

# Catalogue of Flat-Band Stoichiometric Materials

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Topological electronic flatten bands near or at the Fermi level are a promising avenue towards unconventional superconductivity and correlated insulating states. However, the related experiments are mostly limited to the engineered materials, such as moiré systems<sup>1–3</sup>. Here we present a catalogue of all the three-dimensional stoichiometric materials with flat bands around the Fermi level that exist in nature. We consider 55,206 materials from the Inorganic Crystal Structure Database catalogued using the [Topological Quantum Chemistry website](#)<sup>4,5</sup>, which provides their structural parameters, space group, band structure, density of states and topological characterization. We combine several direct signatures and properties of band flatness to a high-throughput analysis of all crystal structures. In particular, we identify materials hosting line-graph or bipartite sublattices - either in two or three dimensions - likely leading to flat bands. From this trove of information, we create the [Materials Flatband Database website](#), a powerful search engine for future theoretical and experimental studies. We use it to extract a curated list of 2,379 materials, with among them 345 promising candidates, potentially hosting flat bands whose charge centers are not strongly localized on the atomic sites. We showcase five representative materials: KAg[CN]<sub>2</sub>, Pb<sub>2</sub>Sb<sub>2</sub>O<sub>7</sub>, Rb<sub>2</sub>CaH<sub>4</sub>, Ca<sub>2</sub>NCl and WO<sub>3</sub>. We provide a theoretical explanation for the origin of their flat bands close to the Fermi energy using the *S*-matrix method introduced in a parallel work<sup>6</sup>.

## I. INTRODUCTION

Electrons whose energy dispersion is bound within a narrow window are conjectured to exhibit a wide-range of interesting physics phenomena. Such electrons form a high density of states “flat band”, where many-body effects dominate over the kinetic energy and where Fermi-surface physics gives way to strongly interacting, non-Fermi liquid behavior<sup>7</sup>. The archetypal - and until recently the only experimentally discovered - such system is the Fractional Quantum Hall effect<sup>8,9</sup> where anyonic (potentially non-Abelian<sup>10</sup>) quasi-particle excitations can appear under a fractional filling of an electronic flat band that develops in the presence of a large magnetic field. New developments in engineered solid-state materials have now shown that flat bands can exist even in the absence of a large magnetic field. In moiré

materials such as (but not limited to) twisted bilayer graphene (TBG)<sup>1–3</sup>, flat electronic bands are obtained by creating large, many nanometer-size moiré unit cell which folds and flattens the initial band structure of the material. This flatness plays a crucial role in the physics of TBG, leading to, e.g., both the correlated insulator states and of the strong-coupling superconductivity that renders the TBG phase diagram akin to that of the high-temperature cuprates. However, as the unit cell is large, the electron density in moiré samples is necessarily low, preventing new type of physics associated with high electron density<sup>11,12</sup>. This renders the yet elusive prediction of flat bands in non-moiré, stoichiometric crystals of immediate importance.

In the present article and its accompanying Supplementary Information (SI), we address for the question of predicting and classifying all the flat bands in all the stoichiometric crystals currently present in nature, keeping in mind that not all flat bands are created equal. Extremely localized orbitals - or large unit cells with well-separated atoms - can easily give rise to mundane flat atomic bands (FAB), as the kinetic energy is suppressed by the vanishing overlap between atomic wave-

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functions, as schematically shown in Fig. 1(a). The FAB is very common in layered and heavy fermion systems. At the opposite side of the spectrum are the flat topological bands (FTB) created by completely extended wavefunctions (such as is the case in TBG), as shown in the schematic Fig. 1(b). (See Appendix B for a more detailed discussion of the FAB and FTB.) There, the quenching of the kinetic energy arises from interference effects despite large electron orbital overlaps and hopping. The latter type of bands can host many exotic quantum phenomena, including magnetism, fractional quantum Hall effect at zero field<sup>13–16</sup>, unconventional superconductivity<sup>2,17,18</sup>, non-Fermi liquid behavior<sup>7</sup> and anomalous Landau level beyond the Onsager’s rule<sup>19</sup>. Such topological bands can enhance the superfluid weight in twisted bilayer graphene<sup>20,21</sup> and could lead to high-temperature superconductivity. Ideal FTB near the Fermi level in crystalline materials has not yet been found; the only experimentally found FTBs are in the engineered TBG. A third type, the flat obstructed atomic band (FOAB) lies at the interface between the polar opposites FAB and FTB: while the electron’s symmetric Wannier function can be localized in real space, the Wannier center is pinned and centered at an empty site<sup>22,23</sup> and hence delocalized from the atomic sites, as illustrated in Fig. 1(c).

We present and implement algorithms for the detection and classification of flat bands near the Fermi level. Using the materials in our database [Topological Quantum Chemistry website \(TQCDB\)](#) (which contains most ICSD stoichiometric structures) obtained in previous works<sup>4,5,22</sup>, we build the complementary [Materials Flat-band Database website \(MFBDB\)](#), where different algorithms and search options for flat bands are provided to the user. First, we perform a brute-force search based on complementary “flatness” criteria such as bandwidth and density of states (DOS), to predict all the (thousands) flat-band materials in the ICSD database. We classify these bands based on their topologies. Second, using a theory that we have developed in Ref.<sup>6</sup> encompassing generic orbital systems with or without SOC, we perform a targeted search of flat-band materials based on the lattice geometry (such as Kagome, pyrochlore, Lieb, bipartite or split sublattices) of the compounds, whose information is present in the X-ray diffraction data on [TQCDB](#) or ICSD. We show that geometry-based theoretical models based on the *S*-matrix method<sup>6</sup> fit our ab-initio calculations of the flat bands remarkably well. Third, we also perform a manual check of thousands of materials for the best flat bands and select 2,379 materials with high-quality flat bands near the Fermi level. In the main text, we showcase our methods, theoretical understanding and predictive power for five represented flat-band materials, while in the Supplementary Material we present thousands of others. Our classification and predictions take into account the different flat band natures, including their topological character, and our database is coupled to the [Materials Project](#) and [NIMS Materials Database](#), providing information about

the magnetic and superconducting properties (including high  $T_c$ ) of the candidate materials.

## II. DATABASE OF FLAT BANDS MATERIALS

In this work, we have used the [TQCDB](#)<sup>4,5</sup> as our materials database. We summarize its main feature in the Methods section and provide its detailed overview in Appendix C1. As we are interested in flat bands near the Fermi energy, we discard materials containing rare-earth elements (with the exception of La atom) and actinides as these elements usually lead to spurious flat bands due to *f* electrons in the ab-initio calculations. In total, 55,206 ICSD entries have been considered for our high-throughput search for flat bands. The automated search is based on two main, complementary, approaches: the detection of flat bands in the band structure and the DOS, and the identification of special sublattices that lead to band flattening. We will now detail each of them.

### A. High-throughput search of flat-bands

For determining band flatness, we rely on calculations where the spin-orbit coupling (SOC) is neglected. While SOC plays an important role in the topological features near the Fermi level, it does not drastically alter the band structure nor the DOS around the Fermi energy  $E_F \pm 2\text{eV}$  region where we focus our search. For each ICSD entry, our database provides the ab-initio paramagnetic-phase electronic band structure along paths made of straight lines in the Brillouin zone connecting high symmetry points (“high symmetry lines”). Each high symmetry line is well defined in every space group (SG) and it has been discretized, irrespective of its length, into 20 equally distant  $k$ -points (*i.e.*, points in the BZ). Since we are interested in low-energy physics, we focus our investigations on the flatness of the two highest/lowest occupied/empty bands around  $E_F$ , which in turn is reached when the occupation number of bands equals half the number of valence electrons. While paramagnetic calculations would fail to capture (anti-)ferromagnetic ground states, we discuss in Appendix G four representative ferromagnetic compounds. Our ferromagnetic calculations both matches the experimental results and while preserving the flat bands obtained in the paramagnetic calculations remain near the Fermi level.

As motivated in Section I, we investigate bands that are flat in *parts* of (but not necessarily over the entire) the BZ. Thus for each ICSD entry, we search for *flat-band segments*: a series of  $L$  consecutive  $k$ -points along the high symmetry lines of the band structure (we use  $L = 10, 20, 30, 40$  or  $50$ ), where the energy band width is smaller than a tunable threshold  $\omega$  (ranging from 25meV to 150meV). The number of such flat segments for every band analyzed provides a convenient signature of band flatness. In Appendix C2a, we provide a full discussion

of the definition, the algorithm and the statistics of flat-band segments around  $E_F$ .

The presence of a flat-band segment alone is not sufficient to predict the presence of interesting physics associated with it: a (quasi) one-dimensional system would equally exhibit a flat-band segment in the directions perpendicular to its dispersive direction. However, peaks (or their absence) in the DOS offer a simple and efficient way to filter out such pathological cases. Thus for each ICSD entry, we map the position and width of all DOS peaks in an energy region of  $\pm 5\text{eV}$  around  $E_F$ . More details about the DOS peak detection are given in Appendix C 2b.

## B. Automated identification of sublattices

Geometric frustration in (line-graph and bipartite) lattices is known to give rise to exact FTBs<sup>24–29</sup>. While initially predicted for *s*-orbitals, this property was recently generalized to a slew of other possible orbital/lattice combinations<sup>6</sup>. This provides a crucial starting point to understand and predict flat bands in crystalline materials: if a material hosts a line-graph or bipartite lattice as a part of its lattice structure (a "sublattice"), and if this sublattice is only weakly perturbed or deformed by the remaining atoms or orbitals, we expect to observe FTBs. To explain the origin of the flat bands found in our high-throughput search, we have automated, using the structural parameters of every ICSD entry, the detection of five types of line-graph or bipartite sublattices: the Kagome, pyrochlore, Lieb, bipartite or split sublattices as detailed in Appendix D and Appendix E.

In 3D, the Kagome, pyrochlore and Lieb lattices can be mathematically characterized by special occupied Wyckoff positions in certain SGs. Using the crystalline structures of materials, we have developed a space-group method to detect the line-graph and Lieb sublattices in the Methods section. Although the space-group method provides a fast way to find the symmetric Kagome, pyrochlore and Lieb sublattices in crystalline materials, the exact sublattice might be spoiled by the presence of other atoms of the *same element* on (or close to) this sublattice. Moreover, the space-group method discards approximate sublattices which could also exhibit quasi-flat bands. To solve these issues, we have further developed a *geometric method* which solely relies on the geometric features of these three sublattice types (discussed in Appendix D 2) and ignores the exact SG restrictions. In Appendix D 3, we have provided a detailed presentation of our algorithms implementing the geometric method for each type of sublattice. Equipped with these methods, we sort all the possible sublattices in a material in two categories: the *rigorous sublattices* which satisfy both methods and the *approximate sublattices* which only satisfy the geometric method but capture weak distortions of rigorous sublattices.

A bipartite lattice with chiral symmetry is formed by two sublattices  $L$  and  $\tilde{L}$  with the kinetic hopping *only*

between  $L$  and  $\tilde{L}$ . As proposed in Ref.<sup>6</sup> and briefly introduced in the Methods section and Appendix E 1, a general method, namely the *S*-matrix method, can be used to explain the origin of flat bands in crystalline materials whose lattice contains a bipartite or split sublattice. We have developed an algorithm (detailed in Appendix E) to search for bipartite lattices from the structural parameters of each ICSD entry with the following necessary simplifying assumptions for a high-throughput analysis. For each crystal structure in the MFBDB, we solely rely on the geometric distance between two atoms to infer the amplitude of kinetic hopping between them. By ignoring the small hopping terms based on a tunable cutoff, we identify if a crystalline material has a bipartite sublattice with a different number of atoms in its  $L$  and  $\tilde{L}$  sublattices. In the algorithm, a special case of bipartite sublattice, namely the split sublattice which has been proposed to host FTBs<sup>28</sup>, is also detected and tagged.

## III. RESULTS

We now summarize the main results obtained in the present high-throughput search. First we discuss the number of geometric sublattices detected by our algorithms and the public website we have developed to search for materials with flat bands based on the criterion in Section II. We discuss a manually curated list of 2,379 materials potentially hosting FTBs, obtained using our toolset. Then, we showcase five best representative flat-band materials and explain the flat-band segments in their band structures using the *S*-matrix method<sup>6</sup>.

### A. Statistics and website

By applying the automated analysis of the lattice structure to the 55,206 ICSD entries of the MFBDB, we have performed a high-throughput search of the rigorous and approximate Kagome, Lieb, pyrochlore sublattices, the bipartite/split lattice with different number of atoms on their further sublattices. 6,120 ICSDs with at least one Kagome (rigorous or approximate) sublattice have been found, including 4,192 ICSDs with a Kagome sublattice labeled as rigorous, 1,666 ICSDs with a pyrochlore sublattice (rigorous or approximate) and 1,541 ICSDs with a rigorous pyrochlore sublattice. For the Lieb lattice, there are 1,590 ICSDs hosting such a sublattice, including 1,202 ICSDs with rigorous Lieb sublattices. At least one bipartite sublattice (irrespective of the cutoffs) is found among 21,175 ICSDs and split sublattices are found in 8,224 ICSDs. A breakdown of these statistics per SG is provided in Appendix C 3. The brute-force scan of the band structures along the high symmetry lines was performed for several threshold parameters. The number of ICSDs exhibiting flat-band segments varies strongly on these parameters; for a detailed statistical analysis see Appendix C 2a.

The data generated through the automated algorithms discussed in Section II is available through our [MFBDB](#)(see Appendix C2 for an overview of the search engine). We actually used this website to perform an extensive investigation of promising candidate materials exhibiting flat bands or large segment of flat bands close to the Fermi energy. The outcome of our search is provided as a list of *curated flat-band materials* in Appendix H1. This list contains 6,338 ICSD entries that can be regrouped into 2,379 unique materials, *i.e.*, ICSDs sharing the same stoichiometric formula, SG and topological property at the Fermi energy (as defined in Appendix C1). The complete set of criteria applied to select these materials is provided in Appendix H1, and it includes the distance to the Fermi energy, the flat band width and topology, and the presence of a peak in the DOS. We have excluded cases where the flat bands were *clear FAB* from the list of curated flat-band materials, and they are listed in Appendix H2. The statistics of detected sublattices among the curated materials are provided in Table I.

## B. Flat-band material candidates

Among the 2,379 high-quality flat-band materials, we select 345 best representative flat-band materials in Appendix H3 for further experimental investigation. Most of the 345 materials host one (or more than one) of the Kagome, pyrochlore, Lieb, bipartite and split sublattices in their crystal structures. For each of the five types of sublattice, we select one representative material, which hosts best flat-band segments on (or close to) the Fermi level, and explain its physical origin using the *S*-matrix method<sup>6</sup>. All of the five representative flat-band materials are chemically realistic, experimentally paramagnetic and not Mott insulators, which is consistent with our paramagnetic calculations.

The five typical materials are KAg[CN]<sub>2</sub> [[ICSD 30275](#), SG 163 (*P*<sub>3</sub>*1c*)] with approximate Kagome sublattice formed by Ag atoms, Pb<sub>2</sub>Sb<sub>2</sub>O<sub>7</sub> [[ICSD 27120](#), SG 227 (*F*<sub>d</sub>*3m*)] with pyrochlore sublattice formed by Pb atoms, Rb<sub>2</sub>CaH<sub>4</sub> [[ICSD 65196](#), SG 139 (*I*<sub>4</sub>/*m*<sub>mm</sub>)] with Lieb sublattice formed by Ca and H atoms, Ca<sub>2</sub>NCl [[ICSD 62555](#), SG 166 (*R*<sub>3</sub>*m*)] with bipartite sublattice formed by Ca and N atoms, and WO<sub>3</sub> [[ICSD 108651](#), SG 221 (*P*<sub>m</sub>*3m*)] with split sublattice formed by W and O atoms. Their crystal structures are shown in Fig. 2(a)-(e) and the orbital characters of the flat bands in the five materials are shown in the orbital-projected band structures in Fig. 2(f)-(j). As detailed in Appendix F, based on the crystal structure and orbital-projected bands of these materials, we have constructed effective tight-binding Hamiltonians using the *S*-matrix method<sup>6</sup> and found that they can successfully explain the origins of flat bands. The flat bands of other materials of similar crystal structures can be found in the [MFBDB](#). In the Methods section, we use Ca<sub>2</sub>NCl to showcase the application of the

*S*-matrix method in explaining the origin of flat bands.

## IV. DISCUSSION

We have performed, for the first time, a high-throughput search for flat electronic bands near the Fermi level and for the detection of line-graph and bipartite sublattices from the crystal structures of stoichiometric crystalline materials. We have further classified the flat bands by their topology, DOS, length of band flatness, and the types of lattices formed by the atoms whose orbitals contribute to the flat band. By successfully applying our algorithms to 55,206 ICSD entries, we have found that 24,052 (43.57%) out of all the ICSD entries host *at least* one of the Kagome, pyrochlore, Lieb, bipartite or split sublattices in their crystal structures. This proportion is raised to 59.26% for our *manually curated list* of 6,338 ICSDs (2,379 unique materials) and 73.87% for the *best representative flat-band materials*. The appearance of flat-bands in materials can be, in large but non-exhaustive part, theoretically understood using the *S*-matrix method<sup>6</sup>, as we have exemplified in five prototypical compounds. All the results obtained in this work and detailed in the supplementary Appendices can be accessed on the [MFBDB](#). Our results pave the way for future theoretical and experimental studies on flat-band materials combining topology and interactions and leading to exotic quantum phenomena, such as magnetism, non-Fermi liquid behavior and superconductivity. Such flat-band investigations are, at present, confined to engineered twisted moire lattices in two dimensions. While the present work studies flat bands in paramagnetic band structures of 3D materials, our methods can be adapted to detect flat bands in magnetic band structures, 2D mono-layer materials, phonons and photonic crystals. Furthermore, the further classification of FOAB's will enlarge the set of flat bands whose center of charge is away from the atomic positions.

## Methods

**Topological Quantum Chemistry website** The database used as an input the structural parameters of stoichiometric materials reported in the Inorganic Crystal Structure Database (ICSD)<sup>30</sup>. For each entry, ab-initio calculations were performed using Density Functional Theory (DFT)<sup>31,32</sup> and its implementation in the Vienna Ab-initio Simulation Package (VASP)<sup>33,34</sup>, with and without accounting for the spin-orbit coupling (SOC). The database provides the structural parameters, the band dispersion along high symmetry lines, the DOS, and the topological characterization for each set of bands in the material's band structure for each of the 69,730 ICSD entries.

**Space-group method of detecting line-graph and Lieb sublattices** To detect a Kagome, pyrochlore or Lieb sublattice in crystalline materials, we have first identified the *minimal* SGs that support these three lattices and the corresponding Wyckoff positions (see details in Appendix D 1). Then, through group-subgroup relations and the split relations between the sets of Wyckoff positions on the *Bilbao Crystallographic Server* (BCS)<sup>35,36</sup>, we have obtained all the SGs which host these lattices. The results are tabulated in the Table V and Table VI of Appendix D. We dub the detection of sublattices using this tabulated information as the *space-group method*.

**A brief introduction of the *S*-matrix method.** Denoting  $|L|$  and  $|\tilde{L}|$  the number of atoms or orbitals in the  $L$  and  $\tilde{L}$  further sublattices of the bipartite or split sublattice of a material (assuming  $|L| \geq |\tilde{L}|$ ), the Bloch Hamiltonian associated to a bipartite sublattice of a material reads

$$H(\mathbf{k}) = \begin{pmatrix} 0 & S^\dagger(\mathbf{k}) \\ S(\mathbf{k}) & 0 \end{pmatrix}. \quad (1)$$

Here  $S(\mathbf{k})$  is a matrix with dimension  $|L| \times |\tilde{L}|$  and  $\mathbf{k}$  is the momentum in the Brillouin zone. A bipartite lattice with  $|L| \neq |\tilde{L}|$  hosts flat bands in its band structure. For example, the Hamiltonian of Eq. 1 has at least  $|L| + |\tilde{L}| - 2 \times \text{rank}(S(\mathbf{k}))$  zero-energy states, *i.e.*, the band structure has at least  $|L| + |\tilde{L}| - 2 \times \text{rank}(S(\mathbf{k}))$  exact flat bands. It is also very likely that these bands exhibit non-trivial topology<sup>6</sup>. While the other  $2 \times \text{rank}(S(\mathbf{k}))$  bands are dispersive, they are related by chiral symmetry. Although in real crystalline materials the chiral symmetry is generally broken by the intra-sublattice hopping, we find in Ref.<sup>6</sup> that this *S*-matrix method goes beyond the chiral symmetry. For a generalized bipartite lattice including the intra-sublattice coupling  $A(k)(B(k))$  of sublattice  $L(\tilde{L})$ , if  $A(k)$  has a momentum-independent eigenvalue  $E = E_0$  with degeneracy  $n_0$  and  $|\tilde{L}| < n_0 \leq |L|$ , then  $H(k)$  also has at least  $n_0 - |\tilde{L}|$  perfectly flat bands at energy  $E = E_0$  irrespective of  $B(k)$ . Moreover, the eigenstates of these  $n_0 - |\tilde{L}|$  flat bands identical to those of the system with chiral symmetry<sup>6</sup>.

**The origin of flat bands in Ca<sub>2</sub>NCl: application of**

**S-matrix method.** As shown in Fig. 2(d) in the main text, the 3D crystal structure of Ca<sub>2</sub>NCl is stacked, composed alternating Ca<sub>2</sub>N and Cl layers. In each Ca<sub>2</sub>N layer, the Ca and N atoms occupy honeycomb (with buckling) and triangular sublattices, respectively. The Cl layer also forms a triangular lattice. As shown in Fig. 2(i), the flat band and the lower dispersive bands next to it are mainly contributed by the  $p$  orbitals of N atoms. By constructing the maximal localized Wannier functions (MLWF)<sup>37</sup>, we extract an effective tight-binding model for these  $p$  bands and find that its hoppings - which are computed from ab-initio methods without any additional theoretical input - obey a set of fine-tuned conditions, which in turn give rise to flatness of the top  $p$  band. As an example, the amplitude of  $\sigma$ -bond comes out to almost exactly the  $-3$  times of  $\pi$ -bond. (See Appendix F 4 for more details.) Since similar flat bands also exist in many other materials of the same structure (*e.g.* Ca<sub>2</sub>NBr, Sr<sub>2</sub>NCl *et al.*), and similar fine-tuned tight-binding ab-initio model, this points to a deeper reason for the fine-tuning conditions.

This deep reason is the *S*-matrix theory. We notice that the nearest neighbors of the N atoms are the Ca atoms and hence that Ca and N atoms form a bipartite sublattice if only the nearest neighbors hoppings are considered in a theoretical model of the bands. As analyzed in Fig. 2(i), the conduction bands around  $E = 3\text{eV}$  are mainly contributed by the  $s$  and  $d$  orbitals on the Ca atoms and the three valence bands in the energy window  $-3 \sim 0\text{eV}$  are mainly contributed by the  $p$  orbitals on N atoms and partially contributed by the hybridized orbitals consisting of  $s$  and  $d_{z^2}$  orbitals on Ca. Since the  $s$  and  $d_{z^2}$  orbitals form the same representation ( $A_1$ ) of the point group symmetry  $C_{3v}$  isomorphic to the site-symmetry group of Ca sites, they hybridize with each other to form two hybridized orbitals. It is a reasonable simplification to only take into account the hybridized orbital with the lowest energy, which we refer to as the  $s$  orbital in the following. A tight-binding model including both the N and Ca atoms is naturally an *S*-matrix theory of a bipartite lattice, where the  $L$  sublattice of the bipartite (sub)-lattice consists of  $p$  orbitals at the triangular lattice formed by N and the  $\tilde{L}$  sublattice consists of (hybridized)  $s$  orbitals at the honeycomb lattice (with buckling) formed by Ca. The onsite energy of  $s$  orbitals ( $\Delta_s$ ) is about 3eV. Following the argument below Eq. 1, there must be  $|L| + |\tilde{L}| - 2 \times \text{rank}(S(\mathbf{k})) = 3 + 2 - 4 = 1$  flat band at  $E = 0$ . (See Appendix F 4 for the explicit form of  $S(\mathbf{k})$ .) As detailed in Appendix F 4, the *S*-matrix band structure matches the first-principles band structure very well. Furthermore, the *S*-matrix theory also explains the fine-tuning conditions in the extracted tight-binding Hamiltonian from the MLWFs: the perturbative effective Hamiltonian for the  $p$  bands,  $-S(\mathbf{k})S^\dagger(\mathbf{k})/\Delta_s$ , perfectly reproduces the fine-tuning conditions of the ab-initio model. Therefore, the *S*-matrix theory is a faithful explanation for the flat band in Ca<sub>2</sub>NCl.

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### Author contribution

B.A.B. and N.R. conceived this work; N.R. and M.R.L. performed the high-throughput calculations with the help from L.E. and Y.X.; Y.X., D.S.M., Z.D.S., M.R.L., L.E. and N.R. worked out the theoretical explanations for the flat-band materials detailed in Appendix F; The material lists in Appendix H were manually selected by Y.X., M.R.L., Z.D.S., M.J. and N.R.; N.R. built the flat-band material database; D.S.M. performed the ab-initio

ferromagnetic calculations advised by Y.X.; M.J., L.S., C.F. helped curate the list of materials to find the most experimentally relevant. All authors discussed the results and wrote the main text and the Methods; Y.X., Z.D.S., M.R.L., D.S.M., M.J., L.E. and N.R. wrote the supplementary materials.

### Competing interests

The authors declare no competing interests.

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**Data availability** All data is available in the Supplementary Information and through our public website Materials Flatband Database website(<https://www.topologicalquantumchemistry.fr/flatbands>).

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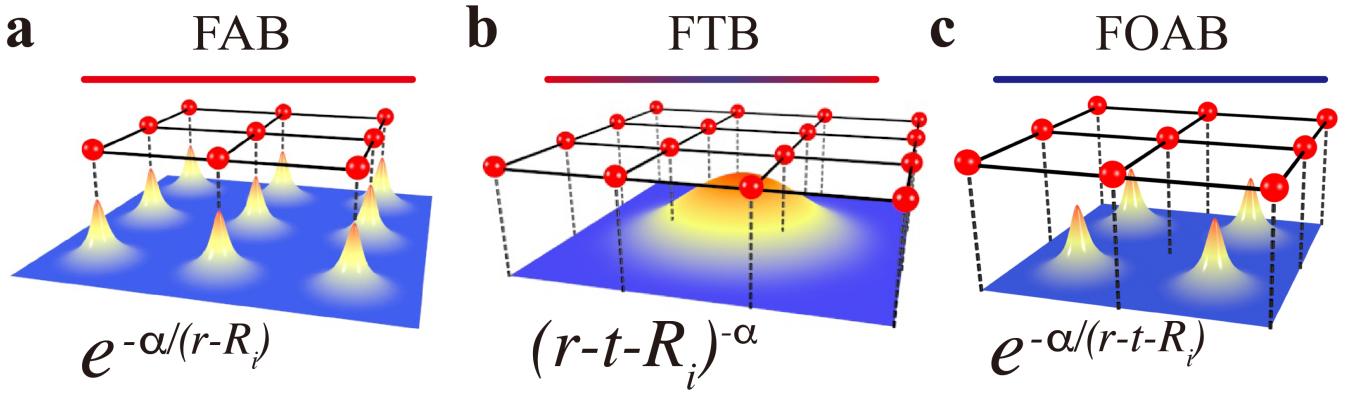


Figure 1. An illustration of the three possible types of flat bands. (a) Flat atomic band (FAB): the Wannier functions associated to the flat bands are exponentially localized on the atoms' sites. (b) Flat topological band (FTB): the Bloch states are extended (with potentially a power law decay) in at least one direction of the lattice. (c) Flat obstructed atomic band (FOAB): as opposed to FAB, the corresponding Wannier functions are exponentially localized but on an empty site. In the figures, the atom sites of the 2D lattices are represented with red spheres. Below the lattices are the Bloch wave functions of the flat bands associated with their decay law, where  $R_i$  is the position of atom  $i$ ,  $t$  is a fractional lattice vector and  $\alpha$  is a positive coefficient.



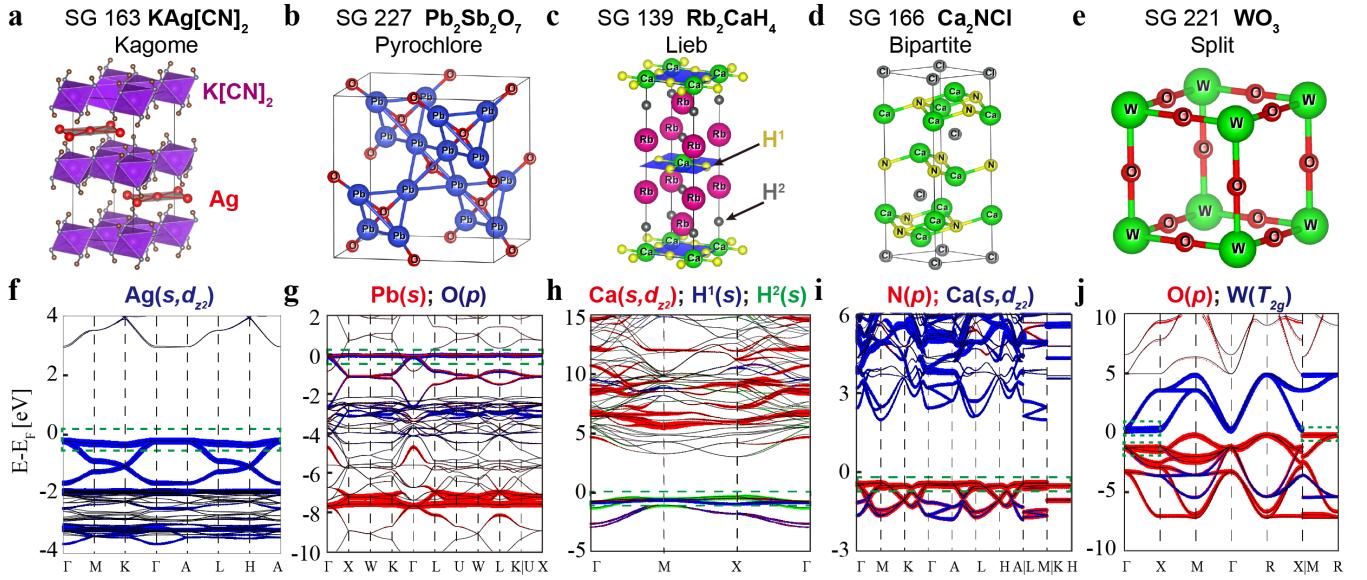


Figure 2. Crystal and band structures of the representative flat-band materials. The crystal structures of (a)  $\text{KAg}[\text{CN}]_2$  which hosts an approximate Kagome sublattice formed by the Ag atoms (in red color), (b)  $\text{Pb}_2\text{Sb}_2\text{O}_7$  with Pb atoms at the Wyckoff position 16d forming a pyrochlore sublattice, (c)  $\text{Rb}_2\text{CaH}_4$  with the H atoms at 4c (i.e., the  $\text{H}^1$  atoms in yellow color) and the Ca atoms at 2a position forming a Lieb sublattice, (d)  $\text{Ca}_2\text{NCl}$  which is stacked by alternating the  $\text{Ca}_2\text{N}$  and Cl layers, where the  $\text{Ca}_2\text{N}$  layer is identified as a bipartite sublattice in our algorithm, (e)  $\text{WO}_3$  with the W and O atoms forming a split lattice. For each material, its band structure and the orbital characterization of the flat bands are plotted and analyzed below its crystal structure. Based on the band structure analysis, the flat bands close to the Fermi level are explained by the  $S$ -matrix method in Appendix F. In the crystal structure plots, SG, chemical formula and the type of sublattice host in the material are provided on the top of each panel. In the band structure plots, the flat-band segments close to the Fermi level are indicated by the dashed green lines. Orbital characters of the colored bands are provided on the top of each panel.



	All ICSDs	Curated	Best
# ICSDs	55,206	6,338	949
# Materials	28,169	2,379	345
Kagome	6,120 (11.09%)	1,699 (26.81%)	516 (54.37%)
Pyrochlore	1,666 (3.02%)	296 (4.67%)	77 (8.11%)
Lieb	1,590 (2.88%)	721 (11.38%)	151 (15.91%)
Bipartite	21,175 (38.36%)	3,138 (49.51%)	432 (45.52%)
Split	8,224 (14.90%)	1,920 (30.29%)	354 (37.30%)
None	31,154 (56.43%)	2,582 (40.74%)	248 (26.13%)

Table I. Statistics of the ICSD entries in the database hosting at least one sublattice for each lattice type. In the first row, we give the number of ICSDs entries for the database (first column), for the list of curated flat-band materials (second column) and for the best representative flat-band materials (third column). The second line provides the number of unique materials for the database, the list of curated flat-band materials and the best representative flat-band materials. The third, fourth, fifth, sixth and seventh rows are the statistics for the Kagome, pyrochlore, Lieb, bipartite with different number of atoms on sublattices and split lattices. An ICSD entry is considered as hosting a given type of lattice if the algorithms discussed in Section II B have found at least one such a lattice irrespective of the cutoffs or being a rigorous or approximate sublattice. Note that an ICSD entry might host more than one type of sublattices. The eighth row provides the statistics for the ICSDs where no sublattices have been detected. For each column, the percentages are computed with respect to the number of ICSDs provided in the first row.

## Supplementary Information for “Catalogue of Flat-Band Stoichiometric Materials”

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## Appendix A: Introduction to the Supplementary Information

In this work, we have presented a catalogue of stoichiometric materials hosting flat bands near the Fermi energy. In addition to the main text, we provide below Supplementary Appendices giving an in-depth discussion of our methodology and several lists of curated materials. Appendix B is devoted to the detailed definition of two types of flat bands: flat atomic bands and flat topological bands. In Appendix C, we give an overview of the [Topological Quantum Chemistry website](#) on which we rely on for our catalogue of flat-band materials. We present the [Materials Flatband Database website](#) and the theory and algorithms for the detection of flat-band segments and density of states peaks. We also provide detailed statistics about the materials hosting the five types of sublattices leading to flat bands (namely the Kagome, pyrochlore, generic bipartite, split and Lieb lattices). We then present Appendices about these five types of sublattices. Appendix D focuses on Kagome, pyrochlore and Lieb sublattices. We cover both the crystal symmetries of these lattices, the three dimensional space groups compatible with them and their geometrical features. We also detail the algorithms we have designed for a high throughput search in our database of materials. In Appendix E, we give a short overview of the bipartite and split lattices and most specifically of our new theoretical method for finding flat bands, the *S*-matrix method, detailed in<sup>6</sup>. We present all the technical details of the algorithms we build in order to automatically look for bipartite and split sublattices in our material database. In Appendix F, we provide the theoretical explanations for the presence of flat bands in seven prototypical materials: WO<sub>3</sub> [[ICSD 108651](#), SG 221 (*Pm* $\bar{3}m)], Pb<sub>2</sub>Sb<sub>2</sub>O<sub>7</sub> [[ICSD 27120](#), SG 227 (*Fd* $\bar{3}m)], CaNi<sub>5</sub> [[ICSD 54474](#), SG 191 (*P6/mmm*)], Ca<sub>2</sub>NCl [[ICSD 62555](#), SG 166 (*R3m*)], Rb<sub>2</sub>CaH<sub>4</sub> [[ICSD 65196](#), SG 139 (*I4/mmm*)], KAg[CN]<sub>2</sub> [[ICSD 30275](#), SG 163 (*P31c*)] and RbMo<sub>3</sub>S<sub>3</sub> [[ICSD 644175](#), SG 176 (*P6<sub>3</sub>/m*)]. To test the validity of our high-throughput search based on paramagnetic calculations for potentially magnetic materials, we study in Appendix G four materials using ab-initio calculation with on-site Hubbard interaction for *d* and *f* electrons, namely SrRuO<sub>3</sub> [[ICSD 69360](#), SG 221 (*Pm* $\bar{3}m)], Rb<sub>2</sub>MnCl<sub>6</sub> [[ICSD 9347](#)] SG 225 (*Fm* $\bar{3}m), Ba<sub>2</sub>MnReO<sub>6</sub> [[ICSD 4169](#)] SG 225 (*Fm* $\bar{3}m) and NiMnSb [[ICSD 54255](#), SG 216 (*F* $\bar{4}3m)]. With magnetizations close to their experimental values, the flat band features are barely affected. Finally in Appendix H, we give a list of 2,379 manually curated materials with flat bands near the Fermi energy. For convenience, materials with flat atomic bands are separated from the ones with flat bands occur from wave function interference. Moreover we have selected 345 compounds hosting the most remarkable flat bands and we provide their band structure and density of states.$$$$$$

## Appendix B: Flat bands with different topologies

In real materials, electronic bands can be flat in the entire Brillouin zone (BZ) or only be flatten along some specific high-symmetry paths. In this appendix, we provide a detailed description of the two types of flat bands, namely the flat atomic bands and the flat topological bands, and provide several mechanisms that could give rise to them.

### 1. Flat atomic bands

In crystalline materials, a set of bands that are flat in all directions or some particular directions is referred to as flat atomic bands if they form a band representation (BR) that can be induced from local orbitals. The flat atomic bands are induced from local orbitals and hence by definition have a *trivial topology*<sup>22,38,39</sup>. However, in practice, it is difficult to fully determine whether a set of bands is a BR: the full determination requires the Bloch wave functions over the whole Brillouin zone. Instead, we use the symmetry eigenvalues (the representations formed by the Bloch bands) to diagnose whether a set of bands is *consistent* with a BR. When the symmetry eigenvalues of a set of flat bands are consistent with a BR induced from local orbitals, we *label* the set of bands as flat atomic bands. With this approach, it is possible that some bands labeled as flat atomic bands are nevertheless topological with some topology not diagnosed by symmetry eigenvalues. A simple example is a 2D Chern insulator with inversion symmetry. When the Chern number is odd, the inversion eigenvalues are not consistent with any BR<sup>40–42</sup>. However, when the Chern number is even, the inversion eigenvalues can be the same as the eigenvalues of some BRs.

When the flat atomic bands are flat in *all* the directions, the flat atomic bands are in the atomic limit, where the hopping between some orbitals of neighboring atoms is infinitesimal, as illustrated in Fig. 1(a) of the main text. In Appendix H 2, we provide a list of manually selected materials hosting flat atomic bands.

