000000 B (24d)
0.0808000000000000 0.0808000000000000 0.0808000000000000 B (32e)
0.0808000000000000 0.0808000000000000 -0.2424000000000000 B (32e)
0.0808000000000000 -0.2424000000000000 0.0808000000000000 B (32e)
-0.2424000000000000 0.0808000000000000 0.0808000000000000 B (32e)
0.5808000000000000 0.5808000000000000 0.5808000000000000 B (32e)
0.5808000000000000 0.5808000000000000 0.2576000000000000 B (32e)
0.2576000000000000 0.5808000000000000 0.5808000000000000 B (32e)
0.5808000000000000 0.2576000000000000 0.5808000000000000 B (32e)
0.2500000000000000 0.2500000000000000 0.2500000000000000 Cl (8b)
0.7500000000000000 0.7500000000000000 0.7500000000000000 Cl (8b)
0.5000000000000000 0.0000000000000000 0.0000000000000000 Mg (24c)
```

0.00000000000000	0.50000000000000	0.50000000000000	Mg (24c)
0.00000000000000	0.50000000000000	0.00000000000000	Mg (24c)
0.50000000000000	0.00000000000000	0.50000000000000	Mg (24c)
0.00000000000000	0.00000000000000	0.50000000000000	Mg (24c)
0.50000000000000	0.00000000000000	0.00000000000000	Mg (24c)
0.00000000000000	0.00000000000000	0.00000000000000	O (8a)
0.50000000000000	0.50000000000000	0.50000000000000	O (8a)
0.10480000000000	0.25940000000000	-0.06200000000000	O (96h)
0.25940000000000	0.10480000000000	-0.30220000000000	O (96h)
-0.06200000000000	-0.30220000000000	0.10480000000000	O (96h)
-0.30220000000000	-0.06200000000000	0.25940000000000	O (96h)
-0.06200000000000	0.10480000000000	0.25940000000000	O (96h)
-0.30220000000000	0.25940000000000	0.10480000000000	O (96h)
0.10480000000000	-0.06200000000000	-0.30220000000000	O (96h)
0.25940000000000	-0.30220000000000	-0.06200000000000	O (96h)
0.25940000000000	-0.06200000000000	0.10480000000000	O (96h)
0.10480000000000	-0.30220000000000	0.25940000000000	O (96h)
-0.30220000000000	0.10480000000000	-0.06200000000000	O (96h)
-0.06200000000000	0.25940000000000	-0.30220000000000	O (96h)
0.75940000000000	0.60480000000000	0.43800000000000	O (96h)
0.60480000000000	0.75940000000000	0.19780000000000	O (96h)
0.19780000000000	0.43800000000000	0.60480000000000	O (96h)
0.43800000000000	0.19780000000000	0.75940000000000	O (96h)
0.19780000000000	0.75940000000000	0.43800000000000	O (96h)
0.43800000000000	0.60480000000000	0.60480000000000	O (96h)
0.19780000000000	0.60480000000000	0.75940000000000	O (96h)
0.60480000000000	0.19780000000000	0.43800000000000	O (96h)
0.75940000000000	0.43800000000000	0.19780000000000	O (96h)

Cu<sub>5</sub>Si<sub>4</sub> (D8<sub>6</sub>): A15B4\_c176\_220\_ae\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Cu5 Si4'

loop_
  _publ_author_name
    'M. Mattern'
    'R. Seyrich'
    'L. Wilde'
    'C. Baehz'
    'M. Knapp'
    'J. Acker'
  _journal_name_full_name
    ;
  Journal of Alloys and Compounds
  ;
  _journal_volume 429
  _journal_year 2007
  _journal_page_first 211
  _journal_page_last 215
  _publ_section_title
    ;
  Phase formation of rapidly quenched Cu-Si alloys
  ;
# Found in Experimental investigation of the Cu-Si phase diagram at x(Cu
↪ )> 0.725, 2011

_aflow_title 'Cu5Si4 Structure'
_aflow_proto 'A15B4_c176_220_ae_c'
_aflow_params 'a, x2, x3, y3, z3'
_aflow_params_values '9.718, -0.042, 0.12, 0.16, -0.04'
_aflow_Strukturbericht 'SD8_{6}S'
_aflow_Pearson 'cI76'

_symmetry_space_group_name_H-M "I -4 3 d"
_symmetry_Int_Tables_number 220

_cell_length_a 9.71800
_cell_length_b 9.71800
_cell_length_c 9.71800
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x, y, z
  2 x, -y, -z+1/2
  3 -x+1/2, y, -z
  4 -x, -y+1/2, z
  5 y, z, x
  6 y, -z, -x+1/2
  7 -y+1/2, z, -x
  8 -y, -z+1/2, x
  9 z, x, y
  10 z, -x, -y+1/2
  11 -z+1/2, x, -y
  12 -z, -x+1/2, y
  13 y+1/4, x+1/4, z+1/4
  14 y+1/4, -x+3/4, -z+1/4
  15 -y+1/4, x+1/4, -z+3/4
  16 -y+3/4, -x+1/4, z+1/4
  17 x+1/4, z+1/4, y+1/4
  18 x+1/4, -z+3/4, -y+1/4
  19 -x+1/4, z+1/4, -y+3/4
  20 -x+3/4, -z+1/4, y+1/4
```

21	z+1/4, y+1/4, x+1/4
22	z+1/4, -y+3/4, -x+1/4
23	-z+1/4, y+1/4, -x+3/4
24	-z+3/4, -y+1/4, x+1/4
25	x+1/2, y+1/2, z+1/2
26	x+1/2, -y+1/2, -z
27	-x, y+1/2, -z+1/2
28	-x+1/2, -y, z+1/2
29	y+1/2, z+1/2, x+1/2
30	y+1/2, -z+1/2, -x
31	-y, z+1/2, -x+1/2
32	-y+1/2, -z, x+1/2
33	z+1/2, x+1/2, y+1/2
34	z+1/2, -x+1/2, -y
35	-z, x+1/2, -y+1/2
36	-z+1/2, -x, y+1/2
37	y+3/4, x+3/4, z+3/4
38	y+3/4, -x+1/4, -z+3/4
39	-y+3/4, x+3/4, -z+1/4
40	-y+1/4, -x+3/4, z+3/4
41	x+3/4, z+3/4, y+3/4
42	x+3/4, -z+1/4, -y+3/4
43	-x+3/4, z+3/4, -y+1/4
44	-x+1/4, -z+3/4, y+3/4
45	z+3/4, y+3/4, x+3/4
46	z+3/4, -y+1/4, -x+3/4
47	-z+3/4, y+3/4, -x+1/4
48	-z+1/4, -y+3/4, x+3/4

```
loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Cu1 Cu 12 a 0.37500 0.00000 0.25000 1.00000
Si1 Si 16 c -0.04200 -0.04200 -0.04200 1.00000
Cu2 Cu 48 e 0.12000 0.16000 -0.04000 1.00000
```

Cu<sub>5</sub>Si<sub>4</sub> (D8<sub>6</sub>): A15B4\_c176\_220\_ae\_c - POSCAR

```
A15B4_c176_220_ae_c & a, x2, x3, y3, z3 --params=9.718, -0.042, 0.12, 0.16, -
↪ 0.04 & I-43d T_{d}^{6} #220 (ace) & cI76 & SD8_{6}S & Cu15Si4 &
↪ & M. Mattern et al., J. Alloys Compd. 429, 211-215 (2007)
1.0000000000000000
-4.8590000000000000 4.8590000000000000 4.8590000000000000
4.8590000000000000 -4.8590000000000000 4.8590000000000000
4.8590000000000000 4.8590000000000000 -4.8590000000000000
Cu Si
30 8
Direct
0.2500000000000000 0.6250000000000000 0.3750000000000000 Cu (12a)
0.7500000000000000 0.8750000000000000 0.1250000000000000 Cu (12a)
0.3750000000000000 0.2500000000000000 0.6250000000000000 Cu (12a)
0.1250000000000000 0.7500000000000000 0.5000000000000000 Cu (12a)
0.6250000000000000 0.3750000000000000 0.2500000000000000 Cu (12a)
0.8750000000000000 0.1250000000000000 0.7500000000000000 Cu (12a)
0.1200000000000000 0.0800000000000000 0.2800000000000000 Cu (48e)
0.3000000000000000 -0.1600000000000000 0.2200000000000000 Cu (48e)
0.2000000000000000 0.4200000000000000 0.5400000000000000 Cu (48e)
0.3800000000000000 0.6600000000000000 -0.0400000000000000 Cu (48e)
0.2800000000000000 0.1200000000000000 0.0800000000000000 Cu (48e)
0.2200000000000000 0.3000000000000000 -0.1600000000000000 Cu (48e)
0.5400000000000000 0.2000000000000000 0.4200000000000000 Cu (48e)
-0.0400000000000000 0.3800000000000000 0.6600000000000000 Cu (48e)
0.0800000000000000 0.2800000000000000 0.1200000000000000 Cu (48e)
-0.1600000000000000 0.2200000000000000 0.3000000000000000 Cu (48e)
0.4200000000000000 0.5400000000000000 0.2000000000000000 Cu (48e)
0.6600000000000000 -0.0400000000000000 0.3800000000000000 Cu (48e)
0.5800000000000000 0.6200000000000000 0.7800000000000000 Cu (48e)
0.3400000000000000 -0.2000000000000000 -0.2800000000000000 Cu (48e)
-0.0800000000000000 0.7000000000000000 0.0400000000000000 Cu (48e)
0.1600000000000000 -0.1200000000000000 0.4600000000000000 Cu (48e)
0.6200000000000000 0.7800000000000000 0.5800000000000000 Cu (48e)
-0.2000000000000000 -0.2800000000000000 0.3400000000000000 Cu (48e)
0.7000000000000000 0.0400000000000000 -0.0800000000000000 Cu (48e)
-0.1200000000000000 0.4600000000000000 0.1600000000000000 Cu (48e)
0.7800000000000000 0.5800000000000000 0.6200000000000000 Cu (48e)
-0.2800000000000000 0.3400000000000000 -0.2000000000000000 Cu (48e)
0.0400000000000000 -0.0800000000000000 0.7000000000000000 Cu (48e)
0.4600000000000000 0.1600000000000000 -0.1200000000000000 Cu (48e)
-0.0840000000000000 -0.0840000000000000 -0.0840000000000000 Si (16c)
0.5000000000000000 0.0000000000000000 0.5840000000000000 Si (16c)
0.0000000000000000 0.5840000000000000 0.5000000000000000 Si (16c)
0.5840000000000000 0.5000000000000000 0.0000000000000000 Si (16c)
0.4160000000000000 0.4160000000000000 0.4160000000000000 Si (16c)
0.5000000000000000 0.0000000000000000 0.0840000000000000 Si (16c)
0.0840000000000000 0.5000000000000000 0.0000000000000000 Si (16c)
0.0000000000000000 0.0840000000000000 0.5000000000000000 Si (16c)
```

Th<sub>3</sub>P<sub>4</sub> (D7<sub>3</sub>): A4B3\_c128\_220\_c\_a - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Th3P4'
_chemical_formula_sum 'P4 Th3'

loop_
  _publ_author_name
    'K. Meisel'
```

```

_journal_name_full_name
:
Zeitschrift fur Anorganische und Allgemeine Chemie
;
_journal_volume 240
_journal_year 1939
_journal_page_first 300
_journal_page_last 312
_publ_Section_title
:
Kristallstrukturen von Thoriumphosphiden
;
_aflow_title 'Th$_{3}$SP$_{4}$ ($D7_{3}$) Structure'
_aflow_proto 'A4B3_c128_220_c_a'
_aflow_params 'a,x_{2}'
_aflow_params_values '8.6,0.08333'
_aflow_Strukturbericht '$D7_{3}$'
_aflow_Pearson 'c128'

_symmetry_space_group_name_H-M "I -4 3 d"
_symmetry_Int_Tables_number 220

_cell_length_a 8.60000
_cell_length_b 8.60000
_cell_length_c 8.60000
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z+1/2
3 -x+1/2,y,-z
4 -x,-y+1/2,z
5 y,z,x
6 y,-z,-x+1/2
7 -y+1/2,z,-x
8 -y,-z+1/2,x
9 z,x,y
10 z,-x,-y+1/2
11 -z+1/2,x,-y
12 -z,-x+1/2,y
13 y+1/4,x+1/4,z+1/4
14 y+1/4,-x+3/4,-z+1/4
15 -y+1/4,x+1/4,-z+3/4
16 -y+3/4,-x+1/4,z+1/4
17 x+1/4,z+1/4,y+1/4
18 x+1/4,-z+3/4,-y+1/4
19 -x+1/4,z+1/4,-y+3/4
20 -x+3/4,-z+1/4,y+1/4
21 z+1/4,y+1/4,x+1/4
22 z+1/4,-y+3/4,-x+1/4
23 -z+1/4,y+1/4,-x+3/4
24 -z+3/4,-y+1/4,x+1/4
25 x+1/2,y+1/2,z+1/2
26 x+1/2,-y+1/2,-z
27 -x,y+1/2,-z+1/2
28 -x+1/2,-y,z+1/2
29 y+1/2,z+1/2,x+1/2
30 y+1/2,-z+1/2,-x
31 -y,z+1/2,-x+1/2
32 -y+1/2,-z,x+1/2
33 z+1/2,x+1/2,y+1/2
34 z+1/2,-x+1/2,-y
35 -z,x+1/2,-y+1/2
36 -z+1/2,-x,y+1/2
37 y+3/4,x+3/4,z+3/4
38 y+3/4,-x+1/4,-z+3/4
39 -y+3/4,x+3/4,-z+1/4
40 -y+1/4,-x+3/4,z+3/4
41 x+3/4,z+3/4,y+3/4
42 x+3/4,-z+1/4,-y+3/4
43 -x+3/4,z+3/4,-y+1/4
44 -x+1/4,-z+3/4,y+3/4
45 z+3/4,y+3/4,x+3/4
46 z+3/4,-y+1/4,-x+3/4
47 -z+3/4,y+3/4,-x+1/4
48 -z+1/4,-y+3/4,x+3/4

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Th1 Th 12 a 0.37500 0.00000 0.25000 1.00000
P1 P 16 c 0.08333 0.08333 0.08333 1.00000

```

Th<sub>3</sub>P<sub>4</sub> (D7<sub>3</sub>): A4B3\_c128\_220\_c\_a - POSCAR

```

A4B3_c128_220_c_a & a,x2 --params=8.6,0.08333 & I-43d T_{d}^{6} #220 (ac
↪ ) & c128 & $D7_{3}$ & Th3P4 & Th3P4 & K. Meisel, Z. Anorg.
↪ Allg. Chem. 240, 300-312 (1939)
1.000000000000000
-4.300000000000000 4.300000000000000 4.300000000000000
4.300000000000000 -4.300000000000000 4.300000000000000
4.300000000000000 4.300000000000000 -4.300000000000000
P Th
8 6

```

Direct				
0.166660000000000	0.166660000000000	0.166660000000000	P	(16c)
0.500000000000000	0.000000000000000	0.333340000000000	P	(16c)
0.000000000000000	0.333340000000000	0.500000000000000	P	(16c)
0.333340000000000	0.500000000000000	0.000000000000000	P	(16c)
0.666660000000000	0.666660000000000	0.666660000000000	P	(16c)
0.500000000000000	0.000000000000000	-0.166660000000000	P	(16c)
-0.166660000000000	0.500000000000000	0.000000000000000	P	(16c)
0.000000000000000	-0.166660000000000	0.500000000000000	P	(16c)
0.250000000000000	0.625000000000000	0.375000000000000	Th	(12a)
0.750000000000000	0.875000000000000	0.125000000000000	Th	(12a)
0.375000000000000	0.250000000000000	0.625000000000000	Th	(12a)
0.125000000000000	0.750000000000000	0.875000000000000	Th	(12a)
0.625000000000000	0.375000000000000	0.250000000000000	Th	(12a)
0.875000000000000	0.125000000000000	0.750000000000000	Th	(12a)

Ca<sub>3</sub>Al<sub>2</sub>O<sub>6</sub> (E9<sub>1</sub>): A2B3C6\_cP33\_221\_cd\_ag\_fh - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ca3Al2O6'
_chemical_formula_sum 'Al2 Ca3 O6'

loop_
_publ_author_name
'F. A. Steele'
'W. P. Davey'
_journal_name_full_name
:
Journal of the American Chemical Society
;
_journal_volume 51
_journal_year 1929
_journal_page_first 689
_journal_page_last 697
_publ_Section_title
:
The Crystal Structure of Tricalcium Aluminate
;

# Found in The crystal structure of tricalcium aluminate, Ca$_{3}$Al$_{2}$O$_{6}$
↪ }$OS_{6}$, 1975

_aflow_title 'Ca$_{3}$Al$_{2}$O$_{6}$ ($E9_{1}$) Structure'
_aflow_proto 'A2B3C6_cP33_221_cd_ag_fh'
_aflow_params 'a,x_{4},x_{5},x_{6}'
_aflow_params_values '7.624,0.3,0.2,0.2'
_aflow_Strukturbericht '$E9_{1}$'
_aflow_Pearson 'cP33'

_symmetry_space_group_name_H-M "P 4/m -3 2/m"
_symmetry_Int_Tables_number 221

_cell_length_a 7.62400
_cell_length_b 7.62400
_cell_length_c 7.62400
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 -y,-x,-z
14 -y,x,z
15 y,-x,z
16 y,x,-z
17 -x,-z,-y
18 -x,z,y
19 x,-z,y
20 x,z,-y
21 -z,-y,-x
22 -z,y,x
23 z,-y,x
24 z,y,-x
25 -x,-y,-z
26 -x,y,z
27 x,-y,z
28 x,y,-z
29 -y,-z,-x
30 -y,z,x
31 y,-z,x
32 y,z,-x
33 -z,-x,-y
34 -z,x,y
35 z,-x,y
36 z,x,-y
37 y,x,z
38 y,-x,-z
39 -y,x,-z
40 -y,-x,z

```

```

41 x,z,y
42 x,-z,-y
43 -x,z,-y
44 -x,-z,y
45 z,y,x
46 z,-y,-x
47 -z,y,-x
48 -z,-y,x

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ca1 Ca 1 a 0.00000 0.00000 0.00000 1.00000
Al1 Al 3 c 0.00000 0.50000 0.50000 1.00000
Al2 Al 3 d 0.50000 0.00000 0.00000 1.00000
O1 O 6 f 0.30000 0.50000 0.50000 1.00000
Ca2 Ca 8 g 0.20000 0.20000 0.20000 1.00000
O2 O 12 h 0.20000 0.50000 0.00000 1.00000

```

Ce<sub>3</sub>Al<sub>2</sub>O<sub>6</sub> (E91): A2B3C6\_cP33\_221\_cd\_ag\_fh - POSCAR

```

A2B3C6_cP33_221_cd_ag_fh & a, x4, x5, x6 --params=7.624, 0.3, 0.2, 0.2 & Pm-3m
↪ O_{h}^{1} #221 (acd fgh) & cP33 & SE9_{1}$ & Ca3Al2O6 &
↪ Ca3Al2O6 & F. A. Steele and W. P. Davey, J. Am. Chem. Soc. 51,
↪ 689-697 (1929)
1.0000000000000000
7.6240000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6240000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.6240000000000000
Al Ca O
6 9 18
Direct
0.0000000000000000 0.5000000000000000 0.5000000000000000 Al (3c)
0.5000000000000000 0.0000000000000000 0.5000000000000000 Al (3c)
0.5000000000000000 0.5000000000000000 0.0000000000000000 Al (3c)
0.5000000000000000 0.0000000000000000 0.0000000000000000 Al (3d)
0.0000000000000000 0.5000000000000000 0.0000000000000000 Al (3d)
0.0000000000000000 0.0000000000000000 0.5000000000000000 Al (3d)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Ca (1a)
0.2000000000000000 0.2000000000000000 0.2000000000000000 Ca (8g)
-0.2000000000000000 -0.2000000000000000 0.2000000000000000 Ca (8g)
-0.2000000000000000 0.2000000000000000 -0.2000000000000000 Ca (8g)
0.2000000000000000 -0.2000000000000000 -0.2000000000000000 Ca (8g)
0.2000000000000000 0.2000000000000000 -0.2000000000000000 Ca (8g)
-0.2000000000000000 -0.2000000000000000 -0.2000000000000000 Ca (8g)
0.2000000000000000 -0.2000000000000000 0.2000000000000000 Ca (8g)
-0.2000000000000000 0.2000000000000000 0.2000000000000000 Ca (8g)
0.3000000000000000 0.5000000000000000 0.5000000000000000 O (6f)
-0.3000000000000000 0.5000000000000000 0.5000000000000000 O (6f)
0.5000000000000000 -0.3000000000000000 0.5000000000000000 O (6f)
0.5000000000000000 0.5000000000000000 0.3000000000000000 O (6f)
0.5000000000000000 0.5000000000000000 -0.3000000000000000 O (6f)
0.2000000000000000 0.5000000000000000 0.0000000000000000 O (12h)
-0.2000000000000000 0.5000000000000000 0.0000000000000000 O (12h)
0.0000000000000000 0.2000000000000000 0.5000000000000000 O (12h)
0.0000000000000000 -0.2000000000000000 0.5000000000000000 O (12h)
0.5000000000000000 0.0000000000000000 0.2000000000000000 O (12h)
0.5000000000000000 0.0000000000000000 -0.2000000000000000 O (12h)
0.5000000000000000 0.2000000000000000 0.0000000000000000 O (12h)
0.5000000000000000 -0.2000000000000000 0.0000000000000000 O (12h)
0.2000000000000000 0.0000000000000000 0.5000000000000000 O (12h)
-0.2000000000000000 0.0000000000000000 0.5000000000000000 O (12h)
0.0000000000000000 0.5000000000000000 -0.2000000000000000 O (12h)
0.0000000000000000 0.5000000000000000 0.2000000000000000 O (12h)

```

Ce<sub>5</sub>Mo<sub>3</sub>O<sub>16</sub>: A5B3C16\_cP96\_222\_ce\_d\_fi - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'Ce5Mo3O16'
_chemical_formula_sum 'Ce5 Mo3 O16'

loop_
_publ_author_name
'P. H. Hubert'
_journal_year 1974
_publ_section_title
;
Contribution {\a} 1 \{\e}tude des molybdites des terres rares: 1.
↪ Bimolybdites Ln_{2}$Mo_{2}$S_{7}$
;

# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'Ce_{5}$Mo_{3}$S_{16}$ Structure'
_aflow_proto 'A5B3C16_cP96_222_ce_d_fi'
_aflow_params 'a, x_{3}, x_{4}, x_{5}, y_{5}, z_{5}'
_aflow_params_values '11.1199004528, 0.0, 0.125, 0.084, 0.166, 0.625'
_aflow_strukturbericht 'None'
_aflow_pearson 'cP96'

_cell_length_a 11.1199004528
_cell_length_b 11.1199004528
_cell_length_c 11.1199004528
_cell_angle_alpha 90.0000000000

```

```

_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "P 4/n -3 2/n (origin choice 2)"
_symmetry_Int_Tables_number 222

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y+1/2, -z+1/2
3 -x+1/2, y, -z+1/2
4 -x+1/2, -y+1/2, z
5 y, z, x
6 y, -z+1/2, -x+1/2
7 -y+1/2, z, -x+1/2
8 -y+1/2, -z+1/2, x
9 z, x, y
10 z, -x+1/2, -y+1/2
11 -z+1/2, x, -y+1/2
12 -z+1/2, -x+1/2, y
13 -y+1/2, -x+1/2, -z+1/2
14 -y+1/2, z, x, z
15 y, -x+1/2, z
16 y, x, -z+1/2
17 -x+1/2, -z+1/2, -y+1/2
18 -x+1/2, z, y
19 x, -z+1/2, y
20 x, z, -y+1/2
21 -z+1/2, -y+1/2, -x+1/2
22 -z+1/2, y, x
23 z, -y+1/2, x
24 z, y, -x+1/2
25 -x, -y, -z
26 -x, y+1/2, z+1/2
27 x+1/2, -y, z+1/2
28 x+1/2, y+1/2, -z
29 -y, -z, -x
30 -y, z+1/2, x+1/2
31 y+1/2, -z, x+1/2
32 y+1/2, z+1/2, -x
33 -z, -x, -y
34 -z, x+1/2, y+1/2
35 z+1/2, -x, y+1/2
36 z+1/2, x+1/2, -y
37 y+1/2, x+1/2, z+1/2
38 y+1/2, -x, -z
39 -y, x+1/2, -z
40 -y, -x, z+1/2
41 x+1/2, z+1/2, y+1/2
42 x+1/2, -z, -y
43 -x, z+1/2, -y
44 -x, -z, y+1/2
45 z+1/2, y+1/2, x+1/2
46 z+1/2, -y, -x
47 -z, y+1/2, -x
48 -z, -y, x+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ce1 Ce 8 c 0.00000 0.00000 0.00000 1.00000
Mo1 Mo 12 d 0.00000 0.75000 0.25000 1.00000
Ce2 Ce 12 e 0.00000 0.25000 0.25000 1.00000
O1 O 16 f 0.12500 0.12500 0.12500 1.00000
O2 O 48 i 0.08400 0.16600 0.62500 1.00000

```

Ce<sub>5</sub>Mo<sub>3</sub>O<sub>16</sub>: A5B3C16\_cP96\_222\_ce\_d\_fi - POSCAR

```

A5B3C16_cP96_222_ce_d_fi & a, x3, x4, x5, y5, z5 --params=11.1199004528, 0.0,
↪ 0.125, 0.084, 0.166, 0.625 & Pn-3n O_{h}^{2} #222 (cdefi) & cP96 &
↪ None & Ce5Mo3O16 & P. H. Hubert, (1974)
1.0000000000000000
11.11990045280000 0.0000000000000000 0.0000000000000000
0.0000000000000000 11.11990045280000 0.0000000000000000
0.0000000000000000 0.0000000000000000 11.11990045280000
Ce Mo O
20 12 64
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 Ce (8c)
0.5000000000000000 0.5000000000000000 0.0000000000000000 Ce (8c)
0.5000000000000000 0.0000000000000000 0.5000000000000000 Ce (8c)
0.0000000000000000 0.5000000000000000 0.5000000000000000 Ce (8c)
0.5000000000000000 0.0000000000000000 0.5000000000000000 Ce (8c)
0.0000000000000000 0.5000000000000000 0.0000000000000000 Ce (8c)
0.5000000000000000 0.0000000000000000 0.0000000000000000 Ce (8c)
0.0000000000000000 0.2500000000000000 0.2500000000000000 Ce (12e)
0.5000000000000000 0.2500000000000000 0.2500000000000000 Ce (12e)
0.2500000000000000 0.0000000000000000 0.2500000000000000 Ce (12e)
0.2500000000000000 0.5000000000000000 0.2500000000000000 Ce (12e)
0.2500000000000000 0.2500000000000000 0.0000000000000000 Ce (12e)
0.2500000000000000 0.2500000000000000 0.5000000000000000 Ce (12e)
0.0000000000000000 0.7500000000000000 0.7500000000000000 Ce (12e)
0.5000000000000000 0.7500000000000000 0.7500000000000000 Ce (12e)
0.7500000000000000 0.0000000000000000 0.7500000000000000 Ce (12e)
0.7500000000000000 0.5000000000000000 0.7500000000000000 Ce (12e)
0.7500000000000000 0.7500000000000000 0.0000000000000000 Ce (12e)
0.7500000000000000 0.7500000000000000 0.5000000000000000 Ce (12e)

```

```

0.000000000000 0.750000000000 0.250000000000 Mo (12d)
0.500000000000 0.750000000000 0.250000000000 Mo (12d)
0.250000000000 0.000000000000 0.750000000000 Mo (12d)
0.250000000000 0.500000000000 0.750000000000 Mo (12d)
0.750000000000 0.250000000000 0.000000000000 Mo (12d)
0.750000000000 0.250000000000 0.500000000000 Mo (12d)
0.750000000000 0.000000000000 0.250000000000 Mo (12d)
0.750000000000 0.500000000000 0.250000000000 Mo (12d)
0.000000000000 0.250000000000 0.750000000000 Mo (12d)
0.500000000000 0.250000000000 0.750000000000 Mo (12d)
0.250000000000 0.750000000000 0.500000000000 Mo (12d)
0.250000000000 0.750000000000 0.000000000000 Mo (12d)
0.125000000000 0.125000000000 0.125000000000 O (16f)
0.375000000000 0.375000000000 0.125000000000 O (16f)
0.375000000000 0.125000000000 0.375000000000 O (16f)
0.125000000000 0.375000000000 0.375000000000 O (16f)
0.125000000000 0.125000000000 0.375000000000 O (16f)
0.375000000000 0.375000000000 0.375000000000 O (16f)
0.125000000000 0.375000000000 0.125000000000 O (16f)
0.375000000000 0.125000000000 0.125000000000 O (16f)
-0.125000000000 -0.125000000000 -0.125000000000 O (16f)
0.625000000000 0.625000000000 -0.125000000000 O (16f)
0.625000000000 -0.125000000000 0.625000000000 O (16f)
-0.125000000000 -0.125000000000 0.625000000000 O (16f)
0.625000000000 0.625000000000 0.625000000000 O (16f)
-0.125000000000 -0.125000000000 0.625000000000 O (16f)
0.625000000000 0.625000000000 0.625000000000 O (16f)
-0.125000000000 -0.125000000000 0.625000000000 O (16f)
0.084000000000 0.166000000000 0.625000000000 O (48i)
0.416000000000 0.334000000000 0.625000000000 O (48i)
0.416000000000 0.166000000000 -0.125000000000 O (48i)
0.084000000000 0.334000000000 -0.125000000000 O (48i)
0.625000000000 0.084000000000 0.166000000000 O (48i)
0.625000000000 0.416000000000 0.334000000000 O (48i)
-0.125000000000 0.416000000000 0.166000000000 O (48i)
-0.125000000000 0.084000000000 0.334000000000 O (48i)
0.166000000000 0.625000000000 0.084000000000 O (48i)
0.334000000000 0.625000000000 0.416000000000 O (48i)
0.166000000000 -0.125000000000 0.416000000000 O (48i)
0.334000000000 -0.125000000000 0.084000000000 O (48i)
0.166000000000 0.084000000000 -0.125000000000 O (48i)
0.334000000000 0.416000000000 -0.125000000000 O (48i)
0.166000000000 0.416000000000 0.625000000000 O (48i)
0.334000000000 0.084000000000 0.625000000000 O (48i)
0.084000000000 0.625000000000 0.334000000000 O (48i)
0.416000000000 0.625000000000 0.166000000000 O (48i)
0.416000000000 -0.125000000000 0.334000000000 O (48i)
0.084000000000 -0.125000000000 0.166000000000 O (48i)
0.625000000000 0.166000000000 0.416000000000 O (48i)
0.625000000000 0.334000000000 0.084000000000 O (48i)
-0.125000000000 0.166000000000 0.084000000000 O (48i)
-0.125000000000 0.334000000000 0.416000000000 O (48i)
-0.084000000000 -0.166000000000 -0.625000000000 O (48i)
0.584000000000 0.666000000000 -0.625000000000 O (48i)
0.584000000000 -0.166000000000 1.125000000000 O (48i)
-0.084000000000 0.666000000000 1.125000000000 O (48i)
-0.625000000000 -0.084000000000 -0.166000000000 O (48i)
-0.625000000000 0.584000000000 -0.166000000000 O (48i)
1.125000000000 0.584000000000 -0.166000000000 O (48i)
1.125000000000 -0.084000000000 0.666000000000 O (48i)
-0.166000000000 -0.625000000000 -0.084000000000 O (48i)
0.666000000000 -0.625000000000 0.584000000000 O (48i)
-0.166000000000 1.125000000000 0.584000000000 O (48i)
0.666000000000 0.584000000000 -0.625000000000 O (48i)
-0.166000000000 -0.084000000000 -0.625000000000 O (48i)
-0.084000000000 -0.625000000000 0.666000000000 O (48i)
0.584000000000 -0.625000000000 -0.166000000000 O (48i)
0.584000000000 1.125000000000 0.666000000000 O (48i)
-0.084000000000 1.125000000000 -0.166000000000 O (48i)
-0.625000000000 -0.166000000000 0.584000000000 O (48i)
-0.625000000000 0.666000000000 -0.084000000000 O (48i)
1.125000000000 -0.166000000000 -0.084000000000 O (48i)
1.125000000000 0.666000000000 0.584000000000 O (48i)

```

Th<sub>6</sub>Mn<sub>23</sub> (D<sub>8h</sub>): A23B6\_cF116\_225\_bd2f\_e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Th6Mn23'
_chemical_formula_sum 'Mn23 Th6'

loop_
  _publ_author_name
    'J. V. Florio'
    'R. E. Rundle'
    'A. I. Snow'
  _journal_name_full_name
    'Acta Crystallographica'
  _journal_volume 5
  _journal_year 1952
  _journal_page_first 445
  _journal_page_last 457
  _publ_Section_title
    'Compounds of thorium with transition metals. I. The thorium-manganese
    ↪ system'

```

# Found in A Handbook of Lattice Spacings and Structures of Metals and Alloys, 1958

```

_aflow_title 'Th$_{6}$Mn$_{23}$ (SD8_{a}$) Structure'
_aflow_proto 'A23B6_cF116_225_bd2f_e'
_aflow_params 'a_x_{3},x_{4},x_{5}'
_aflow_params_values '12.523,0.203,0.178,0.378'
_aflow_Strukturbericht 'SD8_{a}$'
_aflow_Pearson 'cF116'

```

```

_symmetry_space_group_name_H-M "F 4/m -3 2/m"
_symmetry_Int_Tables_number 225

```

```

_cell_length_a 12.52300
_cell_length_b 12.52300
_cell_length_c 12.52300
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

```

```

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz

```

```

1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 -y,-x,-z
14 -y,x,z
15 y,-x,z
16 y,x,-z
17 -x,-z,-y
18 -x,z,y
19 x,-z,y
20 x,z,-y
21 -z,-y,-x
22 -z,y,x
23 z,-y,x
24 z,y,-x
25 -x,-y,-z
26 -x,y,z
27 x,-y,z
28 x,y,-z
29 -y,-z,-x
30 -y,z,x
31 y,-z,x
32 y,z,-x
33 -z,-x,-y
34 -z,x,y
35 z,-x,y
36 z,x,-y
37 y,x,z
38 y,-x,-z
39 -y,x,-z
40 -y,-x,z
41 x,z,y
42 x,-z,-y
43 -x,z,-y
44 -x,-z,y
45 z,y,x
46 z,-y,-x
47 -z,y,-x
48 -z,-y,x
49 x,y+1/2,z+1/2
50 x,-y+1/2,-z+1/2
51 -x,y+1/2,-z+1/2
52 -x,-y+1/2,z+1/2
53 y,z+1/2,x+1/2
54 y,-z+1/2,-x+1/2
55 -y,z+1/2,-x+1/2
56 -y,-z+1/2,x+1/2
57 z,x+1/2,y+1/2
58 z,-x+1/2,-y+1/2
59 -z,x+1/2,-y+1/2
60 -z,-x+1/2,y+1/2
61 -y,-x+1/2,-z+1/2
62 -y,x+1/2,z+1/2
63 y,-x+1/2,z+1/2
64 y,x+1/2,-z+1/2
65 -x,-z+1/2,-y+1/2
66 -x,z+1/2,y+1/2
67 x,-z+1/2,y+1/2
68 x,z+1/2,-y+1/2
69 -z,-y+1/2,-x+1/2
70 -z,y+1/2,x+1/2
71 z,-y+1/2,x+1/2
72 z,y+1/2,-x+1/2
73 -x,-y+1/2,-z+1/2
74 -x,y+1/2,z+1/2
75 x,-y+1/2,z+1/2
76 x,y+1/2,-z+1/2
77 -y,-z+1/2,-x+1/2
78 -y,z+1/2,x+1/2
79 y,-z+1/2,x+1/2
80 y,z+1/2,-x+1/2
81 -z,-x+1/2,-y+1/2
82 -z,x+1/2,y+1/2

```

```

83 z, -x+1/2, y+1/2
84 z, x+1/2, -y+1/2
85 y, x+1/2, z+1/2
86 y, -x+1/2, -z+1/2
87 -y, x+1/2, -z+1/2
88 -y, -x+1/2, z+1/2
89 x, z+1/2, y+1/2
90 x, -z+1/2, -y+1/2
91 -x, z+1/2, -y+1/2
92 -x, -z+1/2, y+1/2
93 z, y+1/2, x+1/2
94 z, -y+1/2, -x+1/2
95 -z, y+1/2, -x+1/2
96 -z, -y+1/2, x+1/2
97 x+1/2, y, z+1/2
98 x+1/2, -y, -z+1/2
99 -x+1/2, y, -z+1/2
100 -x+1/2, -y, z+1/2
101 y+1/2, z, x+1/2
102 y+1/2, -z, -x+1/2
103 -y+1/2, z, -x+1/2
104 -y+1/2, -z, x+1/2
105 z+1/2, x, y+1/2
106 z+1/2, -x, -y+1/2
107 -z+1/2, x, -y+1/2
108 -z+1/2, -x, y+1/2
109 -y+1/2, -x, -z+1/2
110 -y+1/2, x, z+1/2
111 y+1/2, -x, z+1/2
112 y+1/2, x, -z+1/2
113 -x+1/2, -z, -y+1/2
114 -x+1/2, z, y+1/2
115 x+1/2, -z, y+1/2
116 x+1/2, z, -y+1/2
117 -z+1/2, -y, -x+1/2
118 -z+1/2, y, x+1/2
119 z+1/2, -y, x+1/2
120 z+1/2, y, -x+1/2
121 -x+1/2, -y, -z+1/2
122 -x+1/2, y, z+1/2
123 x+1/2, -y, z+1/2
124 x+1/2, y, -z+1/2
125 -y+1/2, -z, -x+1/2
126 -y+1/2, z, x+1/2
127 y+1/2, -z, x+1/2
128 y+1/2, z, -x+1/2
129 -z+1/2, -x, -y+1/2
130 -z+1/2, x, y+1/2
131 z+1/2, -x, y+1/2
132 z+1/2, x, -y+1/2
133 y+1/2, x, z+1/2
134 y+1/2, -x, -z+1/2
135 -y+1/2, x, -z+1/2
136 -y+1/2, -x, z+1/2
137 x+1/2, z, y+1/2
138 x+1/2, -z, -y+1/2
139 -x+1/2, z, -y+1/2
140 -x+1/2, -z, y+1/2
141 z+1/2, y, x+1/2
142 z+1/2, -y, -x+1/2
143 -z+1/2, y, -x+1/2
144 -z+1/2, -y, x+1/2
145 x+1/2, y+1/2, z
146 x+1/2, -y+1/2, -z
147 -x+1/2, y+1/2, -z
148 -x+1/2, -y+1/2, z
149 y+1/2, z+1/2, x
150 y+1/2, -z+1/2, -x
151 -y+1/2, z+1/2, -x
152 -y+1/2, -z+1/2, x
153 z+1/2, x+1/2, y
154 z+1/2, -x+1/2, -y
155 -z+1/2, x+1/2, -y
156 -z+1/2, -x+1/2, y
157 -y+1/2, -x+1/2, -z
158 -y+1/2, x+1/2, z
159 y+1/2, -x+1/2, z
160 y+1/2, x+1/2, -z
161 -x+1/2, -z+1/2, -y
162 -x+1/2, z+1/2, y
163 x+1/2, -z+1/2, y
164 x+1/2, z+1/2, -y
165 -z+1/2, -y+1/2, -x
166 -z+1/2, y+1/2, x
167 z+1/2, -y+1/2, x
168 z+1/2, y+1/2, -x
169 -x+1/2, -y+1/2, -z
170 -x+1/2, y+1/2, z
171 x+1/2, -y+1/2, z
172 x+1/2, y+1/2, -z
173 -y+1/2, -z+1/2, -x
174 -y+1/2, z+1/2, x
175 y+1/2, -z+1/2, x
176 y+1/2, z+1/2, -x
177 -z+1/2, -x+1/2, -y
178 -z+1/2, x+1/2, y
179 z+1/2, -x+1/2, y
180 z+1/2, x+1/2, -y
181 y+1/2, x+1/2, z
182 y+1/2, -x+1/2, -z
183 -y+1/2, x+1/2, -z
184 -y+1/2, -x+1/2, z
185 x+1/2, z+1/2, y
186 x+1/2, -z+1/2, -y
187 -x+1/2, z+1/2, -y

```

```

188 -x+1/2, -z+1/2, y
189 z+1/2, y+1/2, x
190 z+1/2, -y+1/2, -x
191 -z+1/2, y+1/2, -x
192 -z+1/2, -y+1/2, x

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mn1 Mn 4 b 0.50000 0.50000 1.00000
Mn2 Mn 24 d 0.00000 0.25000 0.25000 1.00000
Th1 Th 24 e 0.20300 0.00000 0.00000 1.00000
Mn3 Mn 32 f 0.17800 0.17800 0.17800 1.00000
Mn4 Mn 32 f 0.37800 0.37800 0.37800 1.00000

```

Th<sub>6</sub>Mn<sub>23</sub> (D<sub>8h</sub>): A23B6\_cF116\_225\_bd2f\_e - POSCAR

```

A23B6_cF116_225_bd2f_e & a, x3, x4, x5 --params=12.523, 0.203, 0.178, 0.378 &
↳ Fm-3m O_h[5] #225 (bdef*2) & cF116 & SD8_{a} & Th6Mn23 &
↳ Th6Mn23 & J. V. Florio and R. E. Rundle and A. I. Snow, Acta
↳ Cryst. 5, 445-457 (1952)

```

1.0000000000000000			
0.0000000000000000	6.261500000000000	6.261500000000000	
6.261500000000000	0.000000000000000	6.261500000000000	
6.261500000000000	6.261500000000000	0.000000000000000	
Mn	Th		
23	6		
Direct			
0.500000000000000	0.500000000000000	0.500000000000000	Mn (4b)
0.500000000000000	0.000000000000000	0.000000000000000	Mn (24d)
0.000000000000000	0.500000000000000	0.500000000000000	Mn (24d)
0.000000000000000	0.500000000000000	0.000000000000000	Mn (24d)
0.500000000000000	0.000000000000000	0.500000000000000	Mn (24d)
0.000000000000000	0.000000000000000	0.500000000000000	Mn (24d)
0.500000000000000	0.500000000000000	0.000000000000000	Mn (24d)
0.178000000000000	0.178000000000000	0.178000000000000	Mn (32f)
0.178000000000000	0.178000000000000	-0.534000000000000	Mn (32f)
-0.534000000000000	0.178000000000000	0.178000000000000	Mn (32f)
-0.178000000000000	-0.178000000000000	0.534000000000000	Mn (32f)
-0.178000000000000	-0.178000000000000	-0.178000000000000	Mn (32f)
-0.178000000000000	0.534000000000000	-0.178000000000000	Mn (32f)
0.534000000000000	-0.178000000000000	-0.178000000000000	Mn (32f)
0.378000000000000	0.378000000000000	0.378000000000000	Mn (32f)
0.378000000000000	0.378000000000000	-1.134000000000000	Mn (32f)
0.378000000000000	-1.134000000000000	0.378000000000000	Mn (32f)
-1.134000000000000	0.378000000000000	0.378000000000000	Mn (32f)
-0.378000000000000	-0.378000000000000	1.134000000000000	Mn (32f)
-0.378000000000000	-0.378000000000000	-0.378000000000000	Mn (32f)
-0.378000000000000	1.134000000000000	-0.378000000000000	Mn (32f)
1.134000000000000	-0.378000000000000	-0.378000000000000	Mn (32f)
-0.203000000000000	0.203000000000000	0.203000000000000	Th (24e)
0.203000000000000	-0.203000000000000	-0.203000000000000	Th (24e)
0.203000000000000	-0.203000000000000	0.203000000000000	Th (24e)
-0.203000000000000	0.203000000000000	-0.203000000000000	Th (24e)
0.203000000000000	0.203000000000000	-0.203000000000000	Th (24e)
-0.203000000000000	-0.203000000000000	0.203000000000000	Th (24e)

K<sub>2</sub>PtCl<sub>6</sub> (J<sub>1</sub>): A6B2C\_cF36\_225\_e\_c\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'K2PtCl6'
_chemical_formula_sum 'Cl6 K2 Pt'

loop_
_publ_author_name
'G. Engel'
_journal_name_full_name
;
Zeitschrift f{"u}r Kristallographiya
;
_journal_volume 90
_journal_year 1935
_journal_page_first 341
_journal_page_last 373
_publ_section_title
;
Die Kristallstrukturen einiger Hexachlorokomplexsalze
;

# Found in The American Mineralogist Crystal Structure Database, 2003

_aflow_title 'KS_{2}$PtCl6_{6}$ (SJ1_{1}$) Structure'
_aflow_proto 'A6B2C_cF36_225_e_c_a'
_aflow_params 'a, x_{3}'
_aflow_params_values '9.725, 0.24'
_aflow_Strukturbericht 'SJ1_{1}$'
_aflow_Pearson 'cF36'

_symmetry_space_group_name_H-M "F 4/m -3 2/m"
_symmetry_Int_Tables_number 225

_cell_length_a 9.72500
_cell_length_b 9.72500
_cell_length_c 9.72500
_cell_angle_alpha 90.00000

```

```

_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y, -z
4 -x, -y, z
5 y, z, x
6 y, -z, -x
7 -y, z, -x
8 -y, -z, x
9 z, x, y
10 z, -x, -y
11 -z, x, -y
12 -z, -x, y
13 -y, -x, -z
14 -y, x, z
15 y, -x, z
16 y, x, -z
17 -x, -z, -y
18 -x, z, y
19 x, -z, y
20 x, z, -y
21 -z, -y, -x
22 -z, y, x
23 z, -y, x
24 z, y, -x
25 -x, -y, -z
26 -x, y, z
27 x, -y, z
28 x, y, -z
29 -y, -z, -x
30 -y, z, x
31 y, -z, x
32 y, z, -x
33 -z, -x, -y
34 -z, x, y
35 z, -x, y
36 z, x, -y
37 y, x, z
38 y, -x, -z
39 -y, x, -z
40 -y, -x, z
41 x, z, y
42 x, -z, -y
43 -x, z, -y
44 -x, -z, y
45 z, y, x
46 z, -y, -x
47 -z, y, -x
48 -z, -y, x
49 x, y+1/2, z+1/2
50 x, -y+1/2, -z+1/2
51 -x, y+1/2, -z+1/2
52 -x, -y+1/2, z+1/2
53 y, z+1/2, x+1/2
54 y, -z+1/2, -x+1/2
55 -y, z+1/2, -x+1/2
56 -y, -z+1/2, x+1/2
57 z, x+1/2, y+1/2
58 z, -x+1/2, -y+1/2
59 -z, x+1/2, -y+1/2
60 -z, -x+1/2, y+1/2
61 -y, -x+1/2, -z+1/2
62 -y, x+1/2, z+1/2
63 y, -x+1/2, z+1/2
64 y, x+1/2, -z+1/2
65 -x, -z+1/2, -y+1/2
66 -x, z+1/2, y+1/2
67 x, -z+1/2, y+1/2
68 x, z+1/2, -y+1/2
69 -z, -y+1/2, -x+1/2
70 -z, y+1/2, x+1/2
71 z, -y+1/2, x+1/2
72 z, y+1/2, -x+1/2
73 -x, -y+1/2, -z+1/2
74 -x, y+1/2, z+1/2
75 x, -y+1/2, z+1/2
76 x, y+1/2, -z+1/2
77 -y, -z+1/2, -x+1/2
78 -y, z+1/2, x+1/2
79 y, -z+1/2, x+1/2
80 y, z+1/2, -x+1/2
81 -z, -x+1/2, -y+1/2
82 -z, x+1/2, y+1/2
83 z, -x+1/2, y+1/2
84 z, x+1/2, -y+1/2
85 y, x+1/2, z+1/2
86 y, -x+1/2, -z+1/2
87 -y, x+1/2, -z+1/2
88 -y, -x+1/2, z+1/2
89 x, z+1/2, y+1/2
90 x, -z+1/2, -y+1/2
91 -x, z+1/2, -y+1/2
92 -x, -z+1/2, y+1/2
93 z, y+1/2, x+1/2
94 z, -y+1/2, -x+1/2
95 -z, y+1/2, -x+1/2
96 -z, -y+1/2, x+1/2
97 x+1/2, y, z+1/2
98 x+1/2, -y, -z+1/2
99 -x+1/2, y, -z+1/2

```

```

100 -x+1/2, -y, z+1/2
101 y+1/2, z, x+1/2
102 y+1/2, -z, -x+1/2
103 -y+1/2, z, -x+1/2
104 -y+1/2, -z, x+1/2
105 z+1/2, x, y+1/2
106 z+1/2, -x, -y+1/2
107 -z+1/2, x, -y+1/2
108 -z+1/2, -x, y+1/2
109 -y+1/2, -x, -z+1/2
110 -y+1/2, x, z+1/2
111 y+1/2, -x, z+1/2
112 y+1/2, x, -z+1/2
113 -x+1/2, -z, -y+1/2
114 -x+1/2, z, y+1/2
115 x+1/2, -z, y+1/2
116 x+1/2, z, -y+1/2
117 -z+1/2, -y, -x+1/2
118 -z+1/2, y, x+1/2
119 z+1/2, -y, x+1/2
120 z+1/2, y, -x+1/2
121 -x+1/2, -y, -z+1/2
122 -x+1/2, y, z+1/2
123 x+1/2, -y, z+1/2
124 x+1/2, y, -z+1/2
125 -y+1/2, -z, -x+1/2
126 -y+1/2, z, x+1/2
127 y+1/2, -z, x+1/2
128 y+1/2, z, -x+1/2
129 -z+1/2, -x, -y+1/2
130 -z+1/2, x, y+1/2
131 z+1/2, -x, y+1/2
132 z+1/2, x, -y+1/2
133 y+1/2, x, z+1/2
134 y+1/2, -x, -z+1/2
135 -y+1/2, x, -z+1/2
136 -y+1/2, -x, z+1/2
137 x+1/2, z, y+1/2
138 x+1/2, -z, -y+1/2
139 -x+1/2, z, -y+1/2
140 -x+1/2, -z, y+1/2
141 z+1/2, y, x+1/2
142 z+1/2, -y, -x+1/2
143 -z+1/2, y, -x+1/2
144 -z+1/2, -y, x+1/2
145 x+1/2, y+1/2, z
146 x+1/2, -y+1/2, -z
147 -x+1/2, y+1/2, -z
148 -x+1/2, -y+1/2, z
149 y+1/2, z+1/2, x
150 y+1/2, -z+1/2, -x
151 -y+1/2, z+1/2, -x
152 -y+1/2, -z+1/2, x
153 z+1/2, x+1/2, y
154 z+1/2, -x+1/2, -y
155 -z+1/2, x+1/2, -y
156 -z+1/2, -x+1/2, y
157 -y+1/2, -x+1/2, -z
158 -y+1/2, x+1/2, z
159 y+1/2, -x+1/2, z
160 y+1/2, x+1/2, -z
161 -x+1/2, -z+1/2, -y
162 -x+1/2, z+1/2, y
163 x+1/2, -z+1/2, y
164 x+1/2, z+1/2, -y
165 -z+1/2, -y+1/2, -x
166 -z+1/2, y+1/2, x
167 z+1/2, -y+1/2, x
168 z+1/2, y+1/2, -x
169 -x+1/2, -y+1/2, -z
170 -x+1/2, y+1/2, z
171 x+1/2, -y+1/2, z
172 x+1/2, y+1/2, -z
173 -y+1/2, -z+1/2, -x
174 -y+1/2, z+1/2, x
175 y+1/2, -z+1/2, x
176 y+1/2, z+1/2, -x
177 -z+1/2, -x+1/2, -y
178 -z+1/2, x+1/2, y
179 z+1/2, -x+1/2, y
180 z+1/2, x+1/2, -y
181 y+1/2, x+1/2, z
182 y+1/2, -x+1/2, -z
183 -y+1/2, x+1/2, -z
184 -y+1/2, -x+1/2, z
185 x+1/2, z+1/2, y
186 x+1/2, -z+1/2, -y
187 -x+1/2, z+1/2, -y
188 -x+1/2, -z+1/2, y
189 z+1/2, y+1/2, x
190 z+1/2, -y+1/2, -x
191 -z+1/2, y+1/2, -x
192 -z+1/2, -y+1/2, x

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Pt1 Pt 4 a 0.00000 0.00000 1.00000
K1 K 8 c 0.25000 0.25000 0.25000 1.00000

```

CI1 CI 24 e 0.24000 0.00000 0.00000 1.00000

K<sub>2</sub>PtCl<sub>6</sub> (J1): A6B2C\_cF36\_225\_e\_c\_a - POSCAR

```
A6B2C_cF36_225_e_c_a & a,x3 --params=9.725,0.24 & Fm-3m O_h^{5} #225 (
↪ ace) & cF36 & SJ1_11$ & K2PtCl6 & K2PtCl6 & G. Engel, Z.
↪ Kristallogr. 90, 341-373 (1935)
1.0000000000000000
0.0000000000000000 4.862500000000000 4.862500000000000
4.862500000000000 0.000000000000000 4.862500000000000
4.862500000000000 4.862500000000000 0.000000000000000
Cl K Pt
6 2 1
Direct
-0.240000000000000 0.240000000000000 0.240000000000000 Cl (24e)
0.240000000000000 -0.240000000000000 -0.240000000000000 Cl (24e)
0.240000000000000 -0.240000000000000 0.240000000000000 Cl (24e)
-0.240000000000000 0.240000000000000 -0.240000000000000 Cl (24e)
0.240000000000000 0.240000000000000 -0.240000000000000 Cl (24e)
-0.240000000000000 -0.240000000000000 0.240000000000000 Cl (24e)
0.250000000000000 0.250000000000000 0.250000000000000 K (8c)
0.750000000000000 0.750000000000000 0.750000000000000 K (8c)
0.000000000000000 0.000000000000000 0.000000000000000 Pt (4a)
```

NaZn<sub>13</sub> (D23): AB13\_cF112\_226\_a\_bi - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral ''
_chemical_formula_sum 'Na Zn13'

loop_
_publ_author_name
'D. P. Shoemaker'
'R. E. Marsh'
'F. J. Ewing'
'L. Pauling'
_journal_name_full_name
;
Acta Crystallographica
;
_journal_volume 5
_journal_year 1952
_journal_page_first 637
_journal_page_last 644
_publ_section_title
;
Interatomic distances and atomic valences in NaZn_{13}$
;
_aflow_title 'NaZn_{13}$ (SD2_{3}$) Structure '
_aflow_proto 'AB13_cF112_226_a_bi'
_aflow_params 'a,y_{3},z_{3}'
_aflow_params_values '12.2836 , 0.1806 , 0.1192 '
_aflow_Strukturbericht 'SD2_{3}$'
_aflow_Pearson 'cF112'

_symmetry_space_group_name_H-M "F 4/m -3 2/c"
_symmetry_Int_Tables_number 226

_cell_length_a 12.28360
_cell_length_b 12.28360
_cell_length_c 12.28360
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 -y+1/2,-x+1/2,-z+1/2
14 -y+1/2,x+1/2,z+1/2
15 y+1/2,-x+1/2,z+1/2
16 y+1/2,x+1/2,-z+1/2
17 -x+1/2,-z+1/2,-y+1/2
18 -x+1/2,z+1/2,y+1/2
19 x+1/2,-z+1/2,y+1/2
20 x+1/2,z+1/2,-y+1/2
21 -z+1/2,-y+1/2,-x+1/2
22 -z+1/2,y+1/2,x+1/2
23 z+1/2,-y+1/2,x+1/2
24 z+1/2,y+1/2,-x+1/2
25 -x,-y,-z
26 -x,y,z
27 x,-y,z
28 x,y,-z
29 -y,-z,-x
30 -y,z,x
31 y,-z,x
32 y,z,-x
33 -z,-x,-y
```

```
34 -z,x,y
35 z,-x,y
36 z,x,-y
37 y+1/2,x+1/2,z+1/2
38 y+1/2,-x+1/2,-z+1/2
39 -y+1/2,x+1/2,-z+1/2
40 -y+1/2,-x+1/2,z+1/2
41 x+1/2,z+1/2,y+1/2
42 x+1/2,-z+1/2,-y+1/2
43 -x+1/2,z+1/2,-y+1/2
44 -x+1/2,-z+1/2,y+1/2
45 z+1/2,y+1/2,x+1/2
46 z+1/2,-y+1/2,-x+1/2
47 -z+1/2,y+1/2,-x+1/2
48 -z+1/2,-y+1/2,x+1/2
49 x,y+1/2,z+1/2
50 x,-y+1/2,-z+1/2
51 -x,y+1/2,-z+1/2
52 -x,-y+1/2,z+1/2
53 y,z+1/2,x+1/2
54 y,-z+1/2,-x+1/2
55 -y,z+1/2,-x+1/2
56 -y,-z+1/2,x+1/2
57 z,x+1/2,y+1/2
58 z,-x+1/2,-y+1/2
59 -z,x+1/2,-y+1/2
60 -z,-x+1/2,y+1/2
61 -y+1/2,-x,-z
62 -y+1/2,x,z
63 y+1/2,-x,z
64 y+1/2,x,-z
65 -x+1/2,-z,-y
66 -x+1/2,z,y
67 x+1/2,-z,y
68 x+1/2,z,-y
69 -z+1/2,-y,-x
70 -z+1/2,y,x
71 z+1/2,-y,x
72 z+1/2,y,-x
73 -x,-y+1/2,-z+1/2
74 -x,y+1/2,z+1/2
75 x,-y+1/2,z+1/2
76 x,y+1/2,-z+1/2
77 -y,-z+1/2,-x+1/2
78 -y,z+1/2,x+1/2
79 y,-z+1/2,x+1/2
80 y,z+1/2,-x+1/2
81 -z,-x+1/2,-y+1/2
82 -z,x+1/2,y+1/2
83 z,-x+1/2,y+1/2
84 z,x+1/2,-y+1/2
85 y+1/2,x,z
86 y+1/2,-x,-z
87 -y+1/2,x,-z
88 -y+1/2,-x,z
89 x+1/2,z,y
90 x+1/2,-z,-y
91 -x+1/2,z,-y
92 -x+1/2,-z,y
93 z+1/2,y,x
94 z+1/2,-y,-x
95 -z+1/2,y,-x
96 -z+1/2,-y,x
97 x+1/2,y,z+1/2
98 x+1/2,-y,-z+1/2
99 -x+1/2,y,-z+1/2
100 -x+1/2,-y,z+1/2
101 y+1/2,z,x+1/2
102 y+1/2,-z,-x+1/2
103 -y+1/2,z,-x+1/2
104 -y+1/2,-z,x+1/2
105 z+1/2,x,y+1/2
106 z+1/2,-x,-y+1/2
107 -z+1/2,x,-y+1/2
108 -z+1/2,-x,y+1/2
109 -y,-x+1/2,-z
110 -y,x+1/2,z
111 y,-x+1/2,z
112 y,x+1/2,-z
113 -x,-z+1/2,-y
114 -x,z+1/2,y
115 x,-z+1/2,y
116 x,z+1/2,-y
117 -z,-y+1/2,-x
118 -z,y+1/2,x
119 z,-y+1/2,x
120 z,y+1/2,-x
121 -x+1/2,-y,-z+1/2
122 -x+1/2,y,z+1/2
123 x+1/2,-y,z+1/2
124 x+1/2,y,-z+1/2
125 -y+1/2,-z,-x+1/2
126 -y+1/2,z,x+1/2
127 y+1/2,-z,x+1/2
128 y+1/2,z,-x+1/2
129 -z+1/2,-x,-y+1/2
130 -z+1/2,x,y+1/2
131 z+1/2,-x,y+1/2
132 z+1/2,x,-y+1/2
133 y,x+1/2,z
134 y,-x+1/2,-z
135 -y,x+1/2,-z
136 -y,-x+1/2,z
137 x,z+1/2,y
138 x,-z+1/2,-y
```



```

139 -x, z+1/2, -y
140 -x, -z+1/2, y
141 z, y+1/2, x
142 z, -y+1/2, -x
143 -z, y+1/2, -x
144 -z, -y+1/2, x
145 x+1/2, y+1/2, z
146 x+1/2, -y+1/2, -z
147 -x+1/2, y+1/2, -z
148 -x+1/2, -y+1/2, z
149 y+1/2, z+1/2, x
150 y+1/2, -z+1/2, -x
151 -y+1/2, z+1/2, -x
152 -y+1/2, -z+1/2, x
153 z+1/2, x+1/2, y
154 z+1/2, -x+1/2, -y
155 -z+1/2, x+1/2, -y
156 -z+1/2, -x+1/2, y
157 -y, -x, -z+1/2
158 -y, x, z+1/2
159 y, -x, z+1/2
160 y, x, -z+1/2
161 -x, -z, -y+1/2
162 -x, z, y+1/2
163 x, -z, y+1/2
164 x, z, -y+1/2
165 -z, -y, -x+1/2
166 -z, y, x+1/2
167 z, -y, x+1/2
168 z, y, -x+1/2
169 -x+1/2, -y+1/2, -z
170 -x+1/2, y+1/2, z
171 x+1/2, -y+1/2, z
172 x+1/2, y+1/2, -z
173 -y+1/2, -z+1/2, -x
174 -y+1/2, z+1/2, x
175 y+1/2, -z+1/2, x
176 y+1/2, z+1/2, -x
177 -z+1/2, -x+1/2, -y
178 -z+1/2, x+1/2, y
179 z+1/2, -x+1/2, y
180 z+1/2, x+1/2, -y
181 y, x, z+1/2
182 y, -x, -z+1/2
183 -y, x, -z+1/2
184 -y, -x, z+1/2
185 x, z, y+1/2
186 x, -z, -y+1/2
187 -x, z, -y+1/2
188 -x, -z, y+1/2
189 z, y, x+1/2
190 z, -y, -x+1/2
191 -z, y, -x+1/2
192 -z, -y, x+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Na1 Na 8 a 0.25000 0.25000 0.25000 1.00000
Zn1 Zn 8 b 0.00000 0.00000 0.00000 1.00000
Zn2 Zn 96 i 0.00000 0.18060 0.11920 1.00000

```

NaZn13 (D23): AB13\_cF112\_226\_a\_bi - POSCAR

```

AB13_cF112_226_a_bi & a, y3, z3 --params=12.2836, 0.1806, 0.1192 & Fm-3c O_{
↪ h)^{6} #226 (abi) & cF112 & SD2_{3}$ & NaZn13 & & D. P.
↪ Shoemaker et al., Acta Cryst. 5, 637-644 (1952)
1.0000000000000000
0.0000000000000000 6.141800000000000 6.141800000000000
6.141800000000000 0.000000000000000 6.141800000000000
6.141800000000000 6.141800000000000 0.000000000000000
Na Zn
2 26
Direct
0.250000000000000 0.250000000000000 0.250000000000000 Na (8a)
0.750000000000000 0.750000000000000 0.750000000000000 Na (8a)
0.000000000000000 0.000000000000000 0.000000000000000 Zn (8b)
0.500000000000000 0.500000000000000 0.500000000000000 Zn (8b)
0.299800000000000 -0.061400000000000 0.061400000000000 Zn (96i)
-0.061400000000000 0.299800000000000 -0.299800000000000 Zn (96i)
0.061400000000000 -0.299800000000000 0.299800000000000 Zn (96i)
-0.299800000000000 0.061400000000000 -0.061400000000000 Zn (96i)
0.061400000000000 0.299800000000000 -0.299800000000000 Zn (96i)
-0.299800000000000 -0.061400000000000 0.299800000000000 Zn (96i)
0.299800000000000 -0.061400000000000 -0.299800000000000 Zn (96i)
-0.061400000000000 -0.299800000000000 0.061400000000000 Zn (96i)
-0.061400000000000 0.061400000000000 0.299800000000000 Zn (96i)
0.299800000000000 -0.299800000000000 -0.061400000000000 Zn (96i)
-0.299800000000000 0.299800000000000 0.061400000000000 Zn (96i)
0.061400000000000 -0.061400000000000 -0.299800000000000 Zn (96i)
0.200200000000000 0.561400000000000 0.799800000000000 Zn (96i)
0.561400000000000 0.200200000000000 0.438600000000000 Zn (96i)
0.438600000000000 0.799800000000000 0.561400000000000 Zn (96i)
0.799800000000000 0.438600000000000 0.200200000000000 Zn (96i)
0.438600000000000 0.200200000000000 0.799800000000000 Zn (96i)
0.799800000000000 0.561400000000000 0.438600000000000 Zn (96i)
0.200200000000000 0.438600000000000 0.561400000000000 Zn (96i)
0.561400000000000 0.799800000000000 0.200200000000000 Zn (96i)
0.561400000000000 0.438600000000000 0.799800000000000 Zn (96i)

```

```

0.200200000000000 0.799800000000000 0.438600000000000 Zn (96i)
0.799800000000000 0.200200000000000 0.561400000000000 Zn (96i)
0.438600000000000 0.561400000000000 0.200200000000000 Zn (96i)

```

Pyrochlore Iridate (Eu2Ir2O7): A2B2C7\_cF88\_227\_c\_d\_af - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Pyrochlore Iridate'
_chemical_formula_sum 'Eu2 Ir2 O7'

loop_
_publ_author_name
'H. Sagayama'
'D. Uematsu'
'T. Arima'
'K. Sugimoto'
'J. J. Ishikawa'
'E. O'Farrell'
'S. Nakatsuji'
_journal_name_full_name
;
Physical Review B
;
_journal_volume 87
_journal_year 2013
_journal_page_first 100403
_journal_page_last 100403
_publ_section_title
;
Determination of long-range all-in-all ordering of IrS^{4+}$
↪ moments in a pyrochlore iridate Eu_{2}$Ir_{2}$S_{7}$ by
↪ resonant x-ray diffraction
;

# Found in Magnetic Excitations across the Metal-Insulator Transition in
↪ the Pyrochlore Iridate Eu_{2}$Ir_{2}$S_{7}$, 2018

_aflow_title 'Pyrochlore Iridate (Eu_{2}$Ir_{2}$S_{7}$) Structure'
_aflow_proto 'A2B2C7_cF88_227_c_d_af'
_aflow_params 'a, x_{4}'
_aflow_params_values '10.2663, 0.4157'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cF88'

_symmetry_space_group_name_H-M 'F d -3 m:2'
_symmetry_Int_Tables_number 227

_cell_length_a 10.26630
_cell_length_b 10.26630
_cell_length_c 10.26630
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y+1/4, -z+1/4
3 -x+1/4, y, -z+1/4
4 -x+1/4, -y+1/4, z
5 y, z, x
6 y, -z+1/4, -x+1/4
7 -y+1/4, z, -x+1/4
8 -y+1/4, -z+1/4, x
9 z, x, y
10 z, -x+1/4, -y+1/4
11 -z+1/4, x, -y+1/4
12 -z+1/4, -x+1/4, y
13 -y, -x, -z
14 -y, x+1/4, z+1/4
15 y+1/4, -x, z+1/4
16 y+1/4, x+1/4, -z
17 -x, -z, -y
18 -x, z+1/4, y+1/4
19 x+1/4, -z, y+1/4
20 x+1/4, z+1/4, -y
21 -z, -y, -x
22 -z, y+1/4, x+1/4
23 z+1/4, -y, x+1/4
24 z+1/4, y+1/4, -x
25 -x, -y, -z
26 -x, y+1/4, z+1/4
27 x+1/4, -y, z+1/4
28 x+1/4, y+1/4, -z
29 -y, -z, -x
30 -y, z+1/4, x+1/4
31 y+1/4, -z, x+1/4
32 y+1/4, z+1/4, -x
33 -z, -x, -y
34 -z, x+1/4, y+1/4
35 z+1/4, -x, y+1/4
36 z+1/4, x+1/4, -y
37 y, x, z
38 y, -x+1/4, -z+1/4
39 -y+1/4, x, -z+1/4
40 -y+1/4, -x+1/4, z
41 x, z, y
42 x, -z+1/4, -y+1/4
43 -x+1/4, z, -y+1/4
44 -x+1/4, -z+1/4, y
45 z, y, x

```

```

46 z,-y+1/4,-x+1/4
47 -z+1/4,y,-x+1/4
48 -z+1/4,-y+1/4,x
49 x,y+1/2,z+1/2
50 x,-y+3/4,-z+3/4
51 -x+1/4,y+1/2,-z+3/4
52 -x+1/4,-y+3/4,z+1/2
53 y,z+1/2,x+1/2
54 y,-z+3/4,-x+3/4
55 -y+1/4,z+1/2,-x+3/4
56 -y+1/4,-z+3/4,x+1/2
57 z,x+1/2,y+1/2
58 z,-x+3/4,-y+3/4
59 -z+1/4,x+1/2,-y+3/4
60 -z+1/4,-x+3/4,y+1/2
61 -y,-x+1/2,-z+1/2
62 -y,x+3/4,z+3/4
63 y+1/4,-x+1/2,z+3/4
64 y+1/4,x+3/4,-z+1/2
65 -x,-z+1/2,-y+1/2
66 -x,z+3/4,y+3/4
67 x+1/4,-z+1/2,y+3/4
68 x+1/4,z+3/4,-y+1/2
69 -z,-y+1/2,-x+1/2
70 -z,y+3/4,x+3/4
71 z+1/4,-y+1/2,x+3/4
72 z+1/4,y+3/4,-x+1/2
73 -x,-y+1/2,-z+1/2
74 -x,y+3/4,z+3/4
75 x+1/4,-y+1/2,z+3/4
76 x+1/4,y+3/4,-z+1/2
77 -y,-z+1/2,-x+1/2
78 -y,z+3/4,x+3/4
79 y+1/4,-z+1/2,x+3/4
80 y+1/4,z+3/4,-x+1/2
81 -z,-x+1/2,-y+1/2
82 -z,x+3/4,y+3/4
83 z+1/4,-x+1/2,y+3/4
84 z+1/4,x+3/4,-y+1/2
85 y,x+1/2,z+1/2
86 y,-x+3/4,-z+3/4
87 -y+1/4,x+1/2,-z+3/4
88 -y+1/4,-x+3/4,z+1/2
89 x,z+1/2,y+1/2
90 x,-z+3/4,-y+3/4
91 -x+1/4,z+1/2,-y+3/4
92 -x+1/4,-z+3/4,y+1/2
93 z,y+1/2,x+1/2
94 z,-y+3/4,-x+3/4
95 -z+1/4,y+1/2,-x+3/4
96 -z+1/4,-y+3/4,x+1/2
97 x+1/2,y,z+1/2
98 x+1/2,-y+1/4,-z+3/4
99 -x+3/4,y,-z+3/4
100 -x+3/4,-y+1/4,z+1/2
101 y+1/2,z,x+1/2
102 y+1/2,-z+1/4,-x+3/4
103 -y+3/4,z,-x+3/4
104 -y+3/4,-z+1/4,x+1/2
105 z+1/2,x,y+1/2
106 z+1/2,-x+1/4,-y+3/4
107 -z+3/4,x,-y+3/4
108 -z+3/4,-x+1/4,y+1/2
109 -y+1/2,-x,-z+1/2
110 -y+1/2,x+1/4,z+3/4
111 y+3/4,-x,z+3/4
112 y+3/4,x+1/4,-z+1/2
113 -x+1/2,-z,-y+1/2
114 -x+1/2,z+1/4,y+3/4
115 x+3/4,-z,y+3/4
116 x+3/4,z+1/4,-y+1/2
117 -z+1/2,-y,-x+1/2
118 -z+1/2,y+1/4,x+3/4
119 z+3/4,-y,x+3/4
120 z+3/4,y+1/4,-x+1/2
121 -x+1/2,-y,-z+1/2
122 -x+1/2,y+1/4,z+3/4
123 x+3/4,-y,z+3/4
124 x+3/4,y+1/4,-z+1/2
125 -y+1/2,-z,-x+1/2
126 -y+1/2,z+1/4,x+3/4
127 y+3/4,-z,x+3/4
128 y+3/4,z+1/4,-x+1/2
129 -z+1/2,-x,-y+1/2
130 -z+1/2,x+1/4,y+3/4
131 z+3/4,-x,y+3/4
132 z+3/4,x+1/4,-y+1/2
133 y+1/2,x,z+1/2
134 y+1/2,-x+1/4,-z+3/4
135 -y+3/4,x,-z+3/4
136 -y+3/4,-x+1/4,z+1/2
137 x+1/2,z,y+1/2
138 x+1/2,-z+1/4,-y+3/4
139 -x+3/4,z,-y+3/4
140 -x+3/4,-z+1/4,y+1/2
141 z+1/2,y,x+1/2
142 z+1/2,-y+1/4,-x+3/4
143 -z+3/4,y,-x+3/4
144 -z+3/4,-y+1/4,x+1/2
145 x+1/2,y+1/2,z
146 x+1/2,-y+3/4,-z+1/4
147 -x+3/4,y+1/2,-z+1/4
148 -x+3/4,-y+3/4,z
149 y+1/2,z+1/2,x
150 y+1/2,-z+3/4,-x+1/4

```

```

151 -y+3/4,z+1/2,-x+1/4
152 -y+3/4,-z+3/4,x
153 z+1/2,x+1/2,y
154 z+1/2,-x+3/4,-y+1/4
155 -z+3/4,x+1/2,-y+1/4
156 -z+3/4,-x+3/4,y
157 -y+1/2,-x+1/2,-z
158 -y+1/2,x+3/4,z+1/4
159 y+3/4,-x+1/2,z+1/4
160 y+3/4,x+3/4,-z
161 -x+1/2,-z+1/2,-y
162 -x+1/2,z+3/4,y+1/4
163 x+3/4,-z+1/2,y+1/4
164 x+3/4,z+3/4,-y
165 -z+1/2,-y+1/2,-x
166 -z+1/2,y+3/4,x+1/4
167 z+3/4,-y+1/2,x+1/4
168 z+3/4,y+3/4,-x
169 -x+1/2,-y+1/2,-z
170 -x+1/2,y+3/4,z+1/4
171 x+3/4,-y+1/2,z+1/4
172 x+3/4,y+3/4,-z
173 -y+1/2,-z+1/2,-x
174 -y+1/2,z+3/4,x+1/4
175 y+3/4,-z+1/2,x+1/4
176 y+3/4,z+3/4,-x
177 -z+1/2,-x+1/2,-y
178 -z+1/2,x+3/4,y+1/4
179 z+3/4,-x+1/2,y+1/4
180 z+3/4,x+3/4,-y
181 y+1/2,x+1/2,z
182 y+1/2,-x+3/4,-z+1/4
183 -y+3/4,x+1/2,-z+1/4
184 -y+3/4,-x+3/4,z
185 x+1/2,z+1/2,y
186 x+1/2,-z+3/4,-y+1/4
187 -x+3/4,z+1/2,-y+1/4
188 -x+3/4,-z+3/4,y
189 z+1/2,y+1/2,x
190 z+1/2,-y+3/4,-x+1/4
191 -z+3/4,y+1/2,-x+1/4
192 -z+3/4,-y+3/4,x

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
O1 O 8 a 0.12500 0.12500 0.12500 1.00000
Eu1 Eu 16 c 0.00000 0.00000 0.00000 1.00000
Ir1 Ir 16 d 0.50000 0.50000 0.50000 1.00000
O2 O 48 f 0.41570 0.12500 0.12500 1.00000

```

Pyrochlore Iridate (Eu<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>): A2B2C7\_cF88\_227\_c\_d\_af - POSCAR

```

A2B2C7_cF88_227_c_d_af & a,x4 --params=10.2663,0.4157 & Fd-3m O_{h}^{(7)}
↳ #227 (acfd) & cF88 & None & Eu2Ir2O7 & Pyrochlore Iridate & H.
↳ Sagayama et al., Phys. Rev. B 87, 100403(2013)
1.0000000000000000
0.0000000000000000 5.133150000000000 5.133150000000000
5.133150000000000 0.000000000000000 5.133150000000000
5.133150000000000 5.133150000000000 0.000000000000000
Eu Ir O
4 4 14
Direct
0.000000000000000 0.000000000000000 0.000000000000000 Eu (16c)
0.000000000000000 0.000000000000000 0.500000000000000 Eu (16c)
0.000000000000000 0.500000000000000 0.000000000000000 Eu (16c)
0.500000000000000 0.000000000000000 0.000000000000000 Eu (16c)
0.500000000000000 0.500000000000000 0.500000000000000 Ir (16d)
0.500000000000000 0.500000000000000 0.000000000000000 Ir (16d)
0.500000000000000 0.000000000000000 0.500000000000000 Ir (16d)
0.000000000000000 0.500000000000000 0.500000000000000 Ir (16d)
0.125000000000000 0.125000000000000 0.125000000000000 O (8a)
0.875000000000000 0.875000000000000 0.875000000000000 O (8a)
-0.165700000000000 0.415700000000000 0.415700000000000 O (48f)
0.415700000000000 -0.165700000000000 -0.165700000000000 O (48f)
0.415700000000000 -0.165700000000000 0.415700000000000 O (48f)
-0.165700000000000 0.415700000000000 -0.165700000000000 O (48f)
0.415700000000000 0.415700000000000 -0.165700000000000 O (48f)
-0.165700000000000 -0.165700000000000 0.415700000000000 O (48f)
1.165700000000000 -0.415700000000000 1.165700000000000 O (48f)
-0.415700000000000 1.165700000000000 -0.415700000000000 O (48f)
-0.415700000000000 1.165700000000000 1.165700000000000 O (48f)
1.165700000000000 -0.415700000000000 -0.415700000000000 O (48f)

```

Spinel (Co<sub>3</sub>O<sub>4</sub>, D<sub>72</sub>): A3B4\_cF56\_227\_ad\_e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Spinel'
_chemical_formula_sum 'Co3 O4'

loop_
_publ_author_name
'O. Knop'
'K. I. G. Reid'