As an example of flat atomic bands, we consider the compound Al<sub>12</sub>Ca<sub>8</sub>O<sub>24</sub>S<sub>2</sub> [[ICSD 67589](#), SG 217 (*I* $\bar{4}3m)] shown in Fig. 3. It has several flat bands below the Fermi level (with band index  $-6 \sim -1$ ). The BR of these bands are induced from the orbitals  $\bar{E}_2 \oplus \bar{F}$  at *2a* position, which are occupied by S atoms. In Fig. 3, we plot the atom-projected band structure and density of states of the compound Al<sub>12</sub>Ca<sub>8</sub>O<sub>24</sub>S<sub>2</sub>. We find that the flat bands arise from the S atom orbitals, as indicated by the green lines. The flatness of the *p* bands of S atoms is due to two reasons: on one$

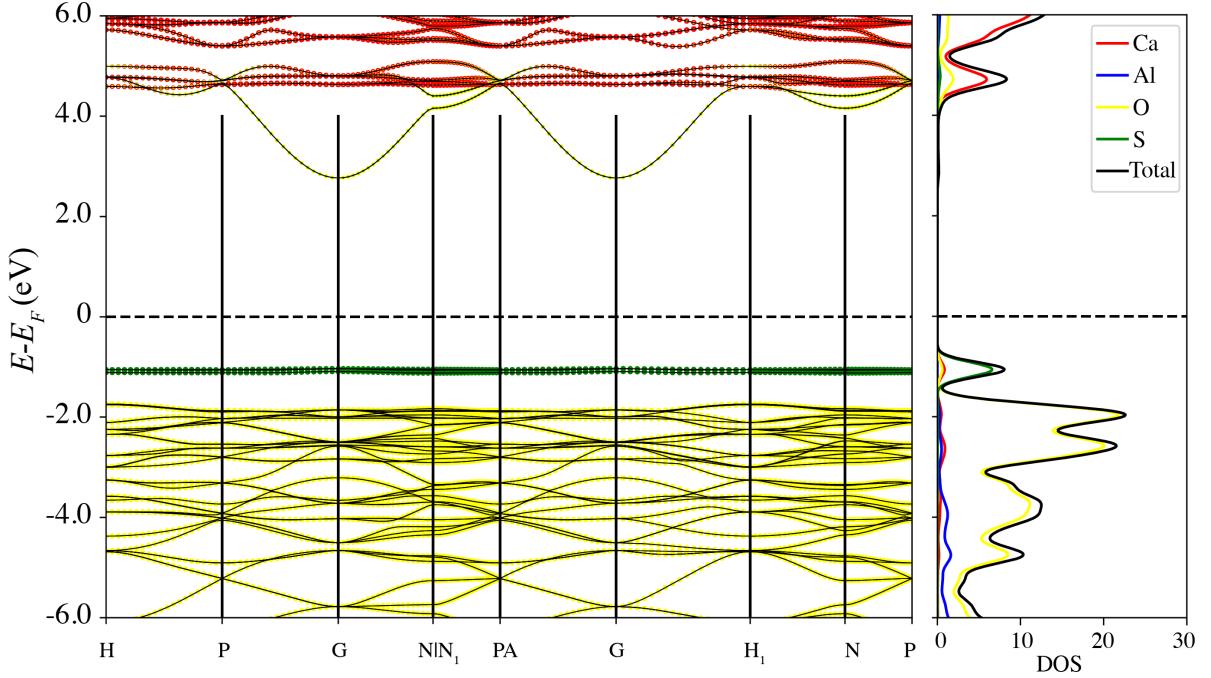


Figure 3. Atom-projected band structure along the high-symmetry path (left panel) and density of states (right panel) for  $\text{Al}_{12}\text{CasO}_{24}\text{S}_2$  [ICSD 67589, SG 217 ( $I\bar{4}3m$ )]. The weight of orbitals on Ca, Al, O and S atoms are represented by the red, blue, yellow and green points and lines, respectively.

hand, there is a big enough difference of the onsite energy between the  $p$  orbitals on S and the orbitals on other atoms; on the other hand, the distance between two neighboring S atoms (about 8 Å) is so large that the kinetic energy between the S  $p$  orbitals is small. Hence, the flat bands contributed by the  $p$  orbitals of S are flat atomic bands.

The flat atomic bands that are flat only in one or two directions can be understood as layered systems, where the inter-layer kinetic energy is weak. In this case, all bands are flat along the inter-layer direction(s). When the bands are flat in one (two) direction(s), each “layer” is a 2D plane (1D chain).

Note that heavy fermion systems may host another class of flat bands in the atomic limit. These bands are formed by localized  $4f$  or  $5f$  orbitals and are extremely flat. As the mean field approximation adopted in the first principle calculations fails to characterize the strong correlation of  $f$  electron, we ignore the heavy fermion systems in this work as we will discuss in Appendix C.

## 2. Flat topological bands

Apart from the flat atomic bands defined in Appendix B1, the flat bands might be topologically nontrivial: when a set of bands that are flat in all or some particular directions do not form any BR, *i.e.*, cannot be induced from local orbitals, the set of bands forms a set of flat topological bands. Since by the definition the topological bands are not equivalent to any local orbitals, the Wannier functions of the topological bands that preserve the symmetry of the system must be extended, *i.e.*, not exponentially localized, as shown in Fig. 1(b) of the main text. In this work and as explained in the last subsection, we only make use of symmetry eigenvalues to diagnose the topology. Hence a set of flat topological bands might potentially be misdiagnosed as flat atomic bands. However, all the diagnosed flat topological bands must be topological.

There are two types of flat topological bands: the stable topological bands and the fragile topological bands<sup>43–49</sup>. The former is realized as a non-integer linear combination (NLC) of elementary BR (EBR) or split elementary BR (SEBR)<sup>22,38,39,50–52</sup>, and the later can be realized as a difference (but not a sum) of EBRs. Since we only rely on symmetry eigenvalues, a flat stable topological band could be labeled as fragile in this work if its symmetry eigenvalues are consistent with a difference of EBRs. On the contrary, all bands labeled as stable topological must be stable topological because by definition their symmetry eigenvalues are not consistent with any BR or difference of BRs. Exact flat fragile bands have been found in several lattice models<sup>29,53,54</sup>. The  $S$ -matrix method introduced in Appendix E and in Ref.<sup>6</sup> is a general mechanism to generate exact flat fragile bands. On the other hand, no examples

of rigorously flat (*i.e.*, dispersionless) stable topological bands have yet been found with compact support hopping. Nevertheless, quasi-flat stable topological bands were recently found in line-graph and split-line-graph lattice models with spin-orbit coupling<sup>28,55</sup>.

## Appendix C: Database of materials with flat bands selected from TQC database

In this Appendix, we will introduce the database of materials that we are relying on for this high-throughput search of flat-band materials. We will also present the [Materials Flatband Database website](#) and the different algorithms and search options that are provided to the user. The tools that we publicly provide through this website have been used to obtain the curated list of flat-band materials that we will present in Appendix H.

### 1. An overview of the Topological material database

For our high-throughput search of materials with flat bands, we have relied on the data and database of the [Topological Quantum Chemistry website](#). It was originally built for Ref.<sup>4</sup> and upgraded both in terms of materials and features in Ref.<sup>5</sup>. Beyond the two original publications related to this database, this database was also used to look for the best candidate materials with fragile bands<sup>56</sup> and to develop machine learning approach to topological feature predictions<sup>57</sup>. We review here some important properties of this database.

The ab-initio calculations of the database were performed using Density Functional Theory (DFT)<sup>31,32</sup> and its implementation in the Vienna Ab-initio Simulation Package (VASP)<sup>33,34</sup>. For each material calculation, we used as input the structural parameters reported on the Inorganic Crystal Structure Database (ICSD)<sup>30</sup>. We treated the interaction between the ion cores and the valence electrons using the projector augmented-wave method<sup>58</sup>. For the exchange-correlation potential, we used the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof parameterization for solids<sup>59</sup>. Effects of spin-orbit coupling were accounted by using the second variation method<sup>60</sup>. For the plane-wave expansion, we employed a  $\Gamma$ -centered  $\mathbf{k}$ -point grid of size (11×11×11) for reciprocal space integration and a 550 eV energy cutoff. The density of states (DOS) was evaluated on a  $\Gamma$ -centered  $\mathbf{k}$ -point grid of size (11×11×11) and using the Methfessel-Paxton algorithm of order 1. We emphasize that all of the first-principle calculations are paramagnetic, *i.e.*, without the onsite spin polarization. The magnetic properties at low temperature reported on [Topological Quantum Chemistry website](#) are extracted from the [Materials Project](#).

The [Topological Quantum Chemistry website](#) is built upon the systematic ab-initio calculation of 85,700 ICSD entries of stoichiometric materials. Among these entries, the calculation with spin-orbit coupling was performed successfully for 73,234 materials. All of them are available through the website. Calculations without spin-orbit coupling are also available although a small fraction (4.78% of the successfully processed ICSD entries with spin-orbit coupling) did not converge. 19,798 of the available materials (*i.e.*, 27.03%) contain rare-earth elements (La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, and Yb) and actinides (Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No and Lr) which may exhibit strong correlation effects and usually lead to spurious flat bands in the DFT calculations. For these reasons, we have discarded these materials from our flat-bandsurvey with one exception, compounds containing La as rare-earth elements. Indeed for the ab-initio calculation, La is always a cation in such compounds and the bands originated from these  $f$  orbitals are usually away from the Fermi energy. In our database, there are 2,689 ICSD entries (*i.e.*, 3.67%) corresponding to this situation. There, the  $f$  bands originated from the La atoms are located at least 1eV above  $E_f$  (typically around 2eV). We have highlighted some of these materials in Appendix H.3.

Many ICSD entries correspond to the same stoichiometric formula and the same space group (SG), leading most of the time (but not always) to, *e.g.*, the same topological properties at the Fermi level. For this reason the [Topological Quantum Chemistry website](#) defines the notion of *unique materials*, including all the ICSD entries having the same stoichiometric formula, SG and topological classification at the Fermi level. This database contains 38,298 such unique materials. While in some cases, all ICSD entries within a given unique materials have band structures and densities of states barely distinguishable by eye, they might in general exhibit some subtle differences for these two quantities. Automated search of flat-band features from the band structure or the density of states should thus be performed on every ICSD belonging to all unique materials.

### 2. The flat-band material database

The website [Materials Flatband Database website](#) relies on the database provided in [Topological Quantum Chemistry website](#). It offers a dedicated search interface to look for materials with flat-band features close to the Fermi

energy. As discussed above, we have filtered out those that contain any rare-earth elements except La. Moreover, to search for flat bands or flat bands along some high symmetry lines, we only focus on the DFT calculations performed without spin-orbit coupling: the band structures and density of states are usually similar with or without spin-orbit coupling, thus only considering the later simplifies the automated search without introducing any bias. Overall, the user has access to 55,206 ICSD entries (28,169 unique materials). The three main tools that we provide to search for flat bands are based on flat segments in the electronic band structure or peaks in the density of states or sublattices. We will now detail these two former, the latter will be discussed in Appendix C3.

#### a. Band structure and flat-band segments

For each ICSD entry, we have access to the electronic band structure computed along high symmetry lines and without spin-orbit coupling. These band structures include all bands up to two times of the number of valence electrons, thus an equal number of bands above and below the last filled one. The notions of filled and empty are defined with respect to the number of electrons and the band index. Each band is evaluated along a path specific to each point group. This path is made of straight lines in the Brillouin zone (BZ) connecting two high symmetry points. The choice of these straight lines is designed to cover all cases required by band connectivity<sup>22,61</sup> while staying connected with the related works and databases. Each straight line is discretized into 20 equally spaced  $\mathbf{k}$  points in the BZ, including the two end high symmetry points. Note that the distance between two consecutive discretized  $\mathbf{k}$  points might differ from one straight line to another: we use a regular mesh with the same number (20) of points for the discretization of each line but the actual distances between two pairs of high symmetry points of the BZ do not have to be equal.

To automatically search for flat segments in a given band structure of an ICSD, we apply the following procedure:

- We only consider at most the last 2 filled bands and 2 empty bands to focus on features near the Fermi level. We require that at least one  $\mathbf{k}$  point with an energy  $E$  in the energy window parameterized by  $\Delta_E$  such that  $|E - E_F| < \Delta_E$ .  $E_F$  is the Fermi energy as computed from the VASP self consistent calculation<sup>5</sup>. If any of the last 2 filled bands and 2 empty bands does not satisfy this constraint, it is discarded.
- We define a flat segment as a series of  $L$  consecutive  $\mathbf{k}$  points along the path in the BZ, whose bandwidth, *i.e.*, the difference between the highest energy and the lowest energy associated to these  $L$  points, is lower than some chosen value  $\omega$ .
- For each band, we test the presence of flat segments starting from every possible discretized  $\mathbf{k}$  points that define the path in the BZ. Notice that segments can overlap (see the purple and green boxes of Fig. 4). Denoting  $N_{\text{BZ}}$  the total number of discretized  $\mathbf{k}$  points that define the path in the BZ, the number of flat segments  $N_{\text{fl}}$  is at most  $N_{\text{BZ}} - L + 1$ . A score is then defined as the ratio

$$\text{score} = \frac{N_{\text{fl}}}{N_{\text{BZ}} - L + 1}. \quad (\text{C1})$$

For example, a perfectly flat band would have a score of 1.

- In addition, we also evaluate  $N_w$  the number of bands that overlap with the energy window defined by  $|E - E_F| < \Delta_E$ . It is used as a proxy to quantify how dense is the band structure in this energy window.

We have applied this procedure to all ICSDs using several discrete values of  $L$  (10, 20, 30, 40 and 50),  $\Delta_E$  (0.5eV, 1.0eV, 1.5eV and 2.0eV), and  $\omega$  (25meV, 50meV, 75meV, 100meV, 125meV and 150meV). We exemplify the search procedure in Fig. 4 for ICSD 62555. In Table II, we provide the number of ICSDs hosting flat-band segments for all values of  $L$  and  $\omega$  that we have considered. Statistics is split into different minimum threshold for the best score (as defined in Eq. (C1) for an ICSD. A score greater than 0 means there is at least one flat-band segment. A score of 1, *i.e.*, the maximum score means that an ICSD has one band out of the (at most) last 2 filled bands and 2 empty bands, where every sequence of  $L$  consecutive  $\mathbf{k}$  points along the path in the BZ with a bandwidth smaller than  $\omega$ . We stress that such a score does not imply that the band has a global bandwidth smaller  $\omega$ .

All the above-mentioned parameters can be selected as search criteria on the [Materials Flatband Database website](#). In addition, a cap on  $N_w$ , the number of bands in the energy window, can be set to look for well separated flat-band segments from other bands. Moreover, the user can require the flat band with the highest score to be topological, either as part of a topological single set of bands or all the bands up to (and including) the best flat band being topological (see Ref.<sup>5</sup> for more details about the difference between these two definitions). The best score as defined

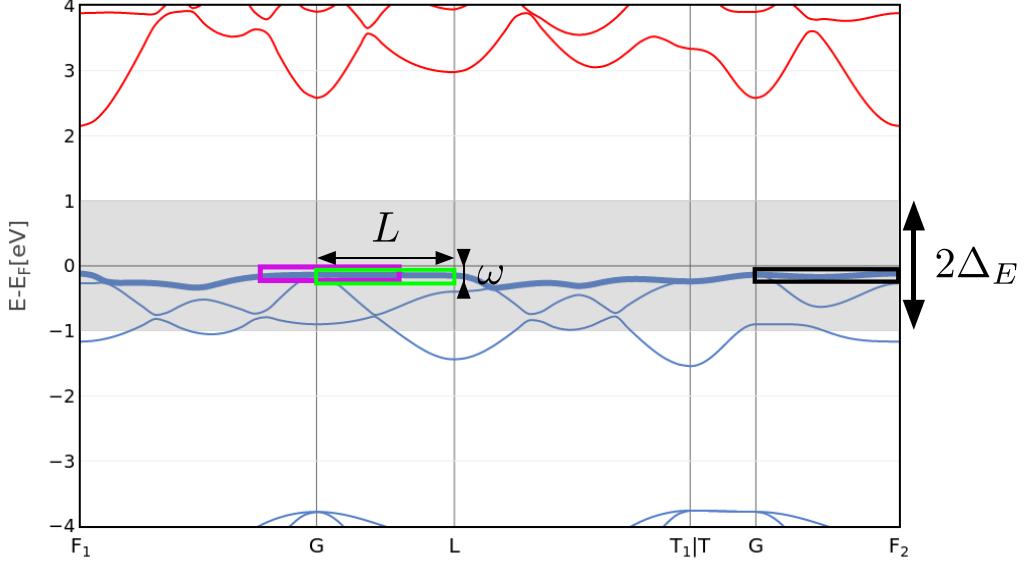


Figure 4. Example of flat-band segments found in the band structure of Ca<sub>2</sub>NCl [ICSD 62555, SG 166 ( $R\bar{3}m$ )] in the space group 166 ( $R\bar{3}m$ ), one of the best flat bands given in Appendix H3. We have set the parameters  $L = 20$ ,  $\omega = 150\text{meV}$  and  $\Delta_E = 1\text{eV}$ . The best flat band closest to the Fermi level is highlight in bold blue and has a score of 0.642. The purple, green and black boxes show three segments satisfying the constraints of the algorithm discussed in Appendix C2a.

in Eq. (C1) is used both as a search criterion and to sort the search results. When selecting a given result, the band having the flat segment closest to the Fermi energy is displayed in bold for convenience (see Fig. 4).

Table II: Statistics about the flat-band segments of all the ICSD entries. Note that we used the energy window  $\Delta_E = 0.5\text{eV}$  but the numbers provided here almost never depend on this parameter. The first column is the minimal best score (as defined in Eq. (C1)) and the second column is the minimum segment length  $L$ . The other columns are the different values for the maximum bandwidth  $\omega$ . We provide both the number of ICSDs hosting such a flat-band segment and the percentage with respect to the total number of ICSDs that we have considered, namely 55,206.

Min. score	$L$	$\omega = 25\text{meV}$	$\omega = 50\text{meV}$	$\omega = 75\text{meV}$	$\omega = 100\text{meV}$	$\omega = 125\text{meV}$	$\omega = 150\text{meV}$
0.01	10	48312 (87.5%)	52693 (95.5%)	54160 (98.1%)	54534 (98.8%)	54752 (99.2%)	54876 (99.4%)
0.01	20	29987 (54.3%)	38914 (70.5%)	43327 (78.5%)	46033 (83.4%)	47939 (86.8%)	49490 (89.7%)
0.01	30	13610 (24.6%)	22700 (41.1%)	29037 (52.6%)	33354 (60.4%)	36537 (66.2%)	38936 (70.5%)
0.01	40	7622 (13.8%)	14472 (26.2%)	19818 (35.9%)	24146 (43.7%)	27701 (50.2%)	30491 (55.2%)
0.01	50	4712 (8.5%)	10179 (18.4%)	14787 (26.8%)	18583 (33.7%)	21508 (39.0%)	24372 (44.1%)
0.25	10	18685 (33.9%)	29936 (54.2%)	36000 (65.2%)	40178 (72.8%)	43345 (78.5%)	45577 (82.6%)
0.25	20	7223 (13.1%)	14525 (26.3%)	20081 (36.4%)	24794 (44.9%)	28636 (51.9%)	31452 (57.0%)
0.25	30	3787 (6.9%)	9079 (16.4%)	13775 (24.9%)	17612 (31.9%)	20739 (37.6%)	23681 (42.9%)
0.25	40	2222 (4.0%)	6160 (11.2%)	9980 (18.1%)	13432 (24.3%)	16390 (29.7%)	18866 (34.2%)
0.25	50	1577 (2.9%)	4815 (8.7%)	8058 (14.6%)	11175 (20.2%)	13989 (25.3%)	16335 (29.6%)
0.50	10	8416 (15.2%)	16617 (30.1%)	22871 (41.4%)	27745 (50.3%)	31376 (56.8%)	34172 (61.9%)
0.50	20	2889 (5.2%)	7691 (13.9%)	12151 (22.0%)	15940 (28.9%)	19095 (34.6%)	22113 (40.1%)
0.50	30	1569 (2.8%)	4866 (8.8%)	8175 (14.8%)	11433 (20.7%)	14286 (25.9%)	16781 (30.4%)
0.50	40	1099 (2.0%)	3686 (6.7%)	6418 (11.6%)	9195 (16.7%)	11768 (21.3%)	14187 (25.7%)
0.50	50	882 (1.6%)	2989 (5.4%)	5467 (9.9%)	7952 (14.4%)	10324 (18.7%)	12541 (22.7%)
0.75	10	3415 (6.2%)	8637 (15.7%)	13323 (24.1%)	17409 (31.5%)	20847 (37.8%)	23861 (43.2%)
0.75	20	1288 (2.3%)	4275 (7.7%)	7345 (13.3%)	10408 (18.9%)	13066 (23.7%)	15519 (28.1%)
0.75	30	868 (1.6%)	2980 (5.4%)	5434 (9.8%)	8006 (14.5%)	10370 (18.8%)	12612 (22.9%)
0.75	40	733 (1.3%)	2490 (4.5%)	4734 (8.6%)	6965 (12.6%)	9202 (16.7%)	11378 (20.6%)
0.75	50	657 (1.2%)	2250 (4.1%)	4330 (7.8%)	6398 (11.6%)	8548 (15.5%)	10634 (19.3%)
1.00	10	895 (1.6%)	3073 (5.6%)	5526 (10.0%)	8005 (14.5%)	10344 (18.7%)	12638 (22.9%)
1.00	20	627 (1.1%)	2162 (3.9%)	4176 (7.6%)	6234 (11.3%)	8342 (15.1%)	10337 (18.7%)

1.00	30	587 (1.1%)	1994 (3.6%)	3922 (7.1%)	5817 (10.5%)	7907 (14.3%)	9873 (17.9%)
1.00	40	552 (1.0%)	1872 (3.4%)	3752 (6.8%)	5568 (10.1%)	7642 (13.8%)	9560 (17.3%)
1.00	50	541 (1.0%)	1813 (3.3%)	3676 (6.7%)	5463 (9.9%)	7508 (13.6%)	9436 (17.1%)

Looking for flat-band segments along the high symmetry lines does not fully take into consideration the 3D structure of a material, whose bands could be dispersive away from high-symmetry paths (as already mentioned in Appendix B 1). A typical example would be a (quasi-)one dimensional system. Any high symmetry line in the BZ perpendicular to the dispersive momentum direction of the one dimensional system would appear flat. For that reason, we also rely on a second indicator: peaks in the density of states.

### b. Peaks in the density of states

The density of states (DOS) calculation is part of the processing applied to each ICSD entry displayed in the [Topological Quantum Chemistry website](#) (see Ref.<sup>5</sup> for in-depth discussion). Similarly with the search for the band structure flat-band segments, we focus on the DOS computed without spin orbit coupling. Note that we do not search for peaks in the DOS directly from the PROCAR output of VASP. Rather, we rely on the output of the python script pydos/pyband which processes the PROCAR files to generate, e.g., the DOS plots on the [Topological Quantum Chemistry website](#).

To look for peaks in the DOS, we consider the energy range  $[-5\text{eV}, 5\text{eV}]$ . We compute the average DOS over this range; this value sets the minimum value to define a peak. We discretize the DOS with a step of  $0.02\text{eV}$  to avoid spurious peaks from fast variations. We then apply the following algorithm:

1. We look for the largest value among the discretized DOS. It should be larger than the average DOS. The energy  $E_{\text{peak}}$  associated to this largest value sets the DOS peak position.
2. We compute  $W_{\text{peak}}$  the peak width as its Gaussian width, *i.e.*, the full width at half maximum of the peak.
3. All points of the discretized DOS within the peak width are discarded.
4. All points around the peak width where the DOS continues to decrease away from the maximum are also discarded (to avoid considering the tails of the peak as other peaks).
5. The procedure is then repeated from the first step until all discretized DOS values have been discarded or are lower than the average DOS.

This crude algorithm offers a reliable and simple way to find DOS peaks. In Fig. 5, we provide an example of DOS peak processed information by this procedure.

All ICSD DOSEs available on [Materials Flatband Database website](#) have been processed with this algorithm. While not directly accessible, the DOS peak information is used by the search engine when activating “Require a DOS peak near  $E_F$ ”. Two search parameters can be tuned: the peak maximum distance to the Fermi level, *i.e.*, the maximal value for  $|E_{\text{peak}} - E_F|$  where  $E_{\text{peak}}$  is the peak position and the maximal Gaussian width  $W_{\text{peak}}$  for the peak closest to Fermi level. These search parameters can be used as the unique criteria or combined with other criteria such as the sublattice features or the existence of flat-band segments along the high symmetry lines.

## 3. Sublattices and database

For all the ICSDs provided in [Materials Flatband Database website](#), we have performed an automated search for five types of sublattices, namely Kagome, pyrochlore, generic bipartite (with a different number of atoms in the two subsets), split and Lieb sublattices. This automated search will be detailed in Appendices D and E. The full list of sublattices for each ICSD are given on their respective webpage on [Materials Flatband Database website](#). Moreover, the presence of sublattices can be used as a search criterion when looking for flat-band materials.

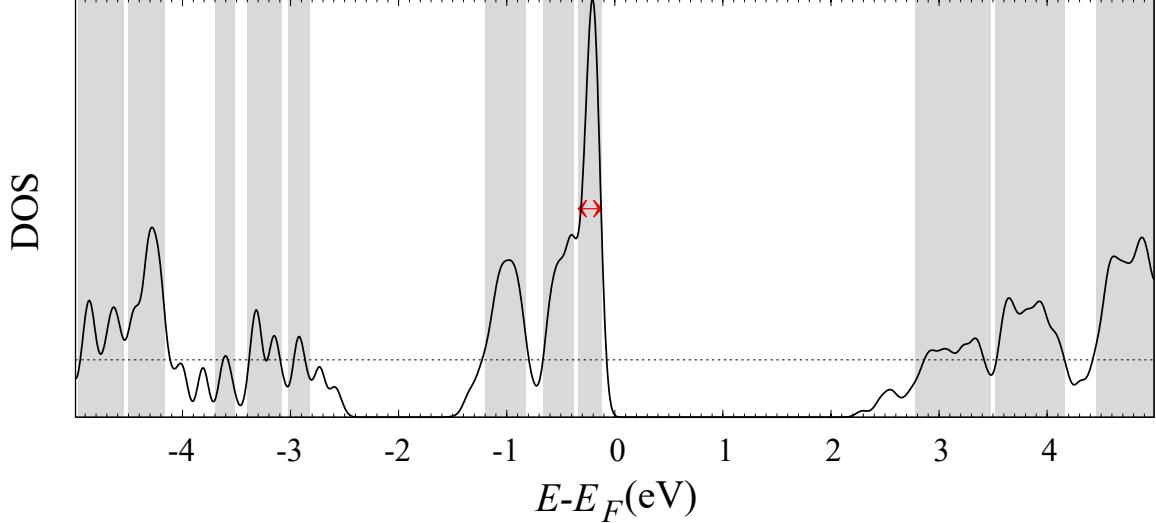


Figure 5. Example of DOS peak information based on the DFT calculations for  $\text{Ca}_2\text{NBr}$  [ICSD 153105, SG 166 ( $R\bar{3}m$ )] in the space group 166 ( $R\bar{3}m$ ), one of the best flat bands given in Appendix H3. The most prominent peak is located at  $E_{\text{peak}} - E_F \simeq -0.22\text{eV}$ . The red double arrows indicates the Gaussian width  $W_{\text{peak}} \simeq 0.22\text{eV}$  of this peak. The dotted line is the average density of states over the energy range  $[-5\text{eV}, 5\text{eV}]$ . The gray areas indicate the extension of each peak.

Table III: *Upper part:* Statistics of the ICSD entries in the database hosting at least one Kagome or Pyrochlore sublattice and an additional sublattice: Lieb, bipartite or split. In the first row, we give the number of ICSDs entries for the database (first column), for the list of curated flat-band materials (second column) and for the best representative flat-band materials (third column). The second and third rows provide the number of ICSD entries with a Kagome (second row) or pyrochlore (third row) for each category (all ICSDs, curated flat-band materials and best representative flat-band materials). The fourth, fifth, and sixth rows are the statistics for ICSD with a Kagome sublattice and either a Lieb, bipartite with different number of atoms on sublattices and split lattices. An ICSD entry is considered as hosting a given type of lattice if the algorithms discussed in Section ‘‘Automated identification of line-graph and bipartite sublattices’’ of the main text have found at least one such a lattice irrespective of the cutoffs or being a rigorous or approximate sublattice. The seventh, eighth, and ninth rows are similar to the fourth, fifth, and sixth rows but for pyrochlore rather than Kagome sublattices. *Lower part:* Statistics of the ICSD entries in the database hosting one type of sublattice. The tenth, eleventh, twelfth and thirteenth rows give the number of ICSDs hosting only a Kagome, pyrochlore, Lieb or bipartite sublattice respectively. All percentage are expressed with respect to the numbers in the second row.

	All ICSDs	Curated	Best
# ICSDs	55,206	6,338	949
Kagome	6,120 (11.09%)	1,699 (26.81%)	516 (54.37%)
Pyrochlore	1,666 (3.02%)	296 (4.67%)	77 (8.11%)
Kagome and Lieb	916 (1.66%)	537 (8.47%)	135 (14.23%)
Kagome and Bipartite	3,244 (5.88%)	1,081 (17.06%)	247 (26.03%)
Kagome and Split	1,974 (3.58%)	904 (14.26%)	228 (24.03%)

Pyrochlore and Lieb	0 (0.00%)	0 (0.00%)	0 (0.00%)
Pyrochlore and Bipartite	968 (1.75%)	172 (2.71%)	16 (1.69%)
Pyrochlore and Split	338 (0.61%)	66 (1.04%)	10 (1.05%)
Only Kagome	2,178 (3.95%)	494 (7.79%)	208 (21.92%)
Only Pyrochlore	698 (1.26%)	124 (1.96%)	61 (6.43%)
Only Lieb	1 (0.00%)	0 (0.00%)	0 (0.00%)
Only Bipartite	17,258 (31.26%)	1,873 (29.55%)	169 (17.81%)

For sake of completeness, we now discuss the frequency of appearance for the sublattice types among the 55,206 ICSD entries in our database. Note that our figures here are based on ICSDs rather than unique materials. Indeed, tiny differences in the atom positions from one ICSD to another one associated to the same unique material might lead to threshold effect: a sublattice close to the maximum error bar of the automated search algorithm for one ICSD might be slightly beyond the error bar for another ICSD. From our survey, we have found that 24,052 ICSDs (43.57%) have at least one sublattice. A large fraction of the ICSDs, 38.36% (*i.e.*, 21,175 ICSDs), have at least one bipartite sublattice. For the Kagome sublattices, 6,120 ICSDs (11.09%), the majority are rigorous Kagome sublattices (4,192 ICSDs, 7.59%) as defined in Appendix D. The approximate Kagome sublattices are found in 2,100 ICSDs (3.80%). Note that an ICSD can have both a rigorous and an approximate Kagome distinct sublattice. A similar analysis can be performed for the Lieb sublattices: there are 1,590 ICSDs (2.88%) with Lieb sublattices, including 1,202 ICSDs (2.18%) with rigorous Lieb sublattices and 438 ICSDs (0.79%) with approximate Lieb sublattices, as defined in Appendix D. Pyrochlore sublattices have been found in 1,666 ICSDs (3.02%), including 1,541 ICSDs hosting (2.79%) rigorous sublattices and 125 ICSDs hosting (0.23%). Finally, split sublattices were detected in 8,224 ICSDs (14.90%). As mentioned in the caption of Table I in the main text, an ICSD entry might host more than one type of sublattices. A trivial example is a pyrochlore sublattice that implies the existence of Kagome sublattices. More interestingly, we provide in Table III the number of ICSDs hosting either a Kagome or a pyrochlore sublattice and any of the three other types of sublattices we have considered: Lieb, bipartite and split sublattices. We also provide in this table, the number of ICSDs hosting a single type of sublattice. Note that the flat bands in a compound hosting solely a bipartite lattice may only be understood in the S-matrix formalism.<sup>6</sup> Additionally, a breakdown of the number of ICSDs per space group that have a given sublattice type among the 5 types we have searched for is available in Table IV.

Table IV: Statistics about ICSD entries with either Kagome, pyrochlore, bipartite, split or Lieb sublattices. The first column is the space group number, the second column is the number of ICSDs that have been processed per SG. The third (seventh) column provides the number of ICSDs per SG having at least one rigorous or approximate Kagome (Lieb) sublattice. The fourth, fifth and sixth columns give the number of ICSDs per SG with at least one pyrochlore, bipartite and split sublattice respectively. Note that we count an ICSD entry as having a bipartite or split sublattice, if it hosts such a sublattice irrespective of the cutoffs defined in Appendix E. Note that not all the 2D Lieb-sublattice materials are labeled as a 3D bipartite/split sublattice in the results of our algorithm and further discussion can be referred to Appendix E 2.