```

```

'Sutarno'
'Y. Nakagawa'
_journal_name_full_name
;
Canadian Journal of Chemistry
;
_journal_volume 46
_journal_year 1968
_journal_page_first 3463
_journal_page_last 3476
_publ_section_title
;
Chalkogenides of the transition elements. VI. X-Ray, neutron, and
  ↳ magnetic investigation of the spinels  $\text{Co}_3\text{SOS}_4$ ,  $\text{NiCo}_2\text{SOS}_4$ 
  ↳  $2\text{SOS}_4$ ,  $\text{Co}_3\text{SSS}_4$ , and  $\text{NiCo}_2\text{SSS}_4$ 
;
_aflow_title 'Spinel ( $\text{Co}_3\text{SOS}_4$ ),  $\text{SD7}_2$ ) Structure'
_aflow_proto 'A3B4_cF56_227_ad_e'
_aflow_params 'a_x_{3}'
_aflow_params_values '8.0835, 0.2642'
_aflow_Strukturbericht 'SD7_{2}'
_aflow_Pearson 'cF56'
;
_symmetry_space_group_name_H-M "F d -3 m:2"
_symmetry_Int_Tables_number 227
;
_cell_length_a 8.08350
_cell_length_b 8.08350
_cell_length_c 8.08350
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000
;
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y+1/4, -z+1/4
3 -x+1/4, y, -z+1/4
4 -x+1/4, -y+1/4, z
5 y, z, x
6 y, -z+1/4, -x+1/4
7 -y+1/4, z, -x+1/4
8 -y+1/4, -z+1/4, x
9 z, x, y
10 z, -x+1/4, -y+1/4
11 -z+1/4, x, -y+1/4
12 -z+1/4, -x+1/4, y
13 -y, -x, -z
14 -y, x+1/4, z+1/4
15 y+1/4, -x, z+1/4
16 y+1/4, x+1/4, -z
17 -x, -z, -y
18 -x, z+1/4, y+1/4
19 x+1/4, -z, y+1/4
20 x+1/4, z+1/4, -y
21 -z, -y, -x
22 -z, y+1/4, x+1/4
23 z+1/4, -y, x+1/4
24 z+1/4, y+1/4, -x
25 -x, -y, -z
26 -x, y+1/4, z+1/4
27 x+1/4, -y, z+1/4
28 x+1/4, y+1/4, -z
29 -y, -z, -x
30 -y, z+1/4, x+1/4
31 y+1/4, -z, x+1/4
32 y+1/4, z+1/4, -x
33 -z, -x, -y
34 -z, x+1/4, y+1/4
35 z+1/4, -x, y+1/4
36 z+1/4, x+1/4, -y
37 y, x, z
38 y, -x+1/4, -z+1/4
39 -y+1/4, x, -z+1/4
40 -y+1/4, -x+1/4, z
41 x, z, y
42 x, -z+1/4, -y+1/4
43 -x+1/4, z, -y+1/4
44 -x+1/4, -z+1/4, y
45 z, y, x
46 z, -y+1/4, -x+1/4
47 -z+1/4, y, -x+1/4
48 -z+1/4, -y+1/4, x
49 x, y+1/2, z+1/2
50 x, -y+3/4, -z+3/4
51 -x+1/4, y+1/2, -z+3/4
52 -x+1/4, -y+3/4, z+1/2
53 y, z+1/2, x+1/2
54 y, -z+3/4, -x+3/4
55 -y+1/4, z+1/2, -x+3/4
56 -y+1/4, -z+3/4, x+1/2
57 z, x+1/2, y+1/2
58 z, -x+3/4, -y+3/4
59 -z+1/4, x+1/2, -y+3/4
60 -z+1/4, -x+3/4, y+1/2
61 -y, -x+1/2, -z+1/2
62 -y, x+3/4, z+3/4
63 y+1/4, -x+1/2, z+3/4
64 y+1/4, x+3/4, -z+1/2
65 -x, -z+1/2, -y+1/2
66 -x, z+3/4, y+3/4
67 x+1/4, -z+1/2, y+3/4
68 x+1/4, z+3/4, -y+1/2

```

```

69 -z, -y+1/2, -x+1/2
70 -z, y+3/4, x+3/4
71 z+1/4, -y+1/2, x+3/4
72 z+1/4, y+3/4, -x+1/2
73 -x, -y+1/2, -z+1/2
74 -x, y+3/4, z+3/4
75 x+1/4, -y+1/2, z+3/4
76 x+1/4, y+3/4, -z+1/2
77 -y, -z+1/2, -x+1/2
78 -y, z+3/4, x+3/4
79 y+1/4, -z+1/2, x+3/4
80 y+1/4, z+3/4, -x+1/2
81 -z, -x+1/2, -y+1/2
82 -z, x+3/4, y+3/4
83 z+1/4, -x+1/2, y+3/4
84 z+1/4, x+3/4, -y+1/2
85 y, x+1/2, z+1/2
86 y, -x+3/4, -z+3/4
87 -y+1/4, x+1/2, -z+3/4
88 -y+1/4, -x+3/4, z+1/2
89 x, z+1/2, y+1/2
90 x, -z+3/4, -y+3/4
91 -x+1/4, z+1/2, -y+3/4
92 -x+1/4, -z+3/4, y+1/2
93 z, y+1/2, x+1/2
94 z, -y+3/4, -x+3/4
95 -z+1/4, y+1/2, -x+3/4
96 -z+1/4, -y+3/4, x+1/2
97 x+1/2, y, z+1/2
98 x+1/2, -y+1/4, -z+3/4
99 -x+3/4, y, -z+3/4
100 -x+3/4, -y+1/4, z+1/2
101 y+1/2, z, x+1/2
102 y+1/2, -z+1/4, -x+3/4
103 -y+3/4, z, -x+3/4
104 -y+3/4, -z+1/4, x+1/2
105 z+1/2, x, y+1/2
106 z+1/2, -x+1/4, -y+3/4
107 -z+3/4, x, -y+3/4
108 -z+3/4, -x+1/4, y+1/2
109 -y+1/2, -x, -z+1/2
110 -y+1/2, x+1/4, z+3/4
111 y+3/4, -x, z+3/4
112 y+3/4, x+1/4, -z+1/2
113 -x+1/2, -z, -y+1/2
114 -x+1/2, z+1/4, y+3/4
115 x+3/4, -z, y+3/4
116 x+3/4, z+1/4, -y+1/2
117 -z+1/2, -y, -x+1/2
118 -z+1/2, y+1/4, x+3/4
119 z+3/4, -y, x+3/4
120 z+3/4, y+1/4, -x+1/2
121 -x+1/2, -y, -z+1/2
122 -x+1/2, y+1/4, z+3/4
123 x+3/4, -y, z+3/4
124 x+3/4, y+1/4, -z+1/2
125 -y+1/2, -z, -x+1/2
126 -y+1/2, z+1/4, x+3/4
127 y+3/4, -z, x+3/4
128 y+3/4, z+1/4, -x+1/2
129 -z+1/2, -x, -y+1/2
130 -z+1/2, x+1/4, y+3/4
131 z+3/4, -x, y+3/4
132 z+3/4, x+1/4, -y+1/2
133 y+1/2, x, z+1/2
134 y+1/2, -x+1/4, -z+3/4
135 -y+3/4, x, -z+3/4
136 -y+3/4, -x+1/4, z+1/2
137 x+1/2, z, y+1/2
138 x+1/2, -z+1/4, -y+3/4
139 -x+3/4, z, -y+3/4
140 -x+3/4, -z+1/4, y+1/2
141 z+1/2, y, x+1/2
142 z+1/2, -y+1/4, -x+3/4
143 -z+3/4, y, -x+3/4
144 -z+3/4, -y+1/4, x+1/2
145 x+1/2, y+1/2, z
146 x+1/2, -y+3/4, -z+1/4
147 -x+3/4, y+1/2, -z+1/4
148 -x+3/4, -y+3/4, z
149 y+1/2, z+1/2, x
150 y+1/2, -z+3/4, -x+1/4
151 -y+3/4, z+1/2, -x+1/4
152 -y+3/4, -z+3/4, x
153 z+1/2, x+1/2, y
154 z+1/2, -x+3/4, -y+1/4
155 -z+3/4, x+1/2, -y+1/4
156 -z+3/4, -x+3/4, y
157 -y+1/2, -x+1/2, -z
158 -y+1/2, x+3/4, z+1/4
159 y+3/4, -x+1/2, z+1/4
160 y+3/4, x+3/4, -z
161 -x+1/2, -z+1/2, -y
162 -x+1/2, z+3/4, y+1/4
163 x+3/4, -z+1/2, y+1/4
164 x+3/4, z+3/4, -y
165 -z+1/2, -y+1/2, -x
166 -z+1/2, y+3/4, x+1/4
167 z+3/4, -y+1/2, x+1/4
168 z+3/4, y+3/4, -x
169 -x+1/2, -y+1/2, -z
170 -x+1/2, y+3/4, z+1/4
171 x+3/4, -y+1/2, z+1/4
172 x+3/4, y+3/4, -z
173 -y+1/2, -z+1/2, -x

```

```

174 -y+1/2, z+3/4, x+1/4
175 y+3/4, -z+1/2, x+1/4
176 y+3/4, z+3/4, -x
177 -z+1/2, -x+1/2, -y
178 -z+1/2, x+3/4, y+1/4
179 z+3/4, -x+1/2, y+1/4
180 z+3/4, x+3/4, -y
181 y+1/2, x+1/2, z
182 y+1/2, -x+3/4, -z+1/4
183 -y+3/4, x+1/2, -z+1/4
184 -y+3/4, -x+3/4, z
185 x+1/2, z+1/2, y
186 x+1/2, -z+3/4, -y+1/4
187 -x+3/4, z+1/2, -y+1/4
188 -x+3/4, -z+3/4, y
189 z+1/2, y+1/2, x
190 z+1/2, -y+3/4, -x+1/4
191 -z+3/4, y+1/2, -x+1/4
192 -z+3/4, -y+3/4, x

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Co1 Co 8 a 0.12500 0.12500 1.00000
Co2 Co 16 d 0.50000 0.50000 0.50000 1.00000
O1 O 32 e 0.26420 0.26420 0.26420 1.00000

```

Spinel (Co<sub>3</sub>O<sub>4</sub>, D<sub>7d</sub>): A3B4\_cF56\_227\_ad\_e - POSCAR

```

A3B4_cF56_227_ad_e & a, x3 --params=8.0835 , 0.2642 & Fd-3m O_{h}^{7} #227
↪ (ade) & cF56 & SD7_{2}$ & Co3O4 & Spinel & O. Knop et al., Can.
↪ J. Chem. 46, 3463-3476 (1968)
1.0000000000000000
0.0000000000000000 4.041750000000000 4.041750000000000
4.041750000000000 0.000000000000000 4.041750000000000
4.041750000000000 4.041750000000000 0.000000000000000
Co O
6 8
Direct
0.125000000000000 0.125000000000000 0.125000000000000 Co (8a)
0.875000000000000 0.875000000000000 0.875000000000000 Co (8a)
0.500000000000000 0.500000000000000 0.500000000000000 Co (16d)
0.500000000000000 0.500000000000000 0.000000000000000 Co (16d)
0.500000000000000 0.000000000000000 0.500000000000000 Co (16d)
0.000000000000000 0.500000000000000 0.500000000000000 Co (16d)
0.264200000000000 0.264200000000000 0.264200000000000 O (32e)
0.264200000000000 0.264200000000000 -0.292600000000000 O (32e)
0.264200000000000 -0.292600000000000 0.264200000000000 O (32e)
-0.292600000000000 0.264200000000000 0.264200000000000 O (32e)
-0.264200000000000 -0.264200000000000 1.292600000000000 O (32e)
-0.264200000000000 -0.264200000000000 -0.264200000000000 O (32e)
-0.264200000000000 1.292600000000000 -0.264200000000000 O (32e)
1.292600000000000 -0.264200000000000 -0.264200000000000 O (32e)

```

CuCrCl<sub>5</sub>[NH<sub>3</sub>]<sub>6</sub>: A5BCD6\_cF416\_228\_eg\_c\_b\_h - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM
_chemical_name_mineral 'CuCrCl5[NH3]6'
_chemical_formula_sum 'Cl5 Cr Cu N6'

loop_
_publ_author_name
'M. Masayasu'
'S. Yoshihiko'
'W. Tokunosok {\ 'e }'
_journal_name_full_name
:
Bulletin of the Chemical Society of Japan
:
_journal_volume 34
_journal_year 1961
_journal_page_first 295
_journal_page_last 296
_publ_section_title
:
The Crystal Structure of [Cr(NH3_{3}$)_{6}$] [CuCl5_{5}$]
:
# Found in Pearson's Crystal Data - Crystal Structure Database for
↪ Inorganic Compounds, 2013

_aflow_title 'CuCrCl5_{5}$[NH3_{3}$]_{6}$ Structure'
_aflow_proto 'A5BCD6_cF416_228_eg_c_b_h'
_aflow_params 'a, x_{3}, y_{4}, x_{5}, y_{5}, z_{5}'
_aflow_params_values '22.2649775014, 0.19, 0.425, 0.05, 0.18, 0.28'
_aflow_strukturbericht 'None'
_aflow_pearson 'cF416'

_cell_length_a 22.2649775014
_cell_length_b 22.2649775014
_cell_length_c 22.2649775014
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "F 41/d -3 2/c (origin choice 2)"

```

\_symmetry\_Int\_Tables\_number 228

```

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y+1/4, -z+1/4
3 -x+1/4, y, -z+1/4
4 -x+1/4, -y+1/4, z
5 y, z, x
6 y, -z+1/4, -x+1/4
7 -y+1/4, z, -x+1/4
8 -y+1/4, -z+1/4, x
9 z, x, y
10 z, -x+1/4, -y+1/4
11 -z+1/4, x, -y+1/4
12 -z+1/4, -x+1/4, y
13 -y+1/2, -x+1/2, -z+1/2
14 -y+1/2, x+1/4, z+1/4
15 y+1/4, -x+1/2, z+1/4
16 y+1/4, x+1/4, -z+1/2
17 -x+1/2, -z+1/2, -y+1/2
18 -x+1/2, z+1/4, y+1/4
19 x+1/4, -z+1/2, y+1/4
20 x+1/4, z+1/4, -y+1/2
21 -z+1/2, -y+1/2, -x+1/2
22 -z+1/2, y+1/4, x+1/4
23 z+1/4, -y+1/2, x+1/4
24 z+1/4, y+1/4, -x+1/2
25 -x, -y, -z
26 -x, y+1/4, z+1/4
27 x+1/4, -y, z+1/4
28 x+1/4, y+1/4, -z
29 -y, -z, -x
30 -y, z+1/4, x+1/4
31 y+1/4, -z, x+1/4
32 y+1/4, z+1/4, -x
33 -z, -x, -y
34 -z, x+1/4, y+1/4
35 z+1/4, -x, y+1/4
36 z+1/4, x+1/4, -y
37 y+1/2, x+1/2, z+1/2
38 y+1/2, -x+1/4, -z+1/4
39 -y+1/4, x+1/2, -z+1/4
40 -y+1/4, -x+1/4, z+1/2
41 x+1/2, z+1/2, y+1/2
42 x+1/2, -z+1/4, -y+1/4
43 -x+1/4, z+1/2, -y+1/4
44 -x+1/4, -z+1/4, y+1/2
45 z+1/2, y+1/2, x+1/2
46 z+1/2, -y+1/4, -x+1/4
47 -z+1/4, y+1/2, -x+1/4
48 -z+1/4, -y+1/4, x+1/2
49 x, y+1/2, z+1/2
50 x, -y+3/4, -z+3/4
51 -x+1/4, y+1/2, -z+3/4
52 -x+1/4, -y+3/4, z+1/2
53 y, z+1/2, x+1/2
54 y, -z+3/4, -x+3/4
55 -y+1/4, z+1/2, -x+3/4
56 -y+1/4, -z+3/4, x+1/2
57 z, x+1/2, y+1/2
58 z, -x+3/4, -y+3/4
59 -z+1/4, x+1/2, -y+3/4
60 -z+1/4, -x+3/4, y+1/2
61 -y+1/2, -x, -z
62 -y+1/2, x+3/4, z+3/4
63 y+1/4, -x, z+3/4
64 y+1/4, x+3/4, -z
65 -x+1/2, -z, -y
66 -x+1/2, z+3/4, y+3/4
67 x+1/4, -z, y+3/4
68 x+1/4, z+3/4, -y
69 -z+1/2, -y, -x
70 -z+1/2, y+3/4, x+3/4
71 z+1/4, -y, x+3/4
72 z+1/4, y+3/4, -x
73 -x, -y+1/2, -z+1/2
74 -x, y+3/4, z+3/4
75 x+1/4, -y+1/2, z+3/4
76 x+1/4, y+3/4, -z+1/2
77 -y, -z+1/2, -x+1/2
78 -y, z+3/4, x+3/4
79 y+1/4, -z+1/2, x+3/4
80 y+1/4, z+3/4, -x+1/2
81 -z, -x+1/2, -y+1/2
82 -z, x+3/4, y+3/4
83 z+1/4, -x+1/2, y+3/4
84 z+1/4, x+3/4, -y+1/2
85 y+1/2, x, z
86 y+1/2, -x+3/4, -z+3/4
87 -y+1/4, x, -z+3/4
88 -y+1/4, -x+3/4, z
89 x+1/2, z, y
90 x+1/2, -z+3/4, -y+3/4
91 -x+1/4, z, -y+3/4
92 -x+1/4, -z+3/4, y
93 z+1/2, y, x
94 z+1/2, -y+3/4, -x+3/4
95 -z+1/4, y, -x+3/4
96 -z+1/4, -y+3/4, x
97 x+1/2, y, z+1/2
98 x+1/2, -y+1/4, -z+3/4
99 -x+3/4, y, -z+3/4
100 -x+3/4, -y+1/4, z+1/2

```

101 y+1/2, z, x+1/2  
 102 y+1/2, -z+1/4, -x+3/4  
 103 -y+3/4, z, -x+3/4  
 104 -y+3/4, -z+1/4, x+1/2  
 105 z+1/2, x, y+1/2  
 106 z+1/2, -x+1/4, -y+3/4  
 107 -z+3/4, x, -y+3/4  
 108 -z+3/4, -x+1/4, y+1/2  
 109 -y, -x+1/2, -z  
 110 -y, x+1/4, z+3/4  
 111 y+3/4, -x+1/2, z+3/4  
 112 y+3/4, x+1/4, -z  
 113 -x, -z+1/2, -y  
 114 -x, z+1/4, y+3/4  
 115 x+3/4, -z+1/2, y+3/4  
 116 x+3/4, z+1/4, -y  
 117 -z, -y+1/2, -x  
 118 -z, y+1/4, x+3/4  
 119 z+3/4, -y+1/2, x+3/4  
 120 z+3/4, y+1/4, -x  
 121 -x+1/2, -y, -z+1/2  
 122 -x+1/2, y+1/4, z+3/4  
 123 x+3/4, -y, z+3/4  
 124 x+3/4, y+1/4, -z+1/2  
 125 -y+1/2, -z, -x+1/2  
 126 -y+1/2, z+1/4, x+3/4  
 127 y+3/4, -z, x+3/4  
 128 y+3/4, z+1/4, -x+1/2  
 129 -z+1/2, -x, -y+1/2  
 130 -z+1/2, x+1/4, y+3/4  
 131 z+3/4, -x, y+3/4  
 132 z+3/4, x+1/4, -y+1/2  
 133 y, x+1/2, z  
 134 y, -x+1/4, -z+3/4  
 135 -y+3/4, x+1/2, -z+3/4  
 136 -y+3/4, -x+1/4, z  
 137 x, z+1/2, y  
 138 x, -z+1/4, -y+3/4  
 139 -x+3/4, z+1/2, -y+3/4  
 140 -x+3/4, -z+1/4, y  
 141 z, y+1/2, x  
 142 z, -y+1/4, -x+3/4  
 143 -z+3/4, y+1/2, -x+3/4  
 144 -z+3/4, -y+1/4, x  
 145 x+1/2, y+1/2, z  
 146 x+1/2, -y+3/4, -z+1/4  
 147 -x+3/4, y+1/2, -z+1/4  
 148 -x+3/4, -y+3/4, z  
 149 y+1/2, z+1/2, x  
 150 y+1/2, -z+3/4, -x+1/4  
 151 -y+3/4, z+1/2, -x+1/4  
 152 -y+3/4, -z+3/4, x  
 153 z+1/2, x+1/2, y  
 154 z+1/2, -x+3/4, -y+1/4  
 155 -z+3/4, x+1/2, -y+1/4  
 156 -z+3/4, -x+3/4, y  
 157 -y, -x, -z+1/2  
 158 -y, x+3/4, z+1/4  
 159 y+3/4, -x, z+1/4  
 160 y+3/4, x+3/4, -z+1/2  
 161 -x, -z, -y+1/2  
 162 -x, z+3/4, y+1/4  
 163 x+3/4, -z, y+1/4  
 164 x+3/4, z+3/4, -y+1/2  
 165 -z, -y, -x+1/2  
 166 -z, y+3/4, x+1/4  
 167 z+3/4, -y, x+1/4  
 168 z+3/4, y+3/4, -x+1/2  
 169 -x+1/2, -y+1/2, -z  
 170 -x+1/2, y+3/4, z+1/4  
 171 x+3/4, -y+1/2, z+1/4  
 172 x+3/4, y+3/4, -z  
 173 -y+1/2, -z+1/2, -x  
 174 -y+1/2, z+3/4, x+1/4  
 175 y+3/4, -z+1/2, x+1/4  
 176 y+3/4, z+3/4, -x  
 177 -z+1/2, -x+1/2, -y  
 178 -z+1/2, x+3/4, y+1/4  
 179 z+3/4, -x+1/2, y+1/4  
 180 z+3/4, x+3/4, -y  
 181 y, x, z+1/2  
 182 y, -x+3/4, -z+1/4  
 183 -y+3/4, x, -z+1/4  
 184 -y+3/4, -x+3/4, z+1/2  
 185 x, z, y+1/2  
 186 x, -z+3/4, -y+1/4  
 187 -x+3/4, z, -y+1/4  
 188 -x+3/4, -z+3/4, y+1/2  
 189 z, y, x+1/2  
 190 z, -y+3/4, -x+1/4  
 191 -z+3/4, y, -x+1/4  
 192 -z+3/4, -y+3/4, x+1/2

loop\_  
 \_atom\_site\_label  
 \_atom\_site\_type\_symbol  
 \_atom\_site\_symmetry\_multiplicity  
 \_atom\_site\_Wyckoff\_label  
 \_atom\_site\_fract\_x  
 \_atom\_site\_fract\_y  
 \_atom\_site\_fract\_z  
 \_atom\_site\_occupancy  
 Cu1 Cu 32 b 0.25000 0.25000 0.25000 1.00000  
 Cr1 Cr 32 c 0.00000 0.00000 0.00000 1.00000  
 Cl1 Cl 64 e 0.19000 0.19000 0.19000 1.00000

C12 Cl 96 g 0.25000 0.42500 0.57500 1.00000  
 N1 N 192 h 0.05000 0.18000 0.28000 1.00000

CuCrCl<sub>5</sub>[NH<sub>3</sub>]<sub>6</sub>; A5BCD6\_cF416\_228\_eg\_c\_b\_h - POSCAR

A5BCD6\_cF416\_228\_eg\_c\_b\_h & a, x3, y4, x5, y5, z5 --params=22.2649775014, 0.19  
 ↪ , 0.425, 0.05, 0.18, 0.28 & Fd-3c O\_{h}^{[8]} #228 (bcegh) & cF416 &  
 ↪ None & CuCrCl<sub>5</sub>[NH<sub>3</sub>]<sub>6</sub> & M. Masayasu and S. Yoshihiko and W.  
 ↪ Tokunosuk {\`e}, Bull. Chem. Soc. Jpn. 34, 295-296 (1961)

	Cl	Cr	Cu	N
	40	8	8	48
Direct				
0.1900000000000000	0.1900000000000000	0.1900000000000000	0.1900000000000000	Cl (64e)
0.1900000000000000	0.1900000000000000	-0.0700000000000000	0.1900000000000000	Cl (64e)
0.1900000000000000	-0.0700000000000000	0.1900000000000000	0.1900000000000000	Cl (64e)
-0.0700000000000000	0.1900000000000000	0.1900000000000000	0.1900000000000000	Cl (64e)
0.3100000000000000	0.3100000000000000	0.5700000000000000	0.3100000000000000	Cl (64e)
0.3100000000000000	0.3100000000000000	0.3100000000000000	0.3100000000000000	Cl (64e)
0.3100000000000000	0.5700000000000000	0.3100000000000000	0.3100000000000000	Cl (64e)
0.5700000000000000	0.3100000000000000	0.3100000000000000	0.3100000000000000	Cl (64e)
-0.1900000000000000	-0.1900000000000000	-0.1900000000000000	-0.1900000000000000	Cl (64e)
-0.1900000000000000	-0.1900000000000000	1.0700000000000000	0.1900000000000000	Cl (64e)
-0.1900000000000000	1.0700000000000000	-0.1900000000000000	-0.1900000000000000	Cl (64e)
1.0700000000000000	-0.1900000000000000	-0.1900000000000000	-0.1900000000000000	Cl (64e)
0.6900000000000000	0.6900000000000000	0.6900000000000000	-0.5700000000000000	Cl (64e)
0.6900000000000000	0.6900000000000000	0.6900000000000000	0.6900000000000000	Cl (64e)
0.6900000000000000	-0.5700000000000000	0.6900000000000000	0.6900000000000000	Cl (64e)
-0.5700000000000000	0.6900000000000000	0.6900000000000000	0.6900000000000000	Cl (64e)
0.0000000000000000	-0.3500000000000000	0.8500000000000000	0.8500000000000000	Cl (96g)
-0.6000000000000000	0.7500000000000000	0.2500000000000000	0.2500000000000000	Cl (96g)
1.1000000000000000	0.2500000000000000	0.7500000000000000	0.7500000000000000	Cl (96g)
0.2500000000000000	1.1000000000000000	-0.6000000000000000	-0.6000000000000000	Cl (96g)
1.1000000000000000	0.7500000000000000	-0.6000000000000000	-0.6000000000000000	Cl (96g)
0.2500000000000000	-0.6000000000000000	0.7500000000000000	0.7500000000000000	Cl (96g)
0.7500000000000000	1.1000000000000000	0.2500000000000000	0.2500000000000000	Cl (96g)
-0.6000000000000000	0.2500000000000000	1.1000000000000000	1.1000000000000000	Cl (96g)
-0.6000000000000000	1.1000000000000000	0.7500000000000000	0.7500000000000000	Cl (96g)
0.7500000000000000	0.2500000000000000	-0.6000000000000000	-0.6000000000000000	Cl (96g)
0.2500000000000000	0.7500000000000000	1.1000000000000000	1.1000000000000000	Cl (96g)
1.1000000000000000	-0.6000000000000000	0.2500000000000000	0.2500000000000000	Cl (96g)
0.2500000000000000	1.6000000000000000	-1.1000000000000000	-1.1000000000000000	Cl (96g)
1.6000000000000000	0.2500000000000000	0.7500000000000000	0.7500000000000000	Cl (96g)
-0.1000000000000000	0.7500000000000000	0.2500000000000000	0.2500000000000000	Cl (96g)
0.7500000000000000	-0.1000000000000000	1.6000000000000000	1.6000000000000000	Cl (96g)
-0.1000000000000000	0.2500000000000000	1.6000000000000000	1.6000000000000000	Cl (96g)
0.7500000000000000	1.6000000000000000	0.2500000000000000	0.2500000000000000	Cl (96g)
0.2500000000000000	-0.1000000000000000	0.7500000000000000	0.7500000000000000	Cl (96g)
1.6000000000000000	0.2500000000000000	0.7500000000000000	0.7500000000000000	Cl (96g)
0.7500000000000000	0.2500000000000000	-0.1000000000000000	-0.1000000000000000	Cl (96g)
-0.1000000000000000	1.6000000000000000	0.7500000000000000	0.7500000000000000	Cl (96g)
0.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000	Cr (32c)
0.0000000000000000	0.0000000000000000	0.5000000000000000	0.5000000000000000	Cr (32c)
0.0000000000000000	0.5000000000000000	0.0000000000000000	0.0000000000000000	Cr (32c)
0.5000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000	Cr (32c)
0.5000000000000000	0.5000000000000000	0.0000000000000000	0.0000000000000000	Cr (32c)
0.5000000000000000	0.0000000000000000	0.5000000000000000	0.5000000000000000	Cr (32c)
0.5000000000000000	0.5000000000000000	0.5000000000000000	0.5000000000000000	Cr (32c)
0.2500000000000000	0.2500000000000000	0.2500000000000000	0.2500000000000000	Cu (32b)
0.2500000000000000	0.2500000000000000	0.7500000000000000	0.7500000000000000	Cu (32b)
0.2500000000000000	0.7500000000000000	0.2500000000000000	0.2500000000000000	Cu (32b)
0.7500000000000000	0.2500000000000000	0.2500000000000000	0.2500000000000000	Cu (32b)
0.7500000000000000	0.7500000000000000	0.7500000000000000	0.7500000000000000	Cu (32b)
0.7500000000000000	0.7500000000000000	0.2500000000000000	0.2500000000000000	Cu (32b)
0.7500000000000000	0.2500000000000000	0.7500000000000000	0.7500000000000000	Cu (32b)
0.1500000000000000	0.4100000000000000	-0.0500000000000000	-0.0500000000000000	N (192h)
-0.0500000000000000	-0.0100000000000000	0.4100000000000000	0.4100000000000000	N (192h)
-0.0100000000000000	-0.0500000000000000	0.1500000000000000	0.1500000000000000	N (192h)
-0.0500000000000000	0.4100000000000000	0.1500000000000000	0.1500000000000000	N (192h)
-0.0100000000000000	0.1500000000000000	0.4100000000000000	0.4100000000000000	N (192h)
-0.0100000000000000	-0.0500000000000000	0.1500000000000000	0.1500000000000000	N (192h)
0.1500000000000000	-0.0100000000000000	-0.0500000000000000	-0.0500000000000000	N (192h)
0.1500000000000000	-0.0500000000000000	0.4100000000000000	0.4100000000000000	N (192h)
0.4100000000000000	-0.0100000000000000	0.1500000000000000	0.1500000000000000	N (192h)
-0.0100000000000000	0.4100000000000000	-0.0500000000000000	-0.0500000000000000	N (192h)
-0.0500000000000000	0.1500000000000000	0.4100000000000000	0.4100000000000000	N (192h)
0.0900000000000000	0.3500000000000000	0.5100000000000000	0.5100000000000000	N (192h)
0.3500000000000000	0.0900000000000000	0.5100000000000000	0.5100000000000000	N (192h)
0.5100000000000000	0.5100000000000000	0.3500000000000000	0.3500000000000000	N (192h)
0.5100000000000000	0.5500000000000000	0.0900000000000000	0.0900000000000000	N (192h)
0.5500000000000000	0.0900000000000000	0.5100000000000000	0.5100000000000000	N (192h)
0.0900000000000000	0.5500000000000000	0.5100000000000000	0.5100000000000000	N (192h)
0.0900000000000000	0.5500000000000000	0.0900000000000000	0.0900000000000000	N (192h)
0.3500000000000000	0.5100000000000000	0.5100000000000000	0.5100000000000000	N (192h)
0.3500000000000000	0.5500000000000000	0.5100000000000000	0.5100000000000000	N (192h)
0.0900000000000000	0.5100000000000000	0.5500000000000000	0.5500000000000000	N (192h)
0.5100000000000000	0.0900000000000000	0.3500000000000000	0.3500000000000000	N (192h)
0.5100000000000000	0.3500000000000000	0.0900000000000000	0.0900000000000000	N (192h)
0.0900000000000000	-0.4100000000000000	0.0500000000000000	0.0500000000000000	N (192h)
-0.4100000000000000	-0.1500000000000000	0.1000000000000000	0.1000000000000000	N (192h)
0.0500000000000000	1.0100000000000000	-0.4100000000000000	-0.4100000000000000	N (192h)
1.0100000000000000	0.0500000000000000	-0.1500000000000000	-0.1500000000000000	N (192h)
0.0500000000000000	-0.4100000000000000	0.1000000000000000	0.1000000000000000	N (192h)
1.0100000000000000	-0.1500000000000000	-0.4100000000000000	-0.4100000000000000	N (192h)
-0.4100000000000000	0.0500000000000000	1.0100000000000000	1.0100000000000000	N

-0.4100000000000000	1.0100000000000000	-0.1500000000000000	N (192h)
1.0100000000000000	-0.4100000000000000	0.0500000000000000	N (192h)
0.0500000000000000	-0.1500000000000000	1.0100000000000000	N (192h)
0.9100000000000000	0.6500000000000000	-0.5100000000000000	N (192h)
0.6500000000000000	0.9100000000000000	0.4500000000000000	N (192h)
0.4500000000000000	-0.5100000000000000	0.6500000000000000	N (192h)
-0.5100000000000000	0.4500000000000000	0.9100000000000000	N (192h)
0.4500000000000000	0.9100000000000000	-0.5100000000000000	N (192h)
-0.5100000000000000	0.6500000000000000	0.4500000000000000	N (192h)
0.9100000000000000	0.4500000000000000	0.6500000000000000	N (192h)
0.6500000000000000	-0.5100000000000000	0.9100000000000000	N (192h)
0.6500000000000000	0.4500000000000000	-0.5100000000000000	N (192h)
0.9100000000000000	-0.5100000000000000	0.4500000000000000	N (192h)
-0.5100000000000000	0.9100000000000000	0.6500000000000000	N (192h)
0.4500000000000000	0.6500000000000000	0.9100000000000000	N (192h)

TeO<sub>6</sub>H<sub>6</sub>: A6B\_cF224\_228\_h\_c - CIF

```
# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'TeO6H6'
_chemical_formula_sum 'O6 Te'

loop_
  _publ_author_name
    'L. M. Kirkpatrick '
    'L. Pauling '
  _journal_name_full_name
    ;
    Zeitschrift f{"u}r Kristallographie - Crystalline Materials
  ;
  _journal_volume 63
  _journal_year 1926
  _journal_page_first 502
  _journal_page_last 506
  _publ_section_title
    ;
    XXVIII. {\ "U}ber die Kristallstruktur der kubischen Tellurs{\ "a}ure
  ;

# Found in Pearson's Crystal Data - Crystal Structure Database for
  ↳ Inorganic Compounds, 2013

_aflow_title 'TeOS_{6}$H6$ Structure '
_aflow_proto 'A6B_cF224_228_h_c'
_aflow_params 'a_x{2},y_{2},z_{2}'
_aflow_params_values '15.4800297791,0.043,0.138,0.278'
_aflow_strukturbericht 'None'
_aflow_pearson 'cF224'

_cell_length_a 15.4800297791
_cell_length_b 15.4800297791
_cell_length_c 15.4800297791
_cell_angle_alpha 90.0000000000
_cell_angle_beta 90.0000000000
_cell_angle_gamma 90.0000000000

_symmetry_space_group_name_H-M "F 41/d -3 2/c (origin choice 2)"
_symmetry_int_tables_number 228

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
  1 x, y, z
  2 x, -y+1/4, -z+1/4
  3 -x+1/4, y, -z+1/4
  4 -x+1/4, -y+1/4, z
  5 y, z, x
  6 y, -z+1/4, -x+1/4
  7 -y+1/4, z, -x+1/4
  8 -y+1/4, -z+1/4, x
  9 z, x, y
  10 z, -x+1/4, -y+1/4
  11 -z+1/4, x, -y+1/4
  12 -z+1/4, -x+1/4, y
  13 -y+1/2, -x+1/2, -z+1/2
  14 -y+1/2, x+1/4, z+1/4
  15 y+1/4, -x+1/2, z+1/4
  16 y+1/4, x+1/4, -z+1/2
  17 -x+1/2, -z+1/2, -y+1/2
  18 -x+1/2, z+1/4, y+1/4
  19 x+1/4, -z+1/2, y+1/4
  20 x+1/4, z+1/4, -y+1/2
  21 -z+1/2, -y+1/2, -x+1/2
  22 -z+1/2, y+1/4, x+1/4
  23 z+1/4, -y+1/2, x+1/4
  24 z+1/4, y+1/4, -x+1/2
  25 -x, -y, -z
  26 -x, y+1/4, z+1/4
  27 x+1/4, -y, z+1/4
  28 x+1/4, y+1/4, -z
  29 -y, -z, -x
  30 -y, z+1/4, x+1/4
  31 y+1/4, -z, x+1/4
  32 y+1/4, z+1/4, -x
  33 -z, -x, -y
  34 -z, x+1/4, y+1/4
  35 z+1/4, -x, y+1/4
  36 z+1/4, x+1/4, -y
  37 y+1/2, x+1/2, z+1/2
  38 y+1/2, -x+1/4, -z+1/4
  39 -y+1/4, x+1/2, -z+1/4
  40 -y+1/4, -x+1/4, z+1/2
```

```
41 x+1/2, z+1/2, y+1/2
42 x+1/2, -z+1/4, -y+1/4
43 -x+1/4, z+1/2, -y+1/4
44 -x+1/4, -z+1/4, y+1/2
45 z+1/2, y+1/2, x+1/2
46 z+1/2, -y+1/4, -x+1/4
47 -z+1/4, y+1/2, -x+1/4
48 -z+1/4, -y+1/4, x+1/2
49 x, y+1/2, z+1/2
50 x, -y+3/4, -z+3/4
51 -x+1/4, y+1/2, -z+3/4
52 -x+1/4, -y+3/4, z+1/2
53 y, z+1/2, x+1/2
54 y, -z+3/4, -x+3/4
55 -y+1/4, z+1/2, -x+3/4
56 -y+1/4, -z+3/4, x+1/2
57 z, x+1/2, y+1/2
58 z, -x+3/4, -y+3/4
59 -z+1/4, x+1/2, -y+3/4
60 -z+1/4, -x+3/4, y+1/2
61 -y+1/2, -x, -z
62 -y+1/2, x+3/4, z+3/4
63 y+1/4, -x, z+3/4
64 y+1/4, x+3/4, -z
65 -x+1/2, -z, -y
66 -x+1/2, z+3/4, y+3/4
67 x+1/4, -z, y+3/4
68 x+1/4, z+3/4, -y
69 -z+1/2, -y, -x
70 -z+1/2, y+3/4, x+3/4
71 z+1/4, -y, x+3/4
72 z+1/4, y+3/4, -x
73 -x, -y+1/2, -z+1/2
74 -x, y+3/4, z+3/4
75 x+1/4, -y+1/2, z+3/4
76 x+1/4, y+3/4, -z+1/2
77 -y, -z+1/2, -x+1/2
78 -y, z+3/4, x+3/4
79 y+1/4, -z+1/2, x+3/4
80 y+1/4, z+3/4, -x+1/2
81 -z, -x+1/2, -y+1/2
82 -z, x+3/4, y+3/4
83 z+1/4, -x+1/2, y+3/4
84 z+1/4, x+3/4, -y+1/2
85 y+1/2, x, z
86 y+1/2, -x+3/4, -z+3/4
87 -y+1/4, x, -z+3/4
88 -y+1/4, -x+3/4, z
89 x+1/2, z, y
90 x+1/2, -z+3/4, -y+3/4
91 -x+1/4, z, -y+3/4
92 -x+1/4, -z+3/4, y
93 z+1/2, y, x
94 z+1/2, -y+3/4, -x+3/4
95 -z+1/4, y, -x+3/4
96 -z+1/4, -y+3/4, x
97 x+1/2, y, z+1/2
98 x+1/2, -y+1/4, -z+3/4
99 -x+3/4, y, -z+3/4
100 -x+3/4, -y+1/4, z+1/2
101 y+1/2, z, x+1/2
102 y+1/2, -z+1/4, -x+3/4
103 -y+3/4, z, -x+3/4
104 -y+3/4, -z+1/4, x+1/2
105 z+1/2, x, y+1/2
106 z+1/2, -x+1/4, -y+3/4
107 -z+3/4, x, -y+3/4
108 -z+3/4, -x+1/4, y+1/2
109 -y, -x+1/2, -z
110 -y, x+1/4, z+3/4
111 y+3/4, -x+1/2, z+3/4
112 y+3/4, x+1/4, -z
113 -x, -z+1/2, -y
114 -x, z+1/4, y+3/4
115 x+3/4, -z+1/2, y+3/4
116 x+3/4, z+1/4, -y
117 -z, -y+1/2, -x
118 -z, y+1/4, x+3/4
119 z+3/4, -y+1/2, x+3/4
120 z+3/4, y+1/4, -x
121 -x+1/2, -y, -z+1/2
122 -x+1/2, y+1/4, z+3/4
123 x+3/4, -y, z+3/4
124 x+3/4, y+1/4, -z+1/2
125 -y+1/2, -z, -x+1/2
126 -y+1/2, z+1/4, x+3/4
127 y+3/4, -z, x+3/4
128 y+3/4, z+1/4, -x+1/2
129 -z+1/2, -x, -y+1/2
130 -z+1/2, x+1/4, y+3/4
131 z+3/4, -x, y+3/4
132 z+3/4, x+1/4, -y+1/2
133 y, x+1/2, z
134 y, -x+1/4, -z+3/4
135 -y+3/4, x+1/2, -z+3/4
136 -y+3/4, -x+1/4, z
137 x, z+1/2, y
138 x, -z+1/4, -y+3/4
139 -x+3/4, z+1/2, -y+3/4
140 -x+3/4, -z+1/4, y
141 z, y+1/2, x
142 z, -y+1/4, -x+3/4
143 -z+3/4, y+1/2, -x+3/4
144 -z+3/4, -y+1/4, x
145 x+1/2, y+1/2, z
```