SG	# ICSDs	# ICSDs with Kagome	# ICSDs with pyrochlore	# ICSDs with bipartite	# ICSDs with split	# ICSDs with Lieb
1	221	2 (0.9%)	—	104 (47.1%)	59 (26.7%)	—
2	1677	8 (0.5%)	—	701 (41.8%)	218 (13.0%)	—
3	14	—	—	7 (50.0%)	3 (21.4%)	—
4	275	—	—	122 (44.4%)	43 (15.6%)	—
5	182	1 (0.6%)	—	91 (50.0%)	37 (20.3%)	—
6	38	2 (5.3%)	—	13 (34.2%)	6 (15.8%)	—
7	141	—	—	77 (54.6%)	45 (31.9%)	—
8	164	8 (4.9%)	—	73 (44.5%)	22 (13.4%)	1 (0.6%)
9	272	3 (1.1%)	1 (0.4%)	145 (53.3%)	44 (16.2%)	—
10	38	2 (5.3%)	—	13 (34.2%)	4 (10.5%)	—

11	677	1 (0.1%)	—	260 (38.4%)	51 (7.5%)	—
12	1528	24 (1.6%)	—	656 (42.9%)	165 (10.8%)	1 (0.1%)
13	246	1 (0.4%)	—	164 (66.7%)	54 (21.9%)	—
14	3370	2 (0.1%)	—	1494 (44.3%)	473 (14.0%)	—
15	2270	5 (0.2%)	—	1303 (57.4%)	449 (19.8%)	—
16	2	—	—	2 (100%)	1 (50.0%)	—
17	8	—	—	3 (37.5%)	3 (37.5%)	1 (12.5%)
18	41	—	—	20 (48.8%)	12 (29.3%)	—
19	327	—	—	116 (35.5%)	25 (7.7%)	—
20	72	1 (1.4%)	—	43 (59.7%)	33 (45.8%)	—
21	10	—	—	4 (40.0%)	4 (40.0%)	—
22	7	—	—	3 (42.9%)	1 (14.3%)	—
23	15	—	—	8 (53.3%)	3 (20.0%)	—
24	3	2 (66.7%)	—	3 (100%)	3 (100%)	—
25	56	—	—	27 (48.2%)	18 (32.1%)	—
26	74	1 (1.4%)	—	41 (55.4%)	18 (24.3%)	1 (1.4%)
27	1	—	—	1 (100%)	1 (100%)	—
28	17	—	—	1 (5.9%)	—	—
29	85	—	—	27 (31.8%)	9 (10.6%)	—
30	6	—	—	5 (83.3%)	1 (16.7%)	1 (16.7%)
31	240	8 (3.3%)	—	89 (37.1%)	13 (5.4%)	—
32	12	—	—	9 (75.0%)	2 (16.7%)	—
33	379	2 (0.5%)	—	200 (52.8%)	70 (18.5%)	—
34	28	2 (7.1%)	—	12 (42.9%)	10 (35.7%)	—
35	8	—	—	6 (75.0%)	3 (37.5%)	—
36	372	1 (0.3%)	—	227 (61.0%)	94 (25.3%)	—
37	7	—	—	7 (100%)	2 (28.6%)	—
38	81	10 (12.3%)	—	33 (40.7%)	19 (23.5%)	13 (16.1%)
39	13	—	—	6 (46.1%)	1 (7.7%)	1 (7.7%)
40	60	—	—	24 (40.0%)	8 (13.3%)	—
41	43	—	—	23 (53.5%)	20 (46.5%)	—
42	4	—	—	—	—	—
43	121	—	—	52 (43.0%)	29 (24.0%)	—
44	80	4 (5.0%)	2 (2.5%)	21 (26.2%)	5 (6.2%)	—
45	11	—	—	8 (72.7%)	5 (45.5%)	2 (18.2%)
46	81	5 (6.2%)	2 (2.5%)	52 (64.2%)	42 (51.9%)	20 (24.7%)
47	62	1 (1.6%)	—	52 (83.9%)	50 (80.7%)	3 (4.8%)
48	2	—	—	1 (50.0%)	1 (50.0%)	—
50	7	—	—	2 (28.6%)	2 (28.6%)	1 (14.3%)
51	115	—	—	46 (40.0%)	16 (13.9%)	2 (1.7%)
52	46	1 (2.2%)	—	37 (80.4%)	15 (32.6%)	—
53	26	—	—	3 (11.5%)	—	—
54	22	—	—	3 (13.6%)	3 (13.6%)	—
55	337	—	—	164 (48.7%)	35 (10.4%)	—
56	29	—	—	21 (72.4%)	14 (48.3%)	—
57	143	1 (0.7%)	—	54 (37.8%)	27 (18.9%)	—
58	461	—	—	162 (35.1%)	27 (5.9%)	—
59	278	—	—	98 (35.2%)	28 (10.1%)	—
60	222	—	—	150 (67.6%)	22 (9.9%)	—
61	211	—	—	84 (39.8%)	25 (11.8%)	—
62	4313	15 (0.3%)	—	1956 (45.4%)	503 (11.7%)	8 (0.2%)
63	1307	9 (0.7%)	—	417 (31.9%)	132 (10.1%)	2 (0.1%)
64	395	8 (2.0%)	—	149 (37.7%)	95 (24.1%)	57 (14.4%)
65	192	4 (2.1%)	—	92 (47.9%)	52 (27.1%)	4 (2.1%)
66	37	—	—	30 (81.1%)	27 (73.0%)	1 (2.7%)
67	40	—	—	5 (12.5%)	3 (7.5%)	—
68	19	—	—	9 (47.4%)	6 (31.6%)	—
69	59	11 (18.6%)	—	26 (44.1%)	8 (13.6%)	—
70	174	5 (2.9%)	5 (2.9%)	81 (46.5%)	38 (21.8%)	—
71	355	5 (1.4%)	—	76 (21.4%)	45 (12.7%)	1 (0.3%)
72	183	—	—	100 (54.6%)	63 (34.4%)	—
73	18	—	—	5 (27.8%)	—	—
74	221	33 (14.9%)	4 (1.8%)	115 (52.0%)	58 (26.2%)	4 (1.8%)
75	5	—	—	4 (80.0%)	4 (80.0%)	—

76	11	—	—	4 (36.4%)	2 (18.2%)	—	
77	2	—	—	—	—	—	
78	1	—	—	—	—	—	
79	13	—	—	3 (23.1%)	1 (7.7%)	—	
80	3	—	—	3 (100%)	2 (66.7%)	—	
81	18	—	—	5 (27.8%)	1 (5.6%)	—	
82	261	—	—	174 (66.7%)	50 (19.2%)	—	
83	6	—	—	1 (16.7%)	1 (16.7%)	—	
84	30	—	—	9 (30.0%)	4 (13.3%)	—	
85	49	—	—	27 (55.1%)	3 (6.1%)	—	
86	43	—	—	5 (11.6%)	2 (4.7%)	—	
87	256	8 (3.1%)	—	140 (54.7%)	115 (44.9%)	—	
88	275	—	—	187 (68.0%)	16 (5.8%)	—	
90	5	—	—	5 (100%)	2 (40.0%)	—	
91	8	—	—	8 (100%)	2 (25.0%)	—	
92	131	—	—	83 (63.4%)	71 (54.2%)	—	
94	1	—	—	1 (100%)	—	—	
95	3	—	—	3 (100%)	1 (33.3%)	—	
96	37	1 (2.7%)	1 (2.7%)	11 (29.7%)	6 (16.2%)	—	
97	1	—	—	—	—	—	
98	7	—	—	3 (42.9%)	2 (28.6%)	—	
99	182	48 (26.4%)	—	158 (86.8%)	152 (83.5%)	45 (24.7%)	
100	37	—	—	32 (86.5%)	17 (46.0%)	—	
102	12	—	—	5 (41.7%)	1 (8.3%)	—	
103	9	—	—	—	—	—	
104	4	—	—	2 (50.0%)	1 (25.0%)	—	
105	4	—	—	—	—	—	
106	1	—	—	1 (100%)	—	—	
107	84	—	—	13 (15.5%)	9 (10.7%)	—	
108	14	—	—	8 (57.1%)	4 (28.6%)	—	
109	33	—	—	6 (18.2%)	—	—	
110	36	—	—	33 (91.7%)	25 (69.4%)	—	
111	24	5 (20.8%)	—	19 (79.2%)	—	—	
112	4	—	—	3 (75.0%)	3 (75.0%)	—	
113	143	—	—	97 (67.8%)	77 (53.9%)	—	
114	41	—	—	19 (46.3%)	11 (26.8%)	—	
115	23	2 (8.7%)	—	6 (26.1%)	2 (8.7%)	—	
116	25	—	—	9 (36.0%)	4 (16.0%)	—	
117	9	—	—	5 (55.6%)	3 (33.3%)	—	
118	11	—	—	3 (27.3%)	2 (18.2%)	—	
119	49	1 (2.0%)	—	24 (49.0%)	10 (20.4%)	—	
120	22	—	—	8 (36.4%)	6 (27.3%)	—	
121	193	—	—	50 (25.9%)	17 (8.8%)	—	
122	502	—	—	78 (15.5%)	53 (10.6%)	—	
123	521	51 (9.8%)	—	177 (34.0%)	146 (28.0%)	119 (22.8%)	
124	33	—	—	6 (18.2%)	—	—	
125	36	—	—	15 (41.7%)	6 (16.7%)	—	
126	9	—	—	5 (55.6%)	4 (44.4%)	—	
127	271	—	—	72 (26.6%)	47 (17.3%)	8 (3.0%)	
128	56	—	—	9 (16.1%)	6 (10.7%)	—	
129	889	3 (0.3%)	—	108 (12.2%)	68 (7.7%)	3 (0.3%)	
130	55	—	—	32 (58.2%)	19 (34.5%)	—	
131	36	—	—	7 (19.4%)	—	—	
132	10	1 (10.0%)	—	5 (50.0%)	1 (10.0%)	—	
133	5	—	—	1 (20.0%)	1 (20.0%)	—	
134	9	2 (22.2%)	—	2 (22.2%)	2 (22.2%)	—	
135	76	—	—	66 (86.8%)	2 (2.6%)	—	
136	710	—	—	552 (77.8%)	14 (2.0%)	2 (0.3%)	
137	126	—	—	104 (82.5%)	34 (27.0%)	—	
138	17	—	—	9 (52.9%)	7 (41.2%)	—	
139	1772	21 (1.2%)	—	502 (28.3%)	406 (22.9%)	338 (19.1%)	
140	777	—	—	228 (29.3%)	145 (18.7%)	40 (5.2%)	
141	403	25 (6.2%)	20 (5.0%)	200 (49.6%)	15 (3.7%)	2 (0.5%)	
142	73	—	—	26 (35.6%)	16 (21.9%)	—	

143	18	2 (11.1%)	—	13 (72.2%)	3 (16.7%)	—
144	31	—	—	13 (41.9%)	12 (38.7%)	—
145	5	—	—	2 (40.0%)	2 (40.0%)	—
146	105	3 (2.9%)	—	59 (56.2%)	10 (9.5%)	—
147	74	1 (1.4%)	—	43 (58.1%)	11 (14.9%)	—
148	740	10 (1.4%)	—	434 (58.6%)	122 (16.5%)	—
149	15	9 (60.0%)	—	15 (100%)	6 (40.0%)	—
150	73	3 (4.1%)	—	57 (78.1%)	27 (37.0%)	—
151	4	—	—	3 (75.0%)	—	—
152	269	—	—	194 (72.1%)	179 (66.5%)	—
153	1	—	—	—	—	—
154	138	—	—	109 (79.0%)	108 (78.3%)	—
155	57	2 (3.5%)	—	25 (43.9%)	7 (12.3%)	—
156	221	5 (2.3%)	—	116 (52.5%)	1 (0.5%)	—
157	26	4 (15.4%)	—	21 (80.8%)	18 (69.2%)	—
158	3	—	—	3 (100%)	1 (33.3%)	—
159	57	7 (12.3%)	—	45 (79.0%)	6 (10.5%)	—
160	291	51 (17.5%)	—	143 (49.1%)	21 (7.2%)	11 (3.8%)
161	246	4 (1.6%)	—	200 (81.3%)	32 (13.0%)	—
162	65	12 (18.5%)	—	60 (92.3%)	27 (41.5%)	—
163	73	6 (8.2%)	—	45 (61.6%)	25 (34.2%)	—
164	789	127 (16.1%)	—	390 (49.4%)	70 (8.9%)	—
165	56	—	—	17 (30.4%)	9 (16.1%)	—
166	1173	292 (24.9%)	2 (0.2%)	392 (33.4%)	125 (10.7%)	—
167	845	7 (0.8%)	—	664 (78.6%)	263 (31.1%)	53 (6.3%)
169	1	—	—	1 (100%)	—	—
173	163	7 (4.3%)	—	115 (70.5%)	46 (28.2%)	—
174	46	—	—	17 (37.0%)	—	—
175	2	—	—	1 (50.0%)	1 (50.0%)	—
176	312	8 (2.6%)	—	145 (46.5%)	15 (4.8%)	—
177	3	—	—	3 (100%)	3 (100%)	—
180	92	—	—	24 (26.1%)	20 (21.7%)	—
181	15	—	—	6 (40.0%)	6 (40.0%)	—
182	48	1 (2.1%)	—	44 (91.7%)	25 (52.1%)	—
183	3	—	—	—	—	—
185	73	1 (1.4%)	—	41 (56.2%)	9 (12.3%)	—
186	716	89 (12.4%)	—	191 (26.7%)	18 (2.5%)	—
187	227	10 (4.4%)	—	22 (9.7%)	1 (0.4%)	—
188	27	—	—	24 (88.9%)	11 (40.7%)	—
189	383	1 (0.3%)	—	80 (20.9%)	14 (3.7%)	—
190	63	—	—	16 (25.4%)	7 (11.1%)	—
191	662	374 (56.5%)	—	59 (8.9%)	25 (3.8%)	—
192	14	13 (92.9%)	—	13 (92.9%)	6 (42.9%)	—
193	362	3 (0.8%)	—	46 (12.7%)	15 (4.1%)	—
194	2643	681 (25.8%)	—	544 (20.6%)	172 (6.5%)	—
195	1	—	—	1 (100%)	1 (100%)	—
196	1	—	—	—	—	—
197	36	—	—	35 (97.2%)	9 (25.0%)	—
198	315	—	—	64 (20.3%)	17 (5.4%)	—
199	37	—	—	27 (73.0%)	12 (32.4%)	—
200	25	6 (24.0%)	—	3 (12.0%)	3 (12.0%)	—
201	6	2 (33.3%)	—	6 (100%)	3 (50.0%)	—
202	26	—	—	—	—	—
203	8	8 (100%)	6 (75.0%)	6 (75.0%)	—	—
204	235	98 (41.7%)	—	126 (53.6%)	26 (11.1%)	8 (3.4%)
205	357	—	—	62 (17.4%)	3 (0.8%)	—
206	154	—	—	131 (85.1%)	1 (0.7%)	—
208	2	—	—	—	—	—
210	1	—	—	1 (100%)	1 (100%)	—
211	1	—	—	1 (100%)	1 (100%)	—
212	29	6 (20.7%)	—	21 (72.4%)	7 (24.1%)	—
213	41	1 (2.4%)	—	22 (53.7%)	21 (51.2%)	—
214	17	—	—	11 (64.7%)	—	—
215	93	54 (58.1%)	—	12 (12.9%)	1 (1.1%)	—

216	1561	108 (6.9%)	79 (5.1%)	58 (3.7%)	7 (0.5%)	—	—
217	150	37 (24.7%)	—	51 (34.0%)	18 (12.0%)	—	—
218	98	—	—	85 (86.7%)	81 (82.7%)	—	—
219	13	12 (92.3%)	—	12 (92.3%)	1 (7.7%)	—	—
220	117	—	—	38 (32.5%)	1 (0.8%)	—	—
221	2271	1344 (59.2%)	—	841 (37.0%)	831 (36.6%)	828 (36.5%)	—
223	451	—	—	13 (2.9%)	—	—	—
224	41	5 (12.2%)	—	36 (87.8%)	35 (85.4%)	—	—
225	4221	647 (15.3%)	9 (0.2%)	320 (7.6%)	245 (5.8%)	8 (0.2%)	—
226	57	1 (1.8%)	—	1 (1.8%)	—	—	—
227	1971	1688 (85.6%)	1535 (77.9%)	1101 (55.9%)	369 (18.7%)	—	—
229	471	14 (3.0%)	—	19 (4.0%)	6 (1.3%)	1 (0.2%)	—
230	6	—	—	1 (16.7%)	1 (16.7%)	—	—
Total	55206	6120 (11.1%)	1666 (3.0%)	21175 (38.4%)	8224 (14.9%)	1590 (2.9%)	—

## Appendix D: Automated search for materials with Kagome, pyrochlore or Lieb sublattice

In Appendix C, we have provided statistics about the crystal sublattices found in the materials of [Topological Quantum Chemistry website](#). These sublattices fall into five classes, namely the Kagome, pyrochlore, bipartite, split or Lieb sublattices. The two line-graph lattices, Kagome and pyrochlore lattices, and Lieb lattice exhibit flat bands in their respective band structure *only* when the related tight-binding Hamiltonian satisfies the following strict condition: the hopping amplitudes between any two nearest-neighbor sites are non-zero and equal. In real crystalline materials, equality between two hopping amplitudes can be guaranteed only when they are related by symmetries. Otherwise such a fine tuning is never achieved exactly. For these reasons, in real crystalline materials, only the Kagome and pyrochlore lattices among the line-graph lattices can be physically realized. For bipartite and split lattices, the condition is: the hopping amplitude is zero between any two unconnected sites.

In this appendix, we first analyze the crystal symmetries and the geometrical features of Kagome, pyrochlore and Lieb lattices. Then, by using their geometrical features, we have designed an algorithm to systematically search for the rigorous and approximate Kagome, pyrochlore or Lieb sublattices in real materials.

### 1. Crystal symmetries of Kagome, pyrochlore and Lieb lattices

As shown in Fig. 6(a), the Kagome lattice in 2D consists of the 3c Wyckoff position of the wallpaper group *p6mm*. Among the 3D space groups, there are three different minimal space groups rigorously compatible with the symmetry of the Kagome lattice: *P*<sup>3</sup> (SG 147), *P*6 (SG 168) and *I*23 (SG 197), of which the Wyckoff positions 3e or 3f, 3c and 6b form a Kagome sublattice, respectively.

Using the group-subgroup relations on the [Bilbao Crystallographic Server](#) (BCS)<sup>35,36</sup>, we have obtained all the space groups that are super-groups of the three minimal space groups for Kagome lattices. We analyzed the subduction of the Wyckoff positions from super-groups to the minimal groups. The Wyckoff positions that form a Kagome sublattice in the super-groups have been obtained and are tabulated in Table V. There, we show all the crystal lattices of the 40 3D space groups that have Kagome sublattices once their corresponding Wyckoff positions provided in this table are occupied by atoms. Note that in the above subduction of Wyckoff positions, if a Wyckoff position of a super-group splits into a Wyckoff position that forms a Kagome sublattice and some other types of Wyckoff positions coplanar to this Kagome sublattice, then the redundant Wyckoff positions spoil the Kagome lattice. Such situation happens, e.g., with the Wyckoff position 12c of *Im*<sup>3</sup>*m*(SG 229). Thus, we have discarded such cases in Table V.

We now turn to the pyrochlore lattice. As shown in Fig. 6(b), a pyrochlore lattice is a 3D lattice. The minimal space groups hosting a pyrochlore lattice are *F*d<sup>3</sup> (SG 203) and *F*4<sub>1</sub>32 (SG 210), of which the Wyckoff positions 16c or 16d with site-symmetry group isomorphic to point group symmetry *3m* form the pyrochlore lattice. Using the same method as of the Kagome lattice, we have obtained all the space groups that are super-groups of the two minimal space groups of the pyrochlore lattice. They are tabulated in Table V, including the corresponding Wyckoff positions that should be occupied to get a pyrochlore lattice. Note that since pyrochlore lattice is a 3D lattice, only the Wyckoff positions tabulated in Table V can be occupied. Any other Wyckoff position occupied by the same element will spoil the exact pyrochlore lattice.

Finally, the Lieb lattice shown in Fig. 6(c), is a 2D lattice associated to the wallpaper group *p4mm*. It is made of two different Wyckoff positions, 1a and 2c. In 3D, the minimal space groups hosting Lieb lattices are *P*4/*m* (SG 83), *P*4<sub>2</sub>/*m* (SG 84) and *P*4/*n* (SG 85). In Table VI, we tabulate these three minimal space groups and their related

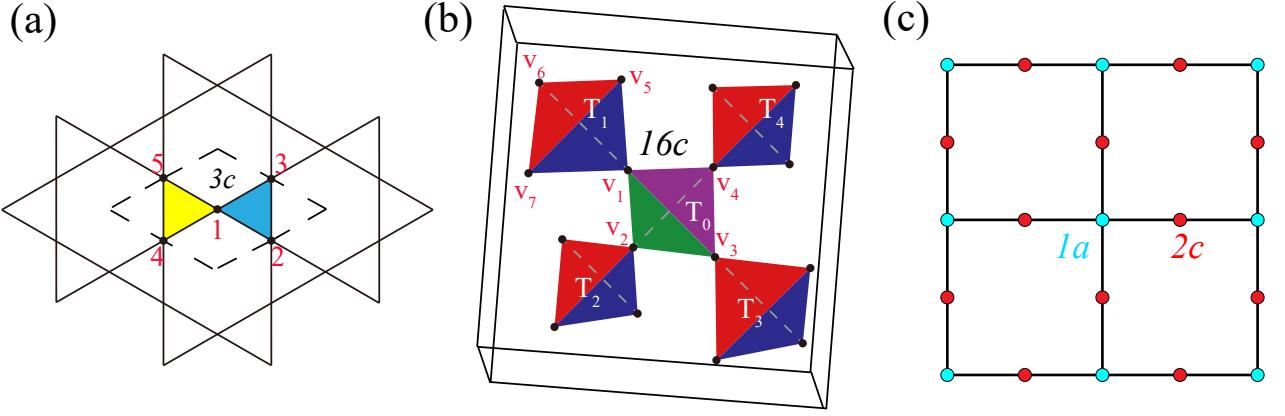


Figure 6. Crystal structures of Kagome, pyrochlore and Lieb lattices. (a) The Wyckoff position  $3c$  of the wallpaper group  $p6mm$  form a Kagome Lattice in 2D. The two equilateral triangles formed by the respective set of sites  $\{1,2,3\}$  and  $\{1,4,5\}$  are related by a vertical two-fold rotational symmetry centered at the site 1. (b) The Wyckoff position  $16c$  in space group  $Fd\bar{3}m$  form a pyrochlore lattice in 3D. The pyrochlore lattice is formed by the regular tetrahedrons which share vertices with each others. For example, the two regular tetrahedrons  $T_0$  and  $T_1$  that formed by the sets of vertices  $\{v_1, v_2, v_3, v_4\}$  and  $\{v_1, v_5, v_6, v_7\}$ , respectively, share the vertex  $v_1$ . Moreover, each site of the pyrochlore sublattice is also shared by three Kagome planes. For example, the triangle formed by the vertices  $\{v_1, v_2, v_3\}$  in  $T_0$  is co-planar with the triangle formed by the vertices  $\{v_1, v_5, v_6\}$  in  $T_1$ . There are four equivalent Kagome sublattices related by the point group symmetry ( $\bar{3}m$ ) of the pyrochlore lattice. (c) The Wyckoff positions  $1a$  and  $2c$  of the wallpaper group  $p4mm$  form a Lieb lattice in 2D. The  $2c$  sites (red) are at the middle point of their two NN  $1a$  sites (blue). The  $1a$  sites have four  $C_4$  symmetry related  $2c$  sites NNs.

super-groups having Lieb sublattice, providing the related Wyckoff positions. We have also discarded the Wyckoff positions of any super-group that split into a Wyckoff position that forms a Lieb sublattice and some other types of Wyckoff positions coplanar to this Lieb sublattice, just like what we have done for the Kagome lattice.

Table V: The Wyckoff positions (WPs) of 3D space groups forming Kagome or pyrochlore sublattice on special Miller plane. For each case of each SG, the column 'WP' provides the WP which form a Kagome or pyrochlore sublattice when it's occupied. The column ' $\overline{WP}$ ' provides all the Wyckoff positions which are defined on the same plane with the Kagome lattice formed by 'WP'. When one (or more than one) of the Wyckoff positions in ' $\overline{WP}$ ' is occupied by the atoms of the same element with 'WP', the Kagome lattice formed by the Wyckoff position in 'WP' will be spoiled. For each case, the column 'Plane' provides the Miller indices of the Kagome sublattice formed by 'WP'. Miller indices are given in the basis of the lattice vector of the conventional unit-cell (using the standard convention of the [Bilbao Crystallographic Server](#)). The column 'Lattice' indicates the type of sublattice formed by the corresponding Wyckoff positions. 'K' and 'P' stand for the Kagome and pyrochlore sublattice, respectively.

SG	WP	$\overline{WP}$	Plane	Lattice	SG	WP	$\overline{WP}$	Plane	Lattice
147 $P\bar{3}$	3e	1a	[0 0 1]	K	147 $P\bar{3}$	3f	1b	[0 0 1]	K
148 $R\bar{3}$	9d	3b	[0 0 1]	K	148 $R\bar{3}$	9e	3a	[0 0 1]	K
162 $P\bar{3}1m$	3f	1a, 2c, 6i	[0 0 1]	K	162 $P\bar{3}1m$	3g	1b, 2d, 6j	[0 0 1]	K
163 $P\bar{3}1c$	6g	2b	[0 0 1]	K	164 $P\bar{3}m1$	3e	1a, 6g	[0 0 1]	K
164 $P\bar{3}m1$	3f	1b, 6h	[0 0 1]	K	165 $P\bar{3}c1$	6e	2b	[0 0 1]	K
166 $R\bar{3}m$	9d	3b, 18g	[0 0 1]	K	166 $R\bar{3}m$	9e	3a, 18f	[0 0 1]	K
167 $R\bar{3}c$	18d	6b	[0 0 1]	K	168 $P6$	3c	1a, 2b, 6d	[0 0 1]	K
175 $P6/m$	3f	1a, 2c, 6j	[0 0 1]	K	175 $P6/m$	3g	1b, 2d, 6k	[0 0 1]	K
175 $P6/m$	6i	2e, 4h, 12l	[0 0 1]	K	176 $P6_3/m$	6g	2b	[0 0 1]	K
177 $P622$	3f	1a, 2c, 6j, 6l	[0 0 1]	K	177 $P622$	3g	1b, 2d, 6k, 6m	[0 0 1]	K
177 $P622$	6i	2e, 4h, 12n	[0 0 1]	K	183 $P6mm$	3c	1a, 2b, 6d, 6e, 12f	[0 0 1]	K
184 $P6cc$	6c	2a, 4b, 12d	[0 0 1]	K	191 $P6/mmm$	3f	1a, 2c, 6j, 6l, 12p	[0 0 1]	K
191 $P6/mmm$	3g	1b, 2d, 6k, 6m, 12q	[0 0 1]	K	191 $P6/mmm$	6i	2e, 4h, 12n, 12o, 24r	[0 0 1]	K
192 $P6/mcc$	6f	2a, 4c, 12j, 12k	[0 0 1]	K	192 $P6/mcc$	6g	2b, 4d, 12l	[0 0 1]	K
192 $P6/mcc$	12i	4e, 8h, 24m	[0 0 1]	K	193 $P6_3/mcm$	6f	2b, 4d, 12i	[0 0 1]	K
194 $P6_3/mmc$	6g	2a, 12i	[0 0 1]	K	195 $P23$	3c	1a	[1 1 1]	K
195 $P23$	3d	1b	[1 1 1]	K	197 $I23$	6b	2a	[1 1 1]	K

200 $Pm\bar{3}$	3c	1a	[1 1 1]	K	200 $Pm\bar{3}$	3d	1b	[1 1 1]	K
201 $Pn\bar{3}$	6d	2a	[1 1 1]	K	202 $Fm\bar{3}$	24d	4b	[1 1 1]	K
202 $Fm\bar{3}$	24d	4a	[1 1 1]	K	203 $Fd\bar{3}$	16c	16d	[1 1 1]	K
203 $Fd\bar{3}$	16d	16c	[1 1 1]	K	204 $Im\bar{3}$	6b	2a	[1 1 1]	K
207 $P4_32$	3c	1a, 12i	[1 1 1]	K	207 $P4_32$	3d	1b, 12j	[1 1 1]	K
208 $P4_232$	6d	2a	[1 1 1]	K	209 $F4_32$	24d	4b, 48h	[1 1 1]	K
209 $F4_32$	24d	4a, 48g	[1 1 1]	K	210 $F4_132$	16c	16d, 48g	[1 1 1]	K
210 $F4_132$	16d	16c, 48g	[1 1 1]	K	211 $I4_32$	6b	2a, 24h	[1 1 1]	K
215 $P\bar{4}3m$	3c	1a	[1 1 1]	K	215 $P\bar{4}3m$	3d	1b	[1 1 1]	K
217 $I\bar{4}3m$	6b	2a	[1 1 1]	K	218 $P\bar{4}3n$	6b	2a	[1 1 1]	K
219 $F\bar{4}3c$	24c	8a	[1 1 1]	K	219 $F\bar{4}3c$	24d	8b	[1 1 1]	K
221 $Pm\bar{3}m$	3c	1a, 12i	[1 1 1]	K	221 $Pm\bar{3}m$	3d	1b, 12j	[1 1 1]	K
222 $Pn\bar{3}n$	6b	2a, 24h	[1 1 1]	K	223 $Pm\bar{3}n$	6b	2a	[1 1 1]	K
224 $Pn\bar{3}m$	6d	2a	[1 1 1]	K	225 $Fm\bar{3}m$	24d	4b, 48i	[1 1 1]	K
225 $Fm\bar{3}m$	24d	4a, 48h	[1 1 1]	K	226 $Fm\bar{3}c$	24c	8a, 96h	[1 1 1]	K
226 $Fm\bar{3}c$	24d	8b	[1 1 1]	K	227 $Fd\bar{3}m$	16c	16d, 96h	[1 1 1]	K
227 $Fd\bar{3}m$	16d	16c, 96h	[1 1 1]	K	228 $Fd\bar{3}c$	48d	16a	[1 1 1]	K
229 $Im\bar{3}m$	6b	2a, 24h	[1 1 1]	K	203 $Fd\bar{3}$	16c	-	-	P
203 $Fd\bar{3}$	16d	-	-	P	210 $F4_132$	16c	-	-	P
210 $F4_132$	16d	-	-	P	227 $Fd\bar{3}m$	16c	-	-	P
227 $Fd\bar{3}m$	16d	-	-	P					

Table VI: The Wyckoff positions (WP) of 3D space groups forming Lieb sublattice on special Miller plane. For each case of each SG, the column 'WP(1a)' is the WP which forms the '1a' site of the Lieb lattice in Figure 6(c). The column 'WP(2c)' provides the list of WPs which form the 2c sites of the Lieb lattice in Figure 6(c). The column 'WP(empty)' provides all the WPs that are defined on the same plane with the WPs in 'WP(1a)' and 'WP(2c)'. If one (or more than one) of the WP in 'WP(empty)' is occupied by any atoms, the Lieb lattice will be spoiled. For each case, the Miller indices are always [0 0 1], given in the basis of the lattice vector of the conventional unit-cell (using the standard convention of the [Bilbao Crystallographic Server](#)).

SG	WP(1a)	WP(2c)	WP(empty)	SG	WP(1a)	WP(2c)	WP(empty)
83 $P4/m$	1c	2e	1a, 4j	83 $P4/m$	1a	2e	1c, 4j
83 $P4/m$	1d	2f	1b, 4k	83 $P4/m$	1b	2f	1d, 4k
84 $P4_2/m$	2d	2a, 2b	2c, 4j	84 $P4_2/m$	2c	2a, 2b	2d, 4j
84 $P4_2/m$	2b	2c, 2d	2a, 4j	84 $P4_2/m$	2a	2c, 2d	2b, 4j
85 $P4/n$	2a	4d		85 $P4/n$	2b	4e	
87 $I4/m$	2b	4c	2a, 8h	87 $I4/m$	2a	4c	2b, 8h
87 $I4/m$	4d	8f		89 $P422$	1c	2e	1a, 4j, 4l, 4o
89 $P422$	1a	2e	1c, 4j, 4l, 4o	89 $P422$	1d	2f	1b, 4k, 4m, 4n
89 $P422$	1b	2f	1d, 4k, 4m, 4n	93 $P4_222$	2d	2a, 2b	2c, 4j, 4k, 4l, 4m
93 $P4_222$	2c	2a, 2b	2d, 4j, 4k, 4l, 4m	93 $P4_222$	2b	2c, 2d	2a, 4j, 4k, 4l, 4m
93 $P4_222$	2a	2c, 2d	2b, 4j, 4k, 4l, 4m	97 $I422$	2b	4c	2a, 8g, 8h, 8i
97 $I422$	2a	4c	2b, 8g, 8h, 8i	111 $P\bar{4}2m$	1d	2e	1a, 4i, 4l
111 $P\bar{4}2m$	1a	2e	1d, 4i, 4l	111 $P\bar{4}2m$	1c	2f	1b, 4j, 4k
111 $P\bar{4}2m$	1b	2f	1c, 4j, 4k	112 $P\bar{4}2c$	2d	2a, 2c	2b, 4g, 4h, 4i, 4j
112 $P\bar{4}2c$	2c	2b, 2d	2a, 4g, 4h, 4i, 4j	112 $P\bar{4}2c$	2b	2a, 2c	2d, 4g, 4h, 4i, 4j
112 $P\bar{4}2c$	2a	2b, 2d	2c, 4g, 4h, 4i, 4j	121 $I\bar{4}2m$	2b	4c	2a, 8f, 8g
121 $I\bar{4}2m$	2a	4c	2b, 8f, 8g	123 $P4/mmm$	1c	2f	1a, 4j, 4l, 4n, 8p
123 $P4/mmm$	1a	2f	1c, 4j, 4l, 4n, 8p	123 $P4/mmm$	1d	2e	1b, 4k, 4m, 4o, 8q
123 $P4/mmm$	1b	2e	1d, 4k, 4m, 4o, 8q	124 $P4/mcc$	2d	4e	2b, 8m
124 $P4/mcc$	2b	4e	2d, 8m	124 $P4/mcc$	2c	4f	2a, 8j, 8k, 8l
124 $P4/mcc$	2a	4f	2c, 8j, 8k, 8l	125 $P4/nbm$	2c	4e	2a, 8i, 8k

125 $P4/nbm$	2a	4e	2c, 8i, 8k	125 $P4/nbm$	2d	4f	2b, 8j, 8l
125 $P4/nbm$	2b	4f	2d, 8j, 8l	126 $P4/nnc$	2b	4c	2a, 8h, 8i, 8j
126 $P4/nnc$	2a	4c	2b, 8h, 8i, 8j	126 $P4/nnc$	4d	8f	
128 $P4/mnc$	2b	4c	2a, 8h	128 $P4/mnc$	2a	4c	2b, 8h
129 $P4/nmm$	2a	4d	8g	129 $P4/nmm$	2b	4e	8h
130 $P4/ncc$	4b	8d		131 $P4_2/mmc$	2d	2a, 2b	2c, 4j, 4k, 4l, 4m, 8q
131 $P4_2/mmc$	2c	2a, 2b	2d, 4j, 4k, 4l, 4m, 8q	131 $P4_2/mmc$	2b	2c, 2d	2a, 4j, 4k, 4l, 4m, 8q
131 $P4_2/mmc$	2a	2c, 2d	2b, 4j, 4k, 4l, 4m, 8q	132 $P4_2/mcm$	2c	4f	2a, 4i, 4j, 8n
132 $P4_2/mcm$	2a	4f	2c, 4i, 4j, 8n	132 $P4_2/mcm$	2d	4e	2b, 8l, 8m
132 $P4_2/mcm$	2b	4e	2d, 8l, 8m	133 $P4_2/nbc$	4b	8e	4a, 8h, 8i
133 $P4_2/nbc$	4a	8e	4b, 8h, 8i	134 $P4_2/nnm$	2b	4c	2a, 8i, 8j
134 $P4_2/nnm$	2a	4c	2b, 8i, 8j	134 $P4_2/nnm$	4d	4e, 4f	8k, 8l
136 $P4_2/nmm$	2b	4c	2a, 4f, 4g, 8i	136 $P4_2/nmm$	2a	4c	2b, 4f, 4g, 8i
138 $P4_2/ncm$	4a	4c, 4d	8g, 8h	139 $I4/mmm$	2b	4c	2a, 8h, 8i, 8j, 16l
139 $I4/mmm$	2a	4c	2b, 8h, 8i, 8j, 16l	139 $I4/mmm$	4d	8f	16k
140 $I4/mcm$	4b	8e	4a, 16i, 16j	140 $I4/mcm$	4a	8e	4b, 16i, 16j
195 $P23$	3c	3d	1a, 6f, 6g, 6h	195 $P23$	3d	3c	1a, 6f, 6g, 6h
195 $P23$	1a	3d	3c, 6f, 6g, 6h	195 $P23$	3c	3d	1b, 6g, 6h, 6i
195 $P23$	3d	3c	1b, 6g, 6h, 6i	195 $P23$	1b	3c	3d, 6g, 6h, 6i
197 $I23$	6b	6b	2a, 12d, 12e	200 $Pm\bar{3}$	3c	3d	1a, 6e, 6f, 6g, 12j
200 $Pm\bar{3}$	3d	3c	1a, 6e, 6f, 6g, 12j	200 $Pm\bar{3}$	1a	3d	3c, 6e, 6f, 6g, 12j
200 $Pm\bar{3}$	3c	3d	1b, 6f, 6g, 6h, 12k	200 $Pm\bar{3}$	3d	3c	1b, 6f, 6g, 6h, 12k
200 $Pm\bar{3}$	1b	3c	3d, 6f, 6g, 6h, 12k	201 $Pn\bar{3}$	6d	6d	2a, 12f, 12g
202 $Fm\bar{3}$	4b	24d	4a, 24e, 48h	202 $Fm\bar{3}$	4a	24d	4b, 24e, 48h
202 $Fm\bar{3}$	8c	24d	48g	204 $Im\bar{3}$	6b	6b	2a, 12d, 12e, 24g
207 $P432$	3c	3d	1a, 6e, 12h, 12i	207 $P432$	3d	3c	1a, 6e, 12h, 12i
207 $P432$	1a	3d	3c, 6e, 12h, 12i	207 $P432$	3c	3d	1b, 6f, 12h, 12j
207 $P432$	3d	3c	1b, 6f, 12h, 12j	207 $P432$	1b	3c	3d, 6f, 12h, 12j
208 $P4_232$	6d	6d	2a, 6e, 6f, 12h, 12i, 12j	208 $P4_232$	6e	4b, 4c	12k, 12l
209 $F432$	4b	24d	4a, 24e, 48g, 48h	209 $F432$	4a	24d	4b, 24e, 48g, 48h
209 $F432$	8c	24d	48i	211 $I432$	6b	6b	2a, 12d, 12e, 24g, 24h
211 $I432$	12d	8c	24i	215 $P43m$	3c	3d	1a, 6f, 12h
215 $P43m$	3d	3c	1a, 6f, 12h	215 $P\bar{4}3m$	1a	3d	3c, 6f, 12h
215 $P\bar{4}3m$	3c	3d	1b, 6g, 12h	215 $P\bar{4}3m$	3d	3c	1b, 6g, 12h
215 $P\bar{4}3m$	1b	3c	3d, 6g, 12h	217 $I\bar{4}3m$	6b	6b	2a, 12d, 12e, 24f
218 $P\bar{4}3n$	6b	6b	2a, 6c, 6d, 12f, 12g, 12h	219 $F\bar{4}3c$	24c	24d	8a, 48f
219 $F\bar{4}3c$	24d	24c	8a, 48f	219 $F\bar{4}3c$	8a	24d	24c, 48f
219 $F\bar{4}3c$	24c	24d	8b, 48g	219 $F\bar{4}3c$	24d	24c	8b, 48g
219 $F\bar{4}3c$	8b	24c	24d, 48g	221 $Pm\bar{3}m$	3c	3d	1a, 6e, 12h, 12i, 24k
221 $Pm\bar{3}m$	3d	3c	1a, 6e, 12h, 12i, 24k	221 $Pm\bar{3}m$	1a	3d	3c, 6e, 12h, 12i, 24k
221 $Pm\bar{3}m$	3c	3d	1b, 6f, 12h, 12j, 24l	221 $Pm\bar{3}m$	3d	3c	1b, 6f, 12h, 12j, 24l
221 $Pm\bar{3}m$	1b	3c	3d, 6f, 12h, 12j, 24l	222 $Pn\bar{3}n$	6b	6b	2a, 12d, 12e, 24g, 24h
222 $Pn\bar{3}n$	12d	8c		223 $Pm\bar{3}n$	6b	6b	2a, 6c, 6d, 12f, 12g, 12h, 24k
223 $Pm\bar{3}n$	6c	6d, 8e	24j	224 $Pn\bar{3}m$	6d	6d	2a, 12f, 12g, 24h
224 $Pn\bar{3}m$	12f	4b, 4c	24i, 24j	225 $Fm\bar{3}m$	4b	24d	4a, 24e, 48h, 48i, 96j
225 $Fm\bar{3}m$	4a	24d	4b, 24e, 48h, 48i, 96j	225 $Fm\bar{3}m$	8c	24d	48g
226 $Fm\bar{3}c$	24c	24d	8b, 48e, 96i	226 $Fm\bar{3}c$	24d	24c	8b, 48e, 96i
226 $Fm\bar{3}c$	8b	24c	24d, 48e, 96i	226 $Fm\bar{3}c$	24c	24d	8a, 48f, 96h
226 $Fm\bar{3}c$	24d	24c	8a, 48f, 96h	226 $Fm\bar{3}c$	8a	24d	24c, 48f, 96h
228 $Fd\bar{3}c$	48d	48d	16a, 96f	229 $Im\bar{3}m$	6b	6b	2a, 12d, 12e, 24g, 24h, 48j
229 $Im\bar{3}m$	12d	8c	48i				

## 2. Geometrical features of standard Kagome, pyrochlore and Lieb lattices

Using the above symmetry analysis, it is straightforward to systematically filter out the crystalline materials exhibiting *rigorous* Kagome, pyrochlore or Lieb sublattices by checking the occupied Wyckoff positions. However, in many of the 3D crystalline materials, there are no rigorous line-graph or Lieb sublattices, only approximate ones. These *approximate* Kagome, pyrochlore or Lieb sublattices are not part of Tables V or VI. Still, they can be obtained from these rigorous sublattices by weak lattice distortion. When this distortion is weak enough, the lattice might still hosts (almost) flat bands. As the *approximate* Kagome, pyrochlore and Lieb sublattices do not satisfy the minimal symmetry groups of the rigorous ones, the only efficient method to identify them is comparing their geometrical structures with those of the rigorous sublattices. In this subsection, we will analyze the key geometrical features of the rigorous Kagome, pyrochlore and Lieb lattices, which are schematically shown in Fig. 6. In the next subsection, we will rely on these features to design numerical algorithms for searching approximate line-graph and Lieb sublattices in real crystalline materials.

**Kagome Lattice** The rigorous Kagome lattice in 2D, as shown in Fig. 6(a), is made of three equivalent sites corresponding to the Wyckoff position  $3c$  in one unit cell with wallpaper group  $p6mm$ . For convenience, we label the five sites of  $3c$  as 1, 2, 3, 4 and 5, where the sites 4 and 5 differ from sites 3 and 2, respectively, by a lattice translation. The 2D point group of  $3c$  is  $2mm$ , which includes a vertical two-fold rotational symmetry and two vertical mirror symmetries. So the two regular triangles formed by sites  $\{1, 2, 3\}$  and sites  $\{1, 4, 5\}$ , respectively, are related by the two-fold rotational symmetry.

Thus, there are two key geometrical features for the rigorous Kagome lattice in Fig. 6(a):

1. For each site on the 2D lattice, it has only four co-planar nearest neighbor (NN) sites on the same plane.
2. Each site and its four NN sites form two equilateral triangles, which are related by a vertical  $C_2$  symmetry.

If a 2D sublattice occupied by the same chemical element of a given material can be characterized by the above two geometrical features within a certain threshold (as will be discussed in the next subsection), then we label it as an approximate Kagome sublattice.

**Pyrochlore Lattice** As shown in Fig. 6(b), the rigorous pyrochlore lattice is a 3D line-graph lattice. Its geometry has the two following features:

1. The unit cell of the 3D lattice is constructed by five regular tetrahedrons, each two of which share one vertex. For example, in Fig. 6(b), the regular tetrahedron  $T_0$  formed by the vertices  $\{v_1, v_2, v_3, v_4\}$  and another regular tetrahedron  $T_1$  formed by the vertices  $\{v_1, v_5, v_6, v_7\}$  share the vertex  $v_1$ .
2. Each of the four triangle surfaces in one tetrahedron is always co-planar with one triangle surface of its NN tetrahedron and the two co-planar triangles form a Kagome sublattice. For example, the triangle formed by the vertices  $\{v_1, v_2, v_3\}$  in  $T_0$  is co-planar with the triangle formed by the vertices  $\{v_1, v_5, v_6\}$  in  $T_1$  and these vertices form a Kagome sublattice. There are four equivalent Kagome sublattices which are related by the point group symmetry of the pyrochlore lattice ( $\bar{3}m$ ).

Thus, for a 3D sublattice which is formed by the same chemical element of a given material, if it can be characterized by the above two geometrical features within a certain threshold, we consider it as an approximate pyrochlore sublattice.

**Lieb lattice** The rigorous Lieb lattice is a 2D lattice formed by two non-equivalent atom sites, the blue and red sites as indicated in Fig. 6(c). The blue sites form a square lattice and the red sites are on the middle of the bonds between two adjacent blue sites.

Lieb lattice has the following three key geometrical features:

1. It has two non-equivalent atom sites,  $\{A_1\}$  and  $\{A_2\}$ , which are co-planar. Each atom in  $\{A_1\}$  always has two NN sites, which belong to  $\{A_2\}$ . Each atom site in  $\{A_2\}$  always has four NN sites, which belong to  $\{A_1\}$ .
2. Each of the atom sites in  $\{A_1\}$  is in the middle of its two NN sites.
3. The four bonds which connect the atom in  $\{A_2\}$  and its four NN sites are related by a four-fold rotational symmetry.

A 2D sublattice occupied by one or two different chemical elements of a given material and satisfying the two above geometrical features within a certain threshold, is labelled as an approximate Lieb sublattice.

### 3. Algorithms to search for Kagome, pyrochlore and Lieb sublattices

The symmetry properties and the key geometrical features of rigorous Kagome, pyrochlore and Lieb lattices enable the high-throughput search for both rigorous and approximate line-graph sublattices in real materials. Using the key geometrical features as discussed in Appendix D 2, we have designed numerical algorithms to search for Kagome, pyrochlore and Lieb sublattices from the crystal lattice of real materials. Whether or not the line-graph and Lieb sublattices also satisfy the symmetry analysis of Appendix D 1, we classify them into rigorous or approximate.

#### a. Kagome and pyrochlore sublattices

There are four steps to identify a Kagome or pyrochlore sublattice from the crystal lattice of a material.

Step 1 For each material, its crystal structure is parsed from the *POSCAR* file, which was used in the first-principle calculations<sup>5</sup>. The crystal symmetry and the list of occupied Wyckoff letters of the non-equivalent atom sites are analyzed by the *Pymatgen* package.

Step 2 By grouping together the atom sites of the same chemical element in one unit cell, the crystal lattice is divided into several sets. For convenience, a set will be denoted by  $\{A_i\}$  where  $A_i$  denotes a single atom. The two following steps are applied to each set until we exhaust all possible sublattices.

Step 3 For each atom site in a certain set  $\{A_i\}$ , we check if it satisfies the following four criteria sequentially:

C1 The atom site has and only has four co-planar nearest neighbor (NN) or next nearest neighbor (NNN) sites, which also belong to  $\{A_i\}$ , *on certain Miller planes*. If true, we refer this atom site as a representative site and obtain the corresponding Miller indices  $[hkl]$ .

C2 By calculating the length of the bonds between the representative atom site and its four NN/NNN sites and the angles between the four bonds, we check whether the five sites form two regular triangles related by a vertical  $C_2$  symmetry, which is centered at the representative atom site.

C3 Each of the four NN/NNN atom sites also satisfies the first two criteria.

C4 Each atom site in the set  $\{A_i\}$  satisfies the criteria C1,C2 and C3 on three different Miller planes.

Step 4 If a set (or part of a set) satisfies the criteria C1, C2 and C3, it is classified as a Kagome sublattice. If it moreover satisfies C4, it is also tagged as a pyrochlore sublattice.

The flow chart of this algorithm is shown in Fig. 7. Based on this algorithm, we have developed a *Python*-based code to identify if the crystal lattice of a material has any Kagome or pyrochlore sublattice. In this code, we rely on several functions of the *Pymatgen* package<sup>62</sup>. The function *Pymatgen.core.structure.get\_neighbors* is used to get the neighboring sites of an atom and the function *pymatgen.core.structure.get\_angle* is used to calculate the angle between two bonds. The Miller indices are obtained using the function *pymatgen.core.lattice.get\_miller\_index\_from\_coords*. Our algorithm requires a set of threshold parameters to distinguish a regular triangle. More precisely, the threshold is set to  $\pm 20\%$  of the NN/NNN bonds' length when identifying two equivalent bonds. A threshold of  $\pm 2^\circ$  is applied to discriminate two identical angles.

#### b. Lieb sublattice

We apply a five-step process to identify a Lieb sublattice from a 3D crystal lattice of material.

Step 1 For each material, its crystal structure is parsed from the *POSCAR* file, which was used in the first-principle calculations<sup>5</sup>. The crystal symmetry and the list of Wyckoff letters of the non-equivalent atom sites are analyzed by the *Pymatgen* package.

Step 2 We obtain all the NN sites for each atom site in the lattice.

Step 3 We select all the atom sites that have only two NN sites of identical element and are at the equal distance of its NN sites. Such atom sites are referred as 'middle sites' and labeled as  $A_1$ . The NN sites of  $A_1$  are labeled as  $A_2$ .

Step 4 For each of the 'middle sites' obtained in Step 3, we check sequentially the following four criteria:

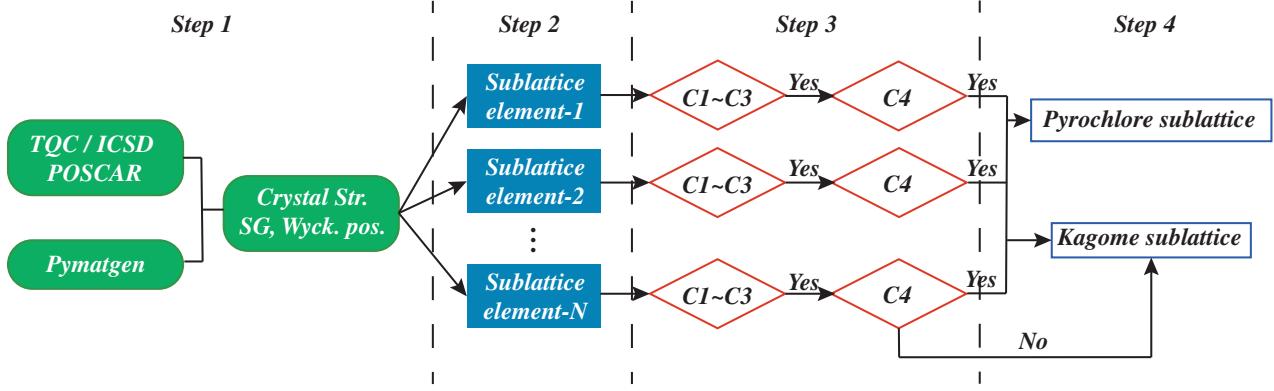


Figure 7. The flow chart of the Kagome or pyrochlore sublattice identification from a 3D crystal lattice. Starting from the crystal structure of material provided as a *POSCAR* file, the crystal symmetry and the Wyckoff positions of each distinct element are analyzed by the *Pymatgen* package. For each sublattice, the criteria C1, C2 and C3 are applied to identify if the sublattice is a Kagome plane. If at this stage, a 2D Kagome sublattice has been identified, the criterion C4 is applied to test if the crystal structure also hosts a 3D pyrochlore sublattice.

- C1 For a given 'middle site'  $A_1$ , each of its two NN sites  $A_2$  has and only has four NN sites, which are *co-planar on certain Miller planes* and are also labeled as  $A_1$  in Step 3.
- C2 The four NNs of  $A_2$  are of identical element. And the four bonds connecting  $A_2$  and its four NN sites are of equal length and the angles between any two neighbor bonds equals to  $90^\circ$ .
- C3 Both of the two NN sites  $A_2$  of a 'middle site'  $A_1$  satisfy the criterion C2 on the same plane.
- C4 All the 'middle sites' on the same plane satisfy simultaneously criteria C1, C2 and C3.

Step 5 If there is a 2D sublattice, of which the atom sites satisfy the criteria C1 to C4 in step 4, it is classified as a Lieb lattice and the Miller indices of the Lieb sublattice are recorded.

The algorithm flow chart is provided in Fig. 8. We have implemented this algorithm in a *Python*-based code. It detects if the crystal lattice of a material has a Lieb sublattice. Our code uses a set of threshold parameters to identify whether two bonds are equal or an angle matches the expected value: a threshold is set to  $\pm 20\%$  of the NN bonds' length to identify two equivalent bonds and a threshold of  $\pm 10^\circ$  is applied to discriminate two identical angles. In real crystalline materials in the [Materials Flatband Database website](#), Lieb sublattices tend to be spoiled by lattice distortion. In this section, a larger threshold is used to identify an approximate Lieb lattice.

### c. Rigorous and approximate sublattices

As discussed in Appendix D 1, rigorous sublattices can be identified from the space group and the corresponding occupied Wyckoff positions in the Table V or VI. Although these two features are analyzed for each crystal structure in the database using *Pymatgen* package<sup>63,64</sup>, they are not enough to confirm that a given material hosts a rigorous sublattice. Indeed, the sublattice might be spoiled by the presence of other in-plane atoms of the *same element* on (or close to) this sublattice. For example, in SG 147 ( $P\bar{3}$ ), the Kagome sublattice formed by the Wyckoff position 3e with atom A occupied will be spoiled by the Wyckoff position 1a if 1a is also occupied by the identical atom. Note that the site of 1a is exactly on the Kagome plane formed by 3e. The two algorithms described in Appendix D 3(a), were designed to detect such situations. Indeed in the geometric method algorithm described above, such cases are discarded when applying criterion C1. Note that if the sublattice has as a nearest neighbor other atoms of *different type*, the flat bands emerging from the sublattice are usually preserved. For example,  $\text{Co}_3\text{Sn}_2\text{S}_2$  [ICSD 5435, SG 166 ( $R\bar{3}m$ )], the Sn atoms sit at the center of the Co Kagome sublattice hexagons. Still flat bands are observed in the band structure (shown in Fig. 9a). Conversely,  $\text{Pt}_2\text{HgSe}_3$  [ICSD 185808, SG 164 ( $P\bar{3}m1$ )] has a Kagome lattice made of Pt atoms at Wyckoff positions 3e. But the Pt atoms at Wyckoff positions 1a spoils the Kagome sublattice and the band structure (shown in Fig. 9b) does not exhibit any flat band. Rather than discarding cases where atoms of a different type are nearest neighbors, we have added on the [Materials Flatband Database website](#) for each sublattice

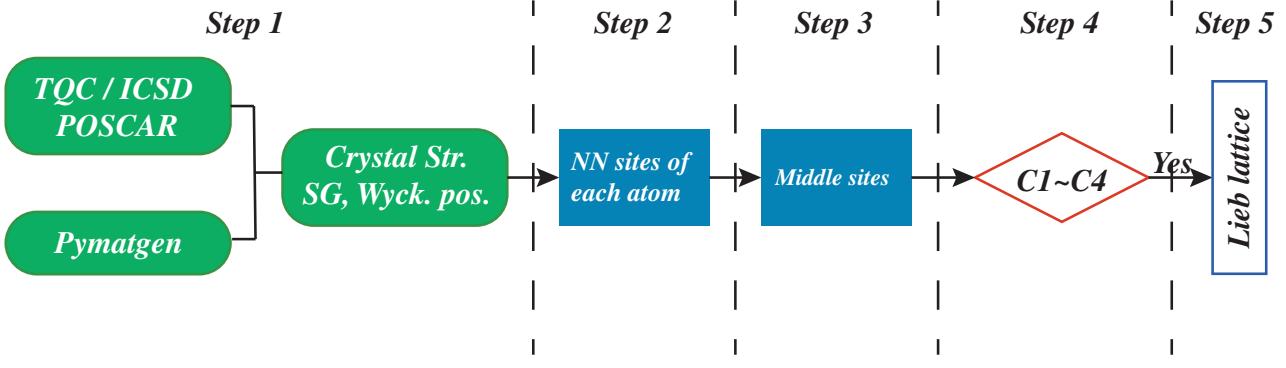


Figure 8. The flow chart of the Lieb sublattice identification from a 3D crystal lattice. Starting from the crystal structure of materials provided as a *POSCAR* file, the crystal symmetry and the Wyckoff positions of each distinct element are analyzed by the *Pymatgen* package. The second step identifies the nearest neighbor(NN) sites of each atom. If an atom is at the middle of its two NN sites, it is referred to as the 'middle-site' (Step 3). Then at Step 4, the criteria from C1 to C4 are applied to check if the *middle sites* and their NN sites form a Lieb sublattice.

description, the location and type of any additional nearest neighbor atoms, (see for example the Kagome sublattice description for [Co<sub>3</sub>Sn<sub>2</sub>S<sub>2</sub>](#)).

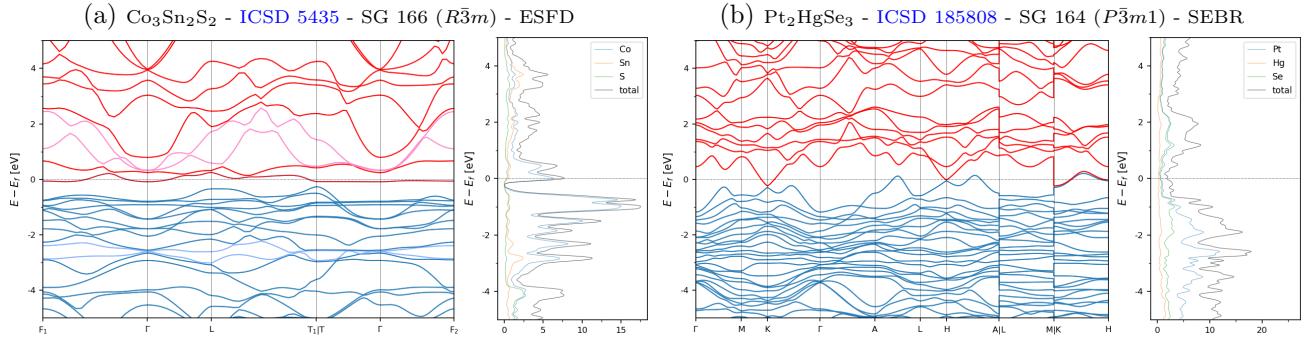


Figure 9. (a) Band structure of Co<sub>3</sub>Sn<sub>2</sub>S<sub>2</sub> [ICSD 5435, SG 166 ( $R\bar{3}m$ )]. (b) Band structure of Pt<sub>2</sub>HgSe<sub>3</sub> [ICSD 185808, SG 164 ( $P\bar{3}m1$ )].

For that reason, a material is tagged as having a *rigorous* Kagome, pyrochlore or Lieb sublattice if, within its space group, its occupied Wyckoff positions belong to the corresponding set of Wyckoff positions in the Table V or VI and if the material successfully passes the corresponding test set by our algorithms. If a material does not satisfy the symmetry features of Appendix D 1 but still successfully passes the corresponding test set by our algorithms, then the material is tagged as having an *approximate* Kagome, pyrochlore or Lieb sublattice.

Among the 55,206 ICSD entries that we have considered, 4,192 ICSDs (7.59%) host at least one rigorous Kagome sublattice, while 2,100 ICSDs (3.80%) host at least one approximate Kagome sublattice. Similarly, we found 1,541 ICSDs (2.79%) with at least one rigorous pyrochlore sublattice, 125 ICSDs (0.23%) with at least one approximate pyrochlore sublattice, 1,202 ICSDs (2.18%) with at least one rigorous Lieb sublattice, 438 ICSDs (0.79%) with at least one approximate Lieb sublattice. Note that an entry might have both a rigorous and an approximate sublattices.

#### Appendix E: Automated search for materials with bipartite or split sublattices

Beyond the line-graph lattices, *i.e.*, Kagome and pyrochlore lattices, and the Lieb lattice that were introduced in Appendix D, split and bipartite lattices could also host exactly flat bands<sup>6</sup>. Recently, these two types of lattices were shown to host topologically non-trivial bands<sup>28</sup>, which indicates that the Wannier states cannot be localized.

A bipartite lattice is a lattice such that all its sites can be divided into two sublattices,  $L$  and  $\tilde{L}$ . Hopping bonds *only* exist in between sites in  $L$  and sites in  $\tilde{L}$ , but do not exist within sites of the same sublattice. Considering the translational symmetry of crystalline materials in 3D, the graph formed by the sites in  $L$  and  $\tilde{L}$  and the bonds connecting them can be either mathematically connected in *at least* one dimension or disconnected in all the dimensions. If the graph of a bipartite sublattice is disconnected, we refer to it as a *disconnected bipartite sublattice*. For example, the three green atoms in Figure 13(a) is typically a group of isolated atoms in the crystal lattice and hence they form a disconnected bipartite sublattice. Otherwise, when the graph of a bipartite sublattice is connected in *at least* one dimension, we refer it to as the *connected bipartite sublattice*. For example, a collection of the one dimensional bipartite chains is considered as a connected bipartite sublattice. In this work, we mainly focus on the bipartite lattice with connected graph and refer the bipartite lattice with disconnected graph as a molecular lattice. A molecular lattice also hosts flat bands but they are in the atomic limit and is thus disregarded as discussed in Appendix B 1. A split lattice is a special case of bipartite lattice: each site  $i$  in sublattice  $\tilde{L}$  has the same hopping term to its two (and exactly two) connected sites in sublattice  $L$ . For example, the Lieb lattice shown in Fig. 6(c) is a two dimensional case of both a bipartite lattice and a split lattice. The red sites correspond to the sublattice  $\tilde{L}$  and the sublattice  $L$  is made of the blue sites. In the Lieb lattice, bonds only connect the blue sites in  $L$  to the red sites in  $\tilde{L}$ , and each site in  $L$  is at the center of its two connected neighbors.

The flat bands that exist in bipartite or split lattice can be explained with the  $S$ -matrix method<sup>6</sup>. In this appendix, we provide a brief introduction to the  $S$ -matrix method that we will use in Appendix F. More details about this method can be found in Ref.<sup>6</sup>. We then detail a numerical algorithm based on geometrical features that allows for a systematic search for crystal structures with bipartite or split sublattices among the stoichiometric materials in [Topological Quantum Chemistry website](#).

## 1. $S$ -matrix method

Given a bipartite lattice with its two sublattices labeled as  $L$  and  $\tilde{L}$ , we assume the number of orbitals per unit cell in  $L$  (denoted  $|L|$ ) is always larger than that in  $\tilde{L}$  (denoted  $|\tilde{L}|$ ), *i.e.*,  $|L| > |\tilde{L}|$ . Since hopping terms only occur between sites of  $L$  and  $\tilde{L}$ , the tight binding Hamiltonian can be expressed in momentum space using the  $S$ -matrix as

$$H(\mathbf{k}) = \begin{pmatrix} 0 & S^\dagger(\mathbf{k}) \\ S(\mathbf{k}) & 0 \end{pmatrix}, \quad (\text{E1})$$

where  $S(\mathbf{k})$  is a matrix with dimension  $|L| \times |\tilde{L}|$  and  $\mathbf{k}$  is the momentum in the Brillouin zone. Thus, the square of the eigenvalues of  $H(\mathbf{k})$  are given by the eigenvalues of  $(H(\mathbf{k}))^2 = \begin{pmatrix} \tilde{T}(\mathbf{k}) & 0 \\ 0 & T(\mathbf{k}) \end{pmatrix}$ , where  $\tilde{T}(\mathbf{k}) = S^\dagger(\mathbf{k})S(\mathbf{k})$ ,  $T(\mathbf{k}) = S(\mathbf{k})S^\dagger(\mathbf{k})$ . Both the matrices  $T(\mathbf{k})$  and  $\tilde{T}(\mathbf{k})$  are positive semidefinite. As shown in the example in the end of this subsection,  $T$  and  $\tilde{T}$  serve as the effective Hamiltonians of  $L$  and  $\tilde{L}$  (after a rescale of energy), respectively, if  $L$  and  $\tilde{L}$  have different on-site energies.

We first prove that  $T(\mathbf{k})$  and  $\tilde{T}(\mathbf{k})$  have the same positive eigenvalues with identical multiplicities. For any eigenstate of  $\tilde{T}(\mathbf{k})$ ,  $\tilde{\phi} = \tilde{\phi}(\mathbf{k})$ , that satisfies  $\tilde{T}(\mathbf{k})\tilde{\phi} = E\tilde{\phi}$  and  $E > 0$ , we can construct  $\phi = S(\mathbf{k})\tilde{\phi}$ . Then we have  $T(\mathbf{k})\phi = S(\mathbf{k})S^\dagger(\mathbf{k})S(\mathbf{k})\tilde{\phi} = S(\mathbf{k})E\tilde{\phi} = ES(\mathbf{k})\tilde{\phi} = E\phi$ , meaning  $\phi$  is an eigenstate of  $T(\mathbf{k})$  with the same eigenvalue  $E$ . Considering two eigenstates of  $\tilde{T}$  satisfying  $\tilde{T}(\mathbf{k})\tilde{\phi}_i = E_i\tilde{\phi}_i$  and  $\tilde{T}(\mathbf{k})\tilde{\phi}_j = E_j\tilde{\phi}_j$ , we have  $\langle \tilde{\phi}_i | \tilde{\phi}_j \rangle = \langle \phi_i | S^\dagger(\mathbf{k})S(\mathbf{k}) | \phi_j \rangle = \langle \phi_i | \tilde{T}(\mathbf{k}) | \phi_j \rangle = E_j \langle \phi_i | \phi_j \rangle \propto \delta_{i,j}$ . Thus  $T(\mathbf{k})$  and  $\tilde{T}(\mathbf{k})$  have identical positive eigenvalues, including their multiplicities. From this property, we deduce that  $T(\mathbf{k})$  and  $\tilde{T}(\mathbf{k})$  lead to the same dispersive bands in the spectrum of  $H(\mathbf{k})$ . Moreover it results in a set of perfectly flat bands at  $E = 0$  with degeneracy  $D = |L| + |\tilde{L}| - 2 \times \text{rank}(S(\mathbf{k}))$ . (As a special case, if  $S(\mathbf{k})S^\dagger(\mathbf{k})$  has full rank, there are  $|L| - |\tilde{L}|$  flat bands in the spectrum of both  $H(\mathbf{k})$  and  $T(\mathbf{k})$ .)

As an example, we consider a two dimensional bipartite lattice formed by  $s$  orbitals at the Kagome sublattice and the honeycomb sublattice, as shown in Fig. 10(a). We refer to the honeycomb sublattice as  $\tilde{L}$  and the Kagome sublattice as  $L$ . Only hopping terms between nearest neighbors are taken into account and all of them are assumed to have the same amplitude. The lattice vectors  $\mathbf{a}_i (i = 1, 2)$  are shown in Fig. 10(a). In this basis and focusing on the unit cell, the atoms in  $\tilde{L}$  are located at  $(\frac{1}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{1}{3})$  and the atoms in  $L$  are at  $(\frac{1}{2}, 0), (\frac{1}{2}, \frac{1}{2}), (0, \frac{1}{2})$ . We can write

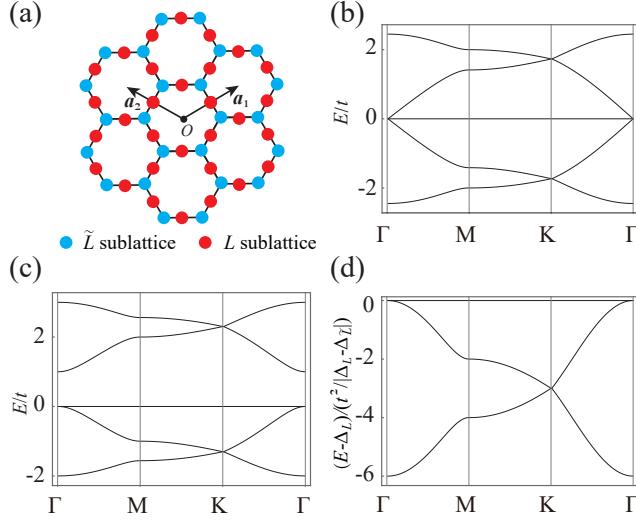


Figure 10. (a) An example of bipartite lattice consists of honeycomb lattice ( $\tilde{L}$  sublattice in blue) and Kagome lattice ( $L$  sublattice in red). (b) Band structure of Hamiltonian  $H_{L\oplus\tilde{L}}$  in Eq. (E3) without any on-site energy, i.e.,  $\Delta_L = \Delta_{\tilde{L}} = 0$ . (c) Band structure of Hamiltonian  $H_{L\oplus\tilde{L}}$  in Eq. (E3) and  $\Delta_L = 0$ ,  $\Delta_{\tilde{L}} = |t|$ . (d) The band structure of the effective Hamiltonian  $H_L$  in Eq. (E7) and  $\Delta_L = 0$ ,  $\Delta_{\tilde{L}} = |t|$ .

the explicit form of the  $S$  matrix as

$$S^\dagger(\mathbf{k}) = t \begin{pmatrix} 1 & 1 & e^{ik_1} \\ e^{ik_2} & 1 & 1 \end{pmatrix}, \quad (\text{E2})$$

with  $t$  being the strength of the nearest neighbor coupling. In the absence of on-site energy, this model is just the split graph lattice of the honeycomb lattice. The Hamiltonian can then be built using Eq. (E1) and the corresponding band structure is shown in Fig. 10(b).

As shown in, e.g. Ref.<sup>6</sup>, flat bands in line-graph lattices might also be understood within the  $S$ -matrix formalism. For pedagogical purposes, we solely focus on the Kagome lattice which is the line-graph lattice of the honeycomb lattice. Starting from the previous example, we further add the on-site energies  $\Delta_{\tilde{L}}$  and  $\Delta_L$  on the sublattices  $\tilde{L}$  and  $L$ . Then the total Hamiltonian of the bipartite lattice  $L \oplus \tilde{L}$  reads

$$H_{L\oplus\tilde{L}}(\mathbf{k}) = \begin{pmatrix} \Delta_{\tilde{L}} \cdot \mathbb{I}_{2 \times 2} & S^\dagger(\mathbf{k}) \\ S(\mathbf{k}) & \Delta_L \cdot \mathbb{I}_{3 \times 3} \end{pmatrix}. \quad (\text{E3})$$

A typical example of band structure associated to this Hamiltonian is shown in Fig. 10(c). Moreover, one has

$$(H_{L\oplus\tilde{L}}(\mathbf{k}) - \Delta_{\tilde{L}} \cdot \mathbb{I}_{5 \times 5}) (H_{L\oplus\tilde{L}}(\mathbf{k}) - \Delta_L \cdot \mathbb{I}_{5 \times 5}) = \begin{pmatrix} S^\dagger(\mathbf{k})S(\mathbf{k}) & 0 \\ 0 & S(\mathbf{k})S^\dagger(\mathbf{k}) \end{pmatrix}. \quad (\text{E4})$$

We assume the eigenvalues of  $S^\dagger S$  are  $\lambda_i (i = 1, 2)$ . Then, the eigenvalues of  $H_{L\oplus\tilde{L}}$  are given by  $\varepsilon^2 - (\Delta_L + \Delta_{\tilde{L}})\varepsilon + \Delta_L \Delta_{\tilde{L}} - \lambda_i = 0$ ,

$$\varepsilon = \frac{(\Delta_L + \Delta_{\tilde{L}}) \pm \sqrt{(\Delta_L - \Delta_{\tilde{L}})^2 + 4\lambda_i}}{2}. \quad (\text{E5})$$

Based on Eq. (E5), when  $\Delta_L \neq \Delta_{\tilde{L}}$ , we can derive the individual effective Hamiltonian for either  $\tilde{L}$  or  $L$  by applying the second-order perturbation theory as

$$H_{\tilde{L}}(\mathbf{k}) \approx \Delta_{\tilde{L}} - S^\dagger(\mathbf{k})S(\mathbf{k})/(\Delta_L - \Delta_{\tilde{L}}), \quad (\text{E6})$$

and

$$H_L(\mathbf{k}) \approx \Delta_L + S(\mathbf{k})S^\dagger(\mathbf{k})/(\Delta_L - \Delta_{\tilde{L}}), \quad (\text{E7})$$

respectively. Hence, the band structures of  $H_L$  and  $H_{\tilde{L}}$  are given by the spectra of  $T(\mathbf{k})$  and  $\tilde{T}(\mathbf{k})$  (after a rescaling of energy), respectively. As shown in Fig. 10(d), there is one flat band of degeneracy  $D = |L| - \text{rank}(S(\mathbf{k})) = 1$  at  $\Delta_L$  in the band structure of  $H_L$ . The effective Hamiltonian for the sublattice  $L$  of Eq. (E7) is nothing else than the Kagome tight binding Hamiltonian, with the nearest coupling  $t^2/(\Delta_L - \Delta_{\tilde{L}})$  and on-site energy  $\Delta_L$ . Thus we have explained the flat band in the Kagome lattice through the  $S$ -matrix formalism.

## 2. Algorithms to search for bipartite and split sublattices in crystalline materials

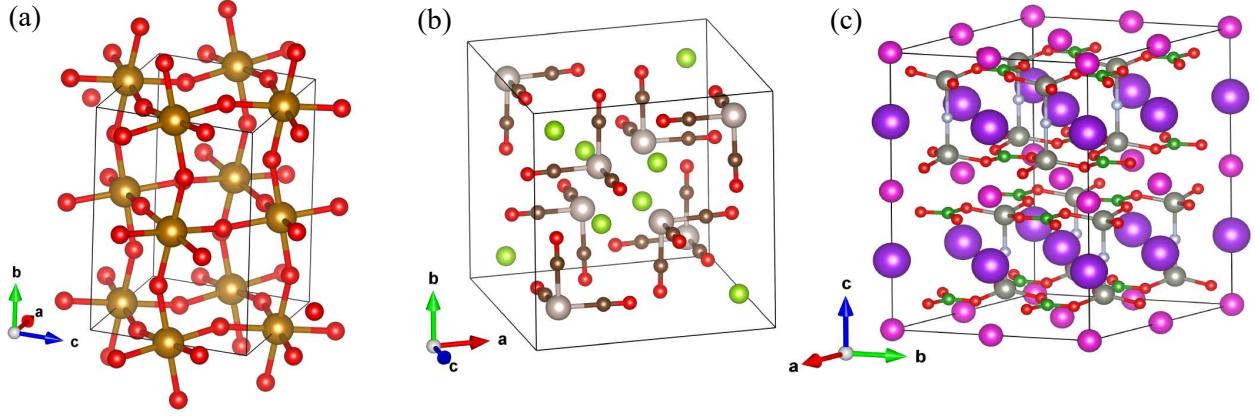


Figure 11. (a) The crystal structure of  $\text{CaFeO}_3$  [ICSD 92330, SG 62 ( $Pnma$ )], where Fe, O are represented by the yellow, red balls and the Ca atoms are ignored. In this material, O and Fe form the sublattices  $L$  and  $\tilde{L}$  respectively, of a bipartite lattice and the number of O and Fe atoms are different:  $|L| = 3$  and  $|\tilde{L}| = 1$ . (b) The crystal structure of  $\text{C}_{12}\text{O}_3\text{Ru}_4\text{Se}_4$  [ICSD 92913, SG 217 ( $I\bar{4}3m$ )], where the Ru, Se, C and O atoms are represented by the grey, green, brown and red balls, respectively. In this material, Ru, C and O form a molecular-cluster which results in the flat atomic bands. The molecular lattices like this one are excluded by the algorithm we have developed. (c) The crystal structure of a  $2 \times 2 \times 1$  supercell of  $\text{CdZn}_2\text{KB}_2\text{O}_6\text{F}$  [ICSD 248025, SG 163 ( $P\bar{3}1c$ )] , where Cd, Zn, K, F, B and O are represented by the purple, grey, blue, white, green and red balls, respectively. In this material, there are two connected subsets along the  $z$  direction. Each connected subset is a bipartite lattice with different number of atoms in its two sublattices. F and O atoms form the  $L$  sublattice and B and Zn atoms form the  $\tilde{L}$  sublattice ( $|L| = 7$  and  $|\tilde{L}| = 4$ ).

In most cases, bipartite sublattices in a crystalline material are not exact if all of the possible hopping terms are considered. There usually exist hoppings between sites of the same sublattice. Nevertheless, a bipartite sublattice dressed by some additional small enough hopping terms could give rise to almost flat bands. For a systematic search of bipartite and split lattices, we solely rely on the geometric distance between two atoms to infer the hopping term amplitude between them. We can then ignore hopping terms which are likely to be small, and identify compounds that have connected bipartite sublattices.

Our algorithm requires a cutoff for the hopping distance above which we assume two atoms are not connected by a hopping term. We base this cutoff on the shortest bond in a crystal structure we want to analyze. Thus for a crystalline material, the first step is to set the cutoff of the hopping distance. In practice, we set the cutoff of the hopping distance  $\tau$  using the following formula:

$$\tau = \lambda \max(d, x), \quad (\text{E8})$$

where  $d$  is the length of the shortest bond in the lattice. To avoid the cases where  $d$  would be too small and thus excluding some non-negligible hopping terms, we also set the lower bound of  $d$  as  $x$ .  $\lambda$  ( $\geq 1$ ) is a multiplicative coefficient to define the cutoff based on the distance  $\max(d, x)$ . For this article and on the [Materials Flatband](#)

[Database website](#), we have considered the values  $\lambda = 1.2, 1.5$  and  $1.7$  and  $x = 1.5, 1.8, 2.1, 2.4$  and  $2.7\text{\AA}$ .

For example in the material  $\text{CaFeO}_3$  [ICSD 92330, SG 62 ( $Pnma$ )] shown in Fig. 11(a), by setting the parameters  $\lambda = 1.2$  and  $x = 1.5\text{\AA}$ , the shortest bond is the Fe – O bond and  $d = 1.91\text{\AA}$ . The hopping distance between Ca and Fe or O are larger than the cutoff  $\tau = 1.2d = 2.29\text{\AA}$ . Hence, Ca atoms are ignored. The bonds lower than  $\tau$  are assumed to be always connected, thus Fe and O form a bipartite sublattice. Indeed, the Fe atoms form the sublattice  $L$  and the O atoms form the sublattice  $\tilde{L}$ . The difference of the atom number between  $L$  and  $\tilde{L}$  is 2.

We now describe the algorithm (see its flow chart in Fig. 14) that we have designed to identify a bipartite sublattice from a crystalline material:

Step 1 We find the shortest bond in the 3D crystal lattice and refer its length as  $d$ . Then, the cutoff of the hopping distance is set as  $\tau = \lambda \max(d, x)$  using the two external parameters  $x$  and  $\lambda$ .

Step 2 For each pair of atoms, if the distance between them is smaller than the cutoff  $\tau$ , we assume the hopping between them is nonzero and we label one as the neighbor of the other one. Otherwise, we consider there is no hopping between them.

Step 3 An atom that has less than two neighbors is considered as a part of a molecular-like cluster, which could contribute to trivial flat atomic bands. We discard such atoms. By repeating this procedure and as shown in Fig. 13, in the end a molecular-like cluster is either deleted (if it was fully disconnected from any other atom) or reduced to a single atom (if the molecular-like cluster was attached to a set of connected atoms via a single atom).

C1 After Step 3, if all the atoms are deleted in the unit cell, there is no bipartite sublattice. Otherwise, the following steps are applied to the remaining atoms.

Step 4 For the set of atoms that are not deleted in Step 3, they can always be divided into several connected subsets, where the hopping term is non-zero between two neighbors within the same subset and is zero between any two atoms in different subsets. Using the results we obtained in Step 2, we can get all the connected subsets. For each connected subset, we apply the following steps.

Step 5 To check if a connected subset  $\mathcal{B}$  is a bipartite sublattice or not, we first define two temporary sets,  $L$  and  $\tilde{L}$ , and a *source set*  $S$ . Then, we choose randomly an atom from  $\mathcal{B}$  and distribute it to  $S$ . We iterate over the following Step 6 and Step 7 to populate  $L$  and  $\tilde{L}$  with the atoms in  $\mathcal{B}$ .

Step 6 From the connected subset  $\mathcal{B}$ , we take all the atoms, which are not in  $L$  or  $\tilde{L}$  but are neighbors of the atoms in  $S$ , as the (new) *target set*  $T$ . We distribute all the atoms in  $S$  to  $L$  and all the atoms in  $T$  to  $\tilde{L}$ . Then we check if  $L$  and  $\tilde{L}$  satisfy the following two criteria:

C2 Any atom in  $L$  (or  $\tilde{L}$ ) is not the neighbor of any other atoms in the same sublattice; Otherwise, the connected subset  $\mathcal{B}$  is not a bipartite lattice and we go back to Step 5, moving to the next connected subset.