```

146 x+1/2,-y+3/4,-z+1/4
147 -x+3/4,y+1/2,-z+1/4
148 -x+3/4,-y+3/4,z
149 y+1/2,-z+1/2,x
150 y+1/2,-z+3/4,-x+1/4
151 -y+3/4,z+1/2,-x+1/4
152 -y+3/4,-z+3/4,x
153 z+1/2,x+1/2,y
154 z+1/2,-x+3/4,-y+1/4
155 -z+3/4,x+1/2,-y+1/4
156 -z+3/4,-x+3/4,y
157 -y,-x,-z+1/2
158 -y,x+3/4,z+1/4
159 y+3/4,-x,z+1/4
160 y+3/4,x+3/4,-z+1/2
161 -x,-z,-y+1/2
162 -x,z+3/4,y+1/4
163 x+3/4,-z,y+1/4
164 x+3/4,z+3/4,-y+1/2
165 -z,-y,-x+1/2
166 -z,y+3/4,x+1/4
167 z+3/4,-y,x+1/4
168 z+3/4,y+3/4,-x+1/2
169 -x+1/2,-y+1/2,-z
170 -x+1/2,y+3/4,z+1/4
171 x+3/4,-y+1/2,z+1/4
172 x+3/4,y+3/4,-z
173 -y+1/2,-z+1/2,-x
174 -y+1/2,z+3/4,x+1/4
175 y+3/4,-z+1/2,x+1/4
176 y+3/4,z+3/4,-x
177 -z+1/2,-x+1/2,-y
178 -z+1/2,x+3/4,y+1/4
179 z+3/4,-x+1/2,y+1/4
180 z+3/4,x+3/4,-y
181 y,x,z+1/2
182 y,-x+3/4,-z+1/4
183 -y+3/4,x,-z+1/4
184 -y+3/4,-x+3/4,z+1/2
185 x,z,y+1/2
186 x,-z+3/4,-y+1/4
187 -x+3/4,z,-y+1/4
188 -x+3/4,-z+3/4,y+1/2
189 z,y,x+1/2
190 z,-y+3/4,-x+1/4
191 -z+3/4,y,-x+1/4
192 -z+3/4,-y+3/4,x+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Te1 Te 32 c 0.00000 0.00000 0.00000 1.00000
O1 O 192 h 0.04300 0.13800 0.27800 1.00000

```

TeO<sub>6</sub>H<sub>6</sub>: A6B\_cF224\_228\_h\_c - POSCAR

```

A6B_cF224_228_h_c & a,x2,y2,z2 --params=15.4800297791,0.043,0.138,0.278
↪ & Fd-3c Oh^{8} #228 (ch) & cF224 & None & TeO6H6 & L. M.
↪ Kirkpatrick and L. Pauling, Zeitschrift f"u;r Kristallographie
↪ - Crystalline Materials 63, 502-506 (1926)
1.0000000000000000
0.0000000000000000 7.74001488955000 7.74001488955000
7.74001488955000 0.0000000000000000 7.74001488955000
7.74001488955000 7.74001488955000 0.0000000000000000
O Te
48 8
Direct
0.3730000000000000 0.1830000000000000 -0.0970000000000000 O (192h)
0.1830000000000000 0.3730000000000000 0.0410000000000000 O (192h)
-0.0970000000000000 0.0410000000000000 0.3730000000000000 O (192h)
0.0410000000000000 -0.0970000000000000 0.1830000000000000 O (192h)
-0.0970000000000000 0.3730000000000000 0.1830000000000000 O (192h)
0.0410000000000000 0.1830000000000000 0.3730000000000000 O (192h)
0.3730000000000000 -0.0970000000000000 0.0410000000000000 O (192h)
0.1830000000000000 0.0410000000000000 -0.0970000000000000 O (192h)
0.1830000000000000 -0.0970000000000000 0.3730000000000000 O (192h)
0.3730000000000000 0.0410000000000000 0.1830000000000000 O (192h)
0.0410000000000000 0.3730000000000000 -0.0970000000000000 O (192h)
-0.0970000000000000 0.1830000000000000 0.0410000000000000 O (192h)
0.1270000000000000 0.3170000000000000 0.4590000000000000 O (192h)
0.3170000000000000 0.1270000000000000 0.5970000000000000 O (192h)
0.5970000000000000 0.4590000000000000 0.3170000000000000 O (192h)
0.4590000000000000 0.5970000000000000 0.1270000000000000 O (192h)
0.5970000000000000 0.1270000000000000 0.4590000000000000 O (192h)
0.4590000000000000 0.3170000000000000 0.5970000000000000 O (192h)
0.1270000000000000 0.5970000000000000 0.3170000000000000 O (192h)
0.3170000000000000 0.4590000000000000 0.1270000000000000 O (192h)
0.3170000000000000 0.5970000000000000 0.4590000000000000 O (192h)
0.1270000000000000 0.4590000000000000 0.5970000000000000 O (192h)
0.4590000000000000 0.1270000000000000 0.3170000000000000 O (192h)
0.5970000000000000 0.3170000000000000 0.1270000000000000 O (192h)
0.3170000000000000 -0.1830000000000000 0.0970000000000000 O (192h)
-0.1830000000000000 -0.3730000000000000 0.9590000000000000 O (192h)
0.0970000000000000 0.9590000000000000 -0.3730000000000000 O (192h)
0.9590000000000000 0.0970000000000000 -0.1830000000000000 O (192h)
0.0970000000000000 -0.3730000000000000 -0.1830000000000000 O (192h)
0.9590000000000000 -0.1830000000000000 -0.3730000000000000 O (192h)
-0.3730000000000000 0.0970000000000000 0.9590000000000000 O (192h)
-0.1830000000000000 0.9590000000000000 0.0970000000000000 O (192h)

```

```

-0.1830000000000000 0.0970000000000000 -0.3730000000000000 O (192h)
-0.3730000000000000 0.9590000000000000 -0.1830000000000000 O (192h)
0.9590000000000000 -0.3730000000000000 0.0970000000000000 O (192h)
0.0970000000000000 -0.1830000000000000 0.9590000000000000 O (192h)
0.8730000000000000 0.6830000000000000 -0.4590000000000000 O (192h)
0.6830000000000000 0.8730000000000000 0.4030000000000000 O (192h)
0.4030000000000000 -0.4590000000000000 0.6830000000000000 O (192h)
-0.4590000000000000 0.4030000000000000 0.8730000000000000 O (192h)
0.4030000000000000 0.8730000000000000 -0.4590000000000000 O (192h)
-0.4590000000000000 0.6830000000000000 0.4030000000000000 O (192h)
0.8730000000000000 0.4030000000000000 0.6830000000000000 O (192h)
0.6830000000000000 -0.4590000000000000 0.8730000000000000 O (192h)
0.6830000000000000 0.4030000000000000 -0.4590000000000000 O (192h)
0.8730000000000000 -0.4590000000000000 0.4030000000000000 O (192h)
-0.4590000000000000 0.8730000000000000 0.6830000000000000 O (192h)
0.4030000000000000 0.6830000000000000 0.8730000000000000 O (192h)
0.0000000000000000 0.0000000000000000 0.0000000000000000 Te (32c)
0.0000000000000000 0.0000000000000000 0.5000000000000000 Te (32c)
0.0000000000000000 0.5000000000000000 0.0000000000000000 Te (32c)
0.5000000000000000 0.0000000000000000 0.0000000000000000 Te (32c)
0.5000000000000000 0.5000000000000000 0.0000000000000000 Te (32c)
0.5000000000000000 0.5000000000000000 0.5000000000000000 Te (32c)
0.5000000000000000 0.0000000000000000 0.5000000000000000 Te (32c)
0.0000000000000000 0.5000000000000000 0.5000000000000000 Te (32c)

```

γ-brass (Fe<sub>3</sub>Zn<sub>10</sub>, D<sub>8h</sub>): A3B10\_cI52\_229\_e\_fh - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '\gamma$-brass Fe_{3}$Zn_{10}$'
_chemical_formula_sum 'Fe3 Zn10'

loop_
_publ_author_name
'J. Schramm'
_journal_name_full_name
;
Zeitschrift fur Metallkunde
;
_journal_volume 30
_journal_year 1938
_journal_page_first 122
_journal_page_last 130
_publ_section_title
;
X-Ray Investigation of Phases and Phase Limits of the Zn Alloy
Systems with Fe, Co and Ni
;

# Found in A Handbook of Lattice Spacings and Structures of Metals and
Alloys, 1958

_aflow_title '\gamma$-brass (Fe_{3}$Zn_{10}$, $D8_{1}$) Structure'
_aflow_proto 'A3B10_cI52_229_e_fh'
_aflow_params 'a,x_{1},x_{2},y_{3}'
_aflow_params_values '8.9822,0.3538,0.13505,0.3045'
_aflow_Strukturbericht '$D8_{1}$'
_aflow_Pearson 'cI52'

_symmetry_space_group_name_H-M "I 4/m -3 2/m"
_symmetry_Int_Tables_number 229

_cell_length_a 8.98220
_cell_length_b 8.98220
_cell_length_c 8.98220
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 -y,-x,-z
14 -y,x,z
15 y,-x,z
16 y,x,-z
17 -x,-z,-y
18 -x,z,y
19 x,-z,y
20 x,z,-y
21 -z,-y,-x
22 -z,y,x
23 z,-y,x
24 z,y,-x
25 -x,-y,-z
26 -x,y,z
27 x,-y,z
28 x,y,-z
29 -y,-z,-x
30 -y,z,x
31 y,-z,x

```

```

32 y,z,-x
33 -z,-x,-y
34 -z,x,y
35 z,-x,y
36 z,x,-y
37 y,x,z
38 y,-x,-z
39 -y,x,-z
40 -y,-x,z
41 x,z,y
42 x,-z,-y
43 -x,z,-y
44 -x,-z,y
45 z,y,x
46 z,-y,-x
47 -z,y,-x
48 -z,-y,x
49 x+1/2,y+1/2,z+1/2
50 x+1/2,-y+1/2,-z+1/2
51 -x+1/2,y+1/2,-z+1/2
52 -x+1/2,-y+1/2,z+1/2
53 y+1/2,z+1/2,x+1/2
54 y+1/2,-z+1/2,-x+1/2
55 -y+1/2,z+1/2,-x+1/2
56 -y+1/2,-z+1/2,x+1/2
57 z+1/2,x+1/2,y+1/2
58 z+1/2,-x+1/2,-y+1/2
59 -z+1/2,x+1/2,-y+1/2
60 -z+1/2,-x+1/2,y+1/2
61 -y+1/2,-x+1/2,-z+1/2
62 -y+1/2,x+1/2,z+1/2
63 y+1/2,-x+1/2,z+1/2
64 y+1/2,x+1/2,-z+1/2
65 -x+1/2,-z+1/2,-y+1/2
66 -x+1/2,z+1/2,y+1/2
67 x+1/2,-z+1/2,y+1/2
68 x+1/2,z+1/2,-y+1/2
69 -z+1/2,-y+1/2,-x+1/2
70 -z+1/2,y+1/2,x+1/2
71 z+1/2,-y+1/2,x+1/2
72 z+1/2,y+1/2,-x+1/2
73 -x+1/2,-y+1/2,-z+1/2
74 -x+1/2,y+1/2,z+1/2
75 x+1/2,-y+1/2,z+1/2
76 x+1/2,y+1/2,-z+1/2
77 -y+1/2,-z+1/2,-x+1/2
78 -y+1/2,z+1/2,x+1/2
79 y+1/2,-z+1/2,x+1/2
80 y+1/2,z+1/2,-x+1/2
81 -z+1/2,-x+1/2,-y+1/2
82 -z+1/2,x+1/2,y+1/2
83 z+1/2,-x+1/2,y+1/2
84 z+1/2,x+1/2,-y+1/2
85 y+1/2,x+1/2,z+1/2
86 y+1/2,-x+1/2,-z+1/2
87 -y+1/2,x+1/2,-z+1/2
88 -y+1/2,-x+1/2,z+1/2
89 x+1/2,z+1/2,y+1/2
90 x+1/2,-z+1/2,-y+1/2
91 -x+1/2,z+1/2,-y+1/2
92 -x+1/2,-z+1/2,y+1/2
93 z+1/2,y+1/2,x+1/2
94 z+1/2,-y+1/2,-x+1/2
95 -z+1/2,y+1/2,-x+1/2
96 -z+1/2,-y+1/2,x+1/2

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_symmetry_multiplicity
  _atom_site_Wyckoff_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
Fe1 Fe 12 e 0.35380 0.00000 0.00000 1.00000
Zn1 Zn 16 f 0.13505 0.13505 0.13505 1.00000
Zn2 Zn 24 h 0.00000 0.30450 0.30450 1.00000

```

$\gamma$ -brass (Fe<sub>3</sub>Zn<sub>10</sub>, D8<sub>1</sub>): A3B10\_cI52\_229\_e\_fh - POSCAR

```

A3B10_cI52_229_e_fh & a, x1, x2, y3 --params=8.9822, 0.3538, 0.13505, 0.3045 &
↳ Im-3m Oh{9} #229 (efh) & cI52 & SD8_{1}$ & Fe3Zn10 & $
↳ gamma$-brass Fe$_{3}$Zn$_{10}$ & J. Schramm, Z. Metallkd. 30,
↳ 122-130 (1938)
1.0000000000000000
-4.491100000000000 4.491100000000000 4.491100000000000
4.491100000000000 -4.491100000000000 4.491100000000000
4.491100000000000 4.491100000000000 -4.491100000000000
Fe Zn
6 20
Direct
0.000000000000000 0.353800000000000 0.353800000000000 Fe (12e)
0.000000000000000 -0.353800000000000 -0.353800000000000 Fe (12e)
0.353800000000000 0.000000000000000 0.353800000000000 Fe (12e)
-0.353800000000000 0.000000000000000 -0.353800000000000 Fe (12e)
0.353800000000000 0.353800000000000 0.000000000000000 Fe (12e)
-0.353800000000000 -0.353800000000000 0.000000000000000 Fe (12e)
0.270100000000000 0.270100000000000 0.270100000000000 Zn (16f)
0.000000000000000 0.000000000000000 -0.270100000000000 Zn (16f)
0.000000000000000 -0.270100000000000 0.000000000000000 Zn (16f)
-0.270100000000000 0.000000000000000 0.000000000000000 Zn (16f)
0.000000000000000 0.000000000000000 0.270100000000000 Zn (16f)
-0.270100000000000 -0.270100000000000 -0.270100000000000 Zn (16f)
0.000000000000000 0.270100000000000 0.000000000000000 Zn (16f)

```

```

0.270100000000000 0.000000000000000 0.000000000000000 Zn (16f)
0.609000000000000 0.304500000000000 0.304500000000000 Zn (24h)
0.000000000000000 0.304500000000000 -0.304500000000000 Zn (24h)
0.000000000000000 -0.304500000000000 0.304500000000000 Zn (24h)
-0.609000000000000 -0.304500000000000 -0.304500000000000 Zn (24h)
0.304500000000000 0.609000000000000 0.304500000000000 Zn (24h)
-0.304500000000000 0.000000000000000 0.304500000000000 Zn (24h)
0.304500000000000 0.000000000000000 -0.304500000000000 Zn (24h)
-0.304500000000000 -0.609000000000000 -0.304500000000000 Zn (24h)
0.304500000000000 0.304500000000000 0.609000000000000 Zn (24h)
0.304500000000000 -0.304500000000000 0.000000000000000 Zn (24h)
-0.304500000000000 0.304500000000000 0.000000000000000 Zn (24h)
-0.304500000000000 -0.304500000000000 -0.609000000000000 Zn (24h)

```

$\beta$ -Hg<sub>4</sub>Pt: A4B\_cI10\_229\_c\_a - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral '$\beta$Hg$_{4}$Pt'
_chemical_formula_sum 'Hg4 Pt'

loop_
  _publ_author_name
  'E. Bauer'
  'H. Nowotny'
  'A. Stempf'
  _journal_name_full_name
  ;
  Monatshefte f{"u}r Chemie - Chemical Monthly
  ;
  _journal_volume 84
  _journal_year 1953
  _journal_page_first 211
  _journal_page_last 212
  _publ_section_title
  ;
  R{"o}ntgenographische Untersuchungen im System: Platin-Quecksilber
  ;

_aflow_title '$\beta$Hg$_{4}$Pt Structure'
_aflow_proto 'A4B_cI10_229_c_a'
_aflow_params 'a'
_aflow_params_values '6.186'
_aflow_Strukturbericht 'None'
_aflow_Pearson 'cI10'

_symmetry_space_group_name_H-M "I m -3 m"
_symmetry_Int_Tables_number 229

_cell_length_a 6.18600
_cell_length_b 6.18600
_cell_length_c 6.18600
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 -y,-x,-z
14 -y,x,z
15 y,-x,z
16 y,x,-z
17 -x,-z,-y
18 -x,z,y
19 x,-z,y
20 x,z,-y
21 -z,-y,-x
22 -z,y,x
23 z,-y,x
24 z,y,-x
25 -x,-y,-z
26 -x,y,z
27 x,-y,z
28 x,y,-z
29 -y,-z,-x
30 -y,z,x
31 y,-z,x
32 y,z,-x
33 -z,-x,-y
34 -z,x,y
35 z,-x,y
36 z,x,-y
37 y,x,z
38 y,-x,-z
39 -y,x,-z
40 -y,-x,z
41 x,z,y
42 x,-z,-y
43 -x,z,-y
44 -x,-z,y

```



```

45 z, y, x
46 z, -y, -x
47 -z, y, -x
48 -z, -y, x
49 x+1/2, y+1/2, z+1/2
50 x+1/2, -y+1/2, -z+1/2
51 -x+1/2, y+1/2, -z+1/2
52 -x+1/2, -y+1/2, z+1/2
53 y+1/2, z+1/2, x+1/2
54 y+1/2, -z+1/2, -x+1/2
55 -y+1/2, z+1/2, -x+1/2
56 -y+1/2, -z+1/2, x+1/2
57 z+1/2, x+1/2, y+1/2
58 z+1/2, -x+1/2, -y+1/2
59 -z+1/2, x+1/2, -y+1/2
60 -z+1/2, -x+1/2, y+1/2
61 -y+1/2, -x+1/2, -z+1/2
62 -y+1/2, x+1/2, z+1/2
63 y+1/2, -x+1/2, z+1/2
64 y+1/2, x+1/2, -z+1/2
65 -x+1/2, -z+1/2, -y+1/2
66 -x+1/2, z+1/2, y+1/2
67 x+1/2, -z+1/2, y+1/2
68 x+1/2, z+1/2, -y+1/2
69 -z+1/2, -y+1/2, -x+1/2
70 -z+1/2, y+1/2, x+1/2
71 z+1/2, -y+1/2, x+1/2
72 z+1/2, y+1/2, -x+1/2
73 -x+1/2, -y+1/2, -z+1/2
74 -x+1/2, y+1/2, z+1/2
75 x+1/2, -y+1/2, z+1/2
76 x+1/2, y+1/2, -z+1/2
77 -y+1/2, -z+1/2, -x+1/2
78 -y+1/2, z+1/2, x+1/2
79 y+1/2, -z+1/2, x+1/2
80 y+1/2, z+1/2, -x+1/2
81 -z+1/2, -x+1/2, -y+1/2
82 -z+1/2, x+1/2, y+1/2
83 z+1/2, -x+1/2, y+1/2
84 z+1/2, x+1/2, -y+1/2
85 y+1/2, x+1/2, z+1/2
86 y+1/2, -x+1/2, -z+1/2
87 -y+1/2, x+1/2, -z+1/2
88 -y+1/2, -x+1/2, z+1/2
89 x+1/2, z+1/2, y+1/2
90 x+1/2, -z+1/2, -y+1/2
91 -x+1/2, z+1/2, -y+1/2
92 -x+1/2, -z+1/2, y+1/2
93 z+1/2, y+1/2, x+1/2
94 z+1/2, -y+1/2, -x+1/2
95 -z+1/2, y+1/2, -x+1/2
96 -z+1/2, -y+1/2, x+1/2

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Pt1 Pt 2 a 0.00000 0.00000 0.00000 1.00000
Hg1 Hg 8 c 0.25000 0.25000 0.25000 1.00000

```

$\beta$ -Hg<sub>4</sub>Pt: A4B\_c110\_229\_c\_a - POSCAR

```

A4B_c110_229_c_a & --params=6.186 & Im-3m O_{h}^{9} #229 (ac) & c110 &
↳ None & Hg4Pt & \beta$-Hg_{4}$Pt & E. Bauer and H. Nowotny
↳ and A. Stempf, Monatsh. Chem. 84, 211-212 (1953)

```

1.0000000000000000				
-3.0930000000000000	3.0930000000000000	3.0930000000000000		
3.0930000000000000	-3.0930000000000000	3.0930000000000000		
3.0930000000000000	3.0930000000000000	-3.0930000000000000		
Hg	Pt			
4	1			
Direct				
0.5000000000000000	0.5000000000000000	0.5000000000000000	Hg	(8c)
0.0000000000000000	0.0000000000000000	0.5000000000000000	Hg	(8c)
0.0000000000000000	0.5000000000000000	0.0000000000000000	Hg	(8c)
0.5000000000000000	0.0000000000000000	0.0000000000000000	Hg	(8c)
0.0000000000000000	0.0000000000000000	0.0000000000000000	Pt	(2a)

Ir<sub>3</sub>Ge<sub>7</sub> (D8<sub>f</sub>): A7B3\_c140\_229\_df\_e - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Ir3Ge7'
_chemical_formula_sum 'Ge7 Ir3'

loop_
_publ_author_name
'U. H\{a}ussermann'
'M. {Elding-Pont\{e}n}'
'C. Svensson'
'S. Lidin'
_journal_name_full_name
;
Chemistry - A European Journal
;
_journal_volume 4
_journal_year 1998
_journal_page_first 1007

```

```

_journal_page_last 1015
_publ_section_title
;
Compounds with the Ir$_{3}$Ge$_{7}$ Structure Type: Interpenetrating
↳ Frameworks with Flexible Bonding Properties
;
# Found in Diffusion of $^{111}$Cd probes in Ga$_{5}$Pt$_{3}$ studied
↳ via nuclear quadrupole relaxation, 2007

_aware_title 'Ir$_{3}$Ge$_{7}$ (SD8_{f}) Structure'
_aware_proto 'A7B3_c140_229_df_e'
_aware_params 'a_{2}, x_{3}'
_aware_params_values '8.735, 0.342, 0.156'
_aware_Strukturbericht 'SD8_{f}'
_aware_Pearson 'c140'

_symmetry_space_group_name_H-M "I 4/m -3 2/m"
_symmetry_Int_Tables_number 229

_cell_length_a 8.73500
_cell_length_b 8.73500
_cell_length_c 8.73500
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x, y, z
2 x, -y, -z
3 -x, y, -z
4 -x, -y, z
5 y, z, x
6 y, -z, -x
7 -y, z, -x
8 -y, -z, x
9 z, x, y
10 z, -x, -y
11 -z, x, -y
12 -z, -x, y
13 -y, -x, -z
14 -y, x, z
15 y, -x, z
16 y, x, -z
17 -x, -z, -y
18 -x, z, y
19 x, -z, y
20 x, z, -y
21 -z, -y, -x
22 -z, y, x
23 z, -y, x
24 z, y, -x
25 -x, -y, -z
26 -x, y, z
27 x, -y, z
28 x, y, -z
29 -y, -z, -x
30 -y, z, x
31 y, -z, x
32 y, z, -x
33 -z, -x, -y
34 -z, x, y
35 z, -x, y
36 z, x, -y
37 y, x, z
38 y, -x, -z
39 -y, x, -z
40 -y, -x, z
41 x, z, y
42 x, -z, -y
43 -x, z, -y
44 -x, -z, y
45 z, y, x
46 z, -y, -x
47 -z, y, -x
48 -z, -y, x
49 x+1/2, y+1/2, z+1/2
50 x+1/2, -y+1/2, -z+1/2
51 -x+1/2, y+1/2, -z+1/2
52 -x+1/2, -y+1/2, z+1/2
53 y+1/2, z+1/2, x+1/2
54 y+1/2, -z+1/2, -x+1/2
55 -y+1/2, z+1/2, -x+1/2
56 -y+1/2, -z+1/2, x+1/2
57 z+1/2, x+1/2, y+1/2
58 z+1/2, -x+1/2, -y+1/2
59 -z+1/2, x+1/2, -y+1/2
60 -z+1/2, -x+1/2, y+1/2
61 -y+1/2, -x+1/2, -z+1/2
62 -y+1/2, x+1/2, z+1/2
63 y+1/2, -x+1/2, z+1/2
64 y+1/2, x+1/2, -z+1/2
65 -x+1/2, -z+1/2, -y+1/2
66 -x+1/2, z+1/2, y+1/2
67 x+1/2, -z+1/2, y+1/2
68 x+1/2, z+1/2, -y+1/2
69 -z+1/2, -y+1/2, -x+1/2
70 -z+1/2, y+1/2, x+1/2
71 z+1/2, -y+1/2, x+1/2
72 z+1/2, y+1/2, -x+1/2
73 -x+1/2, -y+1/2, -z+1/2
74 -x+1/2, y+1/2, z+1/2
75 x+1/2, -y+1/2, z+1/2

```

```

76 x+1/2,y+1/2,-z+1/2
77 -y+1/2,-z+1/2,-x+1/2
78 -y+1/2,z+1/2,x+1/2
79 y+1/2,-z+1/2,x+1/2
80 y+1/2,z+1/2,-x+1/2
81 -z+1/2,-x+1/2,-y+1/2
82 -z+1/2,x+1/2,y+1/2
83 z+1/2,-x+1/2,y+1/2
84 z+1/2,x+1/2,-y+1/2
85 y+1/2,x+1/2,z+1/2
86 y+1/2,-x+1/2,-z+1/2
87 -y+1/2,x+1/2,-z+1/2
88 -y+1/2,-x+1/2,z+1/2
89 x+1/2,z+1/2,y+1/2
90 x+1/2,-z+1/2,-y+1/2
91 -x+1/2,z+1/2,-y+1/2
92 -x+1/2,-z+1/2,y+1/2
93 z+1/2,y+1/2,x+1/2
94 z+1/2,-y+1/2,-x+1/2
95 -z+1/2,y+1/2,-x+1/2
96 -z+1/2,-y+1/2,x+1/2

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ge1 Ge 12 d 0.25000 0.00000 0.50000 1.00000
Ir1 Ir 12 e 0.34200 0.00000 0.00000 1.00000
Ge2 Ge 16 f 0.15600 0.15600 0.15600 1.00000

```

Ir<sub>3</sub>Ge<sub>7</sub> (D8<sub>f</sub>): A7B3\_c140\_229\_df\_e - POSCAR

```

A7B3_c140_229_df_e & a,x2,x3 --params=8.735,0.342,0.156 & Im-3m O_{h}^{19}
↪ } #229 (def) & c140 & $D8_{f}$ & Ir3Ge7 & Ir3Ge7 & U.H\{a}
↪ ussermann et al., Chem. Euro. J. 4, 1007-1015 (1998)
1.0000000000000000
-4.367500000000000 4.367500000000000 4.367500000000000
4.367500000000000 -4.367500000000000 4.367500000000000
4.367500000000000 4.367500000000000 -4.367500000000000
Ge Ir
14 6
Direct
0.500000000000000 0.750000000000000 0.250000000000000 Ge (12d)
0.500000000000000 0.250000000000000 0.750000000000000 Ge (12d)
0.250000000000000 0.500000000000000 0.750000000000000 Ge (12d)
0.750000000000000 0.500000000000000 0.250000000000000 Ge (12d)
0.750000000000000 0.250000000000000 0.500000000000000 Ge (12d)
0.250000000000000 0.750000000000000 0.500000000000000 Ge (12d)
0.312000000000000 0.312000000000000 0.312000000000000 Ge (16f)
0.000000000000000 0.000000000000000 -0.312000000000000 Ge (16f)
0.000000000000000 -0.312000000000000 0.000000000000000 Ge (16f)
-0.312000000000000 0.000000000000000 0.000000000000000 Ge (16f)
0.000000000000000 0.000000000000000 0.312000000000000 Ge (16f)
-0.312000000000000 -0.312000000000000 -0.312000000000000 Ge (16f)
0.000000000000000 0.312000000000000 0.000000000000000 Ge (16f)
0.312000000000000 0.000000000000000 0.000000000000000 Ge (16f)
0.000000000000000 0.342000000000000 0.342000000000000 Ir (12e)
0.000000000000000 -0.342000000000000 -0.342000000000000 Ir (12e)
0.342000000000000 0.000000000000000 0.342000000000000 Ir (12e)
-0.342000000000000 0.000000000000000 -0.342000000000000 Ir (12e)
0.342000000000000 0.342000000000000 0.000000000000000 Ir (12e)
-0.342000000000000 -0.342000000000000 0.000000000000000 Ir (12e)

```

Garnet (Co<sub>3</sub>Al<sub>2</sub>Si<sub>3</sub>O<sub>12</sub>, S1<sub>4</sub>): A2B3C12D3\_c1160\_230\_a\_c\_h\_d - CIF

```

# CIF file
data_findsym-output
_audit_creation_method FINDSYM

_chemical_name_mineral 'Garnet'
_chemical_formula_sum 'Al2 Co3 O12 Si3'

loop_
_publ_author_name
'C. R. {Ross II}'
'H. Keppler'
'D. Canil'
'H. {St.} C. {O\`Neill}'
_journal_name_full_name
;
American Mineralogist
;
_journal_volume 81
_journal_year 1996
_journal_page_first 61
_journal_page_last 66
_publ_section_title
;
Structure and crystal-field spectra of Co3Al2Si3O12 (SiO4)3 and (
↪ Mg,Ni)3Al2Si3O12 (SiO4)3 garnet
;

# Found in The American Mineralogist Crystal Structure Database, 2003
_flow_title 'Garnet (Co3Al2Si3O12)3 Structure'
_flow_proto 'A2B3C12D3_c1160_230_a_c_h_d'
_flow_params 'a_x_{4},y_{4},z_{4}'
_flow_params_values '11.4597,0.3471,0.4664,0.0512'
_flow_Strukturbericht '$S1_{4}$'
_flow_Pearson 'c1160'

```

```

_symmetry_space_group_name_H-M "I 41/a -3 2/d"
_symmetry_Int_Tables_number 230

_cell_length_a 11.45970
_cell_length_b 11.45970
_cell_length_c 11.45970
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000

```

```

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z+1/2
3 -x+1/2,y,-z
4 -x,-y+1/2,z
5 y,z,x
6 y,-z,-x+1/2
7 -y+1/2,z,-x
8 -y,-z+1/2,x
9 z,x,y
10 z,-x,-y+1/2
11 -z+1/2,x,-y
12 -z,-x+1/2,y
13 -y+1/4,-x+1/4,-z+1/4
14 -y+1/4,x+3/4,z+1/4
15 y+1/4,-x+1/4,z+3/4
16 y+3/4,x+1/4,-z+1/4
17 -x+1/4,-z+1/4,-y+1/4
18 -x+1/4,z+3/4,y+1/4
19 x+1/4,-z+1/4,y+3/4
20 x+3/4,z+1/4,-y+1/4
21 -z+1/4,-y+1/4,-x+1/4
22 -z+1/4,y+3/4,x+1/4
23 z+1/4,-y+1/4,x+3/4
24 z+3/4,y+1/4,-x+1/4
25 -x,-y,-z
26 -x,y,z+1/2
27 x+1/2,-y,z
28 x,y+1/2,-z
29 -y,-z,-x
30 -y,z,x+1/2
31 y+1/2,-z,x
32 y,z+1/2,-x
33 -z,-x,-y
34 -z,x,y+1/2
35 z+1/2,-x,y
36 z,x+1/2,-y
37 y+1/4,x+1/4,z+1/4
38 y+1/4,-x+3/4,-z+1/4
39 -y+1/4,x+1/4,-z+3/4
40 -y+3/4,-x+1/4,z+1/4
41 x+1/4,z+1/4,y+1/4
42 x+1/4,-z+3/4,-y+1/4
43 -x+1/4,z+1/4,-y+3/4
44 -x+3/4,-z+1/4,y+1/4
45 z+1/4,y+1/4,x+1/4
46 z+1/4,-y+3/4,-x+1/4
47 -z+1/4,y+1/4,-x+3/4
48 -z+3/4,-y+1/4,x+1/4
49 x+1/2,y+1/2,z+1/2
50 x+1/2,-y+1/2,-z
51 -x,y+1/2,-z+1/2
52 -x+1/2,-y,z+1/2
53 y+1/2,z+1/2,x+1/2
54 y+1/2,-z+1/2,-x
55 -y,z+1/2,-x+1/2
56 -y+1/2,-z,x+1/2
57 z+1/2,x+1/2,y+1/2
58 z+1/2,-x+1/2,-y
59 -z,x+1/2,-y+1/2
60 -z+1/2,-x,y+1/2
61 -y+3/4,-x+3/4,-z+3/4
62 -y+3/4,x+1/4,z+3/4
63 y+3/4,-x+3/4,z+1/4
64 y+1/4,x+3/4,-z+3/4
65 -x+3/4,-z+3/4,-y+3/4
66 -x+3/4,z+1/4,y+3/4
67 x+3/4,-z+3/4,y+1/4
68 x+1/4,z+3/4,-y+3/4
69 -z+3/4,-y+3/4,-x+3/4
70 -z+3/4,y+1/4,x+3/4
71 z+3/4,-y+3/4,x+1/4
72 z+1/4,y+3/4,-x+3/4
73 -x+1/2,-y+1/2,-z+1/2
74 -x+1/2,y+1/2,z
75 x,-y+1/2,z+1/2
76 x+1/2,y,-z+1/2
77 -y+1/2,-z+1/2,-x+1/2
78 -y+1/2,z+1/2,x
79 y,-z+1/2,x+1/2
80 y+1/2,z,-x+1/2
81 -z+1/2,-x+1/2,-y+1/2
82 -z+1/2,x+1/2,y
83 z,-x+1/2,y+1/2
84 z+1/2,x,-y+1/2
85 y+3/4,x+3/4,z+3/4
86 y+3/4,-x+1/4,-z+3/4
87 -y+3/4,x+3/4,-z+1/4
88 -y+1/4,-x+3/4,z+3/4
89 x+3/4,z+3/4,y+3/4
90 x+3/4,-z+1/4,-y+3/4
91 -x+3/4,z+3/4,-y+1/4

```

```

92 -x+1/4,-z+3/4,y+3/4
93 z+3/4,y+3/4,x+3/4
94 z+3/4,-y+1/4,-x+3/4
95 -z+3/4,y+3/4,-x+1/4
96 -z+1/4,-y+3/4,x+3/4

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 16 a 0.00000 0.00000 0.00000 1.00000
Co1 Co 24 c 0.12500 0.00000 0.25000 1.00000
Si1 Si 24 d 0.37500 0.00000 0.25000 1.00000
O1 O 96 h 0.34710 0.46640 0.05120 1.00000

```

```

0.625000000000000 0.375000000000000 0.250000000000000 Si (24d)
0.875000000000000 0.125000000000000 0.750000000000000 Si (24d)
0.625000000000000 0.750000000000000 0.375000000000000 Si (24d)
0.875000000000000 0.250000000000000 0.125000000000000 Si (24d)
0.750000000000000 0.375000000000000 0.625000000000000 Si (24d)
0.250000000000000 0.125000000000000 0.875000000000000 Si (24d)
0.125000000000000 0.875000000000000 0.250000000000000 Si (24d)
0.375000000000000 0.625000000000000 0.750000000000000 Si (24d)

```

Garnet (Co<sub>3</sub>Al<sub>2</sub>Si<sub>3</sub>O<sub>12</sub>, S 1<sub>4</sub>): A2B3C12D3\_c1160\_230\_a\_c\_h\_d - POSCAR

```

A2B3C12D3_c1160_230_a_c_h_d & a,x4,y4,z4 --params=11.4597,0.3471,0.4664,
↪ 0.0512 & Ia-3d O_{h}^{10} #230 (acdh) & c1160 & $S1_{4}$ &
↪ Co3Al2Si3O12 & Garnet & C. R. {Ross II} et al., Am. Mineral. 81
↪ , 61-66 (1996)

```

```

1.000000000000000
-5.729850000000000 5.729850000000000 5.729850000000000
5.729850000000000 -5.729850000000000 5.729850000000000
5.729850000000000 5.729850000000000 -5.729850000000000
Al Co O Si
8 12 48 12
Direct
0.000000000000000 0.000000000000000 0.000000000000000 Al (16a)
0.500000000000000 0.000000000000000 0.500000000000000 Al (16a)
0.000000000000000 0.500000000000000 0.000000000000000 Al (16a)
0.500000000000000 0.000000000000000 0.000000000000000 Al (16a)
0.500000000000000 0.000000000000000 0.000000000000000 Al (16a)
0.500000000000000 0.500000000000000 0.000000000000000 Al (16a)
0.000000000000000 0.000000000000000 0.500000000000000 Al (16a)
0.000000000000000 0.500000000000000 0.000000000000000 Al (16a)
0.250000000000000 0.375000000000000 0.125000000000000 Co (24c)
0.750000000000000 0.125000000000000 0.375000000000000 Co (24c)
0.125000000000000 0.250000000000000 0.375000000000000 Co (24c)
0.375000000000000 0.750000000000000 0.125000000000000 Co (24c)
0.375000000000000 0.125000000000000 0.250000000000000 Co (24c)
0.125000000000000 0.375000000000000 0.750000000000000 Co (24c)
0.750000000000000 0.625000000000000 0.875000000000000 Co (24c)
0.250000000000000 0.875000000000000 0.625000000000000 Co (24c)
0.875000000000000 0.750000000000000 0.625000000000000 Co (24c)
0.625000000000000 0.250000000000000 0.875000000000000 Co (24c)
0.625000000000000 0.875000000000000 0.750000000000000 Co (24c)
0.875000000000000 0.625000000000000 0.250000000000000 Co (24c)
0.517600000000000 0.398300000000000 0.813500000000000 O (96h)
0.084800000000000 -0.295900000000000 -0.313500000000000 O (96h)
0.415200000000000 0.101700000000000 0.619300000000000 O (96h)
-0.017600000000000 0.795900000000000 -0.119300000000000 O (96h)
0.813500000000000 0.517600000000000 0.398300000000000 O (96h)
-0.313500000000000 0.084800000000000 -0.295900000000000 O (96h)
0.619300000000000 0.415200000000000 0.101700000000000 O (96h)
-0.119300000000000 -0.017600000000000 0.795900000000000 O (96h)
0.398300000000000 0.813500000000000 0.517600000000000 O (96h)
-0.295900000000000 -0.313500000000000 0.084800000000000 O (96h)
0.101700000000000 0.619300000000000 0.415200000000000 O (96h)
0.795900000000000 -0.119300000000000 -0.017600000000000 O (96h)
0.795900000000000 0.415200000000000 0.813500000000000 O (96h)
0.101700000000000 -0.017600000000000 -0.313500000000000 O (96h)
-0.295900000000000 0.517600000000000 0.619300000000000 O (96h)
0.398300000000000 0.084800000000000 -0.119300000000000 O (96h)
0.084800000000000 -0.119300000000000 0.398300000000000 O (96h)
0.517600000000000 0.619300000000000 -0.295900000000000 O (96h)
-0.017600000000000 -0.313500000000000 0.101700000000000 O (96h)
0.415200000000000 0.813500000000000 0.795900000000000 O (96h)
0.619300000000000 -0.295900000000000 0.517600000000000 O (96h)
-0.119300000000000 0.398300000000000 0.084800000000000 O (96h)
0.813500000000000 0.795900000000000 0.415200000000000 O (96h)
-0.313500000000000 0.101700000000000 -0.017600000000000 O (96h)
-0.517600000000000 -0.398300000000000 -0.813500000000000 O (96h)
0.915200000000000 0.295900000000000 1.313500000000000 O (96h)
-0.415200000000000 0.898300000000000 0.380700000000000 O (96h)
1.017600000000000 0.204100000000000 0.119300000000000 O (96h)
-0.813500000000000 -0.517600000000000 -0.398300000000000 O (96h)
1.313500000000000 0.915200000000000 0.295900000000000 O (96h)
0.380700000000000 -0.415200000000000 0.898300000000000 O (96h)
0.119300000000000 1.017600000000000 0.204100000000000 O (96h)
-0.398300000000000 -0.813500000000000 -0.517600000000000 O (96h)
0.295900000000000 1.313500000000000 0.915200000000000 O (96h)
0.898300000000000 0.380700000000000 -0.415200000000000 O (96h)
0.204100000000000 0.119300000000000 1.017600000000000 O (96h)
0.204100000000000 -0.415200000000000 -0.813500000000000 O (96h)
0.898300000000000 1.017600000000000 1.313500000000000 O (96h)
0.295900000000000 -0.517600000000000 0.380700000000000 O (96h)
-0.398300000000000 0.915200000000000 0.119300000000000 O (96h)
0.915200000000000 0.119300000000000 -0.398300000000000 O (96h)
-0.517600000000000 0.380700000000000 0.295900000000000 O (96h)
1.017600000000000 1.313500000000000 0.898300000000000 O (96h)
-0.415200000000000 -0.813500000000000 0.204100000000000 O (96h)
0.380700000000000 0.295900000000000 -0.517600000000000 O (96h)
0.119300000000000 -0.398300000000000 0.915200000000000 O (96h)
-0.813500000000000 0.204100000000000 -0.415200000000000 O (96h)
1.313500000000000 0.898300000000000 1.017600000000000 O (96h)
0.250000000000000 0.625000000000000 0.375000000000000 Si (24d)
0.750000000000000 0.875000000000000 0.125000000000000 Si (24d)
0.375000000000000 0.250000000000000 0.625000000000000 Si (24d)
0.125000000000000 0.750000000000000 0.875000000000000 Si (24d)