C3 If all the atoms in the connected subset  $\mathcal{B}$  have been distributed into either  $L$  or  $\tilde{L}$  then we go to C4; otherwise, we go to Step 7.

Step 7 We take all the atoms, which are not in  $L$  or  $\tilde{L}$  but are the neighbors of the atoms in  $T$ , as the new *source set*  $S$ . Then we empty the *target set*  $T$  and repeat Step 6.

C4 If the numbers of atoms in  $L$  and  $\tilde{L}$  are nonzero and different, the connected subset  $\mathcal{B}$  is tagged as a bipartite lattice with different numbers of atoms in its two sublattices and we go to C5.

C5 For the bipartite lattice with two sublattices  $L$  and  $\tilde{L}$  (up to a relabelling, we can always assume  $L > \tilde{L}$ ), we further check if it is a split lattice. If any atom in  $L$  has exactly two neighbors in  $\tilde{L}$ , and is at equal distance to its two neighbors, the bipartite lattice is also a split lattice. For this step, our algorithm uses a threshold corresponding to  $\pm 20\%$  of the length of the shorter bond to test if two distances are identical.

To illustrate how our algorithm works for the bipartite lattice with different number of atoms on sublattices, we apply it to an example of the material  $\text{CdZn}_2\text{KB}_2\text{O}_6\text{F}$  [ICSD 248025, SG 163 ( $P\bar{3}1c$ )] whose crystal structure is shown in both Fig. 11(c) and Fig. 12(a).

Step 1 In the first step, we identify that the bond between O (red atoms in Figure 12(a)) and B (green atoms in Figure 12(a)) is the shortest bond in  $\text{CdZn}_2\text{KB}_2\text{O}_6\text{F}$ . As the length of this shortest bond is  $1.38\text{\AA}$  and less than  $1.5\text{\AA}$ , we set the cutoff of the hopping distance as  $\tau = 1.5 \times 1.5 = 2.25\text{\AA}$ .

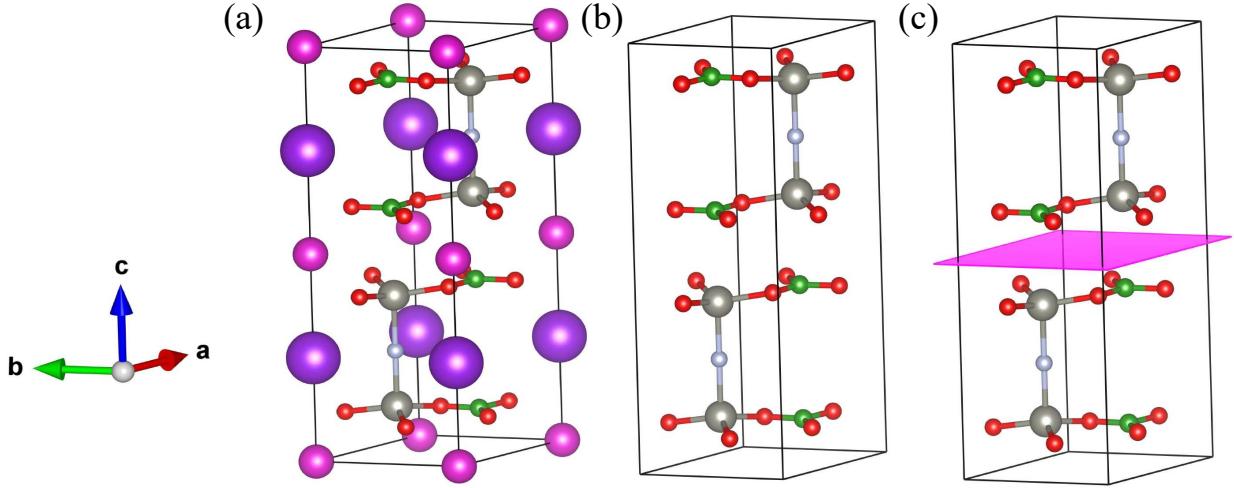


Figure 12. (a) The crystal structure of a unit cell of  $\text{CdZn}_2\text{KB}_2\text{O}_6\text{F}$  [ICSD 248025, SG 163 ( $P\bar{3}1c$ )], where Cd, Zn, K, F, B and O are represented by the purple, grey, blue, white, green and red balls, respectively. Only the bonds whose lengths are smaller than the cutoff  $\tau = 2.25\text{\AA}$  that is considered in Step 2 are shown. (b) The lattice structure after Step 3, all the Cd and K atoms are deleted and all the Zn atoms, B atoms, O atoms and F atoms are left. (c) In Step 3, we identify two connected subsets which are separated by the purple plane. In the explanation of our algorithm for this material we consider the subset above the purple plane first.

Step 2 Then, we discard the bonds of length larger than  $\tau$  and only assume the bonds of length smaller than  $\tau$  to have nonzero hopping amplitude. For example, by ignoring the bonds with zero hopping amplitude, the crystal structure of  $\text{CdZn}_2\text{KB}_2\text{O}_6\text{F}$  is plotted in Fig. 12(a), where the length of each plotted bond is less than the cutoff  $\tau = 2.25\text{\AA}$ .

Step 3 If an atom has no, or only one, bond left, we delete it from the lattice. In the case of  $\text{CdZn}_2\text{KB}_2\text{O}_6\text{F}$ , all of the Cd atoms (the purple atoms in Figure 12(a)) and K atoms (the blue atoms in Figure 12(a)) have no bond left. Thus, they are removed from the lattice. And the lattice structure after this step is shown in Figure 12(b).

C1 As shown in Figure 12(b), following Step 3, all the Zn atoms (the grey atoms in Figure 12(a)), B atoms, O atoms and F atoms (the white atom in Figure 12(a)) are left in the unit cell, so continue to Step 4.

Step 4 Using the results obtained in Step 2, (*i.e.*, which hoppings considered in Figure 12(b)), we find two *connected* subsets, which are separated by the  $[0 \ 0 \ 1]$  Miller plane at  $z = 0.5c$  (where  $c$  is the lattice constant along  $z$  direction) in the lattice, as shown in Figure 12(c).

Step 5 For both of the connected subsets in Figure 12(c), we check whether they are bipartite sublattice separately. Now, we take the one above the purple plane in Figure 12(c) as an example. For convenience, we name this connected subset as  $\mathcal{B}$ . Considering the double counting problem of the O atoms at the unit cell's boundary, there are six O atoms, one F atom, two Zn atoms and two B atoms in  $\mathcal{B}$ . We first define two temporary sets,  $L$  and  $\tilde{L}$ , and a *source set*  $S$ . Then, we choose randomly an atom from  $\mathcal{B}$  and distribute it to  $S$ . Here, we choose one F atom from  $\mathcal{B}$ .

Step 6 From the connected subset  $\mathcal{B}$ , we take the two Zn atoms, which are neighbors of the F atom in  $S$ , as the *target set*  $T$ . We distribute all the atoms in  $S$  (*i.e.*, one F atom) to  $L$  and all the atoms in  $T$  (*i.e.*, two Zn atoms) to  $\tilde{L}$ . Then we check if  $L$  and  $\tilde{L}$  satisfy the C2 and C3.

C2 As obtained in Step 2, the two Zn atoms in  $\tilde{L}$  are not neighbors to each other and there is only one F atom in  $L$ . Thus C2 is satisfied.

C3 In the connected subset  $\mathcal{B}$ , there still are six O and two B atoms left to be distributed, so C3 is not satisfied and we proceed to Step 7.

Step 7 We take the neighbors of the two Zn atoms in  $T$ , *i.e.*, the six O atoms, as the new *source set*  $S$ . Then we empty the *target set*  $T$  and repeat Step 6.

Step 6 From the connected subset  $\mathcal{B}$ , we take the neighbors of the six O atoms of  $S$ , *i.e.*, the two B atoms which are not in  $L$  or  $\tilde{L}$ , as the new *target set*  $T$ . We distribute all the atoms in  $S$  (*i.e.*, the six O atoms) to  $L$  and all the atoms in  $T$  (*i.e.*, two B atoms) to  $\tilde{L}$ . Then we check if  $L$  and  $\tilde{L}$  satisfy C2 and C3.

C2 As obtained in Step 2, the two Zn and the two B atoms in  $\tilde{L}$  are not neighbors to each other. The six O and the F atom in  $L$  are not neighbors to each other. So C2 is satisfied.

C3 All the atoms in  $\mathcal{B}$  have been distributed to either  $L$  or  $\tilde{L}$ . So C3 is satisfied and we move to C4.

C4 The number of atoms in  $L$  is 7 which includes six O atoms and one F atom, while the number of atoms in  $\tilde{L}$  is 4 which includes two Zn atoms and two B atoms. So C4 is satisfied and the connected subset  $\mathcal{B}$  is a bipartite lattice with different numbers of atoms in its two sublattices. Then, we check the criteria in C5.

C5 We further check if this subset is a split lattice. Since none of the atoms in  $L$  are at equal distance to their two neighbors in  $\tilde{L}$  up to our threshold, the bipartite lattice is not a split lattice.

Step5 All the above steps are repeated for the lower connected subset as obtained in Step 4.

Within the above algorithm, we found that the subset  $\mathcal{B}$  is a bipartite lattice with sublattice  $L$  and  $\tilde{L}$ .  $L$  includes six O atoms and one F atom while  $\tilde{L}$  includes two Zn atoms and two B atoms.

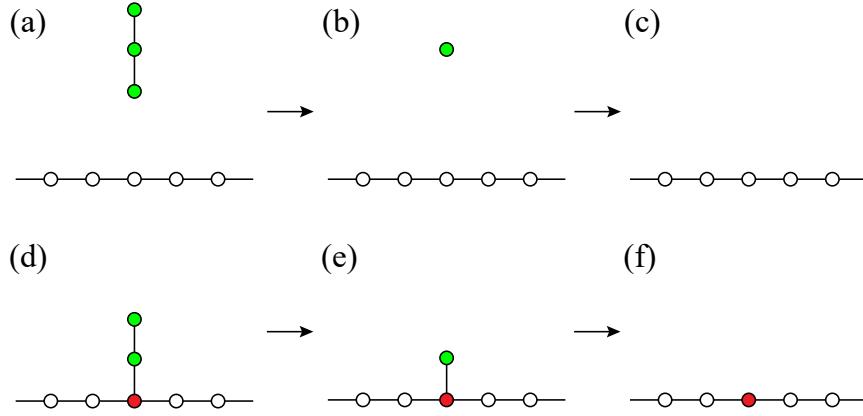


Figure 13. Two of the possible cases when removing a molecular cluster. (a)-(c) The molecular cluster is made of the three green sites and is completely detached from the the fully connected sites (white circles). Acting with Step 3 once, we remove two out of the three green sites. Applying Step 3 a second time, we completely get rid of the molecular cluster. (d)-(f) The molecular cluster is made of the two green sites and one red site belonging to fully connected sites. Repetitively acting on the molecular cluster using Step 3, we end up with a single site of the molecular cluster (in red).

To illustrate how the molecular lattices are excluded, we consider the example  $\text{C}_{12}\text{O}_3\text{Ru}_4\text{Se}_4$ [ICSD 92913, SG 217 ( $I\bar{4}3m$ )], whose crystal structure is shown in Fig. 11(b). Applying our algorithm to this material leads to the following sequence:

Step 1 In the first step, we identify that the bond between C atoms (brown atoms in Figure 11(b)) and O atoms (red atoms in Figure 11(b)) is the shortest bond in  $\text{C}_{12}\text{O}_3\text{Ru}_4\text{Se}_4$ . As the length of this shortest bond is smaller than  $1.5\text{\AA}$ , we set the cutoff of the hopping distance as  $\tau = \lambda 1.5\text{\AA}$ .

Step 2 Then, we discard the bonds of length larger than  $\tau$  and only the bonds of length smaller than  $\tau$  are assumed to have nonzero hopping. For example, by ignoring the bonds with zero hopping, the crystal structure of  $\text{C}_{12}\text{O}_3\text{Ru}_4\text{Se}_4$  is plotted in Fig. 11(b) for  $\tau = 1.5 \times 1.5 = 2.25\text{\AA}$ , where the length of each plotted bond is less than the cutoff  $\tau = 2.25\text{\AA}$ .

Step 3 If an atom has no or only one bond left, we delete it from the lattice. In the case of  $\text{C}_{12}\text{O}_3\text{Ru}_4\text{Se}_4$ , all of the Se atoms (green atoms in Figure 11(b)) have no bond left and every O atom has only one bond. Thus, both of them are removed from the lattice. Then, each of the left C atoms (brown atoms in Figure 11(b)) only has one bond and should be removed. After that, the Ru atoms (grey atoms in Figure 11(b)) get isolated and hence are also removed. Finally, all the atoms are removed from the lattice and this material does not belong to a *connected bipartite lattice*.

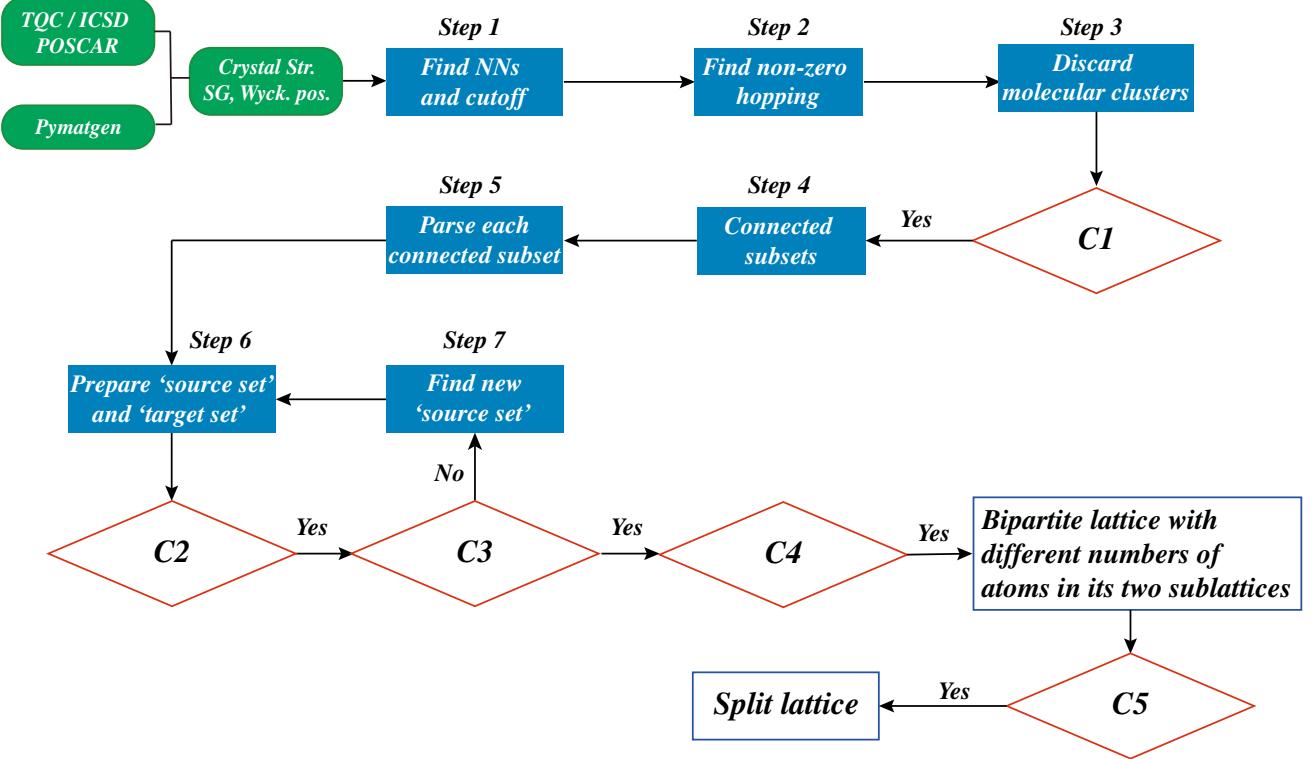


Figure 14. The flow chart of the algorithm identifying bipartite sublattices from a 3D crystal lattice. Starting from the crystal structure of a material given by its *POSCAR* file, we use the *Pymatgen* package to analyze the crystal symmetry and the Wyckoff positions of each distinct element. Step 1 is applied to identify the nearest neighbor(NN) sites of each atom and set the cutoff of the hopping distance. In Step 2, if the hopping distance is within the cutoff, the hopping amplitude is set to non-zero; otherwise, the hopping amplitude is set to zero; In Step 3, the molecular-like clusters are removed and we exit the algorithm through C1 if there has no atom left. In Step 4, for the set of atoms that are not removed in Step 3, they are divided into several connected subsets, where the hopping amplitude is non-zero between two neighbors within the same subset and is zero between any two atoms in different connected subsets. The Steps 5, 6 and 7 and the criteria C2 and C3 are applied to each connected subset to identify the bipartite sublattice based on the neighbors of each atom as extracted in Step 2. The criteria C4 is applied to check whether the numbers of the atoms in the two sublattices  $L$  and  $\tilde{L}$  are different. If a bipartite lattice is detected, an additional test based on the criteria C5 is performed to check if the bipartite lattice is also a split lattice.

In this work, we applied our algorithm using different values for the cutoff parameters  $\lambda$  and  $x$  in Eq. (E8). As we mentioned above, we adopted the values of  $\lambda$  to be 1.2, 1.5 and 1.7 and the values of  $x$  to be 1.5, 1.8, 2.1, 2.4 and 2.7 Å. We have scanned the materials available in the database of Appendix C to search for bipartite sublattices potentially leading to flat bands, *i.e.*,  $|L| \neq |\tilde{L}|$  and split sublattices. The individual results are available on the [Materials Flatband Database website](#). The bipartite sublattice statistics for each setting are provided in Table VII.

Table VII: Statistics for the ICSD entries with either bipartite or split sublattices with respect to the lower bound of  $d$  and the multiplicative factor  $\lambda$  that define the distance cutoff in Eq. (E8). The first and second columns are the values of  $x$  and  $\lambda$ . The third column is the number of ICSD entries hosting at least one bipartite sublattice and the fourth column is the number of ICSD entries hosting at least one split sublattice among the bipartite sublattices. All percentages are computed with respect to the total number of ICSD entries that have been considered (55,206 ICSDs).

$x$	$d$	# ICSDs with bipartite	# ICSDs with split
$x = 1.5\text{\AA}$	$\lambda = 1.2$	15662 (28.4%)	7811 (14.2%)
$x = 1.5\text{\AA}$	$\lambda = 1.5$	6011 (10.9%)	1235 (2.2%)
$x = 1.5\text{\AA}$	$\lambda = 1.7$	217 (0.4%)	31 (0.1%)
$x = 1.8\text{\AA}$	$\lambda = 1.2$	18459 (33.4%)	7282 (13.2%)
$x = 1.8\text{\AA}$	$\lambda = 1.5$	1879 (3.4%)	296 (0.5%)
$x = 1.8\text{\AA}$	$\lambda = 1.7$	64 (0.1%)	6 (0.0%)

$x = 2.1\text{\AA}$	$\lambda = 1.2$	14895 (27.0%)	4721 (8.6%)
$x = 2.1\text{\AA}$	$\lambda = 1.5$	697 (1.3%)	102 (0.2%)
$x = 2.1\text{\AA}$	$\lambda = 1.7$	6 (0.0%)	1 (0.0%)
$x = 2.4\text{\AA}$	$\lambda = 1.2$	4704 (8.5%)	1339 (2.4%)
$x = 2.4\text{\AA}$	$\lambda = 1.5$	245 (0.4%)	22 (0.0%)
$x = 2.4\text{\AA}$	$\lambda = 1.7$	—	—
$x = 2.7\text{\AA}$	$\lambda = 1.2$	2863 (5.2%)	617 (1.1%)
$x = 2.7\text{\AA}$	$\lambda = 1.5$	37 (0.1%)	4 (0.0%)
$x = 2.7\text{\AA}$	$\lambda = 1.7$	—	—

**Discussion** At the end of this section, we comment on the relation between Lieb, bipartite and split sublattices in crystalline materials. As we defined before, the split sublattice is a special case of bipartite sublattice and each of the split sublattices we obtained in our results *has to* be a bipartite sublattice. Mathematically, the Lieb lattice is a special case of both bipartite and split sublattices in 2D. However, in 3D crystalline materials, the conditions in our method to identify a 2D Lieb sublattice is not stringent enough to identify if the 2D Lieb sublattice is also a bipartite or split sublattice in 3D. In our geometric algorithm for Lieb sublattice, we only consider the NN bonds and the atoms on (or close to) a 2D plane. In the algorithm for bipartite sublattice, we set a cutoff  $\tau$  for the hopping distance and consider all the hoppings of distance less than the cutoff  $\tau$ . Hence more hoppings and atoms are involved and it could make a Lieb-sublattice material not a bipartite-sublattice material. Actually we have only found one such case when a Lieb lattice is not a bipartite lattice in our database, *i.e.*,  $\text{H}_3\text{F}_3\text{GaN}$  [ICSD 89503, SG 39 (*Aem2*)].

## Appendix F: Theoretical explanations for flat bands in representative materials

In this appendix, we discuss seven typical materials among the 345 materials that will be presented in Appendix H 3 which host clear flat bands at or near the Fermi level. Here we explain the origins of these flat bands. The seven materials are  $\text{WO}_3$  [ICSD 108651, SG 221 ( $Pm\bar{3}m$ )],  $\text{Pb}_2\text{Sb}_2\text{O}_7$  [ICSD 27120, SG 227 ( $Fd\bar{3}m$ )],  $\text{CaNi}_5$  [ICSD 54474, SG 191 ( $P6/mmm$ )],  $\text{Ca}_2\text{NCl}$  [ICSD 62555, SG 166 ( $R\bar{3}m$ )],  $\text{Rb}_2\text{CaH}_4$  [ICSD 65196, SG 139 ( $I4/mmm$ )],  $\text{KAg}[\text{CN}]_2$  [ICSD 30275, SG 163 ( $P\bar{3}1c$ )], and  $\text{RbMo}_3\text{S}_3$  [ICSD 644175, SG 176 ( $P6_3/m$ )]. The first six materials have a bipartite sublattice in the crystal lattice and the flat bands can be explained using the *S*-matrix method, as introduced in Appendix E and in Ref.<sup>6</sup>. For the last example,  $\text{RbMo}_3\text{S}_3$ , the flat bands are due to the quasi-1D character and the weak inter-chain couplings of this material.

### 1. $\text{WO}_3$

The crystal structure of  $\text{WO}_3$  [ICSD 108651, SG 221 ( $Pm\bar{3}m$ )] is shown in Fig. 15(a). W and O occupy the  $1a$  and  $3c$  Wyckoff positions, respectively. From its band structure without SOC considered, as plotted in Fig. 15(c), there are three connected bands at (and above) the Fermi level. Along the high-symmetry paths  $\Gamma \rightarrow \text{X}$ ,  $\text{X} \rightarrow \text{M}$  and  $\text{M} \rightarrow \text{R}$ , there is always one out of the three bands that is extremely flat (but not necessarily at the Fermi level). By analyzing the orbital-projected band structure obtained from the first-principles calculation, the three bands come from the  $d_{xy}$ ,  $d_{yz}$  and  $d_{xz}$  orbitals of W, which form the 3 dimensional single-valued irrep  $T_{2g}$  of the site-symmetry-group  $O_h$  of the  $1a$  position. Below the  $T_{2g}$  bands of W, there is another set of valence bands coming from  $p$  orbitals of O, as indicated by the red lines in Fig. 15(c), of which the highest bands are also flat. Similar structures of flat bands also exist in the perovskites with the chemical formulae  $\text{ABO}_3$  or  $\text{BO}_3$  in SG 211 ( $Pm\bar{3}m$ )<sup>65–67</sup>, where B is a transition element with  $3d$  electrons in the outer shell sitting at the  $1a$  (or  $1b$ ) Wyckoff position and O sits at the  $3c$  (or  $3d$ ) Wyckoff position.

Both the flat conduction bands (along some paths) and the flat valence bands can be explained using the *S*-matrix method, as introduced in Appendix E. For the case in  $\text{WO}_3$ , we refer to the sublattices of W and O as two sublattices  $\tilde{L}$  and  $L$ . Then, the lattice of  $L \oplus \tilde{L}$  is a bipartite lattice if only the bonds connecting W and its NN O atoms are taken into account. As explained in the above tight-binding method, the bands near the Fermi level come from  $d_{yz}$ ,  $d_{xz}$ , and  $d_{xy}$  orbitals on W and the  $p$  orbitals on O. We introduce the Bloch basis as

$$|\phi_\alpha(\mathbf{k})\rangle = \sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\mathbf{k}} |\alpha, \mathbf{R}\rangle, \quad |\phi_a(\mathbf{k})\rangle = \sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\mathbf{k}} |a, \mathbf{R}\rangle, \quad (\text{F1})$$

where  $\alpha$  indexes the three  $d$  orbitals,  $a$  indexes the nine  $p$  orbitals on the three O atoms, and  $\mathbf{R}$  indexes the lattice

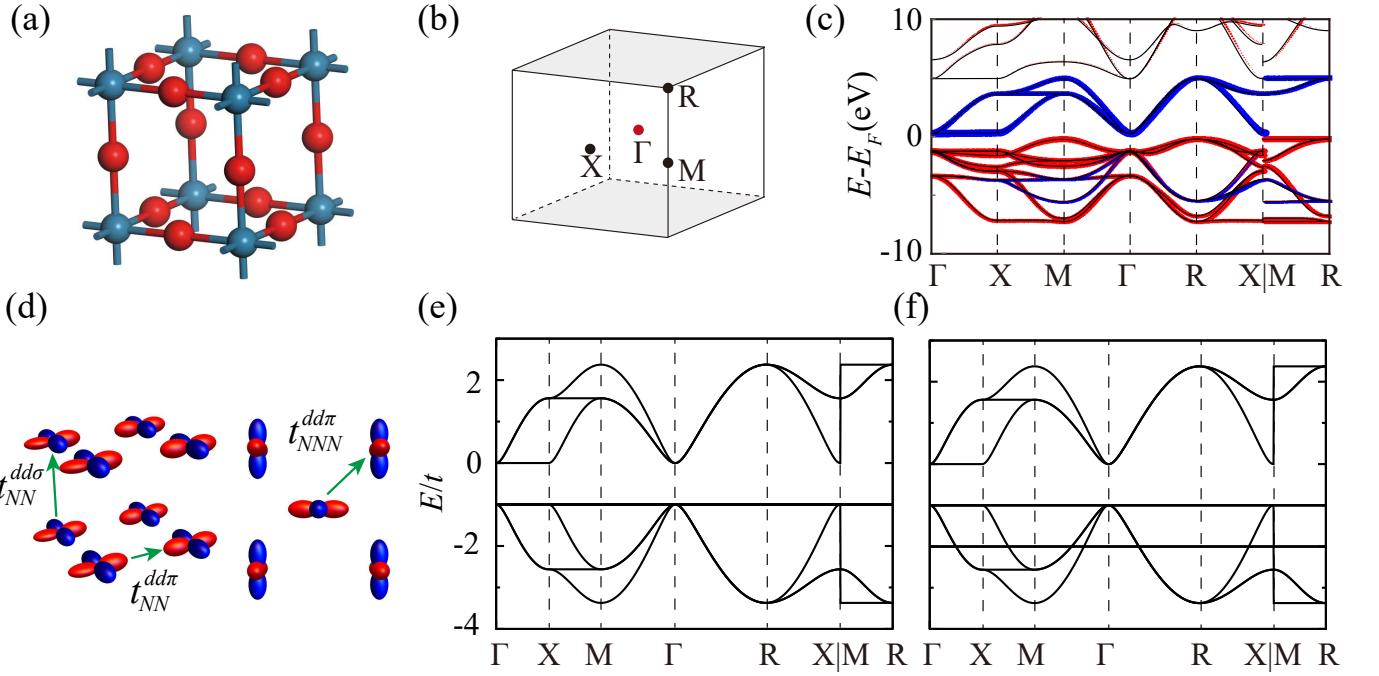


Figure 15. (a) The crystal structure of WO<sub>3</sub>. W and O are represented by the blue and red balls, respectively. (b) The bulk BZ of WO<sub>3</sub>. (c) Orbital-projected band structure of WO<sub>3</sub> without spin-orbit coupling. The weights of  $d_{xy}, d_{yz}$  and  $d_{zx}$  orbitals on W are highlighted in blue, and the weights of the  $p$  orbitals on O are highlighted in red. (d) The schematic of the three different hopping terms that are considered in Eq. (F7). (e) The band structure of the bipartite lattice  $L \oplus \tilde{L}$  constructed from the  $S$  matrix in Eq. (F2). We have chosen  $\Delta = -|t|$  for our calculation. (f) The band structure of the bipartite lattice  $L \oplus \tilde{L}$  with an additional onsite term  $\delta$  that splits the  $A_{2u}$  and  $E_u$  orbitals at the O atoms.

vectors, respectively.  $\alpha = 1, 2, 3$  correspond to the  $d_{xy}$ ,  $d_{yz}$ , and  $d_{xz}$  orbitals, respectively,  $a = i + 3(j - 1)$  correspond to the  $p_x$  ( $i = 1$ ),  $p_y$  ( $i = 2$ ),  $p_z$  ( $i = 3$ ) orbitals at the  $j$ th site of the  $3c$  Wyckoff position, respectively. Here  $j = 1, 2, 3$  correspond to the sites  $(\frac{1}{2}, 0, 0)$ ,  $(0, \frac{1}{2}, 0)$  and  $(0, 0, \frac{1}{2})$ , respectively. Notice that we have chosen a periodic gauge for the basis in Eq. (F1), *i.e.*, the basis is invariant if we change  $\mathbf{k}$  to  $\mathbf{k} + \mathbf{G}$  with  $\mathbf{G}$  being a vector of the reciprocal lattice. We will use this periodic gauge throughout this section. The  $S$  matrix of this bipartite lattice is given by  $S_{\alpha a}^{\dagger}(\mathbf{k}) = \langle \phi_{\alpha}(\mathbf{k}) | \hat{H} | \phi_a(\mathbf{k}) \rangle$ . This  $3 \times 9$ -dimensional  $S^{\dagger}(\mathbf{k})$  matrix is

$$S^{\dagger}(\mathbf{k}) = t \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 - e^{-ik_z} & 0 & 1 - e^{-ik_y} & 0 \\ 0 & 0 & 1 - e^{-ik_z} & 0 & 0 & 0 & 1 - e^{-ik_x} & 0 & 0 \\ 0 & 1 - e^{-ik_y} & 0 & 1 - e^{-ik_x} & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{F2})$$

Here  $t$  is the hopping between the  $d_{xy}$  orbital at  $(0, 0, 0)$  and  $p_x$  orbital at  $(\frac{1}{2}, 0, 0)$  which can be obtained from the maximally localized Wannier function (MLWF) calculations<sup>37</sup> and is  $-1.654$  eV. Here, we build the MLWF by the  $p$  orbitals and the  $T_{2g}$  orbitals of W atom. The inter-sublattice couplings *e.g.* the coupling between  $p_z$  orbitals at  $(0, 0, \frac{1}{2})$  and  $(0, \frac{1}{2}, 0)$  ( $0.179$  eV), and the coupling between  $d_{xy}$  orbitals at  $(0, 0, 0)$  and  $(1, 0, 0)$  ( $-0.222$  eV) are ignored. Since these couplings are much smaller than those we consider, neglecting these couplings is reasonable. Other NN hoppings between  $T_{2g}$  and  $p$  orbitals are equivalent to this hopping due to the symmetries. We further assume the onsite energy of  $p$  orbitals as  $\Delta$  ( $< 0$ ), then the total Hamiltonian reads

$$H_{L \oplus \tilde{L}}(\mathbf{k}) = \begin{pmatrix} 0_{3 \times 3} & S^{\dagger}(\mathbf{k}) \\ S(\mathbf{k}) & \Delta \cdot \mathbb{I}_{9 \times 9} \end{pmatrix}. \quad (\text{F3})$$

To discover the flat valence bands (over the whole Brillouin zone), we consider the SVD decomposition of the  $S(\mathbf{k})$  matrix as  $S(\mathbf{k}) = U(\mathbf{k})\Sigma(\mathbf{k})V^{\dagger}(\mathbf{k})$ , where  $U(\mathbf{k})$  is a nine-by-nine unitary matrix,  $V(\mathbf{k})$  is a three-by-three unitary matrix, and  $\Sigma(\mathbf{k})$  is a nine-by-three rectangular diagonal matrix with real non-negative diagonal elements. We apply

the unitary transformation to the Hamiltonian

$$\begin{pmatrix} V^\dagger(\mathbf{k}) & 0_{3 \times 9} \\ 0_{9 \times 3} & U^\dagger(\mathbf{k}) \end{pmatrix} \cdot H_{L \oplus \tilde{L}}(\mathbf{k}) \cdot \begin{pmatrix} V(\mathbf{k}) & 0_{3 \times 9} \\ 0_{9 \times 3} & U(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} 0_{3 \times 3} & \Sigma^T(\mathbf{k}) \\ \Sigma(\mathbf{k}) & \Delta \cdot \mathbb{I}_{9 \times 9} \end{pmatrix}. \quad (\text{F4})$$

Suppose that the diagonal elements of  $\Sigma(\mathbf{k})$  are  $\xi_n(\mathbf{k})$  with  $n = 1, 2, 3$ , then the system has six branches of dispersive bands  $\frac{\Delta}{2} \pm \sqrt{\xi_n^2(\mathbf{k}) + \Delta^2/4}$  and six flat bands at  $\Delta$ . If one branch of  $\xi_n(\mathbf{k})$  is a constant  $\xi_c$  over the whole Brillouin zone, we would have one more flat band at  $\frac{\Delta}{2} \pm \sqrt{\xi_c^2 + \Delta^2/4}$  and an additional flat band at 0. For a generic Hamiltonian in form of Eq. (F3), there are  $|L| - \text{rank}(S(\mathbf{k}))$  states at  $\Delta$  and  $|\tilde{L}| - \text{rank}(S(\mathbf{k}))$  states at 0. The other  $2 \times \text{rank}(S(\mathbf{k}))$  states must have energies either below (above)  $\Delta$  or above (below) 0 for negative (positive)  $\Delta$ . The particular  $S(\mathbf{k})$  matrix defined in Eq. (F2) has rank three at generic momenta, hence there are 6 flat bands at the energy  $\Delta$ , as shown in Fig. 15(e).

Since the  $T_{2g}$ -bands and  $p$ -bands are well separated in energy, we can derive the individual effective Hamiltonians for them by applying the second-order perturbation theory, already exemplified in Appendix E 1, as

$$H_{\tilde{L}}(\mathbf{k}) \approx -S^\dagger(\mathbf{k})S(\mathbf{k})/\Delta, \quad (\text{F5})$$

and

$$H_L(\mathbf{k}) \approx \Delta + S(\mathbf{k})S^\dagger(\mathbf{k})/\Delta, \quad (\text{F6})$$

respectively (The exact expressions are provided in Appendix E 1). The effective Hamiltonian of  $T_{2g}$ -bands is a diagonal matrix

$$H_{\tilde{L}}(\mathbf{k}) = -2t^2/\Delta \begin{pmatrix} 2 - \cos k_y - \cos k_z & 0 & 0 \\ 0 & 2 - \cos k_x - \cos k_z & 0 \\ 0 & 0 & 2 - \cos k_x - \cos k_y \end{pmatrix}. \quad (\text{F7})$$

With parameters given by  $t_{NN}^{dd\pi} = -t^2/|\Delta|$ ,  $t_{NN}^{dd\delta} = t_{NNN}^{dd\pi} = 0$ ,  $\Delta_d = -\frac{4t^2}{\Delta} = \frac{4t^2}{|\Delta|}$ .  $\Delta_d$  is the onsite energy of  $T_{2g}$  orbitals,  $t_{NN}^{dd\pi}$  ( $t_{NNN}^{dd\pi}$ ) is the amplitude of the NN (NNN) in-plane hopping while  $t_{NN}^{dd\delta}$  is the amplitude of NN out-of-plane hopping, as schematically shown in Fig. 15(d). Taking the  $T_{2g}$  orbitals as basis, we built the MLWF. The values of  $\Delta_d$ ,  $t_{NN}^{dd\pi}$ ,  $t_{NNN}^{dd\pi}$  and  $t_{NN}^{dd\delta}$  are 2.45eV, -0.62eV, 0.01eV and -0.006eV, respectively. Then, the Hamiltonian in Eq. (F7) is a diagonal matrix with elements  $2t_{NN}^{dd\pi} \{ \cos k_y + \cos k_z, \cos k_x + \cos k_z, \cos k_x + \cos k_y \}$  (up to the constant shift  $\Delta_d$ ). We can prove that there is always a flat band along a path parallel to the direction of the  $k_i$  ( $i = x, y, z$ ) axis, and the energy of the flat band is  $E = 2t_{NN}^{dd\pi}(\cos k_j + \cos k_k)$ , where  $i \neq j \neq k$ .

- Along the high-symmetry path  $\Gamma \rightarrow X$ , with  $k_y = k_z = 0$ , the Hamiltonian in Eq. (F7) becomes a diagonal matrix with three diagonal elements,  $2t_{NN}^{dd\pi} \{ 2, 1 + \cos k_x, 1 + \cos k_x \} + \{\Delta_d, \Delta_d, \Delta_d\}$ , resulting in one flat band at  $E = 4t_{NN}^{dd\pi} + \Delta_d = -0.03$ eV. This flat band has a touching point at the  $\Gamma$  point with a double-degenerate dispersive band.
- Along the high-symmetry path  $X \rightarrow M$ , with  $k_x = \pi$  and  $k_z = 0$ , the Hamiltonian in Eq. (F7) becomes a diagonal matrix with three diagonal elements,  $2t_{NN}^{dd\pi} \{ 1 + \cos k_y, 0, -1 + \cos k_y \} + \{\Delta_d, \Delta_d, \Delta_d\}$ , resulting in one flat band at  $E = \Delta_d = 2.45$ eV. This flat band has touching points at  $X$  and  $M$  points with two dispersive bands, respectively.
- Along the high-symmetry path  $R \rightarrow M$ , with  $k_x = k_y = \pi$ , the Hamiltonian in Eq. (F7) becomes a diagonal matrix with three diagonal elements,  $2t_{NN}^{dd\pi} \{ -1 + \cos k_z, -1 + \cos k_z, -2 \} + \{\Delta_d, \Delta_d, \Delta_d\}$ , resulting in a flat bands at  $E = -4t_{NN}^{dd\pi} + \Delta_d = 4.93$ eV. This flat band has a touching point at  $R$  point with a double-degenerate dispersive band.

The dispersion of the valence bands from the first-principle calculations is more complicated than the dispersion of the valence bands in the  $S$ -matrix model, as can be seen by comparing Fig. 15(c) and Fig. 15(e). Indeed, we have omitted several symmetry-allowed terms in the  $S$ -matrix model. For example, the site-symmetry-groups of the O atoms are all  $D_{4h}$ . The  $p_x, p_y, p_z$  orbitals form a two-dimensional irrep  $E_u$  and a one-dimensional irrep  $A_{2u}$  of the point group  $D_{4h}$ . The two irreps in principle should have different onsite energies due to the crystal field splitting.

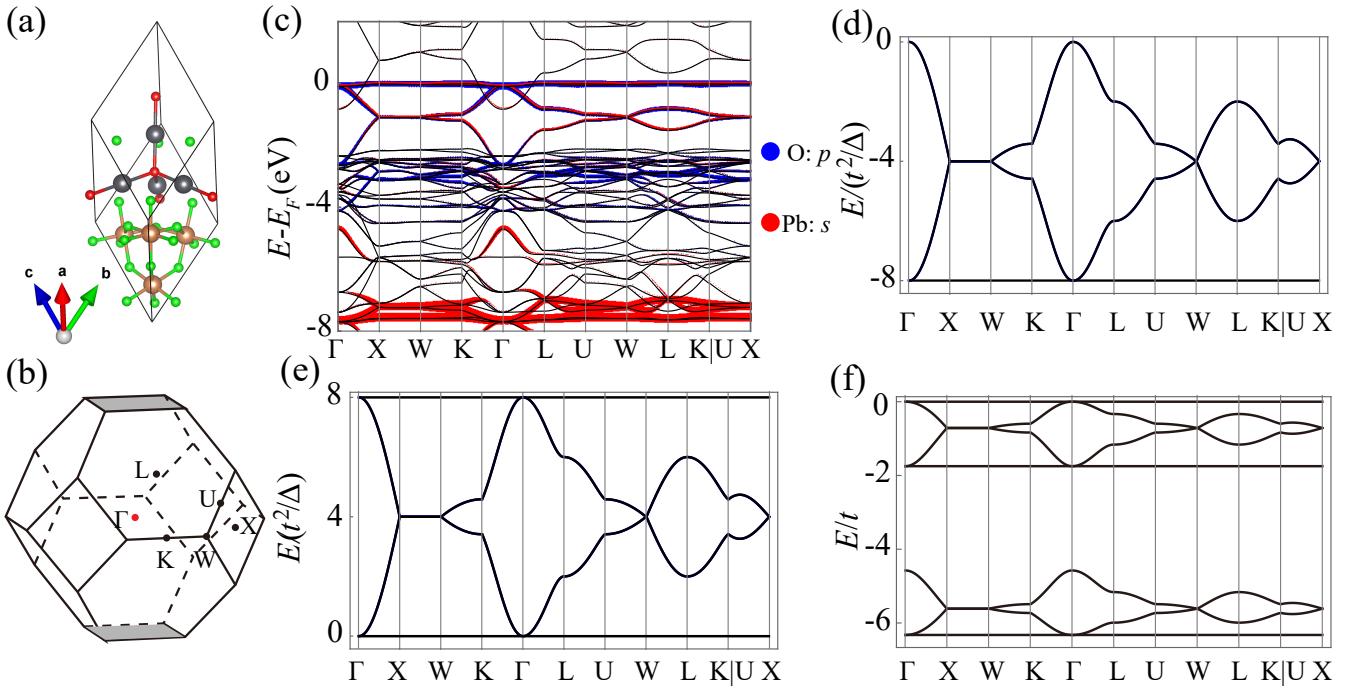


Figure 16. (a) The crystal structure of  $\text{Pb}_2\text{Sb}_2\text{O}_7$ . The Pb and Sb atoms are in gray and brown, respectively. The O atoms at 8b and 48f are in red and green, respectively. (b) The bulk BZ of  $\text{Pb}_2\text{Sb}_2\text{O}_7$ . (c) Band structure calculated by GGA-PBE of  $\text{Pb}_2\text{Sb}_2\text{O}_7$  without spin-orbit coupling. The weights of the  $s$  orbital on Pb and the  $p$  orbitals on O atoms that are located at 8b are highlighted in red and blue, respectively. (d) The band structure of Hamiltonian  $H_{\tilde{L}}$  in Eq. (F10). (e) The band structure of Hamiltonian  $H_L$  in Eq. (F10). (f) The band structure of Hamiltonian  $H_{L \oplus \tilde{L}}$  in Eq. (F9).

In the  $S$ -matrix construction we have set both onsite energies as  $\Delta$  for simplicity. Now we consider splitting the  $A_{2u}$  and  $E_u$  orbitals by adding an additional onsite energy  $\delta$  on the  $A_{2u}$  orbitals. Notice that the  $A_{2u}$  irreps at  $(\frac{1}{2}, 0, 0)$ ,  $(0, \frac{1}{2}, 0)$ ,  $(0, 0, \frac{1}{2})$  are formed by  $p_x$ ,  $p_y$ , and  $p_z$  orbitals, respectively. From the  $S$ -matrix in Eq. (F2), one can see that these  $A_{2u}$  orbitals are decoupled from the other orbitals. Hence, for  $\delta = 0$ , the  $A_{2u}$  orbitals contribute to three of the six flat bands at  $\Delta$ . A nonzero  $\delta$  just shifts the energy of these three flat bands to  $\Delta + \delta$ , as shown in Fig. 15(f), where  $\delta$  is set to  $-|t|$  (note that  $\delta$  does not have to be equal to  $\Delta$ ). The band structure with nonzero  $\delta$  still has perfect flat-band segments in the valence bands. These flat bands will have finite band widths if the (smaller) hopping terms between  $p$  orbitals at different O atoms are taken into account. We leave this discussion for future studies.

The above analysis using the  $S$ -matrix method could be adapted to explain the flat bands of the other perovskites, such as  $\text{ReO}_3$  [ICSD 16810, SG 221 ( $Pm\bar{3}m$ )<sup>68</sup>],  $\text{NbF}_3$  [ICSD 25596, SG 221 ( $Pm\bar{3}m$ )],  $\text{BaTiO}_3$  [ICSD 27971, SG 221 ( $Pm\bar{3}m$ )],  $\text{CaTiO}_3$  [ICSD 162924, SG 221 ( $Pm\bar{3}m$ )],  $\text{SrTiO}_3$  [ICSD 80874, SG 221 ( $Pm\bar{3}m$ )],  $\text{NaNbO}_3$  [ICSD 28588, SG 221 ( $Pm\bar{3}m$ )],  $\text{NaTaO}_3$  [ICSD 88378, SG 221 ( $Pm\bar{3}m$ )],  $\text{CrLaO}_3$  [ICSD 28930, SG 221 ( $Pm\bar{3}m$ )],  $\text{CrSrO}_3$  [ICSD 108903, SG 221 ( $Pm\bar{3}m$ )],  $\text{BaFeO}_3$  [ICSD 29096, SG 221 ( $Pm\bar{3}m$ )],  $\text{SrFeO}_3$  [ICSD 91062, SG 221 ( $Pm\bar{3}m$ )],  $\text{LaFeO}_3$  [ICSD 29118, SG 221 ( $Pm\bar{3}m$ )],  $\text{LaMnO}_3$  [ICSD 674501, SG 221 ( $Pm\bar{3}m$ )],  $\text{SrRuO}_3$  [ICSD 82983, SG 221 ( $Pm\bar{3}m$ )],  $\text{BaRuO}_3$  [ICSD 673893, SG 221 ( $Pm\bar{3}m$ )],  $\text{SrCoO}_3$  [ICSD 77142, SG 221 ( $Pm\bar{3}m$ )],  $\text{SrVO}_3$  [ICSD 88982, SG 221 ( $Pm\bar{3}m$ )],  $\text{CaTcO}_3$  [ICSD 671082, SG 221 ( $Pm\bar{3}m$ )],  $\text{SrTcO}_3$  [ICSD 109076, SG 221 ( $Pm\bar{3}m$ )],  $\text{CaTcO}_3$  [ICSD 671086, SG 221 ( $Pm\bar{3}m$ )],  $\text{TiPbO}_3$  [ICSD 187295, SG 221 ( $Pm\bar{3}m$ )],  $\text{CrPbO}_3$  [ICSD 160196, SG 221 ( $Pm\bar{3}m$ )],  $\text{CaMnO}_3$  [ICSD 168902, SG 221 ( $Pm\bar{3}m$ )],  $\text{SrMnO}_3$  [ICSD 188415, SG 221 ( $Pm\bar{3}m$ )],  $\text{VPbO}_3$  [ICSD 187637, SG 221 ( $Pm\bar{3}m$ )],  $\text{KNbO}_3$  [ICSD 190920, SG 221 ( $Pm\bar{3}m$ )], and  $\text{VBaO}_3$  [ICSD 191203, SG 221 ( $Pm\bar{3}m$ )]. Note that all of these materials are listed in Appendix H1.

## 2. $\text{Pb}_2\text{Sb}_2\text{O}_7$

The crystal structure of  $\text{Pb}_2\text{Sb}_2\text{O}_7$  [ICSD 27120, SG 227 ( $Fd\bar{3}m$ ) (origin choice 1 as defined on the *Bilbao Crystallographic Server*)] is shown in Fig. 16(a). The 16d and 16c Wyckoff positions are occupied by the Pb and Sb atoms, respectively. O atoms occupy two different Wyckoff positions, 8b and 48f. As tabulated in Table V, each of the

sublattices formed by Pb and Sb is a pyrochlore lattice, which is a 3D line-graph lattice that could host flat bands<sup>26</sup>. As shown in the orbital-projected band structure of  $\text{Pb}_2\text{Sb}_2\text{O}_7$  in Fig. 16(c), around the Fermi level, there are two flat bands mainly composed by the  $p$  orbitals of the O located at the  $8b$  position. As indicated in the orbital-projected band structure, the  $p$  orbitals of O are hybridized with the  $s$  orbitals of Pb. The other bands between -8eV and -2eV are mainly contributed by the O atoms at the  $48f$  Wyckoff position. The hybridization between the  $s$  orbitals of O at  $8b$  and these bands is tiny because the distances from the O atoms at  $8b$  to the Sb atoms and O atoms at  $48f$  are larger than those to the Pb atoms. In fact, in [Materials Flatband Database website](#) and Appendix H 1, the crystal structure of  $\text{Pb}_2\text{Sb}_2\text{O}_7$  is identified to have a bipartite lattice formed by Pb and the O at  $8b$ . As shown below, the flat bands come from the  $S$ -matrix of this bipartite lattice.

We refer to the two sublattices formed by O (at  $8b$ ) and Pb (at  $16d$ ) as  $L$  and  $\tilde{L}$ , respectively. Then, the lattice of  $L \oplus \tilde{L}$  is a bipartite lattice if only the bonds connecting Pb and its NN O atoms are taken into account. We construct the  $S$  matrix by putting three  $p$  orbitals at each of the  $8b$  positions  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ ,  $(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$  and an  $s$  orbital at each of the  $16d$  positions  $(\frac{5}{8}, \frac{5}{8}, \frac{5}{8})$ ,  $(\frac{5}{8}, \frac{5}{8}, \frac{1}{8})$ ,  $(\frac{5}{8}, \frac{1}{8}, \frac{5}{8})$  and  $(\frac{1}{8}, \frac{5}{8}, \frac{5}{8})$ , with coordinates given in the primitive unit cell spanned by  $\mathbf{a}_1 = a(0, 1/2, 1/2)$ ,  $\mathbf{a}_2 = a(1/2, 0, 1/2)$ ,  $\mathbf{a}_3 = a(1/2, 1/2, 0)$ , with  $a$  being the lattice parameter. We use  $\alpha$  and  $a$  to label the orbitals in the sublattices  $\tilde{L}$  and  $L$ , respectively. The index  $\alpha = 1, 2, 3, 4$  corresponds to the four  $s$  orbitals at the four sites in  $\tilde{L}$ . The index  $a = i + 2(j-1)$  corresponds to the  $p_x$  ( $j=1$ ),  $p_y$  ( $j=2$ ),  $p_z$  ( $j=3$ ) orbitals at the  $i$ 'th site ( $i=1, 2$ ) in  $L$ . Then the  $S$  matrix can be written as

$$S^\dagger(\mathbf{k}) = t \begin{pmatrix} 1 & -1 & 1 & -1 & 1 & -1 \\ -1 & e^{-ik_3} & -1 & e^{-ik_3} & 1 & -e^{-ik_3} \\ -1 & e^{-ik_2} & 1 & -e^{-ik_2} & -1 & e^{-ik_2} \\ 1 & -e^{-ik_1} & -1 & e^{-ik_1} & -1 & e^{-ik_1} \end{pmatrix}. \quad (\text{F8})$$

Here,  $t$  is the strength of the coupling between  $s$  orbital at  $(\frac{5}{8}, \frac{5}{8}, \frac{5}{8})$  and  $p_x$  orbital at  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ , and  $(k_1, k_2, k_3)$  is the coordinate of the momentum  $\mathbf{k} = \sum_{i=1}^3 k_i \mathbf{b}_i$ , where  $\mathbf{b}_i$  is the reciprocal lattice basis corresponding to the  $\mathbf{a}_i$  given above. We assume the onsite energies of the  $p$  and  $s$  orbitals to be  $\Delta_s$  and  $\Delta_p$ , respectively, and they satisfy  $\Delta_s < \Delta_p < 0$ . Although  $\Delta_s$  and  $\Delta_p$  are free parameters, to simplify the expression of the following Hamiltonian and the associated eigenvalues of flat bands, we choose a set of particular values  $\Delta_p = (\sqrt{2} - \sqrt{10})|t|$ ,  $\Delta_s = -(\sqrt{2} + \sqrt{10})|t|$ . The total Hamiltonian is given by

$$H_{L \oplus \tilde{L}}(\mathbf{k}) = \begin{pmatrix} \Delta_s \mathbb{I}_{4 \times 4} & S^\dagger(\mathbf{k}) \\ S(\mathbf{k}) & \Delta_p \mathbb{I}_{6 \times 6} \end{pmatrix}. \quad (\text{F9})$$

Following the same analysis below Eq. (F3), one can find that there will be  $|L| - \text{rank}(S(\mathbf{k}))$  states at the energy  $\Delta_p$  and  $|\tilde{L}| - \text{rank}(S(\mathbf{k}))$  states at the energy  $\Delta_s$ . While the other  $2 \times \text{rank}(S(\mathbf{k}))$  states have the energies  $\frac{\Delta_s + \Delta_p}{2} \pm \sqrt{\xi_n^2(\mathbf{k}) + (\Delta_s - \Delta_p)^2/4}$ , with  $\xi_n(\mathbf{k})$  being the nonzero singular values of  $S(\mathbf{k})$ . Since  $\text{rank}(S(\mathbf{k})) = |\tilde{L}| = 4$  at generic momenta, there are two flat bands at  $E = \Delta_p \approx -1.75|t|$ , as shown in Fig. 16(e). The effective Hamiltonian for  $L$  ( $p$ -bands) and  $\tilde{L}$  ( $s$ -bands) can be derived through the second order perturbation theory as

$$H_L(\mathbf{k}) \approx \Delta_p + \frac{S(\mathbf{k})S^\dagger(\mathbf{k})}{\Delta_p - \Delta_s}, \quad H_{\tilde{L}}(\mathbf{k}) \approx \Delta_s - \frac{S^\dagger(\mathbf{k})S(\mathbf{k})}{\Delta_p - \Delta_s}, \quad (\text{F10})$$

respectively. The energy spectra of  $H_{\tilde{L}}$  and  $H_L$  are given in Fig. 16(d) and (e), respectively, which qualitatively reproduce the band structures of  $H_{L \oplus \tilde{L}}(\mathbf{k})$ .

One may notice that in addition to the flat bands at  $\Delta_p$ , there are two other sets of flat bands at the top and the bottom of the band structure of  $H_{L \oplus \tilde{L}}$  which are both double-degenerate. They come from the double-degenerate singular value  $2\sqrt{2}t$  of  $S(\mathbf{k})$  at arbitrary  $\mathbf{k}$ . Indeed from the above analysis, this singular value leads to flat bands at  $\frac{\Delta_s + \Delta_p}{2} \pm \sqrt{8t^2 + (\Delta_s - \Delta_p)^2/4}$ , i.e., 0 and  $-2\sqrt{10}|t|$ , respectively. The flat band at zero energy corresponds to the first-principles flat band at the Fermi level (Fig. 16(c)). Hence, the bipartite lattice in this example give rise to the flat bands at  $E = \Delta_p$ , which come from the rank of  $S(\mathbf{k})$ , as well as to the two degenerate extra flat bands which come from the particular singular values of  $S(\mathbf{k})$ .

The band structure features obtained from  $S$ -matrix method is consistent with the first-principle calculations of  $\text{Pb}_2\text{Sb}_2\text{O}_7$ . Such an analysis applies to some other materials with the pyrochlore structure, such as  $\text{Sn}_2\text{Nb}_2\text{O}_7$  [ICSD 163817, SG 227 ( $Fd\bar{3}m$ )],  $\text{Ca}_2\text{Nb}_2\text{O}_7$  [ICSD 22411, SG 227 ( $Fd\bar{3}m$ )],  $\text{Bi}_2\text{Pt}_2\text{O}_7$  [ICSD 202346, SG 227 ( $Fd\bar{3}m$ )],  $\text{Bi}_2\text{Ir}_2\text{O}_7$  [ICSD 161103, SG 227 ( $Fd\bar{3}m$ )],  $\text{Bi}_2\text{Rh}_2\text{O}_7$  [ICSD 161099, SG 227 ( $Fd\bar{3}m$ )],  $\text{Ge}_2\text{In}_2\text{O}_7$  [ICSD 239593, SG 227 ( $Fd\bar{3}m$ )], and  $\text{Sn}_2\text{Ta}_2\text{O}_7$  [ICSD 27119, SG 227 ( $Fd\bar{3}m$ )]. Note that all of these materials are part of the curated

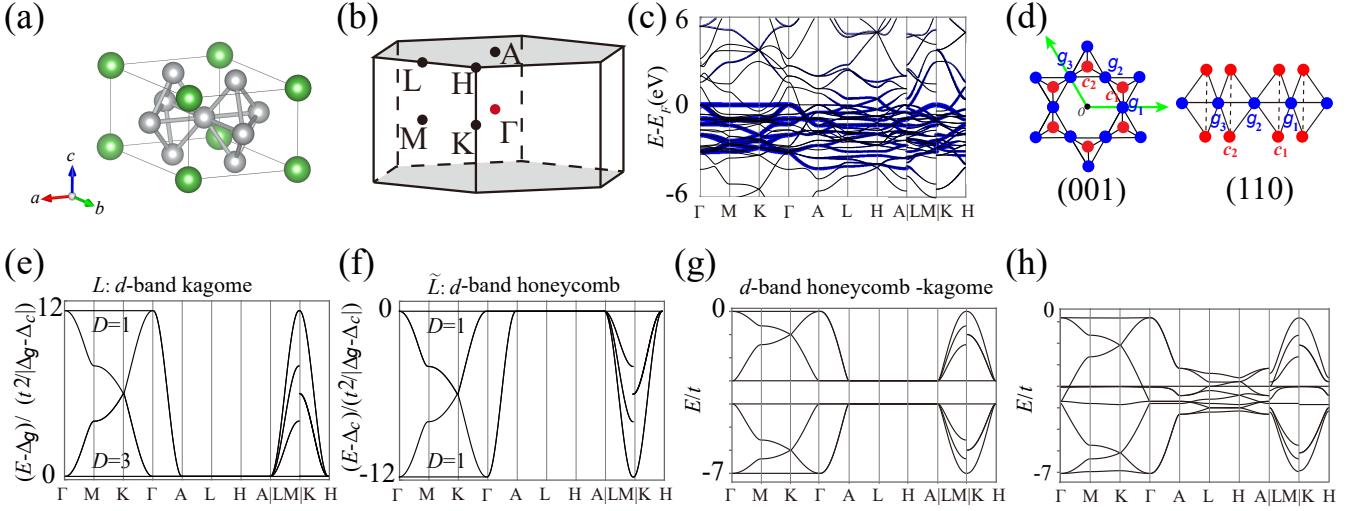


Figure 17. (a) The crystal structure of  $\text{CaNi}_5$ . The Ca and Ni atoms are represented by the green and gray balls, respectively. (b) The bulk BZ of  $\text{CaNi}_5$ . (c) Band structure of  $\text{CaNi}_5$  without spin-orbit coupling, where the weights of  $d_{xz}$  and  $d_{yz}$  orbitals on Ni are highlighted in blue. (d) The schematic pictures of the top- and side-view (*i.e.*, along the respective (001) and (110) directions) of the bipartite lattice in  $\text{CaNi}_5$ . (e) and (f) The band structures of the effective Hamiltonians of  $d_{xz}$ ,  $d_{yz}$  orbitals on Kagome ( $L$ ) and honeycomb ( $\tilde{L}$ ) lattices, where the effective Hamiltonians are obtained from the  $S$ -matrix method through second order perturbation theory. The degeneracy  $D$  of each segment of flat bands is indicated in the plots. (g) The band structure of  $d_{xz}$ ,  $d_{yz}$  orbitals on the bipartite lattice  $\tilde{L} \oplus L$ . (h) The band structure of  $\tilde{L} \oplus L$  with intra-sublattice couplings.

list in Appendix H 1.

### 3. $\text{CaNi}_5$

The crystal structure of  $\text{CaNi}_5$  [ICSD 54474, SG 191 ( $P6/mmm$ )] is shown in Fig. 17(a). The  $1a$  Wyckoff position is occupied by Ca and both the  $3g$  and  $2c$  Wyckoff positions are occupied by Ni. The band structure of  $\text{CaNi}_5$  is plotted in Fig. 17(c), which has an extremely flat band at the Fermi level in the  $k_z = 0$  plane. By analyzing the orbital-projected band structure, we find that the flat bands mainly arise from the  $d_{xz}$  and  $d_{yz}$  orbitals on Ni.

In  $\text{CaNi}_5$ , Ni form two sublattices: Ni atoms at  $2c$  form a honeycomb sublattice, and Ni atoms at  $3g$  form a Kagome sublattice. In the following, to understand the origin of this flat band, we first only consider couplings between two sublattices. We will consider couplings within each sublattice at the end of this subsection. We refer to the sublattices formed by Ni atoms at  $2c$  and  $3g$  as  $\tilde{L}$  and  $L$ , respectively. We label the  $3g$  and  $2c$  positions as  $g_i$  ( $i = 1, 2, 3$ ) and  $c_i$  ( $i = 1, 2$ ), respectively, as shown in Fig. 17(d). They form a bipartite lattice since we ignore the hoppings within each of them. We introduce the  $S$  matrix formed by the  $d_{xz}$  and  $d_{yz}$  orbitals in  $\tilde{L}$  and  $L$  as  $S_{\alpha a}^\dagger = \langle \phi_\alpha(\mathbf{k}) | H | \phi_a(\mathbf{k}) \rangle$ .  $\alpha = i + 2(j - 1)$  corresponds to the  $d_{yz}$  ( $j = 1$ ),  $d_{xz}$  ( $j = 2$ ) orbitals at the  $i$ th site ( $i = 1, 2$ ) in  $\tilde{L}$ .  $a = i + 3(j - 1)$  corresponds to the  $d_{yz}$  ( $j = 1$ ),  $d_{xz}$  ( $j = 2$ ) orbitals at the  $i$ th site ( $i = 1, 2, 3$ ) in  $L$ . Based on the MLWF, we consider the coupling between  $d_{xz}$  orbital at  $c_2$  and  $d_{yz}$  orbital at  $g_3$  and set its strength to  $t$ . The  $S$ -matrix reads

$$S^\dagger(\mathbf{k}) = \frac{t}{4} (1 + e^{ik_3}) \begin{pmatrix} 4 & 1 & e^{ik_1} & 0 & -\sqrt{3} & \sqrt{3}e^{ik_1} \\ 4e^{ik_2} & 1 & 1 & 0 & -\sqrt{3} & \sqrt{3} \\ 0 & -\sqrt{3} & \sqrt{3}e^{ik_1} & 0 & 3 & 3e^{ik_1} \\ 0 & -\sqrt{3} & \sqrt{3} & 0 & 3 & 3 \end{pmatrix}, \quad (\text{F11})$$

where  $(k_1, k_2, k_3)$  are the coordinates of the momentum  $\mathbf{k} = \sum_{i=1}^3 k_i \mathbf{b}_i$ , where  $\mathbf{b}_i$  is the reciprocal lattice basis corresponding to the primitive unit cell spanned by  $\mathbf{a}_1 = b(1, 0, 0)$ ,  $\mathbf{a}_2 = b(-1/2, \sqrt{3}/2, 0)$ ,  $\mathbf{a}_3 = c(0, 0, 1)$ , with  $b$  and  $c$  being the lattice parameters. Note that the values of the hopping amplitudes appearing in  $S_{i,j}^\dagger(\mathbf{k})$  are constrained by the space group symmetries.

The Hamiltonians of the bipartite lattice  $L \oplus \tilde{L}$  and the  $\tilde{L}$  and  $L$  are given by Eqs. (F9) and (F10) except that

$\{\Delta_s, \Delta_p\}$  should be replaced by  $\{\Delta_c, \Delta_g\}$ . Here  $\Delta_c$  is the onsite energy of d orbitals on the honeycomb lattice and  $\Delta_g$  is the onsite energy of d orbitals on the Kagome lattice. In the following we choose  $\Delta_c = -4|t|$  and  $\Delta_g = -3|t|$ . The  $S(\mathbf{k})$  matrix has rank three at generic momentum. Following the same analysis below Eq. (F3), one can find that in the band structure of  $H_{L \oplus \tilde{L}}$  there will be  $|L| - \text{rank}(S(\mathbf{k})) = 3$  states at the energy  $\Delta_g$  and  $|\tilde{L}| - \text{rank}(S(\mathbf{k})) = 1$  states at the energy  $\Delta_c$ , as shown in Fig. 17(g). In addition, since  $S$  has a constant singular value  $2\sqrt{3}|t| \cos \frac{k_3}{2}$  in a horizontal plane with fixed  $k_3$ , due to the discussion below Eq. (F3), there is a set of 2D flat bands at  $\frac{\Delta_g + \Delta_c}{2} \pm \sqrt{12t^2 \cos^2 \frac{k_3}{2} + (\Delta_g - \Delta_c)^2/4}$ . For  $k_3 = 0$ , the two additional flat bands at  $E = 0$  and  $E = -7t$ , respectively.

The effective Hamiltonian  $H_{\tilde{L}} \approx \Delta_c - S^\dagger(\mathbf{k})S(\mathbf{k})/(\Delta_g - \Delta_c)$  describes a 3D system consisting of honeycomb lattice layers. It has single particle dimension four. Since  $S(\mathbf{k})$  has rank three over the whole Brillouin zone (or smaller ranks at high symmetry momenta) and has a constant singular value  $2\sqrt{3}|t| \cos \frac{k_3}{2}$  in a horizontal plane with fixed  $k_3$ , the band structure of  $H_{\tilde{L}}$  has a 3D flat band at  $E = \Delta_c$  and a 2D flat band  $E = \Delta_c - \frac{12t^2}{\Delta_g - \Delta_c} \cos^2 \frac{k_3}{2}$  in any fixed- $k_3$  plane (Fig. 17(f))<sup>69</sup>. Similarly, the effective Hamiltonian of the Kagome lattice ( $H_L \approx \Delta_g - S(\mathbf{k})S^\dagger(\mathbf{k})/(\Delta_c - \Delta_g)$ ), which has dimension six, has a three-fold degenerate 3D flat band at  $E = \Delta_g$  and a 2D flat band at  $E = \Delta_g - \frac{12t^2}{\Delta_c - \Delta_g} \cos^2 \frac{k_3}{2}$  in any fixed- $k_3$  plane (Fig. 17(e)).

Comparing with the band structure from first-principle calculations in Fig. 17(c), we identify the flat band of  $L \oplus \tilde{L}$  at  $E = 0$  as the flat band near the Fermi level in CaNi<sub>5</sub>. To further check the robustness of the flat bands in Fig. 17(g), we consider the couplings within each sublattice. We set the hopping between  $d_{yz}$  orbital at  $c_1$  and  $d_{xz}$  orbital at  $c_2$  ( $d_{yz}$  orbital at  $g_1$  and  $d_{yz}$  orbital at  $g_2$ ), as well as the equivalent hopping terms due to symmetries, to  $0.1t$  ( $0.2t$ ) (Fig. 17(d)). The resulting band structure is shown in Fig. 17(h). One can see that these intra-sublattice hopping terms barely have any effect on the flat band at  $E = 0$  and  $E = -7t$  in the  $k_3 = 0$  plane.

The above explanations of the extremely flat band in CaNi<sub>5</sub> can also be applied to some other materials with AB<sub>5</sub>-type structure in SG 191 ( $P6/mmm$ ), such as LaNi<sub>5</sub> [ICSD 242027, SG 191 ( $P6/mmm$ )], ScNi<sub>5</sub> [ICSD 646468, SG 191 ( $P6/mmm$ )], CaPd<sub>5</sub> [ICSD 106357, SG 191 ( $P6/mmm$ )], SrPd<sub>5</sub> [ICSD 105707, SG 191 ( $P6/mmm$ )], BaPd<sub>5</sub> [ICSD 616030, SG 191 ( $P6/mmm$ )], YNi<sub>5</sub> [ICSD 647075, SG 191 ( $P6/mmm$ )] and YFe<sub>5</sub> [ICSD 103699, SG 191 ( $P6/mmm$ )]. Note that all of these materials are listed in Appendix H1.

#### 4. Ca<sub>2</sub>NCl

The crystal structure and BZ of Ca<sub>2</sub>NCl [ICSD 62555, SG 166 ( $R\bar{3}m$ )] are shown in Figs. 18(a) and (b), respectively. Since it is a layered material, we have chosen to use the conventional unit cell rather than the primitive unit cell for the band structure calculation. The 3a, 3b and 6c Wyckoff positions are occupied by the Cl, N and Ca atoms, respectively. The lattice parameters of the conventional cell are  $a = b = 3.67\text{\AA}$  and  $c = 19.89\text{\AA}$ . As shown in the band structure in Fig. 18(c), the highest valence band is flat along all the high-symmetry paths. From the orbital-projected band structure, we see that the dominant contribution to the flat band comes from the  $p$  orbitals of N. Since the distance between two neighboring N layers is large ( $c/3 = 6.63\text{\AA}$ ), in the following we will omit the inter-layer couplings. This is a reasonable approximation because, as shown in Fig. 18(c), the band dispersion of the non-flat bands in the  $k_z$  direction, e.g. paths FA, LM, KH, is weak compared to the in-plane dispersion.

To explain the flat bands in Fig. 18(c), we first build a 2D tight-binding model consisting of  $p_x, p_y$  and  $p_z$  orbitals on the N atoms in a single N layer. The N atoms in a single layer form a simple triangular lattice. The tight-binding Hamiltonian on the  $p_x, p_y, p_z$  orbitals is given by

$$H(\mathbf{k}) = 2 \begin{pmatrix} H_{12}(\mathbf{k}) & H_3(\mathbf{k}) \\ H_3^\dagger(\mathbf{k}) & \Delta + t_z^{pp\pi} [\cos k_1 + \cos k_2 + \cos(k_1 + k_2)] \end{pmatrix}, \quad (\text{F12})$$

with the terms

$$H_{12}(\mathbf{k}) = \begin{pmatrix} t^{pp\sigma} \cos k_1 + \frac{t^{pp\sigma} + 3t^{pp\pi}}{4} [\cos k_2 + \cos(k_1 + k_2)] & \frac{\sqrt{3}(t^{pp\pi} - t^{pp\sigma})}{4} [\cos k_2 - \cos(k_1 + k_2)] \\ \frac{\sqrt{3}(t^{pp\pi} - t^{pp\sigma})}{4} [\cos k_2 - \cos(k_1 + k_2)] & t^{pp\pi} \cos k_1 + \frac{3t^{pp\sigma} + t^{pp\pi}}{4} [\cos k_2 + \cos(k_1 + k_2)] \end{pmatrix}. \quad (\text{F13})$$

and

$$H_3^\dagger(\mathbf{k}) = \left( \frac{\sqrt{3}t^p}{8} [\cos k_2 - \cos(k_1 + k_2)] \quad \frac{t^p}{8} [-2\cos k_1 + \cos k_2 + \cos(k_1 + k_2)] \right) \quad (\text{F14})$$

Here  $t^{pp\pi}$  and  $t^{pp\sigma}$  are the  $\pi$ -bond and  $\sigma$ -bond strengths between  $p_x$  and  $p_y$  orbitals,  $t_z^{pp\pi}$  is the  $\pi$ -bond strength

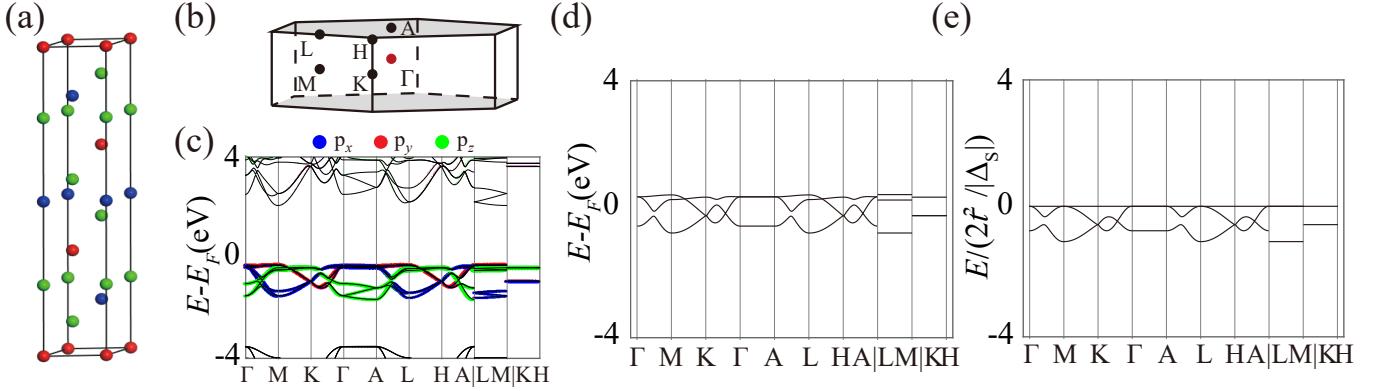


Figure 18. (a) The crystal structure of  $\text{Ca}_2\text{NCl}$ , where the N atoms are represented by the blue balls. (b) The bulk BZ of  $\text{Ca}_2\text{NCl}$ . (c) Band structure of  $\text{Ca}_2\text{NCl}$  without spin-orbit coupling. The weights of the  $p$  orbitals N on the highest set of valence bands are highlighted in blue for the  $p_x$  orbitals, red for the  $p_y$  orbitals and green for the  $p_z$  orbitals. (d) Band structure of the three band Hamiltonian in Eq. (F12) with the parameters extracted from the MLWF calculation. (e) Band structure given by the  $S$ -matrix method given in Eq. (F18).

between  $p_z$  orbitals, and  $t^p/8$  is the strength of coupling between a  $p_y$  orbital at  $(0, 0, 0)$  and a  $p_z$  orbital at  $(0, 1, 0)$ . As mentioned in Appendix F 3, the hopping amplitudes appearing in Eq. (F12) are constrained by the space group symmetries.  $(k_1, k_2)$  is the coordinate of the momentum  $\mathbf{k} = \sum_{i=1}^2 k_i \mathbf{b}_i$ , where  $\mathbf{b}_i$  is the reciprocal lattice basis corresponding to the unit cell spanned by  $\mathbf{a}_1 = a(1, 0)$ ,  $\mathbf{a}_2 = a(-\frac{1}{2}, \frac{\sqrt{3}}{2})$ . We set the difference of the onsite energy of  $p_z$  and  $p_{x,y}$  orbitals as  $\Delta$ . From the MLWF we extract the parameters  $\Delta = 0.04\text{eV}$ ,  $t^{pp\sigma} = 0.21\text{eV}$ ,  $t_z^{pp\pi} = -0.10\text{eV}$ ,  $t^{pp\pi} = -0.08\text{eV}$ , and  $t^p = 0.16\text{eV}$ . The tight-binding band structure is shown in Fig. 18(d). It correctly reproduces the flat band from the first-principles calculation. We find that the flatness comes from a set of conditions for the hopping terms that are approximately satisfied in the MLWF model. As an example, we take the path  $\Gamma\text{M}$  ( $k_1 = 0$ ) to show one such conditions. In this path, the Hamiltonian is simplified to

$$H(0, k_2) = 2 \begin{pmatrix} t^{pp\sigma} + \frac{t^{pp\sigma} + 3t^{pp\pi}}{2} \cos k_2 & 0 & 0 \\ 0 & t^{pp\sigma} + \frac{3t^{pp\sigma} + t^{pp\pi}}{2} \cos k_2 & -\frac{t^p}{4} + \frac{t^p}{4} \cos k_2 \\ 0 & -\frac{t^p}{4} + \frac{t^p}{4} \cos k_2 & \Delta + t_z^{pp\pi}(1 + 2 \cos k_2) \end{pmatrix} \quad (\text{F15})$$

There would be an *exact* flat band at  $E = 2t^{pp\sigma}$  along this path if  $t^{pp\sigma} + 3t^{pp\pi} = 0$ . This condition is approximately satisfied by the actual values extracted from MLWFs ( $t^{pp\sigma} + 3t^{pp\pi} = -0.03\text{eV}$ ). As shown in Fig. 18(d), if the condition  $t^{pp\sigma} + 3t^{pp\pi} = 0$  is not strictly satisfied well, the band near  $E = 2t^{pp\sigma}$  becomes weakly dispersive but is still relatively flat. This follows from the first-principles calculations.