```

## Prototype Index

1. $\alpha$ -Al <sub>2</sub> S <sub>3</sub> : A2B3_hp30_169_2a_3a	547	43. Akermanite: A2BC7D2_tP24_113_e_a_cef_e	380
2. $\alpha$ -CuAlCl <sub>4</sub> : AB4C_tP12_112_b_n_e	378	44. Al <sub>2</sub> CuIr <sup>§</sup> : A2BC_oC16_67_ag_b_g	236
3. $\alpha$ -FeSe <sup>†</sup> : AB_oC8_67_a_g	240	45. Al <sub>2</sub> S <sub>3</sub> : A2B3_hp30_170_2a_3a	550
4. $\alpha$ -Naumannite: A2B_oP12_17_abe_e	75	46. Al <sub>4</sub> C <sub>3</sub> : A4B3_hr7_166_2c_ac	530
5. $\alpha$ -NbO <sub>2</sub> : AB2_tI96_88_2f_4f	296	47. Al <sub>4</sub> U: A4B_oI20_74_beh_e	256
6. $\alpha$ -P <sub>3</sub> N <sub>5</sub> : A5B3_mC32_9_5a_3a	42	48. Al <sub>8</sub> Cr <sub>5</sub> : A8B5_hr26_160_a3bc_a3b	514
7. $\alpha$ -PbO <sup>†</sup> : AB_oC8_67_a_g	242	49. Al <sub>9</sub> Mn <sub>3</sub> Si: A9B3C_hp26_194_hk_h_a	646
8. $\alpha$ -PdCl <sub>2</sub> : A2B_oP6_58_g_a	176	50. AlLi <sub>3</sub> N <sub>2</sub> : AB3C2_cI96_206_c_e_ad	704
9. $\alpha$ -RbPr[MoO <sub>4</sub> ] <sub>2</sub> : A2B8CD_oP24_48_k_2m_d_b	149	51. AlPO <sub>4</sub> : AB2_hp72_192_m_j2kl	635
10. $\alpha$ -Sm <sub>3</sub> Ge <sub>5</sub> : A5B3_hp16_190_bdh_g	626	52. Al[PO <sub>4</sub> ]: AB4C_hp72_168_2d_8d_2d	543
11. $\alpha$ -ThSi <sub>2</sub> : A2B_tI12_141_e_a	457	53. Al[PO <sub>4</sub> ]: AB4C_hp72_184_d_4d_d	594
12. $\alpha$ -Tl <sub>2</sub> TeO <sub>3</sub> : A3BC2_oP48_50_3m_m_2m	157	54. Anhydrite: AB4C_oC24_63_c_fg_c	224
13. $\alpha$ -Toluene: A7B8_mP120_14_14e_16e	64	55. As <sub>2</sub> Ba: A2B_mP18_7_6a_3a	36
14. $\beta$ -Bi <sub>2</sub> O <sub>3</sub> : A2B3_tP20_117_i_adgh	393	56. AsPh <sub>4</sub> CeS <sub>8</sub> P <sub>4</sub> Me <sub>8</sub> : AB32CD4E8_tP184_93_i_16p_af_2p_4p	315
15. $\beta$ -CuI: AB_hp4_156_ac_ac	497	57. AuCN: ABC_hp3_183_a_a_a	590
16. $\beta$ -Hg <sub>4</sub> Pt: A4B_cI10_229_c_a	793	58. AuF <sub>3</sub> : AB3_hp24_178_b_ac	582
17. $\beta$ -NbO <sub>2</sub> : AB2_tI48_80_2b_4b	279	59. AuF <sub>3</sub> : AB3_hp24_179_b_ac	586
18. $\beta$ -PdCl <sub>2</sub> : A2B_hr18_148_2f_f	483	60. BN: AB_oF8_42_a_a	143
19. $\beta$ -RuCl <sub>3</sub> : A3B_hp8_158_d_a	501	61. BPS <sub>4</sub> : ABC <sub>4</sub> _oI12_23_a_b_k	91
20. $\beta$ -RuCl <sub>3</sub> : A3B_hp8_185_c_a	605	62. Ba <sub>5</sub> In <sub>4</sub> Bi <sub>5</sub> : A5B5C4_tP28_104_ac_ac_c	347
21. $\beta$ -SeO <sub>2</sub> <sup>*</sup> : A2B_oP12_26_abc_ab	97	63. Ba <sub>5</sub> Si <sub>3</sub> : A5B3_tP32_130_cg_cf	427
22. $\beta$ -Si <sub>3</sub> N <sub>4</sub> : A4B3_hp14_173_bc_c	562	64. BaCr <sub>2</sub> Ru <sub>4</sub> O <sub>12</sub> : AB2C12D4_tP76_75_2a2b_2d_12d_4d	258
23. $\beta$ -SiO <sub>2</sub> : A2B_hp9_181_j_c	588	65. BaCu <sub>4</sub> [VO][PO <sub>4</sub> ] <sub>4</sub> : AB4C17D4E_tP54_90_a_g_c4g_g_c	310
24. $\beta$ -Ta <sub>2</sub> O <sub>5</sub> : A5B2_oP14_49_dehq_ab	151	66. BaGe <sub>2</sub> As <sub>2</sub> : A2BC2_tP20_105_f_ac_2e	352
25. $\beta$ -ThI <sub>3</sub> : A3B_oC64_66_kl2m_bdl	233	67. BaSi <sub>4</sub> O <sub>9</sub> : AB9C4_hp28_188_e_kl_ak	616
26. $\beta$ -Toluene: A7B8_oP120_60_7d_8d	185	68. Barite: AB4C_oP24_62_c_2cd_c	206
27. $\beta$ -V <sub>3</sub> S: AB3_tP32_133_h_i2j	433	69. Be[BH <sub>4</sub> ] <sub>2</sub> : A2BC8_tI176_110_2b_b_8b	368
28. $\delta$ -PdCl <sub>2</sub> : A2B_mP6_10_mn_bg	46	70. Benzene: AB_oP48_61_3c_3c	191
29. $\delta^I_H$ -NW <sub>2</sub> : AB2_hp9_164_bd_c2d	523	71. Beryl: A2B3C18D6_hp58_192_c_f_lm_l	631
30. $\epsilon$ -NiAl <sub>3</sub> : A3B_oP16_62_cd_c	200	72. Bi <sub>2</sub> O <sub>3</sub> : A2B3_hp20_159_bc_2c	503
31. $\epsilon$ -WO <sub>3</sub> : A3B_mP16_7_6a_2a	38	73. Bi <sub>5</sub> Nb <sub>3</sub> O <sub>15</sub> : A5B3C15_oP46_30_a2c_bc_a7c	112
32. $\gamma$ -Ag <sub>3</sub> SI: A3BC_hr5_146_b_a_a	475	74. BiAl <sub>2</sub> S <sub>4</sub> : A2BC4_tP28_126_cd_e_k	416
33. $\gamma$ -MgNiSn: A7B7C2_tP32_101_bde_ade_d	340	75. BiGaO <sub>3</sub> : ABC3_oP20_54_e_d_cf	168
34. $\gamma$ -PdCl <sub>2</sub> : A2B_mP6_14_e_a	62	76. Boracite: A7BC3D13_cF192_219_de_b_c_ah	749
35. $\gamma$ -brass: A4B9_cP52_215_ei_3efgi	741	77. C: A_tP12_138_bi	449
36. $\gamma$ -brass: A3B10_cI52_229_e_fh	790	78. C <sub>17</sub> FeO <sub>4</sub> Pt: A17BC4D_tP184_89_17p_p_4p_io	300
37. $\kappa$ -alumina: A2B3_oP40_33_4a_6a	120	79. Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> : A2B3C6_cP264_205_2d_ab2c2d_6d	687
38. $\pi$ -FeMg <sub>3</sub> Al <sub>8</sub> Si <sub>6</sub> : A8BC3D6_hp18_189_bfh_a_g_i	619	80. Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> : A2B3C6_cP33_221_cd_ag_fh	758
39. $\pi$ -FeMg <sub>3</sub> Al <sub>9</sub> Si <sub>5</sub> : A9BC3D5_hp18_189_fi_a_g_bh	622	81. Ca <sub>3</sub> PI <sub>3</sub> : A3B3C_cI56_214_g_h_a	736
40. Ag <sub>3</sub> [PO <sub>4</sub> ]: A3B4C_cP16_218_c_e_a	747	82. Ca <sub>4</sub> Al <sub>6</sub> O <sub>16</sub> S: A6B4C16D_oP108_27_abcd4e_4e_16e_e	101
41. Ag <sub>3</sub> Pb <sub>2</sub> O <sub>6</sub> : A5B6C2_hp13_157_2ac_2c_b	499	83. CaRbFe <sub>4</sub> As <sub>4</sub> : A4BC4D_tP10_123_gh_a_i_d	406
42. AgUF <sub>6</sub> : AB6C_tP16_132_d_io_a	431	84. Calomel: AB_tI8_139_e_e	451
		85. Carbonyl Sulphide: ABC_hr3_160_a_a_a	517

<sup>†</sup> $\alpha$ -FeSe and  $\alpha$ -PbO have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters.

<sup>\*</sup>H<sub>2</sub>S and  $\beta$ -SeO<sub>2</sub> have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters.

<sup>§</sup>Al<sub>2</sub>CuIr and HoCu<sub>2</sub> have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

86. CdAs <sub>2</sub> : A2B_tI12_98_f_a	333	131. Gd <sub>3</sub> Al <sub>2</sub> : A2B3_tP20_102_2c_b2c	343
87. CdI <sub>2</sub> : AB2_hp9_156_b2c_3a2bc	493	132. GdSI: ABC_hp12_174_cj_fk_aj	566
88. Ce <sub>3</sub> Si <sub>6</sub> N <sub>11</sub> : A3B11C6_tP40_100_ac_bc2d_cd	337	133. GeAs <sub>2</sub> : A2B_op24_55_2g2h_gh	170
89. Ce <sub>5</sub> Mo <sub>3</sub> O <sub>16</sub> : A5B3C16_cP96_222_ce_d_fi	761	134. GeP: AB_tI4_107_a_a	360
90. CeCo <sub>4</sub> B <sub>4</sub> : A4BC4_tP18_137_g_b_g	445	135. GeSe <sub>2</sub> : AB2_tP12_81_adg_2h	282
91. CeRu <sub>2</sub> B <sub>2</sub> : A2BC2_of40_22_fi_ad_gh	81	136. H <sub>2</sub> S: A2B_ap6_2_aei_i	28
92. CeTe <sub>3</sub> : AB3_oc16_40_b_3b	139	137. H <sub>2</sub> S: A2B_mp12_13_2g_ef	60
93. Co <sub>2</sub> Al <sub>5</sub> : A5B2_hp28_194_ahk_ch	643	138. H <sub>2</sub> S*: A2B_op12_26_abc_ab	95
94. Co <sub>5</sub> Ge <sub>7</sub> : A5B7_tI24_107_ac_abd	358	139. H <sub>2</sub> S: A2B_oc24_64_2f_f	226
95. Cobaltite: ABC_op12_29_a_a_a	110	140. H <sub>2</sub> S III: A2B_tP48_77_8d_4d	270
96. Cr <sub>5</sub> B <sub>3</sub> : A3B5_tI32_140_ah_cl	455	141. H <sub>2</sub> S IV: A2B_mp12_7_4a_2a	34
97. CrCl <sub>3</sub> : A3B_hp24_153_3c_2b	488	142. H <sub>3</sub> Cl: AB3_mC16_9_a_3a	44
98. CrFe <sub>3</sub> NiSn <sub>5</sub> : AB_hp6_183_c_ab	592	143. H <sub>3</sub> Cl: AB3_mp16_10_mn_3m3n	48
99. Cs <sub>2</sub> ZnFe[CN] <sub>6</sub> : A6B2CD6E_cP64_208_m_ad_b_m_c	712	144. H <sub>3</sub> Cl: AB3_mC16_15_e_cf	71
100. Cs <sub>3</sub> P <sub>7</sub> : A3B7_tP40_76_3a_7a	264	145. H <sub>3</sub> Cl: AB3_op16_19_a_3a	77
101. CsPr[MoO <sub>4</sub> ] <sub>2</sub> : AB2C8D_op24_49_g_q_2qr_e	153	146. H <sub>3</sub> S: A3B_oI32_23_ij2k_k	85
102. Cu <sub>15</sub> Si <sub>4</sub> : A15B4_cl76_220_ae_c	753	147. H <sub>3</sub> S: A3B_oc64_66_gi2lm_2l	230
103. Cu <sub>2</sub> Fe[CN] <sub>6</sub> : A12B2C_cF60_196_h_bc_a	652	148. H <sub>3</sub> S: A3B_hr4_160_b_a	512
104. Cu <sub>3</sub> P: A3B_hp24_165_bdg_f	527	149. H-III: A_mc24_15_2e2f	73
105. Cu <sub>3</sub> P <sup>  </sup> : A3B_hp24_185_ab2c_c	602	150. HCl: AB_oc8_36_a_a	129
106. CuBi <sub>2</sub> O <sub>4</sub> : A2BC4_tP28_130_f_c_g	425	151. HgI <sub>2</sub> : AB2_tP12_115_j_egi	389
107. CuBrSe <sub>3</sub> : ABC3_op20_30_2a_c_3c	115	152. HgI <sub>2</sub> <sup>¶</sup> : AB2_tP6_137_a_d	447
108. CuBrSe <sub>3</sub> : ABC3_op20_53_e_g_hi	166	153. HoCuP <sub>2</sub> <sup>§</sup> : ABC2_oc16_67_b_g_ag	238
109. CuCrCl <sub>5</sub> [NH <sub>3</sub> ] <sub>6</sub> : A5BCD6_cF416_228_eg_c_b_h	778	154. Ir <sub>3</sub> Ga <sub>5</sub> : A5B3_tP32_118_g2i_aceh	397
110. CuI: AB_hp12_156_2ab3c_2ab3c	495	155. Ir <sub>3</sub> Ge <sub>7</sub> : A7B3_cI40_229_df_e	795
111. CuNiSb <sub>2</sub> : ABC2_hp4_164_a_b_d	525	156. IrGe <sub>4</sub> : A4B_hp15_144_4a_a	467
112. Cubanite: AB2C3_op24_62_c_d_cd	202	157. K <sub>2</sub> CdPb: AB2C_oc16_40_a_2b_b	137
113. Downeyite: A2B_tP24_135_gh_h	436	158. K <sub>2</sub> PtCl <sub>6</sub> : A6B2C_cF36_225_e_c_a	769
114. Er <sub>3</sub> Ru <sub>2</sub> : A3B2_hp10_176_h_bd	573	159. K <sub>2</sub> SnCl <sub>6</sub> : A6B2C_tP18_128_eh_d_b	420
115. F <sub>6</sub> KP: A24BC_cF104_209_j_a_b	716	160. K <sub>2</sub> Ta <sub>4</sub> O <sub>9</sub> F <sub>4</sub> : A2B13C4_hp57_168_d_c6d_2d	539
116. FCC C <sub>60</sub> Buckminsterfullerene: A_cF240_202_h2i	671	161. KAg[CO <sub>3</sub> ]: ABCD3_oI48_73_d_e_e_ef	252
117. Fe <sub>12</sub> Zr <sub>2</sub> P <sub>7</sub> : A12B7C2_hp21_174_2j2k_ajk_cf	564	162. KAu <sub>4</sub> Sn <sub>2</sub> : A4BC2_tI28_120_i_d_e	404
118. Fe <sub>3</sub> Te <sub>3</sub> Tl: A3B3C_hp14_176_h_h_d	575	163. KB <sub>6</sub> H <sub>6</sub> : A6B6C_cF104_202_h_h_c	669
119. Fe <sub>3</sub> Th <sub>7</sub> : A3B7_hp20_186_c_b2c	610	164. KBO <sub>2</sub> : ABC2_hr24_167_e_e_2e	536
120. FeCu <sub>2</sub> Al <sub>7</sub> : A7B2C_tP40_128_egi_h_e	422	165. KCeSe <sub>4</sub> : ABC4_tP12_125_a_b_m	414
121. FeNi: AB_mp4_6_2b_2a	32	166. KHg <sub>2</sub> : A2B_oI12_74_h_e	254
122. FeOCl: ABC_op6_59_a_b_a	178	167. KNiCl <sub>3</sub> : A3BC_hp30_185_cd_c_ab	599
123. FePSe <sub>3</sub> : ABC3_hr10_146_2a_2a_2b	477	168. KSbO <sub>3</sub> : AB3C_cP60_201_ce_fh_g	666
124. FeS: AB_of8_22_a_c	83	169. La <sub>2</sub> NiO <sub>4</sub> : A2BC4_op28_50_ij_ac_ijm	155
125. FeSb <sub>2</sub> : AB2_op6_34_a_c	125	170. La <sub>2</sub> O <sub>3</sub> : A2B3_hp5_164_d_ad	521
126. Forsterite: A2B4C_op28_62_ac_2cd_c	196	171. La <sub>43</sub> Ni <sub>17</sub> Mg <sub>5</sub> : A43B5C17_oc260_63_c8fg6h_cfg_ce3f2h	212
127. Fresnoite: A2B8C2D_tP26_100_c_abcd_c_a	335	172. LaPtSi: ABC_tI12_109_a_a_a	364
128. GaCl <sub>2</sub> : A2B_op24_52_2e_cd	160	173. LaRhC <sub>2</sub> : A2BC_tP16_76_2a_a_a	262
129. GaSb: AB_tI4_119_c_a	402	174. Li <sub>2</sub> MoF <sub>6</sub> : A6B2C_tP18_94_eg_c_a	325
130. Garnet: A2B3C12D3_cI160_230_a_c_h_d	797	175. Li <sub>2</sub> Sb: A2B_hp18_190_gh_bf	624
		176. Li <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> : A2B5C2_oc36_37_d_c2d_d	131

<sup>||</sup>Cu<sub>3</sub>P and Na<sub>3</sub>As have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

<sup>¶</sup>ZrO<sub>2</sub> and HgI<sub>2</sub> have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

177. LiScI <sub>3</sub> : A3BC_hP10_188_k_a_e	614	223. Pyrite <sup>‡</sup> : AB2_oP12_29_a_2a	108
178. LiSn: AB_mP6_10_en_am	52	224. Pyrochlore: A2BCD3E6_cF208_203_e_c_d_f_g	675
179. M-carbon: A_mC16_12_4i	58	225. Pyrochlore Iridate:	
180. Mavlyanovite: A5B3_hP16_193_dg_g	639	A2B2C7_cF88_227_c_d_af	774
181. Mg <sub>2</sub> Zn <sub>11</sub> : A2B11_cP39_200_f_aghij	663	226. Quaternary Heusler:	
182. MgB <sub>12</sub> H <sub>12</sub> [H <sub>2</sub> O] <sub>12</sub> :		ABCD_cF16_216_c_d_b_a	745
A12B36CD12_cF488_196_2h_6h_ac_fgh	654	227. R-carbon: A_oP16_55_2g2h	174
183. MgSO <sub>4</sub> : AB4C_oC24_63_a_fg_c	222	228. Rasvumite: A2BC3_oC24_63_e_c_cg	210
184. Mg[NH]: ABC_hP36_175_jk_jk_jk	570	229. Rb <sub>2</sub> TiCu <sub>2</sub> S <sub>4</sub> : A2B2C4D_tP18_132_e_i_o_d	429
185. Mn <sub>2</sub> B: AB2_oF48_70_f_fg	246	230. Rb <sub>3</sub> AsSe <sub>16</sub> : AB3C16_cF160_203_b_ad_eg	683
186. MnAl <sub>6</sub> : A6B_oC28_63_efg_c	218	231. RbGa <sub>3</sub> : A3B_tI24_119_b2i_af	400
187. MnF <sub>2</sub> : A2B_tP12_111_2n_adf	374	232. Re <sub>2</sub> O <sub>5</sub> [SO <sub>4</sub> ] <sub>2</sub> : A13B2C2_oP34_32_a6c_c_c	117
188. MnGa <sub>2</sub> Sb <sub>2</sub> : A2BC2_oI20_45_c_b_c	145	233. Re <sub>3</sub> N: AB3_hP4_187_e_fh	612
189. Mo <sub>8</sub> P <sub>5</sub> : A8B5_mP13_6_a7b_3a2b	30	234. Rh <sub>2</sub> Ga <sub>9</sub> : A9B2_mP22_7_9a_2a	40
190. MoS <sub>2</sub> : AB2_hP12_143_cd_ab2d	465	235. Rh <sub>2</sub> S <sub>3</sub> : A2B3_oP20_60_d_cd	180
191. Moissanite-15R: AB_hr10_160_5a_5a	519	236. Rh <sub>3</sub> P <sub>2</sub> : A2B3_tP5_115_g_ag	387
192. Molybdite: AB3_oP16_62_c_3c	204	237. Rh <sub>5</sub> Ge <sub>3</sub> : A3B5_oP16_55_ch_agh	172
193. Muthmannite: ABC2_mP8_10_ac_eh_mn	50	238. Ru <sub>2</sub> Sn <sub>3</sub> : A2B3_tP20_116_bci_fj	391
194. NV: AB_tP8_111_n_n	376	239. RuIn <sub>3</sub> : A3B_tP16_118_ei_f	395
195. Na <sub>3</sub> As <sup>  </sup> : AB3_hP24_185_c_ab2c	607	240. S-II: A_hP9_154_bc	491
196. Na <sub>4</sub> Ti <sub>2</sub> Si <sub>8</sub> O <sub>22</sub> [H <sub>2</sub> O] <sub>4</sub> :		241. S-III: A_tI16_142_f	459
A4B2C13D_tP40_90_g_d_cef2g_c	307	242. S-carbon: A_mP8_10_2m2n	54
197. Na <sub>5</sub> Fe <sub>3</sub> F <sub>14</sub> : A14B3C5_tP44_94_c3g_ad_bg	322	243. Sc-V: A_hP6_178_a	584
198. NaFeS <sub>2</sub> : ABC2_oI16_23_ab_i_k	89	244. ScRh <sub>6</sub> P <sub>4</sub> : A4B6C_hP11_143_bd_2d_a	463
199. NaGdCu <sub>2</sub> F <sub>8</sub> : A2B8CD_tI24_97_d_k_a_b	329	245. SeO <sub>3</sub> : A3B_tP32_114_3e_e	382
200. NaZn <sub>13</sub> : AB13_cF112_226_a_bi	771	246. Sheldrickite:	
201. NaZn[OH] <sub>3</sub> : A3BC3D_tP64_106_3c_c_3c_c	354	A2B3C3DE7_hP48_145_2a_3a_3a_a_7a	471
202. Nb <sub>4</sub> CoSi: AB4C_tP12_124_a_m_c	408	247. SiO <sub>2</sub> : A2B_hP36_177_j2lm_n	579
203. Nb <sub>7</sub> Ru <sub>6</sub> B <sub>8</sub> : A8B7C6_hP21_175_ck_aj_k	568	248. SiO <sub>2</sub> : A2B_cI72_211_hi_i	731
204. NbAs: AB_tI8_109_a_a	366	249. Simple Cubic C <sub>60</sub> Buckminsterfullerine:	
205. NbPS: ABC_oI12_71_h_j_g	250	A_cP240_205_10d	696
206. NbTe <sub>4</sub> : AB4_tP10_103_a_d	345	250. Simpsonite: A4B14C3_hP21_143_bd_ac4d_d	461
207. NbTe <sub>4</sub> : AB4_tP10_124_a_m	410	251. SmSI: ABC_hr6_166_c_c_c	532
208. Ni <sub>3</sub> P: A3B_tI32_82_3g_g	284	252. Sodium Chlorate: ABC3_cP20_198_a_a_b	661
209. Ni <sub>3</sub> Ti: A3B_hP16_194_gh_ac	641	253. Spinel: A3B4_cF56_227_ad_e	776
210. Nierite: A4B3_hP28_159_ab2c_2c	506	254. Sr <sub>2</sub> As <sub>2</sub> O <sub>7</sub> : A2B7C2_tP88_78_4a_14a_4a	273
211. PH <sub>3</sub> : A3B_cP16_208_j_b	710	255. Sr <sub>2</sub> Bi <sub>3</sub> : A3B2_oP20_52_de_cd	162
212. PI <sub>3</sub> : A3B_hP8_173_c_b	560	256. Sr <sub>5</sub> Si <sub>3</sub> : A3B5_tI32_108_ac_a2c	362
213. Pd <sub>17</sub> Se <sub>15</sub> : A17B15_cP64_207_acfk_eij	707	257. SrAl <sub>2</sub> Se <sub>4</sub> : A2B4C_oC28_66_l_kl_a	228
214. Pd <sub>4</sub> Se: A4B_tP10_114_e_a	385	258. SrBr <sub>2</sub> : A2B_tP30_85_ab2g_cg	288
215. PdSn <sub>4</sub> : AB4_oC20_68_a_i	244	259. SrH <sub>2</sub> : A2B_oP12_62_2c_c	198
216. Petzite: A3BC2_cI48_214_f_a_e	739	260. SrSi <sub>2</sub> : A2B_cP12_212_c_a	734
217. Phenakite: A2B4C_hr42_148_2f_4f_f	479	261. Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub> : A10B2C_hP39_171_5c_c_a	553
218. Pinnoite: A2B6CD7_tP64_77_2d_6d_d_ab6d	267	262. Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub> : A10B2C_hP39_172_5c_c_a	557
219. Post-perovskite: AB3C_oC20_63_a_cf_c	220	263. Stannoidite:	
220. PrNiO <sub>3</sub> : AB3C_hr10_167_b_e_a	534	A8B2C12D2E_oI50_23_bcfk_i_3k_j_a	87
221. PrRu <sub>4</sub> P <sub>12</sub> : A12BC4_cP34_195_2j_ab_2e	649	264. Ta <sub>2</sub> H: AB2_oC6_21_a_k	79
222. PtPb <sub>4</sub> : A4B_tP10_125_m_a	412		

<sup>‡</sup>ZrO<sub>2</sub> and Pyrite have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

265.	Ta <sub>2</sub> Se <sub>8</sub> I: AB8C2_tI44_97_e_2k_cd	331
266.	Ta <sub>3</sub> B <sub>4</sub> : A4B3_oI14_71_gh_cg	248
267.	Ta <sub>3</sub> S <sub>2</sub> : A2B3_oC40_39_2d_2c2d	133
268.	TaNiTe <sub>2</sub> : ABC2_oP16_53_h_e_gh	164
269.	TeO <sub>6</sub> H <sub>6</sub> : A6B_cF224_228_h_c	785
270.	TeZn: AB_hp6_144_a_a	469
271.	Te[OH] <sub>6</sub> : A12B6C_cF608_210_4h_2h_e	719
272.	Th <sub>3</sub> P <sub>4</sub> : A4B3_cI28_220_c_a	756
273.	Th <sub>6</sub> Mn <sub>23</sub> : A23B6_cF116_225_bd2f_e	766
274.	ThB <sub>4</sub> : A4B_tP20_127_ehj_g	418
275.	ThBC: ABC_tP24_91_d_d_d	313
276.	ThBC: ABC_tP24_95_d_d_d	327
277.	ThCl <sub>4</sub> : A4B_tI20_88_f_a	294
278.	Thortveitite: A7B2C2_mC22_12_ajj_h_i	56
279.	Ti <sub>2</sub> Ge <sub>3</sub> : A3B2_tP10_83_adk_j	286
280.	Ti <sub>3</sub> O: AB3_hp24_149_acgi_3l	486
281.	Ti <sub>3</sub> P: AB3_tP32_86_g_3g	291
282.	TiAl <sub>2</sub> Br <sub>8</sub> : A2B8C_oP22_34_c_4c_a	123
283.	TiFeSi: ABC_oI36_46_ac_bc_3b	147
284.	Tl <sub>4</sub> HgI <sub>6</sub> : AB6C4_tP22_104_a_2ac_c	350
285.	TlP <sub>5</sub> : A5B_oP24_26_3a3b2c_ab	99
286.	TlZn <sub>2</sub> Sb <sub>2</sub> : A2BC2_tI20_79_c_2a_c	277
287.	Tongbaite: A2B3_oP20_62_2c_3c	194
288.	Troilite: AB_hp24_190_i_afh	628
289.	Tychite: A4B2C6D16E_cF232_203_e_d_f_eg_a	679
290.	UCl <sub>3</sub> : A3B_hp8_176_h_d	577
291.	V <sub>2</sub> MoO <sub>8</sub> : AB8C2_oC22_35_a_ab3e_e	127
292.	VPCl <sub>9</sub> : A9BC_oC44_39_3c3d_a_c	135
293.	W <sub>3</sub> O <sub>10</sub> : A10B3_oF52_42_2abce_ab	141
294.	W <sub>5</sub> Si <sub>3</sub> : A3B5_tI32_140_ah_bk	453
295.	WO <sub>3</sub> : A3B_oP32_60_3d_d	182
296.	Weberite: AB7CD2_oI44_24_a_b3d_c_ac	93
297.	Westerveldite: AB_oP8_62_c_c	208
298.	YbBaCo <sub>4</sub> O <sub>7</sub> : AB4C7D_hp26_159_b_ac_a2c_b	509
299.	Zn <sub>3</sub> P <sub>2</sub> : A2B3_tP40_137_cdf_3g	440
300.	ZnSb <sub>2</sub> O <sub>4</sub> : A4B2C_tP28_135_gh_h_d	438
301.	ZrO <sub>2</sub> <sup>‡</sup> : A2B_oP12_29_2a_a	106
302.	ZrO <sub>2</sub> <sup>¶</sup> : A2B_tP6_137_d_a	443

## Pearson Symbol Index

<b>aP</b>	.....
1. <b>aP6</b>	.....
1.1. H <sub>2</sub> S: A2B_aP6_2_aei_i	28
<b>cF</b>	.....
1. <b>cF16</b>	.....
1.1. Quaternary Heusler: ABCD_cF16_216_c_d_b_a	745
2. <b>cF36</b>	.....
2.1. K <sub>2</sub> PtCl <sub>6</sub> : A6B2C_cF36_225_e_c_a	769
3. <b>cF56</b>	.....
3.1. Spinel: A3B4_cF56_227_ad_e	776
4. <b>cF60</b>	.....
4.1. Cu <sub>2</sub> Fe[CN] <sub>6</sub> : A12B2C_cF60_196_h_bc_a	652
5. <b>cF88</b>	.....
5.1. Pyrochlore Iridate: A2B2C7_cF88_227_c_d_af	774
6. <b>cF104</b>	.....
6.1. KB <sub>6</sub> H <sub>6</sub> : A6B6C_cF104_202_h_h_c	669
6.2. F <sub>6</sub> KP: A24BC_cF104_209_j_a_b	716
7. <b>cF112</b>	.....
7.1. NaZn <sub>13</sub> : AB13_cF112_226_a_bi	771
8. <b>cF116</b>	.....
8.1. Th <sub>6</sub> Mn <sub>23</sub> : A23B6_cF116_225_bd2f_e	766
9. <b>cF160</b>	.....
9.1. Rb <sub>3</sub> AsSe <sub>16</sub> : AB3C16_cF160_203_b_ad_eg	683
10. <b>cF192</b>	.....
10.1. Boracite: A7BC3D13_cF192_219_de_b_c_ah	749
11. <b>cF208</b>	.....
11.1. Pyrochlore: A2BCD3E6_cF208_203_e_c_d_f_g	675
12. <b>cF224</b>	.....
12.1. TeO <sub>6</sub> H <sub>6</sub> : A6B_cF224_228_h_c	785
13. <b>cF232</b>	.....
13.1. Tychite: A4B2C6D16E_cF232_203_e_d_f_eg_a	679
14. <b>cF240</b>	.....
14.1. FCC C <sub>60</sub> Buckminsterfullerene: A_cF240_202_h2i	671
15. <b>cF416</b>	.....
15.1. CuCrCl <sub>5</sub> [NH <sub>3</sub> ] <sub>6</sub> : A5BCD6_cF416_228_eg_c_b_h	778
16. <b>cF488</b>	.....
16.1. MgB <sub>12</sub> H <sub>12</sub> [H <sub>2</sub> O] <sub>12</sub> : A12B36CD12_cF488_196_2h_6h_ac_fgh	654
17. <b>cF608</b>	.....
17.1. Te[OH] <sub>6</sub> : A12B6C_cF608_210_4h_2h_e	719
<b>cI</b>	.....
1. <b>cI10</b>	.....
1.1. β-Hg <sub>4</sub> Pt: A4B_cI10_229_c_a	793
2. <b>cI28</b>	.....
2.1. Th <sub>3</sub> P <sub>4</sub> : A4B3_cI28_220_c_a	756

3.	<b>cI40</b>	3.1. Ir <sub>3</sub> Ge <sub>7</sub> : A7B3_cI40_229_df_e .....	795
4.	<b>cI48</b>	4.1. Petzite: A3BC2_cI48_214_f_a_e .....	739
5.	<b>cI52</b>	5.1. $\gamma$ -brass: A3B10_cI52_229_e_fh .....	790
6.	<b>cI56</b>	6.1. Ca <sub>3</sub> PI <sub>3</sub> : A3B3C_cI56_214_g_h_a .....	736
7.	<b>cI72</b>	7.1. SiO <sub>2</sub> : A2B_cI72_211_hi_i .....	731
8.	<b>cI76</b>	8.1. Cu <sub>15</sub> Si <sub>4</sub> : A15B4_cI76_220_ae_c .....	753
9.	<b>cI96</b>	9.1. AlLi <sub>3</sub> N <sub>2</sub> : AB3C2_cI96_206_c_e_ad .....	704
10.	<b>cI160</b>	10.1. Garnet: A2B3C12D3_cI160_230_a_c_h_d ...	797
<b>cP</b> .....			
1.	<b>cP12</b>	1.1. SrSi <sub>2</sub> : A2B_cP12_212_c_a .....	734
2.	<b>cP16</b>	2.1. PH <sub>3</sub> : A3B_cP16_208_j_b .....	710
		2.2. Ag <sub>3</sub> [PO <sub>4</sub> ]: A3B4C_cP16_218_c_e_a .....	747
3.	<b>cP20</b>	3.1. Sodium Chlorate: ABC3_cP20_198_a_a_b ..	661
4.	<b>cP33</b>	4.1. Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> : A2B3C6_cP33_221_cd_ag_fh ....	758
5.	<b>cP34</b>	5.1. PrRu <sub>4</sub> P <sub>12</sub> : A12BC4_cP34_195_2j_ab_2e ....	649
6.	<b>cP39</b>	6.1. Mg <sub>2</sub> Zn <sub>11</sub> : A2B11_cP39_200_f_aghij .....	663
7.	<b>cP52</b>	7.1. $\gamma$ -brass: A4B9_cP52_215_ei_3efgi .....	741
8.	<b>cP60</b>	8.1. KSbO <sub>3</sub> : AB3C_cP60_201_ce_fh_g .....	666
9.	<b>cP64</b>	9.1. Pd <sub>17</sub> Se <sub>15</sub> : A17B15_cP64_207_acfk_eij .....	707
		9.2. Cs <sub>2</sub> ZnFe[CN] <sub>6</sub> : A6B2CD6E_cP64_208_m_ad_b_m_c .....	712
10.	<b>cP96</b>	10.1. Ce <sub>5</sub> Mo <sub>3</sub> O <sub>16</sub> : A5B3C16_cP96_222_ce_d_fi ...	761
11.	<b>cP240</b>	11.1. Simple Cubic C <sub>60</sub> Buckminsterfullerene: A_cP240_205_10d .....	696
12.	<b>cP264</b>	12.1. Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> : A2B3C6_cP264_205_2d_ab2c2d_6d .....	687
<b>hP</b> .....			
1.	<b>hP3</b>	1.1. AuCN: ABC_hP3_183_a_a_a .....	590
2.	<b>hP4</b>	2.1. $\beta$ -CuI: AB_hP4_156_ac_ac .....	497
		2.2. CuNiSb <sub>2</sub> : ABC2_hP4_164_a_b_d .....	525
		2.3. Re <sub>3</sub> N: AB3_hP4_187_e_fh .....	612
3.	<b>hP5</b>	3.1. La <sub>2</sub> O <sub>3</sub> : A2B3_hP5_164_d_ad .....	521
4.	<b>hP6</b>	4.1. TeZn: AB_hP6_144_a_a .....	469
		4.2. Sc-V: A_hP6_178_a .....	584
		4.3. CrFe <sub>3</sub> NiSn <sub>5</sub> : AB_hP6_183_c_ab .....	592
5.	<b>hP8</b>	5.1. $\beta$ -RuCl <sub>3</sub> : A3B_hP8_158_d_a .....	501
		5.2. PI <sub>3</sub> : A3B_hP8_173_c_b .....	560
		5.3. UCl <sub>3</sub> : A3B_hP8_176_h_d .....	577
		5.4. $\beta$ -RuCl <sub>3</sub> : A3B_hP8_185_c_a .....	605
6.	<b>hP9</b>	6.1. S-II: A_hP9_154_bc .....	491
		6.2. CdI <sub>2</sub> : AB2_hP9_156_b2c_3a2bc .....	493
		6.3. $\delta''_H$ -NW <sub>2</sub> : AB2_hP9_164_bd_c2d .....	523
		6.4. $\beta$ -SiO <sub>2</sub> : A2B_hP9_181_j_c .....	588
7.	<b>hP10</b>	7.1. Er <sub>3</sub> Ru <sub>2</sub> : A3B2_hP10_176_h_bd .....	573
		7.2. LiScI <sub>3</sub> : A3BC_hP10_188_k_a_e .....	614
8.	<b>hP11</b>	8.1. ScRh <sub>6</sub> P <sub>4</sub> : A4B6C_hP11_143_bd_2d_a .....	463
9.	<b>hP12</b>	9.1. MoS <sub>2</sub> : AB2_hP12_143_cd_ab2d .....	465
		9.2. CuI: AB_hP12_156_2ab3c_2ab3c .....	495
		9.3. GdSI: ABC_hP12_174_cj_fk_aj .....	566
10.	<b>hP13</b>	10.1. Ag <sub>5</sub> Pb <sub>2</sub> O <sub>6</sub> : A5B6C2_hP13_157_2ac_2c_b ...	499
11.	<b>hP14</b>	11.1. $\beta$ -Si <sub>3</sub> N <sub>4</sub> : A4B3_hP14_173_bc_c .....	562
		11.2. Fe <sub>3</sub> Te <sub>3</sub> Tl: A3B3C_hP14_176_h_h_d .....	575
12.	<b>hP15</b>	12.1. IrGe <sub>4</sub> : A4B_hP15_144_4a_a .....	467
13.	<b>hP16</b>	13.1. $\alpha$ -Sm <sub>3</sub> Ge <sub>5</sub> : A5B3_hP16_190_bdh_g .....	626
		13.2. Mavlyanovite: A5B3_hP16_193_dg_g .....	639
		13.3. Ni <sub>3</sub> Ti: A3B_hP16_194_gh_ac .....	641
14.	<b>hP18</b>	14.1. $\pi$ -FeMg <sub>3</sub> Al <sub>8</sub> Si <sub>6</sub> : A8BC3D6_hP18_189_bfh_a_g_i .....	619
		14.2. $\pi$ -FeMg <sub>3</sub> Al <sub>9</sub> Si <sub>5</sub> : A9BC3D5_hP18_189_fi_a_g_bh .....	622
		14.3. Li <sub>2</sub> Sb: A2B_hP18_190_gh_bf .....	624
15.	<b>hP20</b>	15.1. Bi <sub>2</sub> O <sub>3</sub> : A2B3_hP20_159_bc_2c .....	503
		15.2. Fe <sub>3</sub> Th <sub>7</sub> : A3B7_hP20_186_c_b2c .....	610
16.	<b>hP21</b>	16.1. Simpsonite: A4B14C3_hP21_143_bd_ac4d_d .....	461
		16.2. Fe <sub>12</sub> Zr <sub>2</sub> P <sub>7</sub> : A12B7C2_hP21_174_2j2k_ajk_cf .....	564
		16.3. Nb <sub>7</sub> Ru <sub>6</sub> B <sub>8</sub> : A8B7C6_hP21_175_ck_aj_k ....	568
17.	<b>hP24</b>	17.1. Ti <sub>3</sub> O: AB3_hP24_149_acgi_3l .....	486
		17.2. CrCl <sub>3</sub> : A3B_hP24_153_3c_2b .....	488
		17.3. Cu <sub>3</sub> P: A3B_hP24_165_bdg_f .....	527