The bands around  $3\text{eV}$  in Fig. 18(c) are mostly due to the Ca atoms. We notice that the nearest neighbors of N atoms are the Ca atoms. Hence the strongest hopping terms in this system are those between N and Ca atoms. In the following, we construct a  $S$ -matrix between the N and Ca atoms and derive Eq. (F12) as an effective Hamiltonian from the second-order perturbation of this  $S$ -matrix model. The set of conditions that guarantee the flat band are automatically implied by the  $S$ -matrix. We refer to the sublattices formed by Ca atoms and N atoms as  $\tilde{L}$  and  $L$ , respectively. We introduce the  $S$  matrix formed by the  $s$  or  $d_z^2$  orbital in  $\tilde{L}$  and  $p$  orbitals in  $L$  as  $S_{\alpha a}^\dagger = \langle \phi_\alpha(\mathbf{k}) | H | \phi_a(\mathbf{k}) \rangle$ . The index  $\alpha = (1, 2)$  corresponds to the  $s$  orbitals at  $(\frac{1}{3}, \frac{2}{3}, x)$  and  $(\frac{1}{3}, \frac{2}{3}, 1-x)$  in  $\tilde{L}$ .  $a = (1, 2, 3)$  corresponds to the  $p_x$ ,  $p_y$  and  $p_z$  orbitals at  $(0, 0, 1/2)$  in  $L$ . The  $S$ -matrix reads

$$S^\dagger(\mathbf{k}) = \frac{t}{4} \begin{pmatrix} -\sqrt{3}(-1 + e^{ik_1}) e^{ik_2} & -e^{i(k_1+k_2)} - e^{ik_2} + 2 & 2\lambda(1 + e^{ik_2} + e^{i(k_1+k_2)}) \\ -\sqrt{3}(-1 + e^{ik_1}) & -2e^{i(k_1+k_2)} + e^{ik_1} + 1 & -2\lambda(1 + e^{ik_1} + e^{i(k_1+k_2)}) \end{pmatrix}, \quad (\text{F16})$$

Here,  $t$  is the strength of coupling between the  $s$  or  $d_z^2$  orbital at  $(\frac{1}{3}, \frac{2}{3}, x)$  and the  $p_y$  orbital at  $(0, 0, 0)$ ,  $\lambda t$  is the strength of coupling between the  $s$  orbital at  $(\frac{1}{3}, \frac{2}{3}, x)$  and the  $p_z$  orbital at  $(0, 0, 0)$ . The Hamiltonians of the bipartite lattice  $L \oplus \tilde{L}$  and the  $\tilde{L}$  and  $L$  are given by Eq. (F9) and Eq. (F10), where  $\Delta_p = 0$  is the onsite energy of  $L$  and

$\Delta_s > 0$  is the onsite energy of  $\tilde{L}$ . The effective Hamiltonian of  $L$  ( $p$ -bands) is given by

$$H_L(\mathbf{k}) \approx -\frac{S(\mathbf{k})S^\dagger(\mathbf{k})}{\Delta_s}, \quad (\text{F17})$$

The explicit form of  $H_L$  is given by

$$\begin{aligned} H_L(\mathbf{k}) &\approx -\frac{S(\mathbf{k})S^\dagger(\mathbf{k})}{\Delta_s} \\ &= \frac{-t^2}{4\Delta_s} \begin{pmatrix} 3 - 3\cos k_1 & \sqrt{3}[\cos k_2 - \cos(k_1 + k_2)] & \sqrt{3}\lambda[\cos k_2 - \cos(k_1 + k_2)] \\ \sqrt{3}[\cos k_2 - \cos(k_1 + k_2)] & 3 + \cos k_1 - 2[\cos k_2 + \cos(k_1 + k_2)] & \lambda[-2\cos k_1 + \cos k_2 + \cos(k_1 + k_2)] \\ \sqrt{3}\lambda[\cos k_2 - \cos(k_1 + k_2)] & \lambda[-2\cos k_1 + \cos k_2 + \cos(k_1 + k_2)] & 4\lambda^2 \left[ \frac{3}{2} + \cos k_1 + \cos k_2 + \cos(k_1 + k_2) \right] \end{pmatrix}. \end{aligned} \quad (\text{F18})$$

From the MLWF we know that the strength of coupling between the  $s$  orbital at  $(\frac{1}{3}, \frac{2}{3}, x)$  and the  $p_y$  orbital at  $(0, 0, 0)$  is bigger than that of coupling between the  $s$  orbital at  $(\frac{1}{3}, \frac{2}{3}, x)$  and the  $p_z$  orbital at  $(0, 0, 0)$ . Meanwhile, they have opposite sign. Thus, we set  $\lambda \simeq -0.71$  in the calculation. The band structure of the  $L$  sublattice is shown in Fig. 18(e). Since the rank of  $S(\mathbf{k})$  is two at generic momentum, there is a single flat band at  $E = 0$ .  $H_L$  has the same form as Eq. (F12) with the five parameters given by  $t^{pp\sigma} = 3t^2/(8\Delta_s)$ ,  $t^{pp\pi} = -t^2/(8\Delta_s)$ ,  $t_z^{pp\pi} = -\lambda^2 t^2/(2\Delta_s)$ ,  $t^p = -\lambda t^2/\Delta_s$ , and  $\Delta = -3t^2/(8\Delta_s)(2\lambda^2 - 1)$ . Since the  $S$ -matrix only has two free parameters, the yielded five parameters will satisfy three conditions which are  $t_p^2 = 16t^{pp\pi}t_z^{pp\pi}$ ,  $3t_p^2 = 32(\Delta + 2t^{pp\pi})t^{pp\pi}$ , and  $t^{pp\sigma} + 3t^{pp\pi} = 0$ . Note that the last condition  $t^{pp\sigma} + 3t^{pp\pi} = 0$ , which is responsible for the flat band in the path  $\Gamma$ M was also derived in Eq. (F15) from the MLWF model.

The bands obtained from first-principle calculations are more complicated than the  $S$ -matrix band. For example, the  $p_z$ -band has a non-negligible bandwidth along the  $k_3$  direction, implying that the hopping terms between  $p_z$  orbitals in different layers are not negligible. Thus, a more realistic model can be obtained by adding these hopping terms to the  $S$ -matrix model.

The explanations that we have developed above can be applied to some other compounds, such as Ca<sub>2</sub>NBr [ICSD 62556, SG 166 ( $R\bar{3}m$ )], Sr<sub>2</sub>NCl [ICSD 172595, SG 166 ( $R\bar{3}m$ )], Sr<sub>2</sub>NBr [ICSD 172601, SG 166 ( $R\bar{3}m$ )], Ca<sub>2</sub>N [ICSD 90632, SG 166 ( $R\bar{3}m$ )]. Note that all of these materials are part of the curated list provided in Appendix H 1.

## 5. Rb<sub>2</sub>CaH<sub>4</sub>

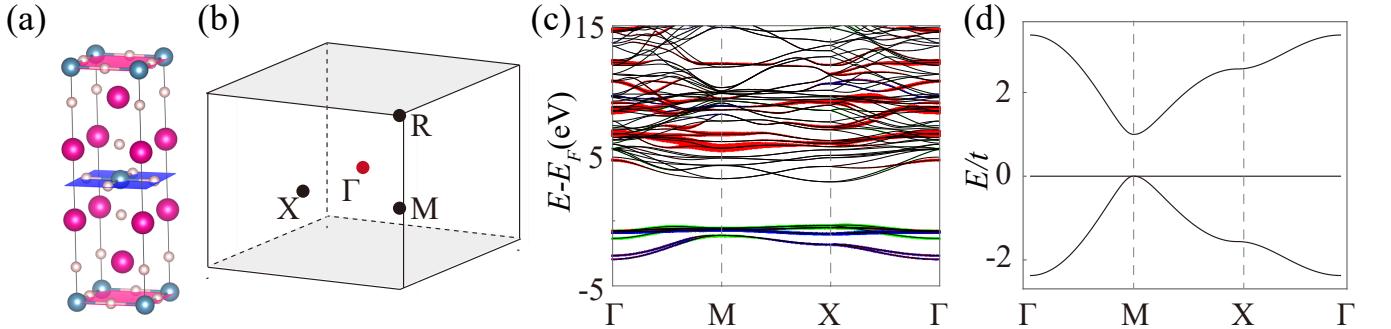


Figure 19. (a) The crystal structure of the unit cell of Rb<sub>2</sub>CaH<sub>4</sub>, where the Ca, H, and Rb atoms are represented by the cyan, pink, and purple balls, respectively. The Ca and H atoms form two Lieb lattices on the (001) Miller plane, as indicated by the pink and blue planes at  $z = 0$  and  $z = 0.5c$  (where  $c$  is the lattice constant along the (001) direction of the unit cell).(b) The 3D bulk BZ of Rb<sub>2</sub>CaH<sub>4</sub>. (c) Orbital-projected band structure along the in-plane high-symmetry  $k$ -paths of Rb<sub>2</sub>CaH<sub>4</sub> in the absence of spin-orbit coupling. The weight of  $s$  orbitals on H atoms sitting at  $4c$  and  $4e$  are highlighted in blue and green, respectively, and the weight of  $s$  and  $d_z^2$  orbitals on Ca atoms at  $2e$  is highlighted in red. (d) The band structure along the in-plane high-symmetry  $k$ -paths of the Lieb lattice given by the  $S$ -matrix method with  $\delta = t$ .

The crystal structure of Rb<sub>2</sub>CaH<sub>4</sub> [ICSD 65196, SG 139 ( $I4/mmm$ )] is shown in Fig. 19(a). The  $4e$  and  $2a$  Wyckoff positions are occupied by the Rb and Ca atoms, respectively. H atoms occupy two non-equivalent Wyckoff positions,  $4c$  and  $4e$ . Ca atoms and the H atoms at  $4e$  form two Lieb sublattices in one unit cell, which could host flat topological bands<sup>28</sup>, as shown in Fig. 19(a).

From the band structures calculations (without SOC) in the [Materials Flatband Database website](#), there are a set of flat bands near the Fermi level. As plotted in Fig. 19(c), we have analyzed the orbital-projected band structure of  $\text{Rb}_2\text{CaH}_4$  and found the flat bands are mainly composed by the  $s$  orbitals on H atoms sitting at the  $4c$  and  $4e$  positions. We also find that all the four bands contributed by the  $s$  orbitals on H atoms at  $4e$  are flat in the whole BZ and they are flat atomic bands, which can be explained by the weak hybridization between H atoms at  $4e$  and the other atoms. While for the four bands which are contributed by the  $s$  orbitals on H atoms sitting at  $4c$ , only two of them are flat and the other two bands are dispersive, implying a larger kinetic energy of the  $s$  electron at  $4c$ . In the following, we discard the flat atomic bands contributed by the H atoms at  $4e$  and explain the origin of the other flat bands contributed by the H atoms at  $4c$  using  $S$ -matrix method.

In the crystal structure of  $\text{Rb}_2\text{CaH}_4$ , the distance between two neighboring Lieb sublattices is so large ( $7.42\text{\AA}$ ) that the coupling between them is weak. Thus, we can simplify the 3D crystal lattice in  $\text{Rb}_2\text{CaH}_4$  with a 2D Lieb lattice, which is indicated by the pink plane in Fig. 19(a). For the 2D lieb lattice, we refer to the two sublattices formed by putting  $s$  orbitals at H sublattice *i.e.*,  $\{(\frac{1}{2}, 0), (0, \frac{1}{2})\}$  and putting  $s$  or  $d_z^2$  orbitals at Ca sublattice *i.e.*,  $(0, 0)$  as  $L$  and  $\tilde{L}$ , respectively. Then the  $S$  matrix can be written as

$$S^\dagger(\mathbf{k}) = t \begin{pmatrix} 1 + e^{-ik_1} & 1 + e^{-ik_2} \end{pmatrix} \quad (\text{F19})$$

where  $t$  is the strength of the coupling between the  $s$  orbital at  $(\frac{1}{2}, 0)$  and the  $s$  or  $d_z^2$  orbital at  $(0, 0)$ ;  $(k_1, k_2)$  are the coordinates of the momentum  $\mathbf{k} = \sum_{i=1}^2 k_i \mathbf{b}_i$ , where  $\mathbf{b}_i$  is the reciprocal lattice vector that corresponds to the in-plane lattice vectors  $\mathbf{a}_1 = a(1, 0)$  and  $\mathbf{a}_2 = a(0, 1)$  (where  $a$  is the in-plane lattice constant). We assume the on-site energy of  $s$  orbital on H is 0 and that of the Ca atom is  $\Delta$ . Then the total Hamiltonian of the bipartite lattice reads

$$H_{L \oplus \tilde{L}}(\mathbf{k}) = \begin{pmatrix} \Delta & S^\dagger(\mathbf{k}) \\ S(\mathbf{k}) & 0_{2 \times 2} \end{pmatrix}. \quad (\text{F20})$$

As the band structure of this Lieb lattice plotted in Fig. 19(d), there is a flat band at 0, which corresponds to the flat bands contributed by the  $s$  orbitals of H at  $4c$  in the first-principles calculations. Note that the weak band splitting of the dispersive bands of energy range from  $-5\text{eV}$  to  $-1\text{eV}$  comes from the weak coupling between the two Lieb lattices in the  $(001)$  direction. The explanations that we have developed above can be applied to some other compounds, such as  $\text{Cs}_2\text{MgH}_4$  [[ICSD 162261](#), SG 139 ( $I4/mmm$ )], and  $\text{K}_2\text{MgH}_4$  [[ICSD 68358](#), SG 139 ( $I4/mmm$ )].

## 6. $\text{KAg}[\text{CN}]_2$

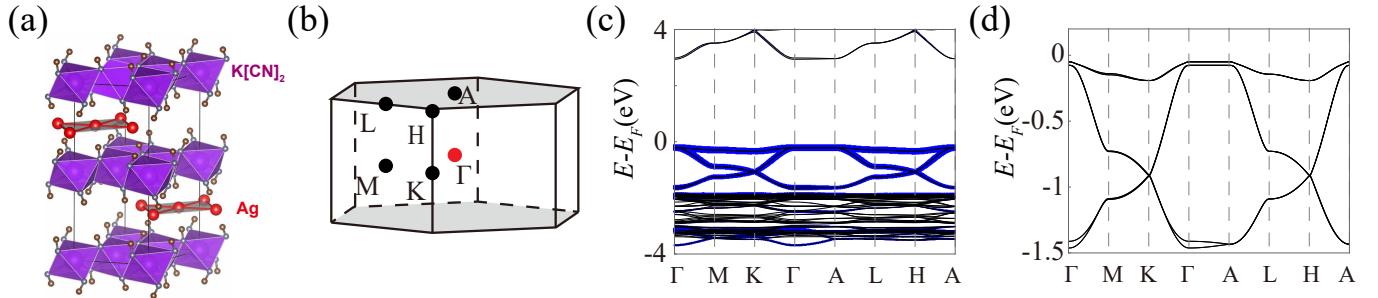


Figure 20. (a) The crystal structure of  $\text{KAg}[\text{CN}]_2$  which is a stacking of alternating molecular layer of  $\text{K}[\text{CN}]_2$  and Kagome layer of Ag atoms (in red color). (b) The bulk BZ of  $\text{KAg}[\text{CN}]_2$  with its high-symmetry  $k$  points. (c) The orbital-projected band structure of  $\text{KAg}[\text{CN}]_2$  along the high-symmetry lines from the first-principle calculation without SOC. The bands contributed by the  $s$  and  $d_{z^2}$  orbitals on Ag atoms are highlighted in blue. (d) The band structure of  $\text{KAg}[\text{CN}]_2$  from the first-principle calculation with SOC (zoomed over the energy range  $-1.5\text{eV}$  and  $0.5\text{eV}$ ), where the minimal direct band gap between the flat bands and the dispersive bands is about  $25\text{ meV}$ .

As shown in the Fig. 20(a), the crystal structure of  $\text{KAg}[\text{CN}]_2$  [[ICSD 30275](#), SG 163 ( $P\bar{3}1c$ )] is a layered structure of alternating molecular layers of  $\text{K}[\text{CN}]_2$  and approximate Kagome layers of Ag atoms. The Ag atoms sitting at  $6h$  Wyckoff position form two layers of *approximate* Kagome sublattices per unit cell on the  $(001)$  plane as indicated by the red spheres in Fig. 20(a). We emphasize that generic  $6h$  positions do not form a Kagome lattice guaranteed by

symmetries. However, the actual positions of the Ag atoms form an approximate Kagome lattice.

As shown in the band structure without SOC in Fig. 20(c) and on the [Materials Flatband Database website](#), there are two spinless flat bands near the Fermi level and the flat bands are mainly contributed by the hybridized orbital of the  $s$  and  $d_{z^2}$  orbitals on Ag atoms. The distance between two neighboring Kagome sublattices is so large (8.90Å) that the coupling between them is weak and hence all the bands along the  $\Gamma$ -A path are flat. Thus, we can simplify the 3D crystal lattice in KAg[CN]<sub>2</sub> to a 2D Kagome lattice. Since the  $s$  and  $d_{z^2}$  orbitals form the same single-value irrep  $A$  of the point group symmetry  $C_2$  at the Wyckoff position 6h, they in general hybridize with each other and form two hybridized orbitals. We model the six bands in the energy range  $-1.5 \sim 0$ eV in Fig. 20(c) by a single hybridized orbital - the one with lower energy - at every Ag atom. In the following we refer to this hybridized orbital as  $s$  orbital because it transforms under the symmetries as an  $s$  orbital. The flat bands of  $s$ -orbital Kagome lattice have been fully studied in several previous works<sup>24,26-28,69</sup>. In Appendix E 1, we have also constructed the effective Hamiltonian of the  $s$ -orbital Kagome model and explained the origin of its flat bands using an alternative  $S$ -matrix method.

In the presence of SOC<sup>28</sup>, the flat bands of the  $s$ -orbital Kagome lattice in 2D are gapped from the dispersive bands in the whole BZ and have a strong topology<sup>22</sup>, *i.e.*, the  $\mathbb{Z}_2$  topological insulator phase protected by time-reversal symmetry. For the 3D material KAg[CN]<sub>2</sub>, as shown in Fig. 20(d), the SOC also fully gaps the flat bands from the dispersive bands. A representation analysis shows that the SOC-gapped flat bands host at least a fragile topology: The irreps of the flat bands at the high-symmetry  $k$  points,  $\{\bar{A}_4\bar{A}_4, \bar{\Gamma}_4\bar{\Gamma}_5 + \bar{\Gamma}_6\bar{\Gamma}_7, \bar{H}_4\bar{H}_5 + \bar{H}_6, \bar{K}_4\bar{K}_5 + \bar{K}_6, \bar{L}_2\bar{L}_2, \bar{M}_3\bar{M}_4 + \bar{M}_5\bar{M}_6\}$ , can only be written as a difference of two BRs, *e.g.*  $\bar{E}_1@c \oplus^1 \bar{E}^2\bar{E}@d \ominus \bar{E}_1@a$ , but not a sum of BRs. The fragile topology has also been identified in Ref.<sup>47</sup>. However, here we argue that the topology of the SOC-gapped flat bands might be a *stable higher-order topology with hinge states* rather than a fragile topology. According to Ref.<sup>28</sup>, the single-layer Kagome lattice with SOC is a 2D  $\mathbb{Z}_2$  topological insulator. Then there will be two layers of 2D topological insulators per unit cell occupying the 6h positions. Because the 6h positions include all the  $C_{2x}$ -axes (and equivalent axes due to  $C_{3z}$  and inversion symmetries), all the  $C_{2x}$ -axes are occupied by the 2D topological insulators. This state is nothing but a layer construction of the  $C_2$  and time-reversal protected higher-order topological insulator<sup>50,70</sup>.

## 7. RbMo<sub>3</sub>S<sub>3</sub>

RbMo<sub>3</sub>S<sub>3</sub> [ICSD 644175, SG 176 ( $P6_3/m$ )] possesses flat bands at the Fermi level. The crystal structure of RbMo<sub>3</sub>S<sub>3</sub> is shown in Fig. 21(a), where Mo and S atoms form a quasi-1D atomic chain along the  $z$  direction. The band structure of RbMo<sub>3</sub>S<sub>3</sub> is shown in Fig. 21(c). There are flat bands on the  $k_z = 0$  and  $k_z = \pi$  planes located at the Fermi level. These flat bands are mainly composed of the  $E_{1g}$  orbitals of Mo atoms. By constructing the MLWF, we find that the maximal hopping strength between the  $E_{1g}$  orbitals of two neighboring chains is about 0.01eV, which is much smaller than the maximal intra-chain hopping (0.76eV). Hence, the flatness of bands at the Fermi level is due to the weak inter-chain coupling of the quasi-1D crystal structure.

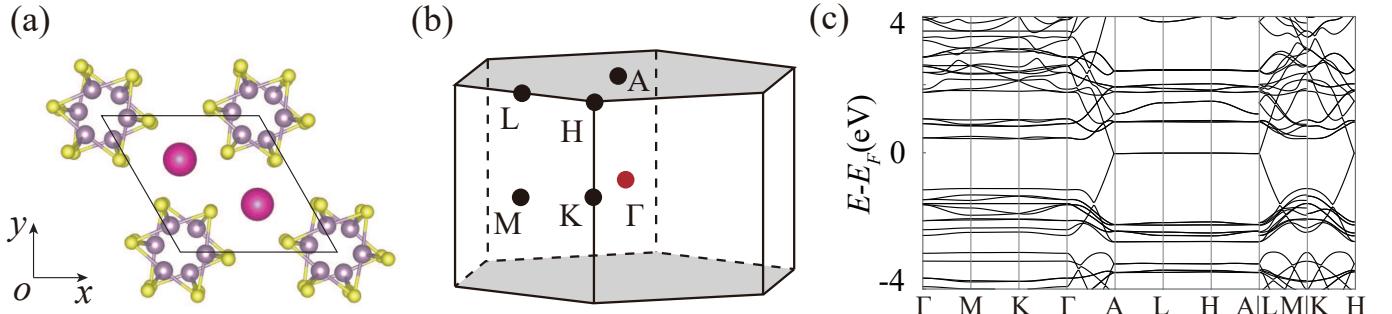


Figure 21. (a) The crystal structure of RbMo<sub>3</sub>S<sub>3</sub>. The Mo (in purple) and S atoms (in yellow) form a 1D atomic chain along the  $z$  direction. (b) The bulk BZ of RbMo<sub>3</sub>S<sub>3</sub>. (c) Band structure of RbMo<sub>3</sub>S<sub>3</sub> from first-principle calculations where spin-orbit coupling is ignored.

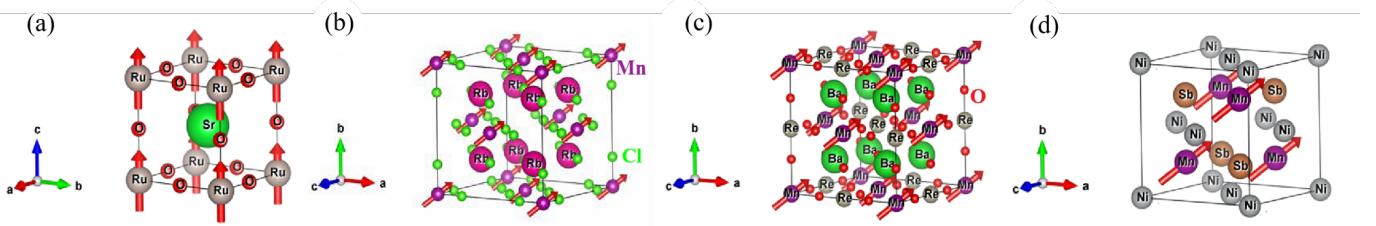


Figure 22. The experimental crystal and magnetic structures of the flat-band materials (a)  $\text{SrRuO}_3$  [ICSD 69360, SG 221 ( $Pm\bar{3}m$ )], (b)  $\text{Rb}_2\text{MnCl}_6$  [ICSD 9347 SG 225 ( $Fm\bar{3}m$ )], (c)  $\text{Ba}_2\text{MnReO}_6$  [ICSD 4169 SG 225 ( $Fm\bar{3}m$ )] and (d)  $\text{NiMnSb}$  [ICSD 54255, SG 216 ( $F\bar{4}3m$ )].

#### Appendix G: Examples of magnetic flat-band materials

In the present work, flat-band materials are obtained from the [Topological Quantum Chemistry website](#) by analyzing their crystal and band structures. As discussed in Appendix C, all the first-principles calculations performed on the [Topological Quantum Chemistry website](#) are forced to be paramagnetic, *i.e.*, without the on-site spin polarization. However, the paramagnetic phase might not be the ground state for all flat-band materials. In Appendix H, we have tagged the materials whose ground states are likely to be magnetic, reporting their magnetic properties found on the [Materials Project](#). To theoretically predict the magnetic properties of materials, we need to compare the total energy of different magnetic configurations in the ab-initio calculations.

In this appendix, we showcase four flat-band materials with experimentally known ferromagnetic ground states and compare the total energies of the paramagnetic and ferromagnetic states obtained from the first-principles calculations. The four materials are  $\text{SrRuO}_3$  [ICSD 69360, SG 221 ( $Pm\bar{3}m$ )],  $\text{Rb}_2\text{MnCl}_6$  [ICSD 9347 SG 225 ( $Fm\bar{3}m$ )],  $\text{Ba}_2\text{MnReO}_6$  [ICSD 4169 SG 225 ( $Fm\bar{3}m$ )] and  $\text{NiMnSb}$  [ICSD 54255, SG 216 ( $F\bar{4}3m$ )]. Their experimental crystal and magnetic structures are shown in Fig. 22.

For the ferromagnetic calculations we adopt the GGA+U method (LDAUTYPE=2, *i.e.*, the simplified (rotationally invariant) approach to the LSDA+U method<sup>71</sup>), which considers the on-site Hubbard  $U$  value of  $d$  or  $f$  electron in the mean-field approximation. By comparing the total energy of the non-magnetic and ferromagnetic phases for different  $U$  values (varying from 0 to 5eV) with and without SOC, as provided in the Tables XI-X, we find that the ferromagnetic phases always have a lower energy and hence the paramagnetic phase is not the ground state of these materials. The theoretically obtained magnetic moments of these four materials are in *good agreement with the experimental results*. Therefore, their magnetic ground states could be captured by the GGA+U method. Here we take  $U = 3$  eV for Ru and  $U = 4$  eV for Mn atom to meet the experimental results of magnetic structure. As shown in Figs. 23-26, with the on-site Hubbard  $U$  value of  $d$  or  $f$  electron in the mean field approximation is considered, the flat bands of the selected materials in the paramagnetic calculations are preserved and remain near the Fermi level. For example, in the ferromagnetic calculations of  $\text{SrRuO}_3$  [ICSD 69360, SG 221 ( $Pm\bar{3}m$ )] shown in Fig. 23 (for two different values of  $U$  and providing both the paramagnetic and the ferromagnetic band structures), the flat bands along high symmetry lines  $\Gamma X$  and  $MR$  at Fermi level are not settling at  $E = 0$  anymore but split into two sets of flat bands near the Fermi level. Similar conclusions hold for the three other ferromagnetic materials that we have considered in this Appendix. While a high-throughput ferromagnetic calculation is out of reach, these examples provide compelling evidence that the flat bands found in the paramagnetic calculations discussed in the results section of the manuscript, will remain in the ferromagnetic calculations.

Table VIII. The total energy comparison for paramagnetic and ferromagnetic states of SrRuO<sub>3</sub>[ICSD 69360, SG 221 ( $Pm\bar{3}m$ )]. In the FM case the magnetization points along the [001] direction of the conventional unit cell. Here, we only provide the  $z$ -component of the magnetic moment  $m_z$  in the last column. The ground state of this material is reported to be ferromagnetic with moment  $2.8 \mu B/Ru$ <sup>72-74</sup>. Our calculations show that the ferromagnetic (FM) state is more stable than the nonmagnetic (NM) state.

			U=0	U=1	U=2	U=3	U=4	U=5
Non-SOC	NM	Total energy (eV)	0	1.046	2.074	3.088	4.091	5.06
	FM	Total energy (eV)	-0.079	0.839	1.730	2.608	3.464	4.271
SOC	NM	Total energy (eV)	0.000	1.032	2.030	2.980	3.828	4.585
	FM	Total energy (eV)	-0.078	0.841	1.731	2.602	3.451	4.265
		$m_z(\mu B)$	1.6077	2.118	2.231	2.244	2.259	2.808

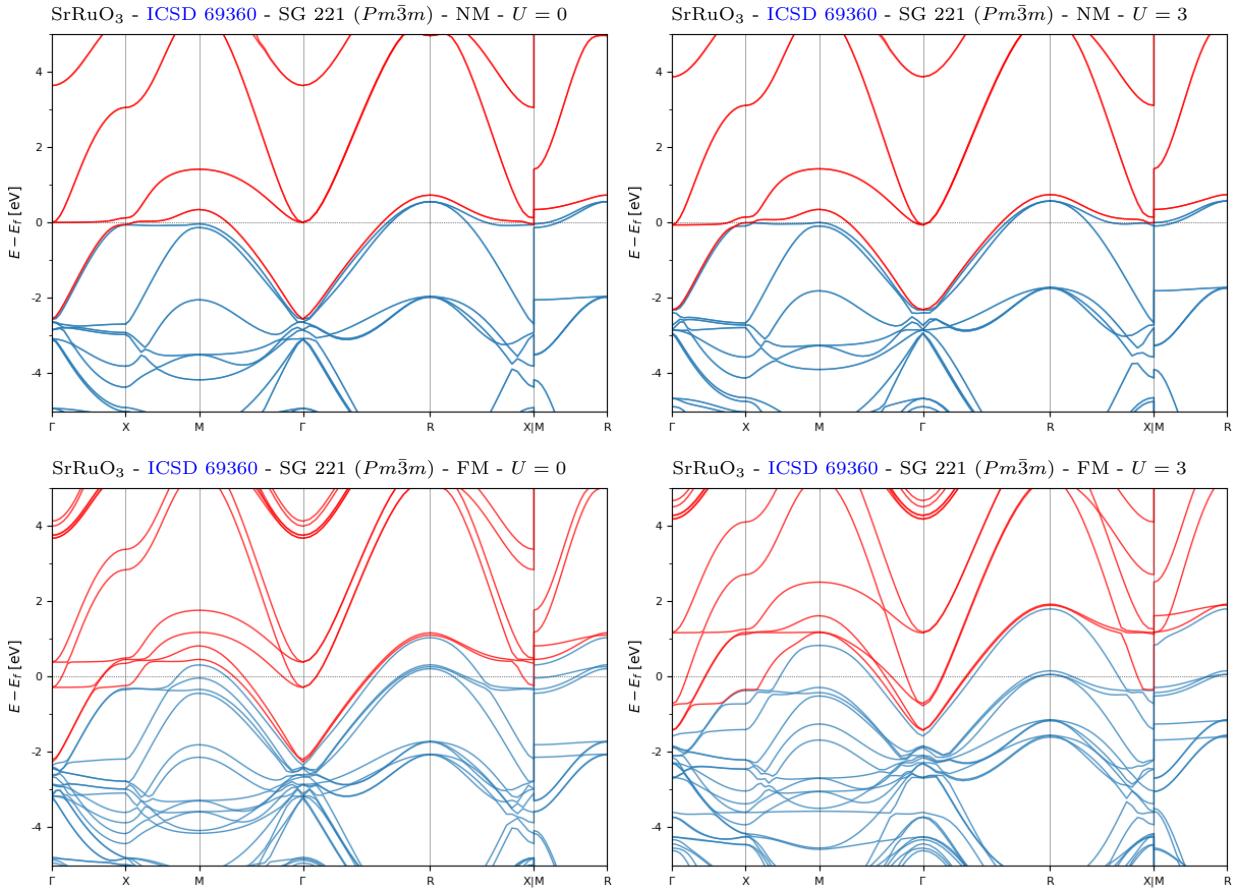


Figure 23. Band structure for SrRuO<sub>3</sub>[ICSD 69360, SG 221 ( $Pm\bar{3}m$ )] obtained with an on-site Hubbard  $U$  value for  $d$  or  $f$  electron in the mean-field approximation and including the spin-orbit coupling. Plots in the upper panel are for paramagnetic calculations (NM) while those of the lower panel are for ferromagnetic calculations (FM). Here we have considered both  $U = 0$  (left panel) and  $U = 3$  (right panel).

Table IX. The total energy comparison for paramagnetic and ferromagnetic states of  $\text{Rb}_2\text{MnCl}_6$ [ICSD 9347, SG 225 ( $Fm\bar{3}m$ )]. In the FM case the magnetization points along the  $[1,1,\bar{1}]$  direction of the conventional unit cell. Here, we only provide the  $x$ -component of the magnetic moment  $m_x$  in the last column. The lattice vectors of the primary unit cell are  $\mathbf{a}_1 = a(0 1/2 1/2)$ ,  $\mathbf{a}_2 = a(1/2 0 1/2)$  and  $\mathbf{a}_3 = a(1/2 1/2 0)$  with  $a$  is the lattice parameter. The total magnetic moment is  $3 \mu\text{B}/\text{Mn}$  which is in good agreement with the experimental  $3.9 \mu\text{B}/\text{Mn}$ <sup>75,76</sup>. The results show that the ferromagnetic (FM) state is more stable than the nonmagnetic (NM) state.

			<b>U=0</b>	<b>U=1</b>	<b>U=2</b>	<b>U=3</b>	<b>U=4</b>	<b>U=5</b>
Non-SOC	NM	Total energy (eV)	0.000	1.219	2.433	3.641	4.841	6.031
	FM	Total energy (eV)	-1.793	-1.092	-0.419	0.224	0.833	1.407
		Mag-mom ( $\mu\text{B}$ )	3.000	3.000	3.000	2.999	3.000	3.000
SOC	NM	Total energy (eV)	0.000	1.051	2.040	2.983	3.845	4.519
	FM	Total energy (eV)	-1.807	-1.102	-0.425	0.222	0.837	1.417
		$m_x(\mu\text{B})$	1.732	1.732	1.732	1.732	1.732	1.732

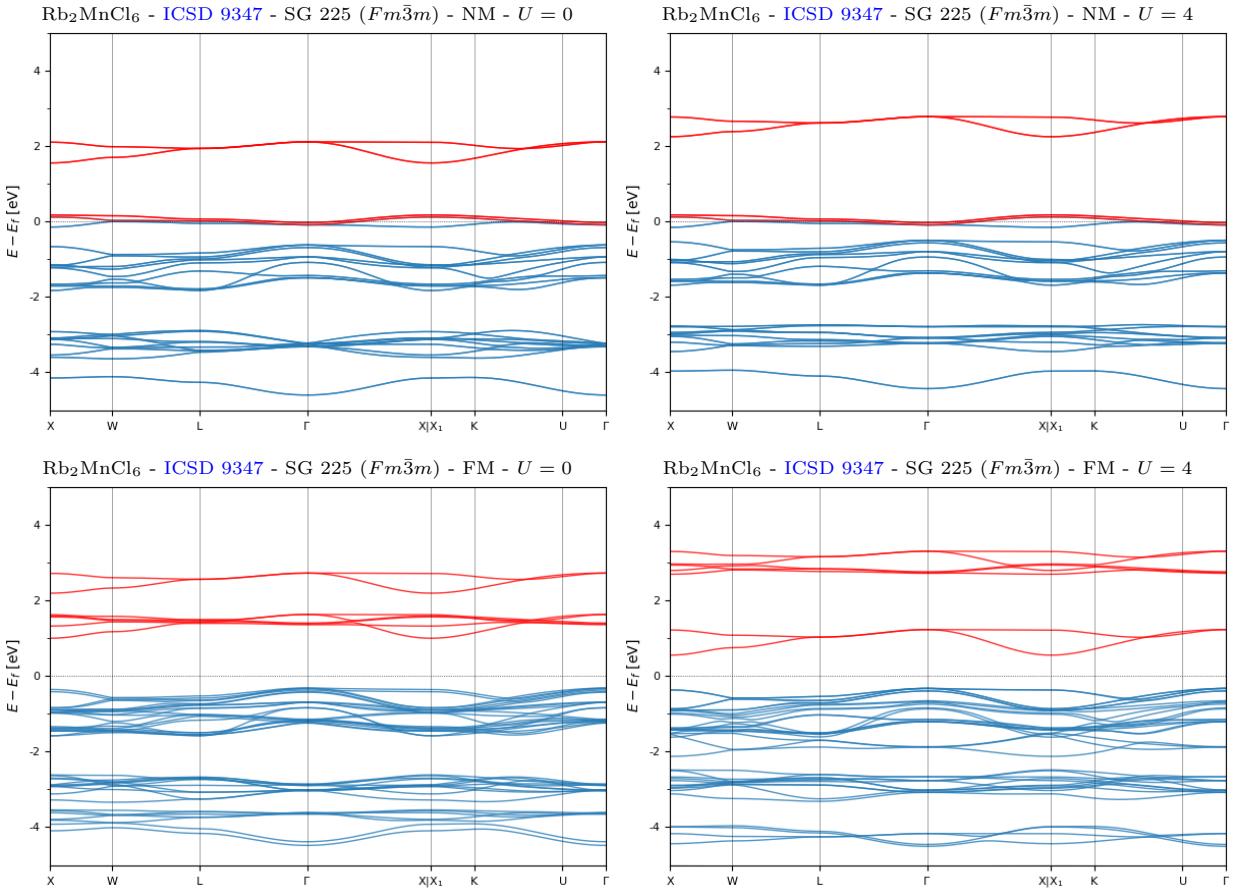


Figure 24. Band structure for  $\text{Rb}_2\text{MnCl}_6$ [ICSD 9347, SG 225 ( $Fm\bar{3}m$ )] obtained with an on-site Hubbard  $U$  value for  $d$  or  $f$  electron in the mean-field approximation and including the spin-orbit coupling. Plots in the upper panel are for paramagnetic calculations (NM) while those of the lower panel are for ferromagnetic calculations (FM). Here we have considered both  $U = 0$  (left panel) and  $U = 4$  (right panel).