17.4.	AuF <sub>3</sub> : AB3_hP24_178_b_ac	582
17.5.	AuF <sub>3</sub> : AB3_hP24_179_b_ac	586
17.6.	Cu <sub>3</sub> P <sup>  </sup> : A3B_hP24_185_ab2c_c	602
17.7.	Na <sub>3</sub> As <sup>  </sup> : AB3_hP24_185_c_ab2c	607
17.8.	Troilite: AB_hP24_190_i_afh	628
18.	<b>hP26</b>	
18.1.	YbBaCo <sub>4</sub> O <sub>7</sub> : AB4C7D_hP26_159_b_ac_a2c_b	509
18.2.	Al <sub>9</sub> Mn <sub>3</sub> Si: A9B3C_hP26_194_hk_h_a	646
19.	<b>hP28</b>	
19.1.	Nierite: A4B3_hP28_159_ab2c_2c	506
19.2.	BaSi <sub>4</sub> O <sub>9</sub> : AB9C4_hP28_188_e_kl_ak	616
19.3.	Co <sub>2</sub> Al <sub>5</sub> : A5B2_hP28_194_ahk_ch	643
20.	<b>hP30</b>	
20.1.	α-Al <sub>2</sub> S <sub>3</sub> : A2B3_hP30_169_2a_3a	547
20.2.	Al <sub>2</sub> S <sub>3</sub> : A2B3_hP30_170_2a_3a	550
20.3.	KNiCl <sub>3</sub> : A3BC_hP30_185_cd_c_ab	599
21.	<b>hP36</b>	
21.1.	Mg[NH]: ABC_hP36_175_jk_jk_jk	570
21.2.	SiO <sub>2</sub> : A2B_hP36_177_j2lm_n	579
22.	<b>hP39</b>	
22.1.	Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub> : A10B2C_hP39_171_5c_c_a	553
22.2.	Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub> : A10B2C_hP39_172_5c_c_a	557
23.	<b>hP48</b>	
23.1.	Sheldrickite: A2B3C3DE7_hP48_145_2a_3a_3a_a_7a	471
24.	<b>hP57</b>	
24.1.	K <sub>2</sub> Ta <sub>4</sub> O <sub>9</sub> F <sub>4</sub> : A2B13C4_hP57_168_d_c6d_2d	539
25.	<b>hP58</b>	
25.1.	Beryl: A2B3C18D6_hP58_192_c_f_lm_l	631
26.	<b>hP72</b>	
26.1.	Al[PO <sub>4</sub> ]: AB4C_hP72_168_2d_8d_2d	543
26.2.	Al[PO <sub>4</sub> ]: AB4C_hP72_184_d_4d_d	594
26.3.	AlPO <sub>4</sub> : AB2_hP72_192_m_j2kl	635
<b>hR</b>		
1.	<b>hR3</b>	
1.1.	Carbonyl Sulphide: ABC_hR3_160_a_a_a	517
2.	<b>hR4</b>	
2.1.	H <sub>3</sub> S: A3B_hR4_160_b_a	512
3.	<b>hR5</b>	
3.1.	γ-Ag <sub>3</sub> SI: A3BC_hR5_146_b_a_a	475
4.	<b>hR6</b>	
4.1.	SmSI: ABC_hR6_166_c_c_c	532
5.	<b>hR7</b>	
5.1.	Al <sub>4</sub> C <sub>3</sub> : A4B3_hR7_166_2c_ac	530
6.	<b>hR10</b>	
6.1.	FePSe <sub>3</sub> : ABC3_hR10_146_2a_2a_2b	477
6.2.	Moissanite-15R: AB_hR10_160_5a_5a	519
6.3.	PrNiO <sub>3</sub> : AB3C_hR10_167_b_e_a	534
7.	<b>hR18</b>	
7.1.	β-PdCl <sub>2</sub> : A2B_hR18_148_2f_f	483
8.	<b>hR24</b>	
8.1.	KBO <sub>2</sub> : ABC2_hR24_167_e_e_2e	536
9.	<b>hR26</b>	
9.1.	Al <sub>8</sub> Cr <sub>5</sub> : A8B5_hR26_160_a3bc_a3b	514
10.	<b>hR42</b>	
10.1.	Phenakite: A2B4C_hR42_148_2f_4f_f	479
<b>mC</b>		
1.	<b>mC16</b>	
1.1.	H <sub>3</sub> Cl: AB3_mC16_9_a_3a	44
1.2.	M-carbon: A_mC16_12_4i	58
1.3.	H <sub>3</sub> Cl: AB3_mC16_15_e_cf	71
2.	<b>mC22</b>	
2.1.	Thortveitite: A7B2C2_mC22_12_aij_h_i	56
3.	<b>mC24</b>	
3.1.	H-III: A_mC24_15_2e2f	73
4.	<b>mC32</b>	
4.1.	α-P <sub>3</sub> N <sub>5</sub> : A5B3_mC32_9_5a_3a	42
<b>mP</b>		
1.	<b>mP4</b>	
1.1.	FeNi: AB_mP4_6_2b_2a	32
2.	<b>mP6</b>	
2.1.	δ-PdCl <sub>2</sub> : A2B_mP6_10_mn_bg	46
2.2.	LiSn: AB_mP6_10_en_am	52
2.3.	γ-PdCl <sub>2</sub> : A2B_mP6_14_e_a	62
3.	<b>mP8</b>	
3.1.	Muthmannite: ABC2_mP8_10_ac_eh_mn	50
3.2.	S-carbon: A_mP8_10_2m2n	54
4.	<b>mP12</b>	
4.1.	H <sub>2</sub> S IV: A2B_mP12_7_4a_2a	34
4.2.	H <sub>2</sub> S: A2B_mP12_13_2g_ef	60
5.	<b>mP13</b>	
5.1.	Mo <sub>8</sub> P <sub>5</sub> : A8B5_mP13_6_a7b_3a2b	30
6.	<b>mP16</b>	
6.1.	ε-WO <sub>3</sub> : A3B_mP16_7_6a_2a	38
6.2.	H <sub>3</sub> Cl: AB3_mP16_10_mn_3m3n	48
7.	<b>mP18</b>	
7.1.	As <sub>2</sub> Ba: A2B_mP18_7_6a_3a	36
8.	<b>mP22</b>	
8.1.	Rh <sub>2</sub> Ga <sub>9</sub> : A9B2_mP22_7_9a_2a	40
9.	<b>mP120</b>	
9.1.	α-Toluene: A7B8_mP120_14_14e_16e	64
<b>oC</b>		
1.	<b>oC6</b>	
1.1.	Ta <sub>2</sub> H: AB2_oC6_21_a_k	79
2.	<b>oC8</b>	
2.1.	HCl: AB_oC8_36_a_a	129

<sup>||</sup>Cu<sub>3</sub>P and Na<sub>3</sub>As have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

2.2.	$\alpha$ -FeSe <sup>†</sup> : AB_oC8_67_a_g	240
2.3.	$\alpha$ -PbO <sup>†</sup> : AB_oC8_67_a_g	242
3.	<b>oC16</b>	
3.1.	K <sub>2</sub> CdPb: AB2C_oC16_40_a_2b_b	137
3.2.	CeTe <sub>3</sub> : AB3_oC16_40_b_3b	139
3.3.	Al <sub>2</sub> CuIr <sup>§</sup> : A2BC_oC16_67_ag_b_g	236
3.4.	HoCuP <sub>2</sub> <sup>§</sup> : ABC2_oC16_67_b_g_ag	238
4.	<b>oC20</b>	
4.1.	Post-perovskite: AB3C_oC20_63_a_cf_c	220
4.2.	PdSn <sub>4</sub> : AB4_oC20_68_a_i	244
5.	<b>oC22</b>	
5.1.	V <sub>2</sub> MoO <sub>8</sub> : AB8C2_oC22_35_a_ab3e_e	127
6.	<b>oC24</b>	
6.1.	Rasvumite: A2BC3_oC24_63_e_c_cg	210
6.2.	MgSO <sub>4</sub> : AB4C_oC24_63_a_fg_c	222
6.3.	Anhydrite: AB4C_oC24_63_c_fg_c	224
6.4.	H <sub>2</sub> S: A2B_oC24_64_2f_f	226
7.	<b>oC28</b>	
7.1.	MnAl <sub>6</sub> : A6B_oC28_63_efg_c	218
7.2.	SrAl <sub>2</sub> Se <sub>4</sub> : A2B4C_oC28_66_1_kl_a	228
8.	<b>oC36</b>	
8.1.	Li <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> : A2B5C2_oC36_37_d_c2d_d	131
9.	<b>oC40</b>	
9.1.	Ta <sub>3</sub> S <sub>2</sub> : A2B3_oC40_39_2d_2c2d	133
10.	<b>oC44</b>	
10.1.	VPCl <sub>9</sub> : A9BC_oC44_39_3c3d_a_c	135
11.	<b>oC64</b>	
11.1.	H <sub>3</sub> S: A3B_oC64_66_gi2lm_2l	230
11.2.	$\beta$ -ThI <sub>3</sub> : A3B_oC64_66_kl2m_bdl	233
12.	<b>oC260</b>	
12.1.	La <sub>43</sub> Ni <sub>17</sub> Mg <sub>5</sub> : A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h	212
<b>oF</b>		
1.	<b>oF8</b>	
1.1.	FeS: AB_oF8_22_a_c	83
1.2.	BN: AB_oF8_42_a_a	143
2.	<b>oF40</b>	
2.1.	CeRu <sub>2</sub> B <sub>2</sub> : A2BC2_oF40_22_fi_ad_gh	81
3.	<b>oF48</b>	
3.1.	Mn <sub>2</sub> B: AB2_oF48_70_f_fg	246
4.	<b>oF52</b>	
4.1.	W <sub>3</sub> O <sub>10</sub> : A10B3_oF52_42_2abce_ab	141
<b>oI</b>		
1.	<b>oI12</b>	
1.1.	BPS <sub>4</sub> : ABC4_oI12_23_a_b_k	91
1.2.	NbPS: ABC_oI12_71_h_j_g	250
1.3.	KHg <sub>2</sub> : A2B_oI12_74_h_e	254
2.	<b>oI14</b>	
2.1.	Ta <sub>3</sub> B <sub>4</sub> : A4B3_oI14_71_gh_cg	248
3.	<b>oI16</b>	
3.1.	NaFeS <sub>2</sub> : ABC2_oI16_23_ab_i_k	89
4.	<b>oI20</b>	
4.1.	MnGa <sub>2</sub> Sb <sub>2</sub> : A2BC2_oI20_45_c_b_c	145
4.2.	Al <sub>4</sub> U: A4B_oI20_74_beh_e	256
5.	<b>oI32</b>	
5.1.	H <sub>3</sub> S: A3B_oI32_23_ij2k_k	85
6.	<b>oI36</b>	
6.1.	TiFeSi: ABC_oI36_46_ac_bc_3b	147
7.	<b>oI44</b>	
7.1.	Weberite: AB7CD2_oI44_24_a_b3d_c_ac	93
8.	<b>oI48</b>	
8.1.	KAg[CO <sub>3</sub> ]: ABCD3_oI48_73_d_e_e_ef	252
9.	<b>oI50</b>	
9.1.	Stannoidite: A8B2C12D2E_oI50_23_bcfk_i_3k_j_a	87
<b>oP</b>		
1.	<b>oP6</b>	
1.1.	FeSb <sub>2</sub> : AB2_oP6_34_a_c	125
1.2.	$\alpha$ -PdCl <sub>2</sub> : A2B_oP6_58_g_a	176
1.3.	FeOCl: ABC_oP6_59_a_b_a	178
2.	<b>oP8</b>	
2.1.	Westerveldite: AB_oP8_62_c_c	208
3.	<b>oP12</b>	
3.1.	$\alpha$ -Naumannite: A2B_oP12_17_abe_e	75
3.2.	H <sub>2</sub> S*: A2B_oP12_26_abc_ab	95
3.3.	$\beta$ -SeO <sub>2</sub> *: A2B_oP12_26_abc_ab	97
3.4.	ZrO <sub>2</sub> <sup>‡</sup> : A2B_oP12_29_2a_a	106
3.5.	Pyrite <sup>‡</sup> : AB2_oP12_29_a_2a	108
3.6.	Cobaltite: ABC_oP12_29_a_a_a	110
3.7.	SrH <sub>2</sub> : A2B_oP12_62_2c_c	198
4.	<b>oP14</b>	
4.1.	$\beta$ -Ta <sub>2</sub> O <sub>5</sub> : A5B2_oP14_49_dehq_ab	151
5.	<b>oP16</b>	
5.1.	H <sub>3</sub> Cl: AB3_oP16_19_a_3a	77
5.2.	TaNiTe <sub>2</sub> : ABC2_oP16_53_h_e_gh	164
5.3.	Rh <sub>5</sub> Ge <sub>3</sub> : A3B5_oP16_55_ch_agh	172
5.4.	R-carbon: A_oP16_55_2g2h	174
5.5.	$\epsilon$ -NiAl <sub>3</sub> : A3B_oP16_62_cd_c	200
5.6.	Molybdate: AB3_oP16_62_c_3c	204
6.	<b>oP20</b>	
6.1.	CuBrSe <sub>3</sub> : ABC3_oP20_30_2a_c_3c	115
6.2.	Sr <sub>2</sub> Bi <sub>3</sub> : A3B2_oP20_52_de_cd	162
6.3.	CuBrSe <sub>3</sub> : ABC3_oP20_53_e_g_hi	166
6.4.	BiGaO <sub>3</sub> : ABC3_oP20_54_e_d_cf	168
6.5.	Rh <sub>2</sub> S <sub>3</sub> : A2B3_oP20_60_d_cd	180

<sup>†</sup> $\alpha$ -FeSe and  $\alpha$ -PbO have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters.

<sup>§</sup>Al<sub>2</sub>CuIr and HoCuP<sub>2</sub> have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

\*H<sub>2</sub>S and  $\beta$ -SeO<sub>2</sub> have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters.

<sup>‡</sup>ZrO<sub>2</sub> and Pyrite have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

6.6. Tongbaite: A2B3_oP20_62_2c_3c	194
7. <b>oP22</b>	
7.1. TiAl <sub>2</sub> Br <sub>8</sub> : A2B8C_oP22_34_c_4c_a	123
8. <b>oP24</b>	
8.1. TiP <sub>5</sub> : A5B_oP24_26_3a3b2c_ab	99
8.2. $\alpha$ -RbPr[MoO <sub>4</sub> ] <sub>2</sub> : A2B8CD_oP24_48_k_2m_d_b	149
8.3. CsPr[MoO <sub>4</sub> ] <sub>2</sub> : AB2C8D_oP24_49_g_q_2qr_e	153
8.4. GaCl <sub>2</sub> : A2B_oP24_52_2e_cd	160
8.5. GeAs <sub>2</sub> : A2B_oP24_55_2g2h_gh	170
8.6. Cubanite: AB2C3_oP24_62_c_d_cd	202
8.7. Barite: AB4C_oP24_62_c_2cd_c	206
9. <b>oP28</b>	
9.1. La <sub>2</sub> NiO <sub>4</sub> : A2BC4_oP28_50_ij_ac_ijm	155
9.2. Forsterite: A2B4C_oP28_62_ac_2cd_c	196
10. <b>oP32</b>	
10.1. WO <sub>3</sub> : A3B_oP32_60_3d_d	182
11. <b>oP34</b>	
11.1. Re <sub>2</sub> O <sub>5</sub> [SO <sub>4</sub> ] <sub>2</sub> : A13B2C2_oP34_32_a6c_c_c	117
12. <b>oP40</b>	
12.1. $\kappa$ -alumina: A2B3_oP40_33_4a_6a	120
13. <b>oP46</b>	
13.1. Bi <sub>5</sub> Nb <sub>3</sub> O <sub>15</sub> : A5B3C15_oP46_30_a2c_bc_a7c	112
14. <b>oP48</b>	
14.1. $\alpha$ -Tl <sub>2</sub> TeO <sub>3</sub> : A3BC2_oP48_50_3m_m_2m	157
14.2. Benzene: AB_oP48_61_3c_3c	191
15. <b>oP108</b>	
15.1. Ca <sub>4</sub> Al <sub>6</sub> O <sub>16</sub> S: A6B4C16D_oP108_27_abcd4e_4e_16e_e	101
16. <b>oP120</b>	
16.1. $\beta$ -Toluene: A7B8_oP120_60_7d_8d	185
<b>tI</b>	
1. <b>tI4</b>	
1.1. GeP: AB_tI4_107_a_a	360
1.2. GaSb: AB_tI4_119_c_a	402
2. <b>tI8</b>	
2.1. NbAs: AB_tI8_109_a_a	366
2.2. Calomel: AB_tI8_139_e_e	451
3. <b>tI12</b>	
3.1. CdAs <sub>2</sub> : A2B_tI12_98_f_a	333
3.2. LaPtSi: ABC_tI12_109_a_a_a	364
3.3. $\alpha$ -ThSi <sub>2</sub> : A2B_tI12_141_e_a	457
4. <b>tI16</b>	
4.1. S-III: A_tI16_142_f	459
5. <b>tI20</b>	
5.1. TiZn <sub>2</sub> Sb <sub>2</sub> : A2BC2_tI20_79_c_2a_c	277
5.2. ThCl <sub>4</sub> : A4B_tI20_88_f_a	294
6. <b>tI24</b>	
6.1. NaGdCu <sub>2</sub> F <sub>3</sub> : A2B8CD_tI24_97_d_k_a_b	329
6.2. Co <sub>5</sub> Ge <sub>7</sub> : A5B7_tI24_107_ac_abd	358
6.3. RbGa <sub>3</sub> : A3B_tI24_119_b2i_af	400
7. <b>tI28</b>	
7.1. KAu <sub>4</sub> Sn <sub>2</sub> : A4BC2_tI28_120_i_d_e	404
8. <b>tI32</b>	
8.1. Ni <sub>3</sub> P: A3B_tI32_82_3g_g	284
8.2. Sr <sub>5</sub> Si <sub>3</sub> : A3B5_tI32_108_ac_a2c	362
8.3. W <sub>5</sub> Si <sub>3</sub> : A3B5_tI32_140_ah_bk	453
8.4. Cr <sub>5</sub> B <sub>3</sub> : A3B5_tI32_140_ah_cl	455
9. <b>tI44</b>	
9.1. Ta <sub>2</sub> Se <sub>8</sub> I: AB8C2_tI44_97_e_2k_cd	331
10. <b>tI48</b>	
10.1. $\beta$ -NbO <sub>2</sub> : AB2_tI48_80_2b_4b	279
11. <b>tI96</b>	
11.1. $\alpha$ -NbO <sub>2</sub> : AB2_tI96_88_2f_4f	296
12. <b>tI176</b>	
12.1. Be[BH <sub>4</sub> ] <sub>2</sub> : A2BC8_tI176_110_2b_b_8b	368
<b>tP</b>	
1. <b>tP5</b>	
1.1. Rh <sub>3</sub> P <sub>2</sub> : A2B3_tP5_115_g_ag	387
2. <b>tP6</b>	
2.1. ZrO <sub>2</sub> <sup>‡</sup> : A2B_tP6_137_d_a	443
2.2. HgI <sub>2</sub> <sup>‡</sup> : AB2_tP6_137_a_d	447
3. <b>tP8</b>	
3.1. NV: AB_tP8_111_n_n	376
4. <b>tP10</b>	
4.1. Ti <sub>2</sub> Ge <sub>3</sub> : A3B2_tP10_83_adk_j	286
4.2. NbTe <sub>4</sub> : AB4_tP10_103_a_d	345
4.3. Pd <sub>4</sub> Se: A4B_tP10_114_e_a	385
4.4. CaRbFe <sub>4</sub> As <sub>4</sub> : A4BC4D_tP10_123_gh_a_i_d	406
4.5. NbTe <sub>4</sub> : AB4_tP10_124_a_m	410
4.6. PtPb <sub>4</sub> : A4B_tP10_125_m_a	412
5. <b>tP12</b>	
5.1. GeSe <sub>2</sub> : AB2_tP12_81_adg_2h	282
5.2. MnF <sub>2</sub> : A2B_tP12_111_2n_adf	374
5.3. $\alpha$ -CuAlCl <sub>4</sub> : AB4C_tP12_112_b_n_e	378
5.4. HgI <sub>2</sub> : AB2_tP12_115_j_egi	389
5.5. Nb <sub>4</sub> CoSi: AB4C_tP12_124_a_m_c	408
5.6. KCeSe <sub>4</sub> : ABC4_tP12_125_a_b_m	414
5.7. C: A_tP12_138_bi	449
6. <b>tP16</b>	
6.1. LaRhC <sub>2</sub> : A2BC_tP16_76_2a_a_a	262
6.2. RuIn <sub>3</sub> : A3B_tP16_118_ei_f	395
6.3. AgUF <sub>6</sub> : AB6C_tP16_132_d_io_a	431
7. <b>tP18</b>	
7.1. Li <sub>2</sub> MoF <sub>6</sub> : A6B2C_tP18_94_eg_c_a	325
7.2. K <sub>2</sub> SnCl <sub>6</sub> : A6B2C_tP18_128_eh_d_b	420
7.3. Rb <sub>2</sub> TiCu <sub>2</sub> S <sub>4</sub> : A2B2C4D_tP18_132_e_i_o_d	429
7.4. CeCo <sub>4</sub> B <sub>4</sub> : A4BC4_tP18_137_g_b_g	445
8. <b>tP20</b>	
8.1. Gd <sub>3</sub> Al <sub>2</sub> : A2B3_tP20_102_2c_b2c	343
8.2. BaGe <sub>2</sub> As <sub>2</sub> : A2BC2_tP20_105_f_ac_2e	352
8.3. Ru <sub>2</sub> Sn <sub>3</sub> : A2B3_tP20_116_bci_fj	391
8.4. $\beta$ -Bi <sub>2</sub> O <sub>3</sub> : A2B3_tP20_117_i_adgh	393
8.5. ThB <sub>4</sub> : A4B_tP20_127_ehj_g	418

<sup>‡</sup>ZrO<sub>2</sub> and HgI<sub>2</sub> have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

9.	<b>tP22</b>	
9.1.	Tl <sub>4</sub> HgI <sub>6</sub> : AB6C4_tP22_104_a_2ac_c	350
10.	<b>tP24</b>	
10.1.	ThBC: ABC_tP24_91_d_d_d	313
10.2.	ThBC: ABC_tP24_95_d_d_d	327
10.3.	Akermanite: A2BC7D2_tP24_113_e_a_cef_e	380
10.4.	Downeyite: A2B_tP24_135_gh_h	436
11.	<b>tP26</b>	
11.1.	Fresnoite: A2B8C2D_tP26_100_c_abcd_c_a	335
12.	<b>tP28</b>	
12.1.	Ba <sub>5</sub> In <sub>4</sub> Bi <sub>5</sub> : A5B5C4_tP28_104_ac_ac_c	347
12.2.	BiAl <sub>2</sub> S <sub>4</sub> : A2BC4_tP28_126_cd_e_k	416
12.3.	CuBi <sub>2</sub> O <sub>4</sub> : A2BC4_tP28_130_f_c_g	425
12.4.	ZnSb <sub>2</sub> O <sub>4</sub> : A4B2C_tP28_135_gh_h_d	438
13.	<b>tP30</b>	
13.1.	SrBr <sub>2</sub> : A2B_tP30_85_ab2g_cg	288
14.	<b>tP32</b>	
14.1.	Ti <sub>3</sub> P: AB3_tP32_86_g_3g	291
14.2.	γ-MgNiSn: A7B7C2_tP32_101_bde_ade_d	340
14.3.	SeO <sub>3</sub> : A3B_tP32_114_3e_e	382
14.4.	Ir <sub>3</sub> Ga <sub>5</sub> : A5B3_tP32_118_g2i_aceh	397
14.5.	Ba <sub>5</sub> Si <sub>3</sub> : A5B3_tP32_130_cg_cf	427
14.6.	β-V <sub>3</sub> S: AB3_tP32_133_h_i2j	433
15.	<b>tP40</b>	
15.1.	Cs <sub>3</sub> P <sub>7</sub> : A3B7_tP40_76_3a_7a	264
15.2.	Na <sub>4</sub> Ti <sub>2</sub> Si <sub>8</sub> O <sub>22</sub> [H <sub>2</sub> O] <sub>4</sub> : A4B2C13D_tP40_90_g_d_cef2g_c	307
15.3.	Ce <sub>3</sub> Si <sub>6</sub> N <sub>11</sub> : A3B11C6_tP40_100_ac_bc2d_cd	337
15.4.	FeCu <sub>2</sub> Al <sub>7</sub> : A7B2C_tP40_128_egi_h_e	422
15.5.	Zn <sub>3</sub> P <sub>2</sub> : A2B3_tP40_137_cdf_3g	440
16.	<b>tP44</b>	
16.1.	Na <sub>5</sub> Fe <sub>3</sub> F <sub>14</sub> : A14B3C5_tP44_94_c3g_ad_bg	322
17.	<b>tP48</b>	
17.1.	H <sub>2</sub> S III: A2B_tP48_77_8d_4d	270
18.	<b>tP54</b>	
18.1.	BaCu <sub>4</sub> [VO][PO <sub>4</sub> ] <sub>4</sub> : AB4C17D4E_tP54_90_a_g_c4g_g_c	310
19.	<b>tP64</b>	
19.1.	Pinnoite: A2B6CD7_tP64_77_2d_6d_d_ab6d	267
19.2.	NaZn[OH] <sub>3</sub> : A3BC3D_tP64_106_3c_c_3c_c	354
20.	<b>tP76</b>	
20.1.	BaCr <sub>2</sub> Ru <sub>4</sub> O <sub>12</sub> : AB2C12D4_tP76_75_2a2b_2d_12d_4d	258
21.	<b>tP88</b>	
21.1.	Sr <sub>2</sub> As <sub>2</sub> O <sub>7</sub> : A2B7C2_tP88_78_4a_14a_4a	273
22.	<b>tP184</b>	
22.1.	C <sub>17</sub> FeO <sub>4</sub> Pt: A17BC4D_tP184_89_17p_p_4p_io	300
22.2.	AsPh <sub>4</sub> CeS <sub>8</sub> P <sub>4</sub> Me <sub>8</sub> : AB32CD4E8_tP184_93_i_16p_af_2p_4p	315

## Strukturbericht Designation Index

<b>B7</b>	1. Moissanite-15R: AB_hR10_160_5a_5a	519
<b>B14</b>	1. Westerveldite: AB_oP8_62_c_c	208
<b>C13</b>	1. HgI <sub>2</sub> <sup>‡</sup> : AB2_tP6_137_a_d	447
<b>C29</b>	1. SrH <sub>2</sub> : A2B_oP12_62_2c_c	198
<b>C47</b>	1. Downeyite: A2B_tP24_135_gh_h	436
<b>C50</b>	1. α-PdCl <sub>2</sub> : A2B_oP6_58_g_a	176
<b>Cc</b>	1. α-ThSi <sub>2</sub> : A2B_tI12_141_e_a	457
<b>D08</b>	1. Molybdate: AB3_oP16_62_c_3c	204
<b>D020</b>	1. ε-NiAl <sub>3</sub> : A3B_oP16_62_cd_c	200
<b>D021</b>	1. Cu <sub>3</sub> P: A3B_hp24_165_bdg_f	527
<b>D024</b>	1. Ni <sub>3</sub> Ti: A3B_hp16_194_gh_ac	641
<b>D0e</b>	1. Ni <sub>3</sub> P: A3B_tI32_82_3g_g	284
<b>D1b</b>	1. Al <sub>4</sub> U: A4B_oI20_74_beh_e	256
<b>D1e</b>	1. ThB <sub>4</sub> : A4B_tP20_127_ehj_g	418
<b>D1f</b>	1. Mn <sub>2</sub> B: AB2_of48_70_f_fg	246
<b>D23</b>	1. NaZn <sub>13</sub> : AB13_cF112_226_a_bi	771
<b>D2h</b>	1. MnAl <sub>6</sub> : A6B_oC28_63_efg_c	218
<b>D31</b>	1. Calomel: AB_tI8_139_e_e	451
<b>D52</b>	1. La <sub>2</sub> O <sub>3</sub> : A2B3_hp5_164_d_ad	521
<b>D59</b>	1. Zn <sub>3</sub> P <sub>2</sub> : A2B3_tP40_137_cdf_3g	440
<b>D510</b>	1. Tongbaite: A2B3_oP20_62_2c_3c	194
<b>D71</b>	1. Al <sub>4</sub> C <sub>3</sub> : A4B3_hR7_166_2c_ac	530
<b>D72</b>	1. Spinel: A3B4_cF56_227_ad_e	776
<b>D73</b>		

<sup>‡</sup>ZrO<sub>2</sub> and HgI<sub>2</sub> have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

1. Th <sub>3</sub> P <sub>4</sub> : A4B3_cI28_220_c_a	756	1. Phenakite: A2B4C_hR42_148_2f_4f_f	479
<b>D7<sub>b</sub></b>		<b>S1<sub>4</sub></b>	
1. Ta <sub>3</sub> B <sub>4</sub> : A4B3_oI14_71_gh_cg	248	1. Garnet: A2B3C12D3_cI160_230_a_c_h_d	797
<b>D8<sub>1</sub></b>		<b>S2<sub>1</sub></b>	
1. $\gamma$ -brass: A3B10_cI52_229_e_fh	790	1. Thortveitite: A7B2C2_mC22_12_ajj_h_i	56
<b>D8<sub>3</sub></b>		<b>S5<sub>3</sub></b>	
1. $\gamma$ -brass: A4B9_cP52_215_ei_3efgi	741	1. Akermanite: A2BC7D2_tP24_113_e_a_cef_e	380
<b>D8<sub>6</sub></b>		<b>None</b>	
1. Cu <sub>15</sub> Si <sub>4</sub> : A15B4_cI76_220_ae_c	753	1. H <sub>2</sub> S: A2B_aP6_2_aei_i	28
<b>D8<sub>10</sub></b>		2. Mo <sub>8</sub> P <sub>5</sub> : A8B5_mP13_6_a7b_3a2b	30
1. Al <sub>8</sub> Cr <sub>5</sub> : A8B5_hR26_160_a3bc_a3b	514	3. FeNi: AB_mP4_6_2b_2a	32
<b>D8<sub>11</sub></b>		4. H <sub>2</sub> S IV: A2B_mP12_7_4a_2a	34
1. Co <sub>2</sub> Al <sub>5</sub> : A5B2_hP28_194_ahk_ch	643	5. As <sub>2</sub> Ba: A2B_mP18_7_6a_3a	36
<b>D8<sub>a</sub></b>		6. $\epsilon$ -WO <sub>3</sub> : A3B_mP16_7_6a_2a	38
1. Th <sub>6</sub> Mn <sub>23</sub> : A23B6_cF116_225_bd2f_e	766	7. Rh <sub>2</sub> Ga <sub>9</sub> : A9B2_mP22_7_9a_2a	40
<b>D8<sub>f</sub></b>		8. $\alpha$ -P <sub>3</sub> N <sub>5</sub> : A5B3_mC32_9_5a_3a	42
1. Ir <sub>3</sub> Ge <sub>7</sub> : A7B3_cI40_229_df_e	795	9. H <sub>3</sub> Cl: AB3_mC16_9_a_3a	44
<b>D8<sub>l</sub></b>		10. $\delta$ -PdCl <sub>2</sub> : A2B_mP6_10_mn_bg	46
1. Cr <sub>5</sub> B <sub>3</sub> : A3B5_tI32_140_ah_cl	455	11. H <sub>3</sub> Cl: AB3_mP16_10_mn_3m3n	48
<b>D8<sub>m</sub></b>		12. Muthmannite: ABC2_mP8_10_ac_ah_mn	50
1. W <sub>5</sub> Si <sub>3</sub> : A3B5_tI32_140_ah_bk	453	13. LiSn: AB_mP6_10_en_am	52
<b>D10<sub>2</sub></b>		14. S-carbon: A_mP8_10_2m2n	54
1. Fe <sub>3</sub> Th <sub>7</sub> : A3B7_hP20_186_c_b2c	610	15. M-carbon: A_mC16_12_4i	58
<b>E9<sub>1</sub></b>		16. H <sub>2</sub> S: A2B_mP12_13_2g_ef	60
1. Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> : A2B3C6_cP33_221_cd_ag_fh	758	17. $\gamma$ -PdCl <sub>2</sub> : A2B_mP6_14_e_a	62
<b>E9<sub>a</sub></b>		18. $\alpha$ -Toluene: A7B8_mP120_14_14e_16e	64
1. FeCu <sub>2</sub> Al <sub>7</sub> : A7B2C_tP40_128_egi_h_e	422	19. H <sub>3</sub> Cl: AB3_mC16_15_e_cf	71
<b>E9<sub>b</sub></b>		20. H-III: A_mC24_15_2e2f	73
1. $\pi$ -FeMg <sub>3</sub> Al <sub>8</sub> Si <sub>6</sub> : A8BC3D6_hP18_189_bfh_a_g_i	619	21. $\alpha$ -Naumannite: A2B_oP12_17_abe_e	75
<b>E9<sub>c</sub></b>		22. H <sub>3</sub> Cl: AB3_oP16_19_a_3a	77
1. Al <sub>9</sub> Mn <sub>3</sub> Si: A9B3C_hP26_194_hk_h_a	646	23. Ta <sub>2</sub> H: AB2_oC6_21_a_k	79
<b>E9<sub>d</sub></b>		24. CeRu <sub>2</sub> B <sub>2</sub> : A2BC2_oF40_22_fi_ad_gh	81
1. AlLi <sub>3</sub> N <sub>2</sub> : AB3C2_cI96_206_c_e_ad	704	25. FeS: AB_oF8_22_a_c	83
<b>E9<sub>e</sub></b>		26. H <sub>3</sub> S: A3B_oI32_23_ij2k_k	85
1. Cubanite: AB2C3_oP24_62_c_d_cd	202	27. Stannoidite: A8B2C12D2E_oI50_23_bcfk_i_3k_j_a	87
<b>F0<sub>2</sub></b>		28. NaFeS <sub>2</sub> : ABC2_oI16_23_ab_i_k	89
1. Carbonyl Sulphide: ABC_hR3_160_a_a_a	517	29. BPS <sub>4</sub> : ABC4_oI12_23_a_b_k	91
<b>F5<sub>13</sub></b>		30. Weberite: AB7CD2_oI44_24_a_b3d_c_ac	93
1. KBO <sub>2</sub> : ABC2_hR24_167_e_e_2e	536	31. H <sub>2</sub> S*: A2B_oP12_26_abc_ab	95
<b>G3</b>		32. $\beta$ -SeO <sub>2</sub> *: A2B_oP12_26_abc_ab	97
1. Sodium Chlorate: ABC3_cP20_198_a_a_b	661	33. TIP <sub>5</sub> : A5B_oP24_26_3a3b2c_ab	99
<b>G3<sub>1</sub></b>		34. Ca <sub>4</sub> Al <sub>6</sub> O <sub>16</sub> S: A6B4C16D_oP108_27_abcd4e_4e_16e_e	101
1. Beryl: A2B3C18D6_hP58_192_c_f_lm_l	631	35. ZrO <sub>2</sub> <sup>‡</sup> : A2B_oP12_29_2a_a	106
<b>H0<sub>1</sub></b>			
1. Anhydrite: AB4C_oC24_63_c_fg_c	224		
<b>H0<sub>2</sub></b>			
1. Barite: AB4C_oP24_62_c_2cd_c	206		
<b>J1<sub>1</sub></b>			
1. K <sub>2</sub> PtCl <sub>6</sub> : A6B2C_cF36_225_e_c_a	769		
<b>S1<sub>2</sub></b>			
1. Forsterite: A2B4C_oP28_62_ac_2cd_c	196		
<b>S1<sub>3</sub></b>			

\*H<sub>2</sub>S and  $\beta$ -SeO<sub>2</sub> have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters.

<sup>‡</sup>ZrO<sub>2</sub> and Pyrite have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

36. Pyrite <sup>‡</sup> : AB2_oP12_29_a_2a	108	82. HoCuP <sub>2</sub> <sup>§</sup> : ABC2_oC16_67_b_g_ag	238
37. Cobaltite: ABC_oP12_29_a_a_a	110	83. $\alpha$ -FeSe <sup>†</sup> : AB_oC8_67_a_g	240
38. Bi <sub>5</sub> Nb <sub>3</sub> O <sub>15</sub> : A5B3C15_oP46_30_a2c_bc_a7c	112	84. $\alpha$ -PbO <sup>†</sup> : AB_oC8_67_a_g	242
39. CuBrSe <sub>3</sub> : ABC3_oP20_30_2a_c_3c	115	85. PdSn <sub>4</sub> : AB4_oC20_68_a_i	244
40. Re <sub>2</sub> O <sub>5</sub> [SO <sub>4</sub> ] <sub>2</sub> : A13B2C2_oP34_32_a6c_c_c	117	86. NbPS: ABC_oI12_71_h_j_g	250
41. $\kappa$ -alumina: A2B3_oP40_33_4a_6a	120	87. KAg[CO <sub>3</sub> ]: ABCD3_oI48_73_d_e_e_ef	252
42. TiAl <sub>2</sub> Br <sub>8</sub> : A2B8C_oP22_34_c_4c_a	123	88. KHg <sub>2</sub> : A2B_oI12_74_h_e	254
43. FeSb <sub>2</sub> : AB2_oP6_34_a_c	125	89. BaCr <sub>2</sub> Ru <sub>4</sub> O <sub>12</sub> :	
44. V <sub>2</sub> MoO <sub>8</sub> : AB8C2_oC22_35_a_ab3e_e	127	AB2C12D4_tP76_75_2a2b_2d_12d_4d	258
45. HCl: AB_oC8_36_a_a	129	90. LaRhC <sub>2</sub> : A2BC_tP16_76_2a_a_a	262
46. Li <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> : A2B5C2_oC36_37_d_c2d_d	131	91. Cs <sub>3</sub> P <sub>7</sub> : A3B7_tP40_76_3a_7a	264
47. Ta <sub>3</sub> S <sub>2</sub> : A2B3_oC40_39_2d_2c2d	133	92. Pinnoite: A2B6CD7_tP64_77_2d_6d_d_ab6d	267
48. VPCl <sub>9</sub> : A9BC_oC44_39_3c3d_a_c	135	93. H <sub>2</sub> S III: A2B_tP48_77_8d_4d	270
49. K <sub>2</sub> CdPb: AB2C_oC16_40_a_2b_b	137	94. Sr <sub>2</sub> As <sub>2</sub> O <sub>7</sub> : A2B7C2_tP88_78_4a_14a_4a	273
50. CeTe <sub>3</sub> : AB3_oC16_40_b_3b	139	95. TlZn <sub>2</sub> Sb <sub>2</sub> : A2BC2_tI20_79_c_2a_c	277
51. W <sub>3</sub> O <sub>10</sub> : A10B3_oF52_42_2abce_ab	141	96. $\beta$ -NbO <sub>2</sub> : AB2_tI48_80_2b_4b	279
52. BN: AB_oF8_42_a_a	143	97. GeSe <sub>2</sub> : AB2_tP12_81_adg_2h	282
53. MnGa <sub>2</sub> Sb <sub>2</sub> : A2BC2_oI20_45_c_b_c	145	98. Ti <sub>2</sub> Ge <sub>3</sub> : A3B2_tP10_83_adk_j	286
54. TiFeSi: ABC_oI36_46_ac_bc_3b	147	99. SrBr <sub>2</sub> : A2B_tP30_85_ab2g_cg	288
55. $\alpha$ -RbPr[MoO <sub>4</sub> ] <sub>2</sub> :		100. Ti <sub>3</sub> P: AB3_tP32_86_g_3g	291
A2B8CD_oP24_48_k_2m_d_b	149	101. ThCl <sub>4</sub> : A4B_tI20_88_f_a	294
56. $\beta$ -Ta <sub>2</sub> O <sub>5</sub> : A5B2_oP14_49_dehq_ab	151	102. $\alpha$ -NbO <sub>2</sub> : AB2_tI96_88_2f_4f	296
57. CsPr[MoO <sub>4</sub> ] <sub>2</sub> : AB2C8D_oP24_49_g_q_2qr_e	153	103. C <sub>17</sub> FeO <sub>4</sub> Pt: A17BC4D_tP184_89_17p_p_4p_io	300
58. La <sub>2</sub> NiO <sub>4</sub> : A2BC4_oP28_50_ij_ac_ijm	155	104. Na <sub>4</sub> Ti <sub>2</sub> Si <sub>8</sub> O <sub>22</sub> [H <sub>2</sub> O] <sub>4</sub> :	
59. $\alpha$ -Tl <sub>2</sub> TeO <sub>3</sub> : A3BC2_oP48_50_3m_m_2m	157	A4B2C13D_tP40_90_g_d_cef2g_c	307
60. GaCl <sub>2</sub> : A2B_oP24_52_2e_cd	160	105. BaCu <sub>4</sub> [VO][PO <sub>4</sub> ] <sub>4</sub> :	
61. Sr <sub>2</sub> Bi <sub>3</sub> : A3B2_oP20_52_de_cd	162	AB4C17D4E_tP54_90_a_g_c4g_g_c	310
62. TaNiTe <sub>2</sub> : ABC2_oP16_53_h_e_gh	164	106. ThBC: ABC_tP24_91_d_d_d	313
63. CuBrSe <sub>3</sub> : ABC3_oP20_53_e_g_hi	166	107. AsPh <sub>4</sub> CeS <sub>8</sub> P <sub>4</sub> Me <sub>8</sub> :	
64. BiGaO <sub>3</sub> : ABC3_oP20_54_e_d_cf	168	AB32CD4E8_tP184_93_i_16p_af_2p_4p	315
65. GeAs <sub>2</sub> : A2B_oP24_55_2g2h_gh	170	108. Na <sub>5</sub> Fe <sub>3</sub> F <sub>14</sub> : A14B3C5_tP44_94_c3g_ad_bg	322
66. Rh <sub>5</sub> Ge <sub>3</sub> : A3B5_oP16_55_ch_agh	172	109. Li <sub>2</sub> MoF <sub>6</sub> : A6B2C_tP18_94_eg_c_a	325
67. R-carbon: A_oP16_55_2g2h	174	110. ThBC: ABC_tP24_95_d_d_d	327
68. FeOCl: ABC_oP6_59_a_b_a	178	111. NaGdCu <sub>2</sub> F <sub>8</sub> : A2B8CD_tI24_97_d_k_a_b	329
69. Rh <sub>2</sub> S <sub>3</sub> : A2B3_oP20_60_d_cd	180	112. Ta <sub>2</sub> Se <sub>8</sub> I: AB8C2_tI44_97_e_2k_cd	331
70. WO <sub>3</sub> : A3B_oP32_60_3d_d	182	113. CdAs <sub>2</sub> : A2B_tI12_98_f_a	333
71. $\beta$ -Toluene: A7B8_oP120_60_7d_8d	185	114. Fresnoite: A2B8C2D_tP26_100_c_abcd_c_a	335
72. Benzene: AB_oP48_61_3c_3c	191	115. Ce <sub>3</sub> Si <sub>6</sub> N <sub>11</sub> : A3B11C6_tP40_100_ac_bc2d_cd	337
73. Rasvumite: A2BC3_oC24_63_e_c_cg	210	116. $\gamma$ -MgNiSn: A7B7C2_tP32_101_bde_ade_d	340
74. La <sub>43</sub> Ni <sub>17</sub> Mg <sub>5</sub> :		117. Gd <sub>3</sub> Al <sub>2</sub> : A2B3_tP20_102_2c_b2c	343
A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h	212	118. NbTe <sub>4</sub> : AB4_tP10_103_a_d	345
75. Post-perovskite: AB3C_oC20_63_a_cf_c	220	119. Ba <sub>5</sub> In <sub>4</sub> Bi <sub>5</sub> : A5B5C4_tP28_104_ac_ac_c	347
76. MgSO <sub>4</sub> : AB4C_oC24_63_a_fg_c	222	120. Tl <sub>4</sub> HgI <sub>6</sub> : AB6C4_tP22_104_a_2ac_c	350
77. H <sub>2</sub> S: A2B_oC24_64_2f_f	226	121. BaGe <sub>2</sub> As <sub>2</sub> : A2BC2_tP20_105_f_ac_2e	352
78. SrAl <sub>2</sub> Se <sub>4</sub> : A2B4C_oC28_66_l_kl_a	228	122. NaZn[OH] <sub>3</sub> : A3BC3D_tP64_106_3c_c_3c_c	354
79. H <sub>3</sub> S: A3B_oC64_66_gi2lm_2l	230	123. Co <sub>5</sub> Ge <sub>7</sub> : A5B7_tI24_107_ac_abd	358
80. $\beta$ -ThI <sub>3</sub> : A3B_oC64_66_kl2m_bdl	233	124. GeP: AB_tI4_107_a_a	360
81. Al <sub>2</sub> CuIr <sup>§</sup> : A2BC_oC16_67_ag_b_g	236	125. Sr <sub>5</sub> Si <sub>3</sub> : A3B5_tI32_108_ac_a2c	362

<sup>§</sup>Al<sub>2</sub>CuIr and HoCuP<sub>2</sub> have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

<sup>†</sup> $\alpha$ -FeSe and  $\alpha$ -PbO have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters.

126. LaPtSi: ABC_tI12_109_a_a_a	364	177. Bi <sub>2</sub> O <sub>3</sub> : A2B3_hP20_159_bc_2c	503
127. NbAs: AB_tI8_109_a_a	366	178. Nierite: A4B3_hP28_159_ab2c_2c	506
128. Be[BH <sub>4</sub> ] <sub>2</sub> : A2BC8_tI176_110_2b_b_8b	368	179. YbBaCo <sub>4</sub> O <sub>7</sub> : AB4C7D_hP26_159_b_ac_a2c_b	509
129. MnF <sub>2</sub> : A2B_tP12_111_2n_adf	374	180. H <sub>3</sub> S: A3B_hR4_160_b_a	512
130. NV: AB_tP8_111_n_n	376	181. $\delta_H^I$ -NW <sub>2</sub> : AB2_hP9_164_bd_c2d	523
131. $\alpha$ -CuAlCl <sub>4</sub> : AB4C_tP12_112_b_n_e	378	182. CuNiSb <sub>2</sub> : ABC2_hP4_164_a_b_d	525
132. SeO <sub>3</sub> : A3B_tP32_114_3e_e	382	183. SmSI: ABC_hR6_166_c_c_c	532
133. Pd <sub>4</sub> Se: A4B_tP10_114_e_a	385	184. PrNiO <sub>3</sub> : AB3C_hR10_167_b_e_a	534
134. Rh <sub>3</sub> P <sub>2</sub> : A2B3_tP5_115_g_ag	387	185. K <sub>2</sub> Ta <sub>4</sub> O <sub>9</sub> F <sub>4</sub> : A2B13C4_hP57_168_d_c6d_2d	539
135. HgI <sub>2</sub> : AB2_tP12_115_j_egi	389	186. Al[PO <sub>4</sub> ]: AB4C_hP72_168_2d_8d_2d	543
136. Ru <sub>2</sub> Sn <sub>3</sub> : A2B3_tP20_116_bci_fj	391	187. $\alpha$ -Al <sub>2</sub> S <sub>3</sub> : A2B3_hP30_169_2a_3a	547
137. $\beta$ -Bi <sub>2</sub> O <sub>3</sub> : A2B3_tP20_117_i_adgh	393	188. Al <sub>2</sub> S <sub>3</sub> : A2B3_hP30_170_2a_3a	550
138. RuIn <sub>3</sub> : A3B_tP16_118_ei_f	395	189. Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub> : A10B2C_hP39_171_5c_c_a	553
139. Ir <sub>3</sub> Ga <sub>5</sub> : A5B3_tP32_118_g2i_aceh	397	190. Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub> : A10B2C_hP39_172_5c_c_a	557
140. RbGa <sub>3</sub> : A3B_tI24_119_b2i_af	400	191. PI <sub>3</sub> : A3B_hP8_173_c_b	560
141. GaSb: AB_tI4_119_c_a	402	192. $\beta$ -Si <sub>3</sub> N <sub>4</sub> : A4B3_hP14_173_bc_c	562
142. KAu <sub>4</sub> Sn <sub>2</sub> : A4BC2_tI28_120_i_d_e	404	193. Fe <sub>12</sub> Zr <sub>2</sub> P <sub>7</sub> : A12B7C2_hP21_174_2j2k_ajk_cf	564
143. CaRbFe <sub>4</sub> As <sub>4</sub> : A4BC4D_tP10_123_gh_a_i_d	406	194. GdSI: ABC_hP12_174_cj_fk_aj	566
144. Nb <sub>4</sub> CoSi: AB4C_tP12_124_a_m_c	408	195. Nb <sub>7</sub> Ru <sub>6</sub> B <sub>8</sub> : A8B7C6_hP21_175_ck_aj_k	568
145. NbTe <sub>4</sub> : AB <sub>4</sub> _tP10_124_a_m	410	196. Mg[NH]: ABC_hP36_175_jk_jk_jk	570
146. PtPb <sub>4</sub> : A4B_tP10_125_m_a	412	197. Er <sub>3</sub> Ru <sub>2</sub> : A3B2_hP10_176_h_bd	573
147. KCeSe <sub>4</sub> : ABC <sub>4</sub> _tP12_125_a_b_m	414	198. Fe <sub>3</sub> Te <sub>3</sub> Tl: A3B3C_hP14_176_h_h_d	575
148. BiAl <sub>2</sub> S <sub>4</sub> : A2BC <sub>4</sub> _tP28_126_cd_e_k	416	199. UCl <sub>3</sub> : A3B_hP8_176_h_d	577
149. K <sub>2</sub> SnCl <sub>6</sub> : A6B2C_tP18_128_eh_d_b	420	200. SiO <sub>2</sub> : A2B_hP36_177_j2lm_n	579
150. CuBi <sub>2</sub> O <sub>4</sub> : A2BC <sub>4</sub> _tP28_130_f_c_g	425	201. AuF <sub>3</sub> : AB <sub>3</sub> _hP24_178_b_ac	582
151. Ba <sub>5</sub> Si <sub>3</sub> : A5B3_tP32_130_cg_cf	427	202. Sc-V: A_hP6_178_a	584
152. Rb <sub>2</sub> TiCu <sub>2</sub> S <sub>4</sub> : A2B2C4D_tP18_132_e_i_o_d	429	203. AuF <sub>3</sub> : AB <sub>3</sub> _hP24_179_b_ac	586
153. AgUF <sub>6</sub> : AB6C_tP16_132_d_io_a	431	204. $\beta$ -SiO <sub>2</sub> : A2B_hP9_181_j_c	588
154. $\beta$ -V <sub>3</sub> S: AB <sub>3</sub> _tP32_133_h_i2j	433	205. AuCN: ABC_hP3_183_a_a_a	590
155. ZnSb <sub>2</sub> O <sub>4</sub> : A4B2C_tP28_135_gh_h_d	438	206. CrFe <sub>3</sub> NiSn <sub>5</sub> : AB_hP6_183_c_ab	592
156. ZrO <sub>2</sub> <sup>II</sup> : A2B_tP6_137_d_a	443	207. Al[PO <sub>4</sub> ]: AB4C_hP72_184_d_4d_d	594
157. CeCo <sub>4</sub> B <sub>4</sub> : A4BC <sub>4</sub> _tP18_137_g_b_g	445	208. KNiCl <sub>3</sub> : A3BC_hP30_185_cd_c_ab	599
158. C: A_tP12_138_bi	449	209. Cu <sub>3</sub> P <sup>II</sup> : A3B_hP24_185_ab2c_c	602
159. S-III: A_tI16_142_f	459	210. $\beta$ -RuCl <sub>3</sub> : A3B_hP8_185_c_a	605
160. Simpsonite: A4B14C3_hP21_143_bd_ac4d_d	461	211. Na <sub>3</sub> As <sup>II</sup> : AB <sub>3</sub> _hP24_185_c_ab2c	607
161. ScRh <sub>6</sub> P <sub>4</sub> : A4B6C_hP11_143_bd_2d_a	463	212. Re <sub>3</sub> N: AB <sub>3</sub> _hP4_187_e_fh	612
162. MoS <sub>2</sub> : AB <sub>2</sub> _hP12_143_cd_ab2d	465	213. LiScI <sub>3</sub> : A3BC_hP10_188_k_a_e	614
163. IrGe <sub>4</sub> : A4B_hP15_144_4a_a	467	214. BaSi <sub>4</sub> O <sub>9</sub> : AB9C <sub>4</sub> _hP28_188_e_kl_ak	616
164. TeZn: AB_hP6_144_a_a	469	215. $\pi$ -FeMg <sub>3</sub> Al <sub>9</sub> Si <sub>5</sub> : A9BC3D5_hP18_189_fi_a_g_bh	622
165. Sheldrickite: A2B3C3DE7_hP48_145_2a_3a_3a_a_7a	471	216. Li <sub>2</sub> Sb: A2B_hP18_190_gh_bf	624
166. $\gamma$ -Ag <sub>3</sub> SI: A3BC_hR5_146_b_a_a	475	217. $\alpha$ -Sm <sub>3</sub> Ge <sub>5</sub> : A5B3_hP16_190_bdh_g	626
167. FePSe <sub>3</sub> : ABC <sub>3</sub> _hR10_146_2a_2a_2b	477	218. Troilite: AB_hP24_190_i_afh	628
168. $\beta$ -PdCl <sub>2</sub> : A2B_hR18_148_2f_f	483	219. AlPO <sub>4</sub> : AB <sub>2</sub> _hP72_192_m_j2kl	635
169. Ti <sub>3</sub> O: AB <sub>3</sub> _hP24_149_acgi_3l	486	220. Mavlyanovite: A5B3_hP16_193_dg_g	639
170. CrCl <sub>3</sub> : A3B_hP24_153_3c_2b	488	221. PrRu <sub>4</sub> P <sub>12</sub> : A12BC <sub>4</sub> _cP34_195_2j_ab_2e	649
171. S-II: A_hP9_154_bc	491	222. Cu <sub>2</sub> Fe[CN] <sub>6</sub> : A12B2C_cF60_196_h_bc_a	652
172. CdI <sub>2</sub> : AB <sub>2</sub> _hP9_156_b2c_3a2bc	493		
173. CuI: AB_hP12_156_2ab3c_2ab3c	495		
174. $\beta$ -CuI: AB_hP4_156_ac_ac	497		
175. Ag <sub>5</sub> Pb <sub>2</sub> O <sub>6</sub> : A5B6C <sub>2</sub> _hP13_157_2ac_2c_b	499		
176. $\beta$ -RuCl <sub>3</sub> : A3B_hP8_158_d_a	501		

<sup>II</sup>Cu<sub>3</sub>P and Na<sub>3</sub>As have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

223. MgB <sub>12</sub> H <sub>12</sub> [H <sub>2</sub> O] <sub>12</sub> :	
A12B36CD12_cF488_196_2h_6h_ac_fgh	654
224. Mg <sub>2</sub> Zn <sub>11</sub> : A2B11_cP39_200_f_ghij	663
225. KSbO <sub>3</sub> : AB3C_cP60_201_ce_fh_g	666
226. KB <sub>6</sub> H <sub>6</sub> : A6B6C_cF104_202_h_h_c	669
227. FCC C <sub>60</sub> Buckminsterfullerine:	
A_cF240_202_h2i	671
228. Pyrochlore: A2BCD3E6_cF208_203_e_c_d_f_g	675
229. Tychite: A4B2C6D16E_cF232_203_e_d_f_eg_a	679
230. Rb <sub>3</sub> AsSe <sub>16</sub> : AB3C16_cF160_203_b_ad_eg	683
231. Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> : A2B3C6_cP264_205_2d_ab2c2d_6d	687
232. Simple Cubic C <sub>60</sub> Buckminsterfullerine:	
A_cP240_205_10d	696
233. Pd <sub>17</sub> Se <sub>15</sub> : A17B15_cP64_207_acfk_eij	707
234. PH <sub>3</sub> : A3B_cP16_208_j_b	710
235. Cs <sub>2</sub> ZnFe[CN] <sub>6</sub> :	
A6B2CD6E_cP64_208_m_ad_b_m_c	712
236. F <sub>6</sub> KP: A24BC_cF104_209_j_a_b	716
237. Te[OH] <sub>6</sub> : A12B6C_cF608_210_4h_2h_e	719
238. SiO <sub>2</sub> : A2B_cI72_211_hi_i	731
239. SrSi <sub>2</sub> : A2B_cP12_212_c_a	734
240. Ca <sub>3</sub> PI <sub>3</sub> : A3B3C_cI56_214_g_h_a	736
241. Petzite: A3BC2_cI48_214_f_a_e	739
242. Quaternary Heusler:	
ABCD_cF16_216_c_d_b_a	745
243. Ag <sub>3</sub> [PO <sub>4</sub> ]: A3B4C_cP16_218_c_e_a	747
244. Boracite: A7BC3D13_cF192_219_de_b_c_ah	749
245. Ce <sub>5</sub> Mo <sub>3</sub> O <sub>16</sub> : A5B3C16_cP96_222_ce_d_fi	761
246. Pyrochlore Iridate:	
A2B2C7_cF88_227_c_d_af	774
247. CuCrCl <sub>5</sub> [NH <sub>3</sub> ] <sub>6</sub> : A5BCD6_cF416_228_eg_c_b_h	778
248. TeO <sub>6</sub> H <sub>6</sub> : A6B_cF224_228_h_c	785
249. β-Hg <sub>4</sub> Pt: A4B_cI10_229_c_a	793

### Duplicate AFLOW Label Index

<b>A2B_oP12_26_abc_ab</b>	
1. H <sub>2</sub> S	95
2. β-SeO <sub>2</sub>	97
<b>AB_oC8_67_a_g</b>	
1. α-FeSe	240
2. α-PbO	242

### Similar AFLOW Label Index

<b>A2B_oP12_29_2a_a</b>	
1. ZrO <sub>2</sub> : A2B_oP12_29_2a_a	106
2. Pyrite: AB2_oP12_29_a_2a	108
<b>A2BC_oC16_67_ag_b_g</b>	
1. Al <sub>2</sub> CuIr: A2BC_oC16_67_ag_b_g	236
2. HoCuP <sub>2</sub> : ABC2_oC16_67_b_g_ag	238
<b>A2B_tP6_137_d_a</b>	
1. ZrO <sub>2</sub> : A2B_tP6_137_d_a	443
2. HgI <sub>2</sub> : AB2_tP6_137_a_d	447
<b>A3B_hP24_185_ab2c_c</b>	
1. Cu <sub>3</sub> P: A3B_hP24_185_ab2c_c	602
2. Na <sub>3</sub> As: AB3_hP24_185_c_ab2c	607

### CIF Index

1. α-Al <sub>2</sub> S <sub>3</sub> : A2B3_hP30_169_2a_3a	923
2. α-CuAlCl <sub>4</sub> : AB4C_tP12_112_b_n_e	884
3. α-FeSe <sup>†</sup> : AB_oC8_67_a_g	852
4. α-Naumannite: A2B_oP12_17_abe_e	812
5. α-NbO <sub>2</sub> : AB2_tI96_88_2f_4f	866
6. α-P <sub>3</sub> N <sub>5</sub> : A5B3_mC32_9_5a_3a	805
7. α-PbO <sup>†</sup> : AB_oC8_67_a_g	853
8. α-PdCl <sub>2</sub> : A2B_oP6_58_g_a	837
9. α-RbPr[MoO <sub>4</sub> ] <sub>2</sub> :	
A2B8CD_oP24_48_k_2m_d_b	830
10. α-Sm <sub>3</sub> Ge <sub>5</sub> : A5B3_hP16_190_bdh_g	940
11. α-ThSi <sub>2</sub> : A2B_tI12_141_e_a	904
12. α-Tl <sub>2</sub> TeO <sub>3</sub> : A3BC2_oP48_50_3m_m_2m	833
13. α-Toluene: A7B8_mP120_14_14e_16e	810
14. β-Bi <sub>2</sub> O <sub>3</sub> : A2B3_tP20_117_i_adgh	887
15. β-CuI: AB_hP4_156_ac_ac	912
16. β-Hg <sub>4</sub> Pt: A4B_cI10_229_c_a	984
17. β-NbO <sub>2</sub> : AB2_tI48_80_2b_4b	862
18. β-PdCl <sub>2</sub> : A2B_hR18_148_2f_f	909
19. β-RuCl <sub>3</sub> : A3B_hP8_158_d_a	913
20. β-RuCl <sub>3</sub> : A3B_hP8_185_c_a	935
21. β-SeO <sub>2</sub> <sup>*</sup> : A2B_oP12_26_abc_ab	818
22. β-Si <sub>3</sub> N <sub>4</sub> : A4B3_hP14_173_bc_c	926
23. β-SiO <sub>2</sub> : A2B_hP9_181_j_c	932
24. β-Ta <sub>2</sub> O <sub>5</sub> : A5B2_oP14_49_dehq_ab	831
25. β-ThI <sub>3</sub> : A3B_oC64_66_kl2m_bdl	851
26. β-Toluene: A7B8_oP120_60_7d_8d	839
27. β-V <sub>3</sub> S: AB3_tP32_133_h_i2j	897
28. δ-PdCl <sub>2</sub> : A2B_mP6_10_mn_bg	806
29. δ <sub>H</sub> <sup>II</sup> -NW <sub>2</sub> : AB2_hP9_164_bd_c2d	918
30. ε-NiAl <sub>3</sub> : A3B_oP16_62_cd_c	843
31. ε-WO <sub>3</sub> : A3B_mP16_7_6a_2a	804
32. γ-Ag <sub>3</sub> SI: A3BC_hR5_146_b_a_a	908
33. γ-MgNiSn: A7B7C2_tP32_101_bde_ade_d	875
34. γ-PdCl <sub>2</sub> : A2B_mP6_14_e_a	810
35. γ-brass: A4B9_cP52_215_ei_3efgi	966
36. γ-brass: A3B10_cI52_229_e_fh	983
37. κ-alumina: A2B3_oP40_33_4a_6a	823
38. π-FeMg <sub>3</sub> Al <sub>8</sub> Si <sub>6</sub> :	
A8BC3D6_hP18_189_bfh_a_g_i	938
39. π-FeMg <sub>3</sub> Al <sub>9</sub> Si <sub>5</sub> :	
A9BC3D5_hP18_189_fi_a_g_bh	939
40. Ag <sub>3</sub> [PO <sub>4</sub> ]: A3B4C_cP16_218_c_e_a	968
41. Ag <sub>3</sub> Pb <sub>2</sub> O <sub>6</sub> : A5B6C2_hP13_157_2ac_2c_b	913
42. AgUF <sub>6</sub> : AB6C_tP16_132_d_io_a	897

<sup>†</sup>α-FeSe and α-PbO have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters.

<sup>\*</sup>H<sub>2</sub>S and β-SeO<sub>2</sub> have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters.



43. Akermanite: A2BC7D2_tP24_113_e_a_cef_e	884	86. CdAs <sub>2</sub> : A2B_tI12_98_f_a	874
44. Al <sub>2</sub> CuIr <sup>§</sup> : A2BC_oC16_67_ag_b_g	851	87. CdI <sub>2</sub> : AB2_hP9_156_b2c_3a2bc	911
45. Al <sub>2</sub> S <sub>3</sub> : A2B3_hP30_170_2a_3a	924	88. Ce <sub>3</sub> Si <sub>6</sub> N <sub>11</sub> : A3B11C6_tP40_100_ac_bc2d_cd	875
46. Al <sub>4</sub> C <sub>3</sub> : A4B3_hR7_166_2c_ac	919	89. Ce <sub>5</sub> Mo <sub>3</sub> O <sub>16</sub> : A5B3C16_cP96_222_ce_d_fi	972
47. Al <sub>4</sub> U: A4B_oI20_74_beh_e	856	90. CeCo <sub>4</sub> B <sub>4</sub> : A4BC4_tP18_137_g_b_g	900
48. Al <sub>8</sub> Cr <sub>5</sub> : A8B5_hR26_160_a3bc_a3b	916	91. CeRu <sub>2</sub> B <sub>2</sub> : A2BC2_oF40_22_fi_ad_gh	814
49. Al <sub>9</sub> Mn <sub>3</sub> Si: A9B3C_hP26_194_hk_h_a	944	92. CeTe <sub>3</sub> : AB3_oC16_40_b_3b	828
50. AlLi <sub>3</sub> N <sub>2</sub> : AB3C2_cI96_206_c_e_ad	958	93. Co <sub>2</sub> Al <sub>5</sub> : A5B2_hP28_194_ahk_ch	944
51. AlPO <sub>4</sub> : AB2_hP72_192_m_j2kl	942	94. Co <sub>5</sub> Ge <sub>7</sub> : A5B7_tI24_107_ac_abd	879
52. Al[PO <sub>4</sub> ]: AB4C_hP72_168_2d_8d_2d	922	95. Cobaltite: ABC_oP12_29_a_a_a	821
53. Al[PO <sub>4</sub> ]: AB4C_hP72_184_d_4d_d	933	96. Cr <sub>5</sub> B <sub>3</sub> : A3B5_tI32_140_ah_cl	903
54. Anhydrite: AB4C_oC24_63_c_fg_c	849	97. CrCl <sub>3</sub> : A3B_hP24_153_3c_2b	911
55. As <sub>2</sub> Ba: A2B_mP18_7_6a_3a	803	98. CrFe <sub>3</sub> NiSn <sub>5</sub> : AB_hP6_183_c_ab	933
56. AsPh <sub>4</sub> CeS <sub>8</sub> P <sub>4</sub> Me <sub>8</sub> : AB32CD4E8_tP184_93_i_16p_af_2p_4p	870	99. Cs <sub>2</sub> ZnFe[CN] <sub>6</sub> : A6B2CD6E_cP64_208_m_ad_b_m_c	960
57. AuCN: ABC_hP3_183_a_a_a	932	100. Cs <sub>3</sub> P <sub>7</sub> : A3B7_tP40_76_3a_7a	858
58. AuF <sub>3</sub> : AB3_hP24_178_b_ac	930	101. CsPr[MoO <sub>4</sub> ] <sub>2</sub> : AB2C8D_oP24_49_g_q_2qr_e	832
59. AuF <sub>3</sub> : AB3_hP24_179_b_ac	931	102. Cu <sub>15</sub> Si <sub>4</sub> : A15B4_cl76_220_ae_c	970
60. BN: AB_oF8_42_a_a	829	103. Cu <sub>2</sub> Fe[CN] <sub>6</sub> : A12B2C_cF60_196_h_bc_a	945
61. BPS <sub>4</sub> : ABC4_oI12_23_a_b_k	816	104. Cu <sub>3</sub> P: A3B_hP24_165_bdg_f	919
62. Ba <sub>5</sub> In <sub>4</sub> Bi <sub>5</sub> : A5B5C4_tP28_104_ac_ac_c	877	105. Cu <sub>3</sub> P <sup>  </sup> : A3B_hP24_185_ab2c_c	935
63. Ba <sub>5</sub> Si <sub>3</sub> : A5B3_tP32_130_cg_cf	896	106. CuBi <sub>2</sub> O <sub>4</sub> : A2BC4_tP28_130_f_c_g	895
64. BaCr <sub>2</sub> Ru <sub>4</sub> O <sub>12</sub> : AB2C12D4_tP76_75_2a2b_2d_12d_4d	857	107. CuBrSe <sub>3</sub> : ABC3_oP20_30_2a_c_3c	822
65. BaCu <sub>4</sub> [VO][PO <sub>4</sub> ] <sub>4</sub> : AB4C17D4E_tP54_90_a_g_c4g_g_c	868	108. CuBrSe <sub>3</sub> : ABC3_oP20_53_e_g_hi	835
66. BaGe <sub>2</sub> As <sub>2</sub> : A2BC2_tP20_105_f_ac_2e	878	109. CuCrCl <sub>5</sub> [NH <sub>3</sub> ] <sub>6</sub> : A5BCD6_cF416_228_eg_c_b_h	980
67. BaSi <sub>4</sub> O <sub>9</sub> : AB9C4_hP28_188_e_kl_ak	938	110. CuI: AB_hP12_156_2ab3c_2ab3c	912
68. Barite: AB4C_oP24_62_c_2cd_c	844	111. CuNiSb <sub>2</sub> : ABC2_hP4_164_a_b_d	918
69. Be[BH <sub>4</sub> ] <sub>2</sub> : A2BC8_tI176_110_2b_b_8b	882	112. Cubanite: AB2C3_oP24_62_c_d_cd	843
70. Benzene: AB_oP48_61_3c_3c	841	113. Downeyite: A2B_tP24_135_gh_h	898
71. Beryl: A2B3C18D6_hP58_192_c_f_lm_l	941	114. Er <sub>3</sub> Ru <sub>2</sub> : A3B2_hP10_176_h_bd	929
72. Bi <sub>2</sub> O <sub>3</sub> : A2B3_hP20_159_bc_2c	914	115. F <sub>6</sub> KP: A24BC_cF104_209_j_a_b	961
73. Bi <sub>5</sub> Nb <sub>3</sub> O <sub>15</sub> : A5B3C15_oP46_30_a2c_bc_a7c	821	116. FCC C <sub>60</sub> Buckminsterfullerine: A_cF240_202_h2i	950
74. BiAl <sub>2</sub> S <sub>4</sub> : A2BC4_tP28_126_cd_e_k	893	117. Fe <sub>12</sub> Zr <sub>2</sub> P <sub>7</sub> : A12B7C2_hP21_174_2j2k_ajk_cf	926
75. BiGaO <sub>3</sub> : ABC3_oP20_54_e_d_cf	835	118. Fe <sub>3</sub> Te <sub>3</sub> Tl: A3B3C_hP14_176_h_h_d	929
76. Boracite: A7BC3D13_cF192_219_de_b_c_ah	969	119. Fe <sub>3</sub> Th <sub>7</sub> : A3B7_hP20_186_c_b2c	936
77. C: A_tP12_138_bi	901	120. FeCu <sub>2</sub> Al <sub>7</sub> : A7B2C_tP40_128_egi_h_e	895
78. C <sub>17</sub> FeO <sub>4</sub> Pt: A17BC4D_tP184_89_17p_p_4p_io	866	121. FeNi: AB_mP4_6_2b_2a	802
79. Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> : A2B3C6_cP264_205_2d_ab2c2d_6d	955	122. FeOCl: ABC_oP6_59_a_b_a	838
80. Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> : A2B3C6_cP33_221_cd_ag_fh	971	123. FePSe <sub>3</sub> : ABC3_hR10_146_2a_2a_2b	908
81. Ca <sub>3</sub> PI <sub>3</sub> : A3B3C_cI56_214_g_h_a	965	124. FeS: AB_oF8_22_a_c	814
82. Ca <sub>4</sub> Al <sub>6</sub> O <sub>16</sub> S: A6B4C16D_oP108_27_abcd4e_4e_16e_e	819	125. FeSb <sub>2</sub> : AB2_oP6_34_a_c	825
83. CaRbFe <sub>4</sub> As <sub>4</sub> : A4BC4D_tP10_123_gh_a_i_d	890	126. Forsterite: A2B4C_oP28_62_ac_2cd_c	842
84. Calomel: AB_tI8_139_e_e	902	127. Fresnoite: A2B8C2D_tP26_100_c_abcd_c_a	874
85. Carbonyl Sulphide: ABC_hR3_160_a_a_a	916	128. GaCl <sub>2</sub> : A2B_oP24_52_2e_cd	833
		129. GaSb: AB_tI4_119_c_a	889
		130. Garnet: A2B3C12D3_cI160_230_a_c_h_d	986

<sup>§</sup>Al<sub>2</sub>CuIr and HoCuP<sub>2</sub> have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

<sup>||</sup>Cu<sub>3</sub>P and Na<sub>3</sub>As have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

131. Gd <sub>3</sub> Al <sub>2</sub> : A2B3_tP20_102_2c_b2c	876	177. LiScI <sub>3</sub> : A3BC_hP10_188_k_a_e	937
132. GdSI: ABC_hP12_174_cj_fk_aj	927	178. LiSn: AB_mP6_10_en_am	807
133. GeAs <sub>2</sub> : A2B_oP24_55_2g2h_gh	836	179. M-carbon: A_mC16_12_4i	809
134. GeP: AB_tI4_107_a_a	880	180. Mavlyanovite: A5B3_hP16_193_dg_g	943
135. GeSe <sub>2</sub> : AB2_tP12_81_adg_2h	862	181. Mg <sub>2</sub> Zn <sub>11</sub> : A2B11_cP39_200_f_aghij	948
136. H <sub>2</sub> S: A2B_aP6_2_aei_i	802	182. MgB <sub>12</sub> H <sub>12</sub> [H <sub>2</sub> O] <sub>12</sub> : A12B36CD12_cF488_196_2h_6h_ac_fgh	946
137. H <sub>2</sub> S: A2B_mP12_13_2g_ef	809	183. MgSO <sub>4</sub> : AB4C_oC24_63_a_fg_c	848
138. H <sub>2</sub> S*: A2B_oP12_26_abc_ab	817	184. Mg[NH]: ABC_hP36_175_jk_jk_jk	928
139. H <sub>2</sub> S: A2B_oC24_64_2f_f	849	185. Mn <sub>2</sub> B: AB2_oF48_70_f_fg	854
140. H <sub>2</sub> S III: A2B_tP48_77_8d_4d	860	186. MnAl <sub>6</sub> : A6B_oC28_63_efg_c	847
141. H <sub>2</sub> S IV: A2B_mP12_7_4a_2a	803	187. MnF <sub>2</sub> : A2B_tP12_111_2n_adf	883
142. H <sub>3</sub> Cl: AB3_mC16_9_a_3a	806	188. MnGa <sub>2</sub> Sb <sub>2</sub> : A2BC2_oI20_45_c_b_c	829
143. H <sub>3</sub> Cl: AB3_mP16_10_mn_3m3n	806	189. Mo <sub>8</sub> P <sub>5</sub> : A8B5_mP13_6_a7b_3a2b	802
144. H <sub>3</sub> Cl: AB3_mC16_15_e_cf	811	190. MoS <sub>2</sub> : AB2_hP12_143_cd_ab2d	906
145. H <sub>3</sub> Cl: AB3_oP16_19_a_3a	813	191. Moissanite-15R: AB_hR10_160_5a_5a	917
146. H <sub>3</sub> S: A3B_oI32_23_ij2k_k	815	192. Molybdate: AB3_oP16_62_c_3c	844
147. H <sub>3</sub> S: A3B_oC64_66_gi2lm_2l	850	193. Muthmannite: ABC2_mP8_10_ac_eh_mn	807
148. H <sub>3</sub> S: A3B_hR4_160_b_a	915	194. NV: AB_tP8_111_n_n	883
149. H-III: A_mC24_15_2e2f	812	195. Na <sub>3</sub> As <sup>  </sup> : AB3_hP24_185_c_ab2c	936
150. HCl: AB_oC8_36_a_a	825	196. Na <sub>4</sub> Ti <sub>2</sub> Si <sub>8</sub> O <sub>22</sub> [H <sub>2</sub> O] <sub>4</sub> : A4B2C13D_tP40_90_g_d_cef2g_c	868
151. HgI <sub>2</sub> : AB2_tP12_115_j_egi	886	197. Na <sub>5</sub> Fe <sub>3</sub> F <sub>14</sub> : A14B3C5_tP44_94_c3g_ad_bg	871
152. HgI <sub>2</sub> <sup>  </sup> : AB2_tP6_137_a_d	901	198. NaFeS <sub>2</sub> : ABC2_oI16_23_ab_i_k	816
153. HoCuP <sub>2</sub> <sup>§</sup> : ABC2_oC16_67_b_g_ag	852	199. NaGdCu <sub>2</sub> F <sub>8</sub> : A2B8CD_tI24_97_d_k_a_b	873
154. Ir <sub>3</sub> Ga <sub>5</sub> : A5B3_tP32_118_g2i_aceh	888	200. NaZn <sub>13</sub> : AB13_cF112_226_a_bi	976
155. Ir <sub>3</sub> Ge <sub>7</sub> : A7B3_cI40_229_df_e	985	201. NaZn[OH] <sub>3</sub> : A3BC3D_tP64_106_3c_c_3c_c	879
156. IrGe <sub>4</sub> : A4B_hP15_144_4a_a	906	202. Nb <sub>4</sub> CoSi: AB4C_tP12_124_a_m_c	891
157. K <sub>2</sub> CdPb: AB2C_oC16_40_a_2b_b	828	203. Nb <sub>7</sub> Ru <sub>6</sub> B <sub>8</sub> : A8B7C6_hP21_175_ck_aj_k	927
158. K <sub>2</sub> PtCl <sub>6</sub> : A6B2C_cF36_225_e_c_a	974	204. NbAs: AB_tI8_109_a_a	881
159. K <sub>2</sub> SnCl <sub>6</sub> : A6B2C_tP18_128_eh_d_b	894	205. NbPS: ABC_oI12_71_h_j_g	855
160. K <sub>2</sub> Ta <sub>4</sub> O <sub>9</sub> F <sub>4</sub> : A2B13C4_hP57_168_d_c6d_2d	922	206. NbTe <sub>4</sub> : AB4_tP10_103_a_d	877
161. KAg[CO <sub>3</sub> ]: ABCD3_oI48_73_d_e_e_ef	855	207. NbTe <sub>4</sub> : AB4_tP10_124_a_m	891
162. KAu <sub>4</sub> Sn <sub>2</sub> : A4BC2_tI28_120_i_d_e	890	208. Ni <sub>3</sub> P: A3B_tI32_82_3g_g	863
163. KB <sub>6</sub> H <sub>6</sub> : A6B6C_cF104_202_h_h_c	949	209. Ni <sub>3</sub> Ti: A3B_hP16_194_gh_ac	943
164. KBO <sub>2</sub> : ABC2_hR24_167_e_e_2e	921	210. Nierite: A4B3_hP28_159_ab2c_2c	914
165. KCeSe <sub>4</sub> : ABC4_tP12_125_a_b_m	892	211. PH <sub>3</sub> : A3B_cP16_208_j_b	960
166. KHg <sub>2</sub> : A2B_oI12_74_h_e	856	212. PI <sub>3</sub> : A3B_hP8_173_c_b	925
167. KNiCl <sub>3</sub> : A3BC_hP30_185_cd_c_ab	934	213. Pd <sub>17</sub> Se <sub>15</sub> : A17B15_cP64_207_acfk_eij	959
168. KSbO <sub>3</sub> : AB3C_cP60_201_ce_fh_g	949	214. Pd <sub>4</sub> Se: A4B_tP10_114_e_a	885
169. La <sub>2</sub> NiO <sub>4</sub> : A2BC4_oP28_50_ij_ac_ijm	832	215. PdSn <sub>4</sub> : AB4_oC20_68_a_i	853
170. La <sub>2</sub> O <sub>3</sub> : A2B3_hP5_164_d_ad	917	216. Petzite: A3BC2_cI48_214_f_a_e	966
171. La <sub>43</sub> Ni <sub>17</sub> Mg <sub>5</sub> : A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h	846	217. Phenakite: A2B4C_hR42_148_2f_4f_f	909
172. LaPtSi: ABC_tI12_109_a_a_a	881	218. Pinnoite: A2B6CD7_tP64_77_2d_6d_d_ab6d	859
173. LaRhC <sub>2</sub> : A2BC_tP16_76_2a_a_a	858	219. Post-perovskite: AB3C_oC20_63_a_cf_c	848
174. Li <sub>2</sub> MoF <sub>6</sub> : A6B2C_tP18_94_eg_c_a	872	220. PrNiO <sub>3</sub> : AB3C_hR10_167_b_e_a	920
175. Li <sub>2</sub> Sb: A2B_hP18_190_gh_bf	939	221. PrRu <sub>4</sub> P <sub>12</sub> : A12BC4_cP34_195_2j_ab_2e	945
176. Li <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> : A2B5C2_oC36_37_d_c2d_d	826	222. PtPb <sub>4</sub> : A4B_tP10_125_m_a	892

<sup>||</sup>ZrO<sub>2</sub> and HgI<sub>2</sub> have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

223. Pyrite <sup>‡</sup> : AB2_oP12_29_a_2a .....	820	265. Ta <sub>2</sub> Se <sub>8</sub> I: AB8C2_tI44_97_e_2k_cd .....	873
224. Pyrochlore: A2BCD3E6_cF208_203_e_c_d_f_g ...	951	266. Ta <sub>3</sub> B <sub>4</sub> : A4B3_oI14_71_gh_cg .....	854
225. Pyrochlore Iridate: A2B2C7_cF88_227_c_d_af .....	977	267. Ta <sub>3</sub> S <sub>2</sub> : A2B3_oC40_39_2d_2c2d .....	826
226. Quaternary Heusler: ABCD_cF16_216_c_d_b_a .....	967	268. TaNiTe <sub>2</sub> : ABC2_oP16_53_h_e_gh .....	834
227. R-carbon: A_oP16_55_2g2h .....	837	269. TeO <sub>6</sub> H <sub>6</sub> : A6B_cF224_228_h_c .....	982
228. Rasvumite: A2BC3_oC24_63_e_c_cg .....	845	270. TeZn: AB_hp6_144_a_a .....	907
229. Rb <sub>2</sub> TiCu <sub>2</sub> S <sub>4</sub> : A2B2C4D_tP18_132_e_i_o_d .....	896	271. Te[OH] <sub>6</sub> : A12B6C_cF608_210_4h_2h_e .....	962
230. Rb <sub>3</sub> AsSe <sub>16</sub> : AB3C16_cF160_203_b_ad_eg .....	954	272. Th <sub>3</sub> P <sub>4</sub> : A4B3_cI28_220_c_a .....	970
231. RbGa <sub>3</sub> : A3B_tI24_119_b2i_af .....	889	273. Th <sub>6</sub> Mn <sub>23</sub> : A23B6_cF116_225_bd2f_e .....	973
232. Re <sub>2</sub> O <sub>5</sub> [SO <sub>4</sub> ] <sub>2</sub> : A13B2C2_oP34_32_a6c_c_c .....	823	274. ThB <sub>4</sub> : A4B_tP20_127_ehj_g .....	893
233. Re <sub>3</sub> N: AB3_hp4_187_e_fh .....	937	275. ThBC: ABC_tP24_91_d_d_d .....	869
234. Rh <sub>2</sub> Ga <sub>9</sub> : A9B2_mP22_7_9a_2a .....	804	276. ThBC: ABC_tP24_95_d_d_d .....	872
235. Rh <sub>2</sub> S <sub>3</sub> : A2B3_oP20_60_d_cd .....	838	277. ThCl <sub>4</sub> : A4B_tI20_88_f_a .....	865
236. Rh <sub>3</sub> P <sub>2</sub> : A2B3_tP5_115_g_ag .....	886	278. Thortveitite: A7B2C2_mC22_12_aij_h_i .....	808
237. Rh <sub>5</sub> Ge <sub>3</sub> : A3B5_oP16_55_ch_agh .....	836	279. Ti <sub>2</sub> Ge <sub>3</sub> : A3B2_tP10_83_adk_j .....	863
238. Ru <sub>2</sub> Sn <sub>3</sub> : A2B3_tP20_116_bci_fj .....	887	280. Ti <sub>3</sub> O: AB3_hp24_149_acgi_3l .....	910
239. RuIn <sub>3</sub> : A3B_tP16_118_ei_f .....	888	281. Ti <sub>3</sub> P: AB3_tP32_86_g_3g .....	865
240. S-II: A_hp9_154_bc .....	911	282. TiAl <sub>2</sub> Br <sub>8</sub> : A2B8C_oP22_34_c_4c_a .....	824
241. S-III: A_tI16_142_f .....	904	283. TiFeSi: ABC_oI36_46_ac_bc_3b .....	830
242. S-carbon: A_mP8_10_2m2n .....	808	284. Tl <sub>4</sub> HgI <sub>6</sub> : AB6C4_tP22_104_a_2ac_c .....	878
243. Sc-V: A_hp6_178_a .....	931	285. TIP <sub>5</sub> : A5B_oP24_26_3a3b2c_ab .....	818
244. ScRh <sub>6</sub> P <sub>4</sub> : A4B6C_hp11_143_bd_2d_a .....	905	286. TlZn <sub>2</sub> Sb <sub>2</sub> : A2BC2_tI20_79_c_2a_c .....	861
245. SeO <sub>3</sub> : A3B_tP32_114_3e_e .....	885	287. Tongbaite: A2B3_oP20_62_2c_3c .....	841
246. Sheldrickite: A2B3C3DE7_hp48_145_2a_3a_3a_a_7a .....	907	288. Troilite: AB_hp24_190_i_afh .....	940
247. SiO <sub>2</sub> : A2B_hp36_177_j2lm_n .....	930	289. Tychite: A4B2C6D16E_cF232_203_e_d_f_eg_a ...	953
248. SiO <sub>2</sub> : A2B_cI72_211_hi_i .....	964	290. UCl <sub>3</sub> : A3B_hp8_176_h_d .....	930
249. Simple Cubic C <sub>60</sub> Buckminsterfullerene: A_cP240_205_10d .....	957	291. V <sub>2</sub> MoO <sub>8</sub> : AB8C2_oC22_35_a_ab3e_e .....	825
250. Simpsonite: A4B14C3_hp21_143_bd_ac4d_d .....	905	292. VPCl <sub>9</sub> : A9BC_oC44_39_3c3d_a_c .....	827
251. SmSI: ABC_hr6_166_c_c_c .....	920	293. W <sub>3</sub> O <sub>10</sub> : A10B3_oF52_42_2abce_ab .....	828
252. Sodium Chlorate: ABC3_cP20_198_a_a_b .....	947	294. W <sub>5</sub> Si <sub>3</sub> : A3B5_tI32_140_ah_bk .....	902
253. Spinel: A3B4_cF56_227_ad_e .....	978	295. WO <sub>3</sub> : A3B_oP32_60_3d_d .....	839
254. Sr <sub>2</sub> As <sub>2</sub> O <sub>7</sub> : A2B7C2_tP88_78_4a_14a_4a .....	860	296. Weberite: AB7CD2_oI44_24_a_b3d_c_ac .....	817
255. Sr <sub>2</sub> Bi <sub>3</sub> : A3B2_oP20_52_de_cd .....	834	297. Westerveldite: AB_oP8_62_c_c .....	845
256. Sr <sub>5</sub> Si <sub>3</sub> : A3B5_tI32_108_ac_a2c .....	880	298. YbBaCo <sub>4</sub> O <sub>7</sub> : AB4C7D_hp26_159_b_ac_a2c_b ...	915
257. SrAl <sub>2</sub> Se <sub>4</sub> : A2B4C_oC28_66_l_kl_a .....	850	299. Zn <sub>3</sub> P <sub>2</sub> : A2B3_tP40_137_cdf_3g .....	899
258. SrBr <sub>2</sub> : A2B_tP30_85_ab2g_cg .....	864	300. ZnSb <sub>2</sub> O <sub>4</sub> : A4B2C_tP28_135_gh_h_d .....	899
259. SrH <sub>2</sub> : A2B_oP12_62_2c_c .....	842	301. ZrO <sub>2</sub> <sup>‡</sup> : A2B_oP12_29_2a_a .....	820
260. SrSi <sub>2</sub> : A2B_cP12_212_c_a .....	965	302. ZrO <sub>2</sub> <sup>¶</sup> : A2B_tP6_137_d_a .....	900
261. Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub> : A10B2C_hp39_171_5c_c_a .....	924		
262. Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub> : A10B2C_hp39_172_5c_c_a .....	925		
263. Stannoidite: A8B2C12D2E_oI50_23_bcfk_i_3k_j_a .....	815		
264. Ta <sub>2</sub> H: AB2_oC6_21_a_k .....	813		

<sup>‡</sup>ZrO<sub>2</sub> and Pyrite have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

## POSCAR Index

1. $\alpha$ -Al <sub>2</sub> S <sub>3</sub> : A2B3_hp30_169_2a_3a	924	43. Akermanite: A2BC7D2_tP24_113_e_a_cef_e	885
2. $\alpha$ -CuAlCl <sub>4</sub> : AB4C_tP12_112_b_n_e	884	44. Al <sub>2</sub> CuIr <sup>§</sup> : A2BC_oC16_67_ag_b_g	852
3. $\alpha$ -FeSe <sup>†</sup> : AB_oC8_67_a_g	853	45. Al <sub>2</sub> S <sub>3</sub> : A2B3_hp30_170_2a_3a	924
4. $\alpha$ -Naumannite: A2B_oP12_17_abe_e	813	46. Al <sub>4</sub> C <sub>3</sub> : A4B3_hr7_166_2c_ac	920
5. $\alpha$ -NbO <sub>2</sub> : AB2_tI96_88_2f_4f	866	47. Al <sub>4</sub> U: A4B_oI20_74_beh_e	857
6. $\alpha$ -P <sub>3</sub> N <sub>5</sub> : A5B3_mC32_9_5a_3a	805	48. Al <sub>8</sub> Cr <sub>5</sub> : A8B5_hr26_160_a3bc_a3b	916
7. $\alpha$ -PbO <sup>†</sup> : AB_oC8_67_a_g	853	49. Al <sub>9</sub> Mn <sub>3</sub> Si: A9B3C_hp26_194_hk_h_a	945
8. $\alpha$ -PdCl <sub>2</sub> : A2B_oP6_58_g_a	838	50. AlLi <sub>3</sub> N <sub>2</sub> : AB3C2_cI96_206_c_e_ad	959
9. $\alpha$ -RbPr[MoO <sub>4</sub> ] <sub>2</sub> : A2B8CD_oP24_48_k_2m_d_b	831	51. AlPO <sub>4</sub> : AB2_hp72_192_m_j2kl	942
10. $\alpha$ -Sm <sub>3</sub> Ge <sub>5</sub> : A5B3_hp16_190_bdh_g	940	52. Al[PO <sub>4</sub> ]: AB4C_hp72_168_2d_8d_2d	923
11. $\alpha$ -ThSi <sub>2</sub> : A2B_tI12_141_e_a	904	53. Al[PO <sub>4</sub> ]: AB4C_hp72_184_d_4d_d	934
12. $\alpha$ -Tl <sub>2</sub> TeO <sub>3</sub> : A3BC2_oP48_50_3m_m_2m	833	54. Anhydrite: AB4C_oC24_63_c_fg_c	849
13. $\alpha$ -Toluene: A7B8_mP120_14_14e_16e	811	55. As <sub>2</sub> Ba: A2B_mP18_7_6a_3a	804
14. $\beta$ -Bi <sub>2</sub> O <sub>3</sub> : A2B3_tP20_117_i_adgh	888	56. AsPh <sub>4</sub> CeS <sub>8</sub> P <sub>4</sub> Me <sub>8</sub> : AB32CD4E8_tP184_93_i_16p_af_2p_4p	870
15. $\beta$ -CuI: AB_hp4_156_ac_ac	913	57. AuCN: ABC_hp3_183_a_a_a	933
16. $\beta$ -Hg <sub>4</sub> Pt: A4B_cI10_229_c_a	985	58. AuF <sub>3</sub> : AB3_hp24_178_b_ac	931
17. $\beta$ -NbO <sub>2</sub> : AB2_tI48_80_2b_4b	862	59. AuF <sub>3</sub> : AB3_hp24_179_b_ac	932
18. $\beta$ -PdCl <sub>2</sub> : A2B_hr18_148_2f_f	910	60. BN: AB_oF8_42_a_a	829
19. $\beta$ -RuCl <sub>3</sub> : A3B_hp8_158_d_a	913	61. BPS <sub>4</sub> : ABC4_oI12_23_a_b_k	817
20. $\beta$ -RuCl <sub>3</sub> : A3B_hp8_185_c_a	935	62. Ba <sub>5</sub> In <sub>4</sub> Bi <sub>5</sub> : A5B5C4_tP28_104_ac_ac_c	877
21. $\beta$ -SeO <sub>2</sub> <sup>*</sup> : A2B_oP12_26_abc_ab	818	63. Ba <sub>5</sub> Si <sub>3</sub> : A5B3_tP32_130_cg_cf	896
22. $\beta$ -Si <sub>3</sub> N <sub>4</sub> : A4B3_hp14_173_bc_c	926	64. BaCr <sub>2</sub> Ru <sub>4</sub> O <sub>12</sub> : AB2C12D4_tP76_75_2a2b_2d_12d_4d	857
23. $\beta$ -SiO <sub>2</sub> : A2B_hp9_181_j_c	932	65. BaCu <sub>4</sub> [VO][PO <sub>4</sub> ] <sub>4</sub> : AB4C17D4E_tP54_90_a_g_c4g_g_c	869
24. $\beta$ -Ta <sub>2</sub> O <sub>5</sub> : A5B2_oP14_49_dehq_ab	831	66. BaGe <sub>2</sub> As <sub>2</sub> : A2BC2_tP20_105_f_ac_2e	878
25. $\beta$ -ThI <sub>3</sub> : A3B_oC64_66_kl2m_bdl	851	67. BaSi <sub>4</sub> O <sub>9</sub> : AB9C4_hp28_188_e_kl_ak	938
26. $\beta$ -Toluene: A7B8_oP120_60_7d_8d	840	68. Barite: AB4C_oP24_62_c_2cd_c	845
27. $\beta$ -V <sub>3</sub> S: AB3_tP32_133_h_i2j	898	69. Be[BH <sub>4</sub> ] <sub>2</sub> : A2BC8_tI176_110_2b_b_8b	882
28. $\delta$ -PdCl <sub>2</sub> : A2B_mP6_10_mn_bg	806	70. Benzene: AB_oP48_61_3c_3c	841
29. $\delta_{H}^{II}$ -NW <sub>2</sub> : AB2_hp9_164_bd_c2d	918	71. Beryl: A2B3C18D6_hp58_192_c_f_lm_l	941
30. $\epsilon$ -NiAl <sub>3</sub> : A3B_oP16_62_cd_c	843	72. Bi <sub>2</sub> O <sub>3</sub> : A2B3_hp20_159_bc_2c	914
31. $\epsilon$ -WO <sub>3</sub> : A3B_mP16_7_6a_2a	804	73. Bi <sub>5</sub> Nb <sub>3</sub> O <sub>15</sub> : A5B3C15_oP46_30_a2c_bc_a7c	822
32. $\gamma$ -Ag <sub>3</sub> SI: A3BC_hr5_146_b_a_a	908	74. BiAl <sub>2</sub> S <sub>4</sub> : A2BC4_tP28_126_cd_e_k	893
33. $\gamma$ -MgNiSn: A7B7C2_tP32_101_bde_ade_d	876	75. BiGaO <sub>3</sub> : ABC3_oP20_54_e_d_cf	836
34. $\gamma$ -PdCl <sub>2</sub> : A2B_mP6_14_e_a	810	76. Boracite: A7BC3D13_cF192_219_de_b_c_ah	969
35. $\gamma$ -brass: A4B9_cP52_215_ei_3efgi	967	77. C: A_tP12_138_bi	902
36. $\gamma$ -brass: A3B10_cI52_229_e_fh	984	78. C <sub>17</sub> FeO <sub>4</sub> Pt: A17BC4D_tP184_89_17p_p_4p_io	867
37. $\kappa$ -alumina: A2B3_oP40_33_4a_6a	824	79. Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> : A2B3C6_cP264_205_2d_ab2c2d_6d	955
38. $\pi$ -FeMg <sub>3</sub> Al <sub>8</sub> Si <sub>6</sub> : A8BC3D6_hp18_189_bfh_a_g_i	939	80. Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> : A2B3C6_cP33_221_cd_ag_fh	972
39. $\pi$ -FeMg <sub>3</sub> Al <sub>9</sub> Si <sub>5</sub> : A9BC3D5_hp18_189_fi_a_g_bh	939	81. Ca <sub>3</sub> PI <sub>3</sub> : A3B3C_cI56_214_g_h_a	966
40. Ag <sub>3</sub> [PO <sub>4</sub> ]: A3B4C_cP16_218_c_e_a	968	82. Ca <sub>4</sub> Al <sub>6</sub> O <sub>16</sub> S: A6B4C16D_oP108_27_abcd4e_4e_16e_e	819
41. Ag <sub>3</sub> Pb <sub>2</sub> O <sub>6</sub> : A5B6C2_hp13_157_2ac_2c_b	913	83. CaRbFe <sub>4</sub> As <sub>4</sub> : A4BC4D_tP10_123_gh_a_i_d	891
42. AgUF <sub>6</sub> : AB6C_tP16_132_d_io_a	897	84. Calomel: AB_tI8_139_e_e	902
		85. Carbonyl Sulphide: ABC_hr3_160_a_a_a	917

<sup>†</sup> $\alpha$ -FeSe and  $\alpha$ -PbO have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters.

<sup>\*</sup>H<sub>2</sub>S and  $\beta$ -SeO<sub>2</sub> have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters.

<sup>§</sup>Al<sub>2</sub>CuIr and HoCu<sub>2</sub> have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

86. CdAs <sub>2</sub> : A2B_tI12_98_f_a	874	131. Gd <sub>3</sub> Al <sub>2</sub> : A2B3_tP20_102_2c_b2c	876
87. CdI <sub>2</sub> : AB2_hp9_156_b2c_3a2bc	912	132. GdSI: ABC_hp12_174_cj_fk_aj	927
88. Ce <sub>3</sub> Si <sub>6</sub> N <sub>11</sub> : A3B11C6_tP40_100_ac_bc2d_cd	875	133. GeAs <sub>2</sub> : A2B_op24_55_2g2h_gh	836
89. Ce <sub>5</sub> Mo <sub>3</sub> O <sub>16</sub> : A5B3C16_cP96_222_ce_d_fi	972	134. GeP: AB_tI4_107_a_a	880
90. CeCo <sub>4</sub> B <sub>4</sub> : A4BC4_tP18_137_g_b_g	901	135. GeSe <sub>2</sub> : AB2_tP12_81_adg_2h	863
91. CeRu <sub>2</sub> B <sub>2</sub> : A2BC2_of40_22_fi_ad_gh	814	136. H <sub>2</sub> S: A2B_ap6_2_aei_i	802
92. CeTe <sub>3</sub> : AB3_oc16_40_b_3b	828	137. H <sub>2</sub> S: A2B_mp12_13_2g_ef	810
93. Co <sub>2</sub> Al <sub>5</sub> : A5B2_hp28_194_ahk_ch	944	138. H <sub>2</sub> S*: A2B_op12_26_abc_ab	818
94. Co <sub>5</sub> Ge <sub>7</sub> : A5B7_tI24_107_ac_abd	880	139. H <sub>2</sub> S: A2B_oc24_64_2f_f	849
95. Cobaltite: ABC_op12_29_a_a_a	821	140. H <sub>2</sub> S III: A2B_tP48_77_8d_4d	860
96. Cr <sub>5</sub> B <sub>3</sub> : A3B5_tI32_140_ah_cl	903	141. H <sub>2</sub> S IV: A2B_mp12_7_4a_2a	803
97. CrCl <sub>3</sub> : A3B_hp24_153_3c_2b	911	142. H <sub>3</sub> Cl: AB3_mC16_9_a_3a	806
98. CrFe <sub>3</sub> NiSn <sub>5</sub> : AB_hp6_183_c_ab	933	143. H <sub>3</sub> Cl: AB3_mp16_10_mn_3m3n	807
99. Cs <sub>2</sub> ZnFe[CN] <sub>6</sub> : A6B2CD6E_cP64_208_m_ad_b_m_c	961	144. H <sub>3</sub> Cl: AB3_mC16_15_e_cf	812
100. Cs <sub>3</sub> P <sub>7</sub> : A3B7_tP40_76_3a_7a	859	145. H <sub>3</sub> Cl: AB3_op16_19_a_3a	813
101. CsPr[MoO <sub>4</sub> ] <sub>2</sub> : AB2C8D_op24_49_g_q_2qr_e	832	146. H <sub>3</sub> S: A3B_oI32_23_ij2k_k	815
102. Cu <sub>15</sub> Si <sub>4</sub> : A15B4_cl76_220_ae_c	970	147. H <sub>3</sub> S: A3B_oc64_66_gi2lm_2l	850
103. Cu <sub>2</sub> Fe[CN] <sub>6</sub> : A12B2C_cF60_196_h_bc_a	946	148. H <sub>3</sub> S: A3B_hr4_160_b_a	916
104. Cu <sub>3</sub> P: A3B_hp24_165_bdg_f	919	149. H-III: A_mc24_15_2e2f	812
105. Cu <sub>3</sub> P <sup>  </sup> : A3B_hp24_185_ab2c_c	935	150. HCl: AB_oc8_36_a_a	826
106. CuBi <sub>2</sub> O <sub>4</sub> : A2BC4_tP28_130_f_c_g	896	151. HgI <sub>2</sub> : AB2_tP12_115_j_egi	887
107. CuBrSe <sub>3</sub> : ABC3_op20_30_2a_c_3c	822	152. HgI <sub>2</sub> <sup>¶</sup> : AB2_tP6_137_a_d	901
108. CuBrSe <sub>3</sub> : ABC3_op20_53_e_g_hi	835	153. HoCuP <sub>2</sub> <sup>§</sup> : ABC2_oc16_67_b_g_ag	852
109. CuCrCl <sub>5</sub> [NH <sub>3</sub> ] <sub>6</sub> : A5BCD6_cF416_228_eg_c_b_h	981	154. Ir <sub>3</sub> Ga <sub>5</sub> : A5B3_tP32_118_g2i_aceh	889
110. CuI: AB_hp12_156_2ab3c_2ab3c	912	155. Ir <sub>3</sub> Ge <sub>7</sub> : A7B3_cI40_229_df_e	986
111. CuNiSb <sub>2</sub> : ABC2_hp4_164_a_b_d	919	156. IrGe <sub>4</sub> : A4B_hp15_144_4a_a	907
112. Cubanite: AB2C3_op24_62_c_d_cd	844	157. K <sub>2</sub> CdPb: AB2C_oc16_40_a_2b_b	828
113. Downeyite: A2B_tP24_135_gh_h	898	158. K <sub>2</sub> PtCl <sub>6</sub> : A6B2C_cF36_225_e_c_a	976
114. Er <sub>3</sub> Ru <sub>2</sub> : A3B2_hp10_176_h_bd	929	159. K <sub>2</sub> SnCl <sub>6</sub> : A6B2C_tP18_128_eh_d_b	894
115. F <sub>6</sub> KP: A24BC_cF104_209_j_a_b	962	160. K <sub>2</sub> Ta <sub>4</sub> O <sub>9</sub> F <sub>4</sub> : A2B13C4_hp57_168_d_c6d_2d	922
116. FCC C <sub>60</sub> Buckminsterfullerene: A_cF240_202_h2i	951	161. KAg[CO <sub>3</sub> ]: ABCD3_oI48_73_d_e_e_ef	856
117. Fe <sub>12</sub> Zr <sub>2</sub> P <sub>7</sub> : A12B7C2_hp21_174_2j2k_ajk_cf	927	162. KAu <sub>4</sub> Sn <sub>2</sub> : A4BC2_tI28_120_i_d_e	890
118. Fe <sub>3</sub> Te <sub>3</sub> Tl: A3B3C_hp14_176_h_h_d	929	163. KB <sub>6</sub> H <sub>6</sub> : A6B6C_cF104_202_h_h_c	950
119. Fe <sub>3</sub> Th <sub>7</sub> : A3B7_hp20_186_c_b2c	937	164. KBO <sub>2</sub> : ABC2_hr24_167_e_e_2e	921
120. FeCu <sub>2</sub> Al <sub>7</sub> : A7B2C_tP40_128_egi_h_e	895	165. KCeSe <sub>4</sub> : ABC4_tP12_125_a_b_m	893
121. FeNi: AB_mp4_6_2b_2a	803	166. KHg <sub>2</sub> : A2B_oI12_74_h_e	856
122. FeOCl: ABC_op6_59_a_b_a	838	167. KNiCl <sub>3</sub> : A3BC_hp30_185_cd_c_ab	934
123. FePSe <sub>3</sub> : ABC3_hr10_146_2a_2a_2b	909	168. KSbO <sub>3</sub> : AB3C_cP60_201_ce_fh_g	949
124. FeS: AB_of8_22_a_c	815	169. La <sub>2</sub> NiO <sub>4</sub> : A2BC4_op28_50_ij_ac_ijm	832
125. FeSb <sub>2</sub> : AB2_op6_34_a_c	825	170. La <sub>2</sub> O <sub>3</sub> : A2B3_hp5_164_d_ad	918
126. Forsterite: A2B4C_op28_62_ac_2cd_c	842	171. La <sub>43</sub> Ni <sub>17</sub> Mg <sub>5</sub> : A43B5C17_oc260_63_c8fg6h_cfg_ce3f2h	846
127. Fresnoite: A2B8C2D_tP26_100_c_abcd_c_a	875	172. LaPtSi: ABC_tI12_109_a_a_a	881
128. GaCl <sub>2</sub> : A2B_op24_52_2e_cd	834	173. LaRhC <sub>2</sub> : A2BC_tP16_76_2a_a_a	858
129. GaSb: AB_tI4_119_c_a	890	174. Li <sub>2</sub> MoF <sub>6</sub> : A6B2C_tP18_94_eg_c_a	872
130. Garnet: A2B3C12D3_cI160_230_a_c_h_d	987	175. Li <sub>2</sub> Sb: A2B_hp18_190_gh_bf	940
		176. Li <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> : A2B5C2_oc36_37_d_c2d_d	826

<sup>||</sup>Cu<sub>3</sub>P and Na<sub>3</sub>As have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

<sup>¶</sup>ZrO<sub>2</sub> and HgI<sub>2</sub> have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

177. LiScI <sub>3</sub> : A3BC_hP10_188_k_a_e	938	223. Pyrite <sup>‡</sup> : AB2_oP12_29_a_2a	821
178. LiSn: AB_mP6_10_en_am	808	224. Pyrochlore: A2BCD3E6_cF208_203_e_c_d_f_g	952
179. M-carbon: A_mC16_12_4i	809	225. Pyrochlore Iridate:	
180. Mavlyanovite: A5B3_hP16_193_dg_g	943	A2B2C7_cF88_227_c_d_af	978
181. Mg <sub>2</sub> Zn <sub>11</sub> : A2B11_cP39_200_f_aghij	948	226. Quaternary Heusler:	
182. MgB <sub>12</sub> H <sub>12</sub> [H <sub>2</sub> O] <sub>12</sub> :		ABCD_cF16_216_c_d_b_a	968
A12B36CD12_cF488_196_2h_6h_ac_fgh	947	227. R-carbon: A_oP16_55_2g2h	837
183. MgSO <sub>4</sub> : AB4C_oC24_63_a_fg_c	848	228. Rasvumite: A2BC3_oC24_63_e_c_cg	846
184. Mg[NH]: ABC_hP36_175_jk_jk_jk	928	229. Rb <sub>2</sub> TiCu <sub>2</sub> S <sub>4</sub> : A2B2C4D_tP18_132_e_i_o_d	897
185. Mn <sub>2</sub> B: AB2_oF48_70_f_fg	854	230. Rb <sub>3</sub> AsSe <sub>16</sub> : AB3C16_cF160_203_b_ad_eg	954
186. MnAl <sub>6</sub> : A6B_oC28_63_efg_c	847	231. RbGa <sub>3</sub> : A3B_tI24_119_b2i_af	889
187. MnF <sub>2</sub> : A2B_tP12_111_2n_adf	883	232. Re <sub>2</sub> O <sub>5</sub> [SO <sub>4</sub> ] <sub>2</sub> : A13B2C2_oP34_32_a6c_c_c	823
188. MnGa <sub>2</sub> Sb <sub>2</sub> : A2BC2_oI20_45_c_b_c	830	233. Re <sub>3</sub> N: AB3_hP4_187_e_fh	937
189. Mo <sub>8</sub> P <sub>5</sub> : A8B5_mP13_6_a7b_3a2b	802	234. Rh <sub>2</sub> Ga <sub>9</sub> : A9B2_mP22_7_9a_2a	805
190. MoS <sub>2</sub> : AB2_hP12_143_cd_ab2d	906	235. Rh <sub>2</sub> S <sub>3</sub> : A2B3_oP20_60_d_cd	839
191. Moissanite-15R: AB_hr10_160_5a_5a	917	236. Rh <sub>3</sub> P <sub>2</sub> : A2B3_tP5_115_g_ag	886
192. Molybdite: AB3_oP16_62_c_3c	844	237. Rh <sub>5</sub> Ge <sub>3</sub> : A3B5_oP16_55_ch_agh	837
193. Muthmannite: ABC2_mP8_10_ac_eh_mn	807	238. Ru <sub>2</sub> Sn <sub>3</sub> : A2B3_tP20_116_bci_fj	887
194. NV: AB_tP8_111_n_n	884	239. RuIn <sub>3</sub> : A3B_tP16_118_ei_f	888
195. Na <sub>3</sub> As <sup>  </sup> : AB3_hP24_185_c_ab2c	936	240. S-II: A_hP9_154_bc	911
196. Na <sub>4</sub> Ti <sub>2</sub> Si <sub>8</sub> O <sub>22</sub> [H <sub>2</sub> O] <sub>4</sub> :		241. S-III: A_tI16_142_f	905
A4B2C13D_tP40_90_g_d_cef2g_c	868	242. S-carbon: A_mP8_10_2m2n	808
197. Na <sub>5</sub> Fe <sub>3</sub> F <sub>14</sub> : A14B3C5_tP44_94_c3g_ad_bg	871	243. Sc-V: A_hP6_178_a	931
198. NaFeS <sub>2</sub> : ABC2_oI16_23_ab_i_k	816	244. ScRh <sub>6</sub> P <sub>4</sub> : A4B6C_hP11_143_bd_2d_a	906
199. NaGdCu <sub>2</sub> F <sub>8</sub> : A2B8CD_tI24_97_d_k_a_b	873	245. SeO <sub>3</sub> : A3B_tP32_114_3e_e	885
200. NaZn <sub>13</sub> : AB13_cF112_226_a_bi	977	246. Sheldrickite:	
201. NaZn[OH] <sub>3</sub> : A3BC3D_tP64_106_3c_c_3c_c	879	A2B3C3DE7_hP48_145_2a_3a_3a_a_7a	907
202. Nb <sub>4</sub> CoSi: AB4C_tP12_124_a_m_c	891	247. SiO <sub>2</sub> : A2B_hP36_177_j2lm_n	930
203. Nb <sub>7</sub> Ru <sub>6</sub> B <sub>8</sub> : A8B7C6_hP21_175_ck_aj_k	928	248. SiO <sub>2</sub> : A2B_cI72_211_hi_i	964
204. NbAs: AB_tI8_109_a_a	882	249. Simple Cubic C <sub>60</sub> Buckminsterfullerine:	
205. NbPS: ABC_oI12_71_h_j_g	855	A_cP240_205_10d	957
206. NbTe <sub>4</sub> : AB4_tP10_103_a_d	877	250. Simpsonite: A4B14C3_hP21_143_bd_ac4d_d	905
207. NbTe <sub>4</sub> : AB4_tP10_124_a_m	892	251. SmSI: ABC_hr6_166_c_c_c	920
208. Ni <sub>3</sub> P: A3B_tI32_82_3g_g	863	252. Sodium Chlorate: ABC3_cP20_198_a_a_b	948
209. Ni <sub>3</sub> Ti: A3B_hP16_194_gh_ac	943	253. Spinel: A3B4_cF56_227_ad_e	980
210. Nierite: A4B3_hP28_159_ab2c_2c	914	254. Sr <sub>2</sub> As <sub>2</sub> O <sub>7</sub> : A2B7C2_tP88_78_4a_14a_4a	861
211. PH <sub>3</sub> : A3B_cP16_208_j_b	960	255. Sr <sub>2</sub> Bi <sub>3</sub> : A3B2_oP20_52_de_cd	834
212. PI <sub>3</sub> : A3B_hP8_173_c_b	926	256. Sr <sub>5</sub> Si <sub>3</sub> : A3B5_tI32_108_ac_a2c	881
213. Pd <sub>17</sub> Se <sub>15</sub> : A17B15_cP64_207_acfk_eij	960	257. SrAl <sub>2</sub> Se <sub>4</sub> : A2B4C_oC28_66_l_kl_a	850
214. Pd <sub>4</sub> Se: A4B_tP10_114_e_a	886	258. SrBr <sub>2</sub> : A2B_tP30_85_ab2g_cg	864
215. PdSn <sub>4</sub> : AB4_oC20_68_a_i	854	259. SrH <sub>2</sub> : A2B_oP12_62_2c_c	843
216. Petzite: A3BC2_cI48_214_f_a_e	966	260. SrSi <sub>2</sub> : A2B_cP12_212_c_a	965
217. Phenakite: A2B4C_hr42_148_2f_4f_f	909	261. Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub> : A10B2C_hP39_171_5c_c_a	925
218. Pinnoite: A2B6CD7_tP64_77_2d_6d_d_ab6d	859	262. Sr[S <sub>2</sub> O <sub>6</sub> ][H <sub>2</sub> O] <sub>4</sub> : A10B2C_hP39_172_5c_c_a	925
219. Post-perovskite: AB3C_oC20_63_a_cf_c	848	263. Stannoidite:	
220. PrNiO <sub>3</sub> : AB3C_hr10_167_b_e_a	921	A8B2C12D2E_oI50_23_bcfk_i_3k_j_a	816
221. PrRu <sub>4</sub> P <sub>12</sub> : A12BC4_cP34_195_2j_ab_2e	945	264. Ta <sub>2</sub> H: AB2_oC6_21_a_k	814
222. PtPb <sub>4</sub> : A4B_tP10_125_m_a	892		

<sup>‡</sup>ZrO<sub>2</sub> and Pyrite have similar AFLOW prototype labels (*i.e.*, same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters.

265.	Ta <sub>2</sub> Se <sub>8</sub> I: AB8C2_tI44_97_e_2k_cd	874
266.	Ta <sub>3</sub> B <sub>4</sub> : A4B3_oI14_71_gh_cg	855
267.	Ta <sub>3</sub> S <sub>2</sub> : A2B3_oC40_39_2d_2c2d	827
268.	TaNiTe <sub>2</sub> : ABC2_oP16_53_h_e_gh	835
269.	TeO <sub>6</sub> H <sub>6</sub> : A6B_cF224_228_h_c	983
270.	TeZn: AB_hp6_144_a_a	907
271.	Te[OH] <sub>6</sub> : A12B6C_cF608_210_4h_2h_e	963
272.	Th <sub>3</sub> P <sub>4</sub> : A4B3_cI28_220_c_a	971
273.	Th <sub>6</sub> Mn <sub>23</sub> : A23B6_cF116_225_bd2f_e	974
274.	ThB <sub>4</sub> : A4B_tP20_127_ehj_g	894
275.	ThBC: ABC_tP24_91_d_d_d	869
276.	ThBC: ABC_tP24_95_d_d_d	872
277.	ThCl <sub>4</sub> : A4B_tI20_88_f_a	865
278.	Thortveitite: A7B2C2_mC22_12_aij_h_i	809
279.	Ti <sub>2</sub> Ge <sub>3</sub> : A3B2_tP10_83_adk_j	864
280.	Ti <sub>3</sub> O: AB3_hp24_149_acgi_3l	910
281.	Ti <sub>3</sub> P: AB3_tP32_86_g_3g	865
282.	TiAl <sub>2</sub> Br <sub>8</sub> : A2B8C_oP22_34_c_4c_a	824
283.	TiFeSi: ABC_oI36_46_ac_bc_3b	830
284.	Tl <sub>4</sub> HgI <sub>6</sub> : AB6C4_tP22_104_a_2ac_c	878
285.	TlP <sub>5</sub> : A5B_oP24_26_3a3b2c_ab	819
286.	TlZn <sub>2</sub> Sb <sub>2</sub> : A2BC2_tI20_79_c_2a_c	862
287.	Tongbaite: A2B3_oP20_62_2c_3c	842
288.	Troilite: AB_hp24_190_i_afh	941
289.	Tychite: A4B2C6D16E_cF232_203_e_d_f_eg_a	953
290.	UCl <sub>3</sub> : A3B_hp8_176_h_d	930
291.	V <sub>2</sub> MoO <sub>8</sub> : AB8C2_oC22_35_a_ab3e_e	825
292.	VPCl <sub>9</sub> : A9BC_oC44_39_3c3d_a_c	827
293.	W <sub>3</sub> O <sub>10</sub> : A10B3_oF52_42_2abce_ab	829
294.	W <sub>5</sub> Si <sub>3</sub> : A3B5_tI32_140_ah_bk	903
295.	WO <sub>3</sub> : A3B_oP32_60_3d_d	839
296.	Weberite: AB7CD2_oI44_24_a_b3d_c_ac	817
297.	Westerveldite: AB_oP8_62_c_c	845
298.	YbBaCo <sub>4</sub> O <sub>7</sub> : AB4C7D_hp26_159_b_ac_a2c_b	915
299.	Zn <sub>3</sub> P <sub>2</sub> : A2B3_tP40_137_cdf_3g	900
300.	ZnSb <sub>2</sub> O <sub>4</sub> : A4B2C_tP28_135_gh_h_d	899
301.	ZrO <sub>2</sub> <sup>‡</sup> : A2B_oP12_29_2a_a	820
302.	ZrO <sub>2</sub> <sup>¶</sup> : A2B_tP6_137_d_a	900