Table X. The total energy comparison for paramagnetic and ferromagnetic states of  $\text{Ba}_2\text{MnReO}_6$ [ICSD 4169, SG 225 ( $Fm\bar{3}m$ )]. In the FM case the magnetization points along the  $[1,1,\bar{1}]$  direction of the conventional cell. Here, we only give the  $x$ -component of the magnetic moment  $m_x$  in the last column. The lattice vectors of the primary unit cell are  $\mathbf{a}_1 = a \begin{pmatrix} 0 & 1/2 & 1/2 \end{pmatrix}$ ,  $\mathbf{a}_2 = a \begin{pmatrix} 1/2 & 0 & 1/2 \end{pmatrix}$  and  $\mathbf{a}_3 = a \begin{pmatrix} 1/2 & 1/2 & 0 \end{pmatrix}$  with  $a$  is the lattice parameter. The theoretical magnetic moment is  $4 \mu\text{B}/\text{Mn}$  which is in good agreement with the experimental  $3.9 \mu\text{B}/\text{Mn}$ <sup>77</sup>. It shows that the ferromagnetic (FM) state is more stable than the nonmagnetic (NM) state.

			<b>U=0</b>	<b>U=1</b>	<b>U=2</b>	<b>U=3</b>	<b>U=4</b>	<b>U=5</b>
Non-SOC	NM	Total energy (eV)	0.000	0.902	1.760	2.572	3.337	4.056
	FM	Total energy (eV)	-1.331	-0.869	-0.502	-0.201	0.053	0.278
		Mag-mom ( $\mu\text{B}$ )	3.124	3.506	3.8272	3.999	4.000	4.000
SOC	NM	Total energy (eV)	0.000	0.903	1.762	2.571	3.331	4.044
	FM	Total energy (eV)	-1.269	-0.804	-0.431	-0.126	0.131	0.357
		$m_x(\mu\text{B})$	1.828	2.044	2.207	2.321	2.332	2.335

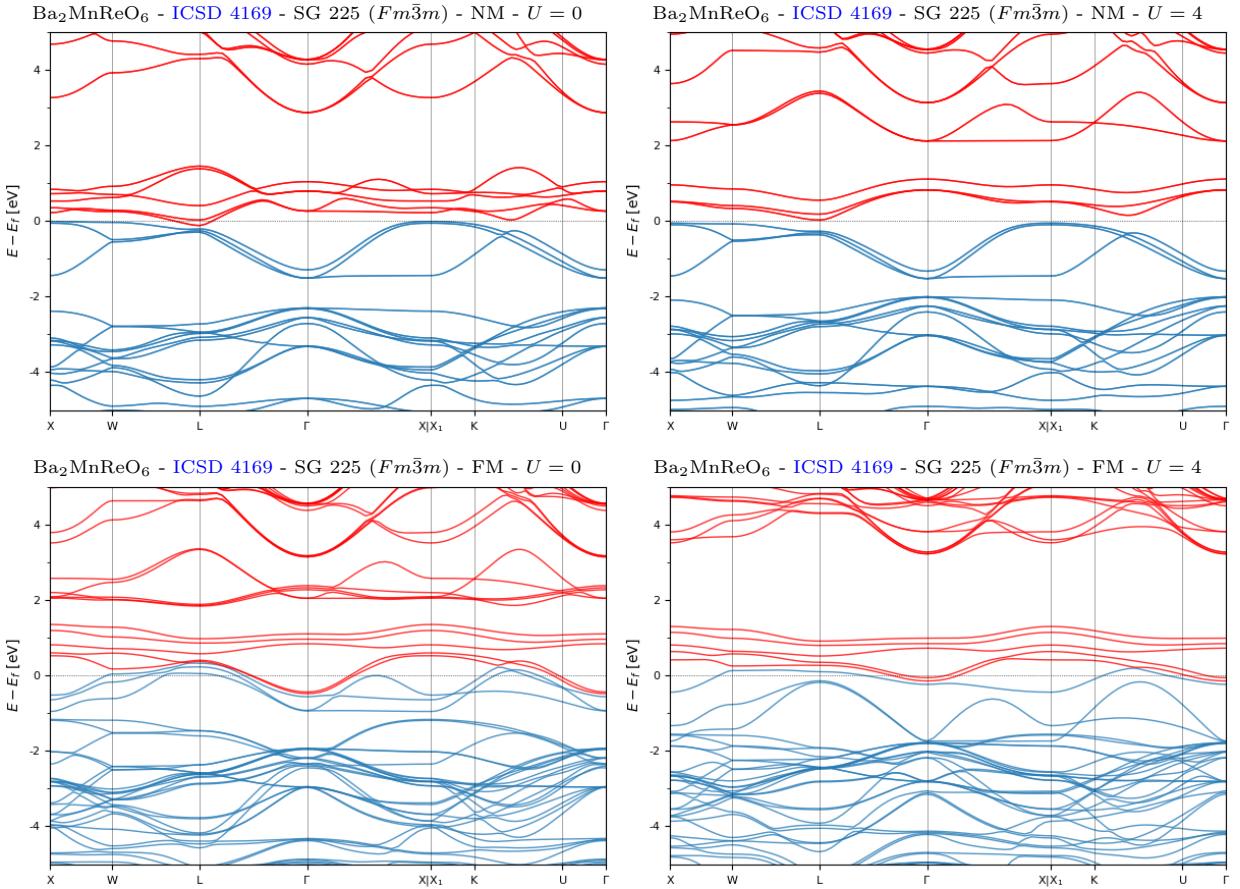


Figure 25. Band structure for  $\text{Ba}_2\text{MnReO}_6$ [ICSD 4169, SG 225 ( $Fm\bar{3}m$ )] obtained with an on-site Hubbard  $U$  value for  $d$  or  $f$  electron in the mean-field approximation and including the spin-orbit coupling. Plots in the upper panel are for paramagnetic calculations (NM) while those of the lower panel are for ferromagnetic calculations (FM). Here we have considered both  $U = 0$  (left panel) and  $U = 4$  (right panel).

Table XI. The total energy comparison for paramagnetic and ferromagnetic states of NiMnSb[ICSD 54255, SG 216 ( $F\bar{4}3m$ )]. In the FM case the magnetization points along the  $[1,1,\bar{1}]$  direction of the conventional cell. Here, we only provide the  $x$ -component of the magnetic moment  $m_x$  in the last column. The lattice vectors of the primary unit cell are  $\mathbf{a}_1 = a \begin{pmatrix} 0 & 1/2 & 1/2 \end{pmatrix}$ ,  $\mathbf{a}_2 = a \begin{pmatrix} 1/2 & 0 & 1/2 \end{pmatrix}$  and  $\mathbf{a}_3 = a \begin{pmatrix} 1/2 & 1/2 & 0 \end{pmatrix}$  with  $a$  is the lattice parameter. The total magnetic moment is  $4 \mu B/Mn$  and is in good agreement with the experiments ( $4.2 \mu B/Mn$ )<sup>78</sup>. The results show that the ferromagnetic (FM) state is more stable than the nonmagnetic or paramagnetic (NM) state.

			<b>U=0</b>	<b>U=1</b>	<b>U=2</b>	<b>U=3</b>	<b>U=4</b>	<b>U=5</b>
Non-SOC	NM	Total energy (eV)	0	1.246	2.488	3.658	5.003	6.247
	FM	Total energy (eV)	-1.445	-0.842	-0.301	0.176	0.59	0.954
		Mag-mom ( $\mu B$ )	4.000	4.000	4.040	4.150	4.225	4.289
SOC	NM	Total energy (eV)	0	1.236	2.399	3.405	4.300	5.115
	FM	Total energy (eV)	-1.434	-0.833	-0.292	0.185	0.598	0.965
		$m_x(\mu B)$	2.309	2.310	2.335	2.396	2.441	2.481

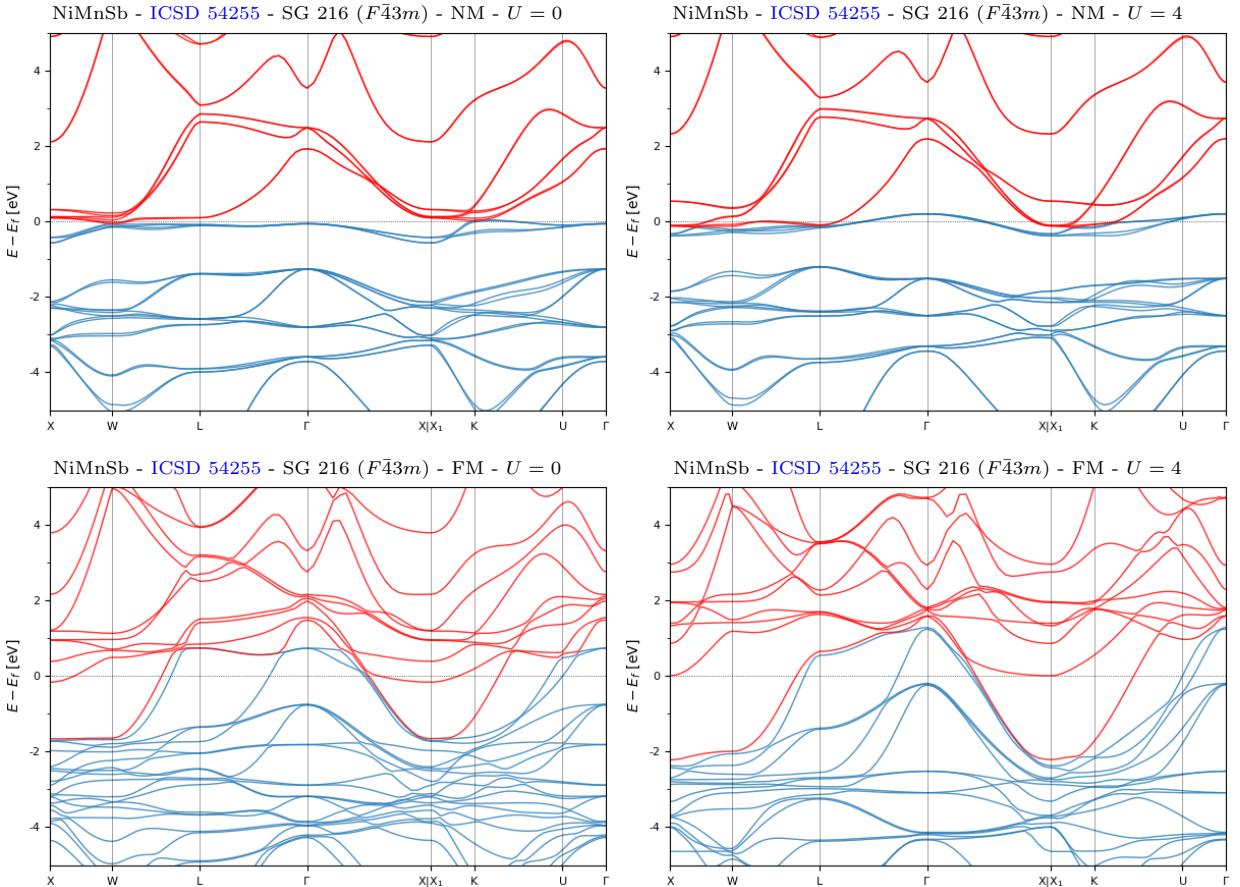


Figure 26. Band structure for NiMnSb[ICSD 54255, SG 216 ( $F\bar{4}3m$ )] obtained with an on-site Hubbard  $U$  value for  $d$  or  $f$  electron in the mean-field approximation and including the spin-orbit coupling. Plots in the upper panel are for paramagnetic calculations (NM) while those of the lower panel are for ferromagnetic calculations (FM). Here we have considered both  $U = 0$  (left panel) and  $U = 4$  (right panel).

## Appendix H: Disconnected flat bands manually selected from flat-band database

In this appendix, we provide a list of curated materials with flat bands. The analysis was manually performed on the database presented in Appendix C1. For convenience, materials with flat atomic bands are handled separately. We highlight 345 compounds hosting the most interesting flat-band features by providing their band structure and DOS.

### 1. List of curated materials with flat bands

We start with the list of 2,379 curated unique materials (as defined in Appendix C1), corresponding to 6,338 ICSD entries. This list is available in Table XII. It was obtained by performing a manual search in our database, using the tools available on [Materials Flatband Database website](#). We have applied several criteria to obtain this list:

- We required that the region of  $\Delta_E = 0.5\text{eV}$  around the Fermi level (as defined in Appendix C2a) to host only a few bands along the high symmetry lines so that the flat bands can be easily distinguished from the dispersing bands.
- Materials with trivial flat atomic bands, of which the BRs are classified as topologically trivial (*i.e.*, LCEBR), have been excluded at this stage. The methodology to detect these materials will be detailed in Appendix H2, including a complete list of candidates.
- We fixed the band width of the flat-band segment to be less than  $\omega = 0.1\text{eV}$  (see Appendix C2a).
- We requested to have at least one DOS peak in the region  $[-1\text{eV}, 1\text{eV}]$  around Fermi level with a Gaussian width  $W_{\text{peak}}$  smaller than  $1\text{eV}$  (see Appendix C2b).

Note that for a given unique compound, we might have one ICSD fulfilling all these criteria and another ICSD not satisfying one of them. Indeed, we use sharp cutoffs and different ICSD entries of a unique compound might have slightly different band structure or DOS (as explained in Appendix C). One such example is  $\text{K}_2\text{O}_7\text{Zn}_6$  [ICSD 1120, SG 102 ( $P4_2nm$ )] and [ICSD 2496, SG 102 ( $P4_2nm$ )]. The former fulfills our conditions, the latter does not. Since the differences are barely noticeable, we include all the ICSD entries of a unique compound as soon as one of them satisfies all the criteria defined above.

For each entry in Table XII, we provide the chemical formula, space group, all related ICSD numbers and possible sublattices that we have found using the procedures described in Appendices D and E. We also provide three additional attributes. First, we rely on the [Materials Project](#)<sup>79</sup> to give the magnetic properties (when available). Similarly, we indicate if a material is known to be superconductor based on the information from the [NIMS Materials Database](#)<sup>80</sup>. Finally, we tag some materials as “high quality”. These materials have a structure determination including refinement (in case of powder data including Rietveld refinement), temperature factors, pressure in the range of  $0.09 - 0.11\text{MPa}$ , temperature within the range of  $285 - 300\text{K}$  and standard deviation given for cell parameters. These are basically compounds whose crystallographic structure has been well-determined and are easy to synthesize.

Among the 2,379 curated unique materials, some of them have already been theoretically analyzed or experimentally probed in the context of flat-band materials. While we cannot pretend to be exhaustive, we list below 11 such materials, their related references and the main features of their studies.

- $\text{RuO}_2$  [ICSD 172178, SG 136 ( $P4_2/mnm$ )] was studied by angle-resolved photoemission spectroscopy (ARPES) experiments in Ref.<sup>81</sup> and was reported to host topologically trivial flat-band surface state.
- The electronic structure properties of  $\text{Y}_2\text{Ni}_7$  [ICSD 647060, SG 166 ( $R\bar{3}m$ )] have been theoretically studied in Ref.<sup>82</sup>, pointing toward the presence of flat bands to explain the magnetic properties of these materials.
- $\text{AlFe}_2\text{B}_2$  [ICSD 241907, SG 65 ( $Cmmm$ )] is a layered ferromagnet studied by ARPES in Ref.<sup>83</sup> and have been shown to host flat bands near the Fermi energy.
- Flat bands near the Fermi level have been observed in ARPES for  $\text{CaCu}_3\text{Ru}_4\text{O}_{12}$  [ICSD 95715, SG 204 ( $I\bar{m}\bar{3}$ )] in Ref.<sup>84</sup>.
- In Ref.<sup>85</sup>, a scanning tunneling microscopy (STM) experiment was performed on the ferromagnetic  $\text{Co}_3\text{Sn}_2\text{S}_2$  [ICSD 624867, SG 166 ( $R\bar{3}m$ )]. A pronounced conductance peak near the Fermi level was observed and identified as arising from the flat bands. In Ref.<sup>86</sup>, the flat bands of ferromagnetic  $\text{Co}_3\text{Sn}_2\text{S}_2$  were also associated to a sharp peak in the optical conductivity measurement.

- Topological flat bands in the vicinity of the Fermi level in CoSn [ICSD 161118, SG 191 ( $P6/mmm$ )] were studied theoretically and observed in the ARPES experiments in Ref.<sup>87,88</sup>. The tuning of the flat bands in doped CoSn was also reported experimentally in Ref.<sup>89</sup>.
- The material MgV<sub>2</sub>O<sub>4</sub> [ICSD 674693, SG 216 ( $F\bar{4}3m$ )] in its ferromagnetic phase was predicted by first-principles calculations in Ref.<sup>90</sup> to host a three-dimensional flat band near the Fermi energy.
- Pd<sub>3</sub>P<sub>2</sub>S<sub>8</sub> [ICSD 16296, SG 164 ( $P\bar{3}m1$ )] with a Kagome van-der-Waals structure was experimentally studied in Ref.<sup>91</sup> where the magnetic measurements were explained by the flat bands predicted in the first-principles calculations.
- Pd<sub>3</sub>Pb [ICSD 42600, SG 221 ( $Pm\bar{3}m$ )] was studied theoretically in Ref.<sup>92</sup> and experimentally by Shubnikov–de Haas oscillations in Ref.<sup>93</sup>, pointing toward a flat-band semimetal.
- A minimal microscopic model within a large- $S$  expansion based was built for Sr<sub>2</sub>FeMoO<sub>6</sub> [ICSD 181752, SG 225 ( $Fm\bar{3}m$ )] in Ref.<sup>94</sup>, leading to the spin-polarized flat bands and four massive or massless Dirac dispersions.
- YCr<sub>6</sub>Ge<sub>6</sub> [ICSD 658018, SG 191 ( $P6/mmm$ )] has been probed by ARPES in Ref.<sup>95</sup> to unveil planar flat bands associated to the Kagome sublattice.

Table XII: Manually curated list of materials with flat bands. We provide in this table the list of the 2,379 entries of curately chosen flat-band materials, indexed by the first column. The second column gives the chemical formula, the third column the space group symbol (and number in parentheses). The fourth column indicates the topological classification at the Fermi level: topological insulator (TI), topological semi-metal (SM) or trivial insulator (Triv.). The fifth column indicates if the material also belongs to the list of best materials given in Appendix H 3 and the figure displaying its band structure and DOS. The sixth column details the sublattices found for each material and common to every ICSD entries of this material. Here 'k' stands for Kagome, 'p' for pyrochlore, 'b' for bipartite, 's' for split lattice and 'l' for Lieb sublattice. A star superscript after 'k' ('l') indicate that only approximate Kagome (Lieb) sublattices were found (as defined in Appendix D). The seventh column gives the magnetic properties as obtained from [Materials Project](#) (NM for non-magnetic, FM for ferromagnetic, AFM for anti-ferromagnetic, FIM for ferrimagnetic, ‘—’ when the information is not available). The eighth column indicates if the material is known to be superconductor according to the [NIMS Materials Database](#). ‘SC’ stands for superconductor while ‘SC\*’ means that alloys based on this material are superconductor. The ninth column tells which material are “high-quality” as defined in Appendix H 1. The last column gives all the ICSD entries related to each material. If a given ICSD has additional sublattices compared to those common to all ICSD entries, a superscript label provides the list of these additional sublattices.

Num.	chem. formula	space group	Topo. at $E_f$	best	sublat.	magn.	super-conduct.	high quality	ICSDs
1	Al <sub>2</sub> O <sub>3</sub>	$P1$ (1)	Triv.	—	—	NM	—	HQ	<a href="#">173014</a>
2	AgBrO <sub>2</sub>	$P1$ (1)	Triv.	<a href="#">Fig. 28</a>	—	—	—	—	<a href="#">670051</a>
3	LiNa <sub>5</sub> N <sub>2</sub>	$P1$ (1)	Triv.	—	—	—	—	—	<a href="#">92316</a>
4	AgHO <sub>2</sub>	$P1$ (1)	Triv.	<a href="#">Fig. 28</a>	—	—	—	—	<a href="#">670060</a>
5	CaNi <sub>5</sub> H	$P1$ (1)	SM	—	—	FM	—	—	<a href="#">189752(k)</a> <a href="#">189753</a>
6	Na <sub>4</sub> Sn <sub>2</sub> Ge <sub>4</sub> O <sub>12</sub> (OH) <sub>4</sub>	$P\bar{1}$ (2)	Triv.	—	—	NM	—	—	<a href="#">15017</a>
7	NaI(H <sub>2</sub> O) <sub>2</sub>	$P\bar{1}$ (2)	Triv.	—	—	NM	—	—	<a href="#">23134</a>
8	(S <sub>2</sub> N <sub>3</sub> )VCl <sub>2</sub>	$P\bar{1}$ (2)	Triv.	—	(b)	NM	—	HQ	<a href="#">30742</a> <a href="#">61351</a>
9	Cu(SeO <sub>4</sub> )(H <sub>2</sub> O)	$P\bar{1}$ (2)	TI	—	—	FM	—	HQ	<a href="#">39887</a>
10	Na <sub>6</sub> Li <sub>2</sub> (W <sub>2</sub> O <sub>10</sub> )	$P\bar{1}$ (2)	Triv.	—	(b)	NM	—	HQ	<a href="#">49027</a>
11	K <sub>2</sub> Cu <sub>3</sub> (SeO <sub>3</sub> ) <sub>4</sub>	$P\bar{1}$ (2)	SM	—	(b,s)	FM	—	HQ	<a href="#">50541</a>
12	Cu(F(AuF <sub>4</sub> ))	$P\bar{1}$ (2)	SM	<a href="#">Fig. 28</a>	(b,s)	FM	—	—	<a href="#">62544</a>
13	K <sub>3</sub> Cu <sub>2</sub> ((P <sub>2</sub> O <sub>7</sub> )H(P <sub>2</sub> O <sub>7</sub> ))	$P\bar{1}$ (2)	TI	—	(b)	FM	—	HQ	<a href="#">62742</a>
14	((NO)(HF <sub>2</sub> ))(IF <sub>5</sub> )	$P\bar{1}$ (2)	Triv.	—	—	—	—	—	<a href="#">71582</a>
15	Cu <sub>3</sub> Bi <sub>4</sub> V <sub>2</sub> O <sub>14</sub>	$P\bar{1}$ (2)	SM	<a href="#">Fig. 28</a>	(b,s)	FM	—	HQ	<a href="#">75222</a>
16	Ca(SnF <sub>3</sub> ) <sub>2</sub>	$P\bar{1}$ (2)	Triv.	—	(b)	NM	—	HQ	<a href="#">92907</a>
17	K <sub>2</sub> Cu(Fe(CN) <sub>6</sub> )	$P\bar{1}$ (2)	SM	—	—	FM	—	HQ	<a href="#">99499</a>
18	Na <sub>2</sub> (Cu <sub>2</sub> Si <sub>4</sub> O <sub>11</sub> )(H <sub>2</sub> O) <sub>2</sub>	$P\bar{1}$ (2)	Triv.	<a href="#">Fig. 28</a>	(b,s)	FM	—	HQ	<a href="#">154123</a> <a href="#">414048</a>
19	(CH <sub>3</sub> ) <sub>2</sub> SeO	$P\bar{1}$ (2)	Triv.	—	—	NM	—	HQ	<a href="#">171011</a>
20	Cd(HCO(NH <sub>2</sub> )) <sub>2</sub> I <sub>2</sub>	$P\bar{1}$ (2)	Triv.	—	—	NM	—	HQ	<a href="#">192774</a>
21	RbSbBrF <sub>3</sub>	$P\bar{1}$ (2)	Triv.	—	—	NM	—	—	<a href="#">200109</a>
22	Na <sub>2</sub> Cu <sub>2</sub> (Si <sub>4</sub> O <sub>11</sub> )	$P\bar{1}$ (2)	Triv.	—	(b,s)	FM	—	HQ	<a href="#">240930</a>
23	Ti <sub>2</sub> P <sub>2</sub> O <sub>9</sub>	$P\bar{1}$ (2)	Triv.	—	(b)	—	—	—	<a href="#">243672</a>
24	Pb <sub>2</sub> (HgO <sub>2</sub> )(CrO <sub>4</sub> )	$P\bar{1}$ (2)	Triv.	—	(b)	NM	—	HQ	<a href="#">280778</a>
25	Rb(VO <sub>2</sub> (IO <sub>3</sub> ) <sub>2</sub> )	$P\bar{1}$ (2)	Triv.	—	—	NM	—	HQ	<a href="#">281304</a>
26	K <sub>2</sub> Cu <sub>3</sub> (Ge <sub>5</sub> O <sub>14</sub> )	$P\bar{1}$ (2)	SM	—	(b)	FM	—	HQ	<a href="#">410828</a>

27	(Hg <sub>2</sub> )((H <sub>4</sub> TeO <sub>6</sub> )(H <sub>6</sub> TeO <sub>6</sub> ))(H <sub>2</sub> O) <sub>2</sub>	P $\bar{1}$ (2)	Triv.	—	—	NM	—	—	412799
28	W <sub>2</sub> NCls <sub>8</sub>	P $\bar{1}$ (2)	SM	—	(b,s)	FM	—	HQ	415768
29	Na <sub>2</sub> (SO <sub>4</sub> )(BF <sub>3</sub> )	P $\bar{1}$ (2)	Triv.	—	—	NM	—	HQ	424150
30	SrHg(As <sub>2</sub> O <sub>7</sub> )	P $\bar{1}$ (2)	Triv.	—	(b)	NM	—	—	430291
31	BaHg(As <sub>2</sub> O <sub>7</sub> )	P $\bar{1}$ (2)	Triv.	—	(b)	NM	—	—	430292
32	Nb <sub>2</sub> Se <sub>9</sub>	P $\bar{1}$ (2)	Triv.	—	—	NM	—	—	645386 8179 62538 670020 34870 34871 34872 68913 77421 77422 77423 77424 77425 109006 171090 171091 171092
33	NaAlSi <sub>3</sub> O <sub>8</sub>	P $\bar{1}$ (2)	Triv.	—	(b,s)	—	—	—	65186
34	Ag(SbF <sub>6</sub> ) <sub>2</sub>	P $\bar{1}$ (2)	SM	—	(b,s)	FM	—	—	164050 164049
35	Al(OH) <sub>3</sub>	P $\bar{1}$ (2)	Triv.	—	—	NM	—	—	66534
36	BaCu(P <sub>2</sub> O <sub>7</sub> )	P $\bar{1}$ (2)	TI	—	(b)	FM	—	HQ	192060
37	BaCu(P <sub>2</sub> O <sub>7</sub> )	P $\bar{1}$ (2)	TI	—	(b)	—	—	HQ	56791
38	Bi <sub>2</sub> Pb <sub>2</sub> V <sub>2</sub> O <sub>10</sub>	P $\bar{1}$ (2)	Triv.	—	(b)	NM	—	HQ	419126 419121
39	PbBiO(VO <sub>4</sub> )	P $\bar{1}$ (2)	Triv.	—	(b)	NM	—	—	8061
40	CaCl <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub>	P $\bar{1}$ (2)	Triv.	—	—	NM	—	—	14005 151568 151569 151570 151571 151572 151573 151574 151575 151576 151577 151586
41	Ca(Ge <sub>2</sub> O <sub>5</sub> )	P $\bar{1}$ (2)	Triv.	—	(b,s)	NM	—	—	166589
42	(Zn(H <sub>2</sub> O) <sub>6</sub> )(SnF <sub>3</sub> ) <sub>2</sub>	P $\bar{1}$ (2)	Triv.	—	—	—	—	HQ	24789 79721
43	Mg <sub>2</sub> B <sub>2</sub> O <sub>5</sub>	P $\bar{1}$ (2)	Triv.	—	(b)	NM	—	—	73008
44	Cs <sub>2</sub> (Sn <sub>2</sub> S <sub>4</sub> (S <sub>2</sub> ))	P $\bar{1}$ (2)	Triv.	—	—	NM	—	HQ	173748
45	V <sub>2</sub> Te <sub>2</sub> O <sub>7</sub> F <sub>2</sub>	P $\bar{1}$ (2)	Triv.	—	(b)	FM	—	HQ	249506
46	Na <sub>2</sub> Pd(SeO <sub>4</sub> ) <sub>2</sub>	P $\bar{1}$ (2)	Triv.	—	(b)	NM	—	HQ	51507
47	Ag(PdF <sub>6</sub> )	P $\bar{1}$ (2)	TI	—	(b,s)	FM	—	HQ	98686
48	K <sub>2</sub> Co(SeO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P $\bar{1}$ (2)	SM	—	—	AFM	—	HQ	180389 182944 194597
49	Na(BSi <sub>3</sub> O <sub>8</sub> )	P $\bar{1}$ (2)	Triv.	—	(b,s)	NM	—	—	71446
50	PbBiO(PO <sub>4</sub> )	P $\bar{1}$ (2)	Triv.	—	—	NM	—	HQ	419125
51	LiFe(SO <sub>4</sub> )F	P $\bar{1}$ (2)	Triv.	—	(b)	AFM	—	—	201436
52	InAsO <sub>4</sub> (H <sub>2</sub> O)	P $\bar{1}$ (2)	Triv.	—	—	NM	—	HQ	10509 57975
53	Al <sub>11</sub> Mn <sub>4</sub>	P $\bar{1}$ (2)	SM	—	—	FM	—	—	431533
54	Na <sub>2</sub> Cu(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P $\bar{1}$ (2)	SM	—	—	FM	—	HQ	40090
55	Sc(PS <sub>4</sub> )	P $\bar{1}$ (2)	Triv.	—	(b)	NM	—	HQ	84868
56	Au <sub>4</sub> Cl <sub>8</sub>	P $\bar{1}$ (2)	Triv.	—	—	NM	—	HQ	238656 238657 238658 238659 238660 238661
57	NaY <sub>2</sub> P <sub>2</sub> S <sub>6</sub>	P $\bar{1}$ (2)	Triv.	—	—	—	—	—	428802
58	NaZnP <sub>2</sub> O <sub>6</sub> OH	P $\bar{1}$ (2)	Triv.	—	—	NM	—	HQ	4327
59	PbPt <sub>2</sub> O <sub>4</sub>	P $\bar{1}$ (2)	TI	—	(k*,b)	NM	—	HQ	60935
60	Sr <sub>2</sub> MgMoO <sub>6</sub>	P $\bar{1}$ (2)	Triv.	—	(b,s)	—	—	HQ	173119
61	Sr(OH)Cl(H <sub>2</sub> O) <sub>4</sub>	P $\bar{1}$ (2)	Triv.	—	—	NM	—	—	416653
62	YBr(MoO <sub>4</sub> )	P $\bar{1}$ (2)	Triv.	—	(b)	—	—	—	2523 191342
63	YBr(WO <sub>4</sub> )	P $\bar{1}$ (2)	Triv.	—	(b)	NM	—	HQ	29359 67604 <sup>(b)</sup> 67605 <sup>(b)</sup> 69800 <sup>(b)</sup>
64	As <sub>2</sub> O <sub>3</sub>	P <sub>2</sub> (3)	Triv.	—	—	—	—	HQ	72991
65	Na <sub>2</sub> (ZnSi <sub>3</sub> O <sub>8</sub> )	P <sub>2</sub> (4)	Triv.	—	(b,s)	NM	—	HQ	924 20114 200440
66	CaCuO <sub>2</sub>	P <sub>2</sub> (4)	Triv.	—	(b,s)	NM	—	—	85786
67	BaCu <sub>2</sub> Cl <sub>2</sub> (Te <sub>2</sub> O <sub>6</sub> )	P <sub>2</sub> (4)	Triv.	—	(b)	FM	—	HQ	189155
68	PbCu <sub>2</sub> (TeO <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	P <sub>2</sub> (4)	Triv.	—	(b)	FM	—	HQ	4327
69	SrCu <sub>2</sub> (TeO <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	P <sub>2</sub> (4)	Triv.	—	(b)	FM	—	HQ	674160
70	Cu(IO <sub>3</sub> ) <sub>2</sub>	P <sub>2</sub> (4)	SM	—	(b,s)	FM	—	HQ	29359 67604 <sup>(b)</sup> 67605 <sup>(b)</sup> 69800 <sup>(b)</sup>
71	LiIn(P <sub>2</sub> O <sub>7</sub> )	P <sub>2</sub> (4)	Triv.	—	(b)	NM	—	HQ	95439
72	LiSc(P <sub>2</sub> O <sub>7</sub> )	P <sub>2</sub> (4)	Triv.	—	(b)	NM	—	HQ	416669
73	Na(BSi <sub>3</sub> O <sub>8</sub> )(OH) <sub>2</sub>	P <sub>2</sub> (4)	Triv.	—	—	NM	—	HQ	12134
74	Te <sub>2</sub> O <sub>5</sub>	P <sub>2</sub> (4)	Triv.	—	(b,s)	NM	—	—	40185 40186
75	NbOI <sub>2</sub>	C <sub>2</sub> (5)	Triv.	Fig. 28	(b,s)	NM	—	HQ	36255
76	NbOBr <sub>2</sub>	C <sub>2</sub> (5)	Triv.	Fig. 28	(b,s)	NM	—	HQ	238656 238657 238658 238659 238660 238661
77	Pb <sub>3</sub> (VO <sub>4</sub> ) <sub>2</sub>	C <sub>2</sub> (5)	Triv.	—	—	NM	—	HQ	171091 171092
78	Sr <sub>4</sub> Zn <sub>3</sub> F <sub>14</sub>	C <sub>m</sub> (8)	Triv.	—	(k*,b)	—	—	HQ	4327
79	Ca <sub>2</sub> CoO <sub>3</sub>	C <sub>m</sub> (8)	SM	—	—	FM	—	HQ	674163
80	SbTaON <sub>2</sub>	C <sub>m</sub> (8)	Triv.	—	(b,s)	—	—	—	674153
81	SbNbN <sub>2</sub> O	C <sub>m</sub> (8)	Triv.	—	(b,s)	—	—	—	674160
82	TeGeN <sub>2</sub> O	C <sub>m</sub> (8)	Triv.	—	(b,s)	—	—	—	419125
83	Cd <sub>2</sub> O(OH) <sub>2</sub> (H <sub>2</sub> O)	C <sub>m</sub> (8)	Triv.	—	—	NM	—	HQ	238656 238657 238658 238659 238660 238661

84	Na <sub>4</sub> (CO <sub>4</sub> )	<i>Cm</i> (8)	Triv.	—	—	NM	—	—	245413 245414 245410(b)
85	K <sub>4</sub> (CO <sub>4</sub> )	<i>Cm</i> (8)	Triv.	—	—	NM	—	—	245424 245426 245421
86	SiO <sub>2</sub>	<i>Cc</i> (9)	Triv.	—	(b,s)	NM	—	—	75662 81381 413210
87	Ba <sub>2</sub> WO <sub>3</sub> F <sub>4</sub>	<i>Cc</i> (9)	Triv.	—	—	NM	—	HQ	201653 33271 673319
88	KSbB <sub>2</sub> O <sub>6</sub>	<i>Cc</i> (9)	Triv.	—	(b)	NM	—	HQ	238073
89	Cs <sub>2</sub> CuP <sub>2</sub> O <sub>7</sub>	<i>Cc</i> (9)	SM	—	(b)	FM	—	—	430123
90	LiVO <sub>3</sub>	<i>Cc</i> (9)	Triv.	—	—	—	—	HQ	23477
91	TiZrSe <sub>4</sub>	<i>P2/m</i> (10)	TI	—	(b)	NM	—	—	104188
92	CrAuTe <sub>4</sub>	<i>P2/m</i> (10)	SM	Fig. 29	—	FM	—	HQ	150279
93	Cu(IO <sub>3</sub> ) <sub>2</sub>	<i>P21/m</i> (11)	SM	—	(b)	FM	—	HQ	2232
94	Ca <sub>3</sub> VN <sub>3</sub>	<i>P21/m</i> (11)	Triv.	—	(b)	NM	—	—	41060
95	CuWO <sub>3</sub> F <sub>2</sub>	<i>P21/m</i> (11)	SM	—	(b,s)	FM	—	HQ	60759
96	K(VO)H(SeO <sub>3</sub> ) <sub>2</sub>	<i>P21/m</i> (11)	SM	—	(b)	FM	—	HQ	82535
97	(NH <sub>4</sub> )(H(VO)(SeO <sub>3</sub> ) <sub>2</sub> )	<i>P21/m</i> (11)	SM	—	—	FM	—	—	97400
98	PbPdSi(P <sub>2</sub> O <sub>7</sub> ) <sub>2</sub>	<i>P21/m</i> (11)	Triv.	—	(b,s)	NM	—	—	195306 420535
99	Na <sub>3</sub> Ni(PO <sub>4</sub> )(CO <sub>3</sub> )	<i>P21/m</i> (11)	Triv.	—	(b)	AFM	—	HQ	237798
100	K <sub>3</sub> (Ru(P <sub>2</sub> Se <sub>6</sub> )(P <sub>3</sub> Se <sub>4</sub> ))	<i>P21/m</i> (11)	Triv.	—	—	NM	—	—	406200
101	(NO)Cu(NO <sub>3</sub> ) <sub>3</sub>	<i>P21/m</i> (11)	SM	—	—	—	—	HQ	422033
102	Cu <sub>3</sub> GeP <sub>2</sub> O <sub>10</sub>	<i>P21/m</i> (11)	SM	—	(b)	FM	—	—	426627
103	As <sub>4</sub> S <sub>5</sub>	<i>P21/m</i> (11)	Triv.	—	—	NM	—	HQ	16107 98901
104	Ba <sub>2</sub> (Zn <sub>2</sub> F <sub>7</sub> Cl)	<i>P21/m</i> (11)	Triv.	—	(b,s)	NM	—	HQ	79478
105	Ba <sub>2</sub> (Co <sub>2</sub> F <sub>7</sub> Cl)	<i>P21/m</i> (11)	Triv.	Fig. 29	(b,s)	FM	—	HQ	79479
106	Ba <sub>2</sub> Ni <sub>2</sub> F <sub>7</sub> Cl	<i>P21/m</i> (11)	Triv.	Fig. 29	(b,s)	FM	—	HQ	84782
107	CuZnCl(OH) <sub>3</sub>	<i>P21/m</i> (11)	SM	—	(b)	FM	—	—	252429
108	Cu <sub>2</sub> Sc <sub>2</sub> (Ge <sub>4</sub> O <sub>13</sub> )	<i>P21/m</i> (11)	Triv.	—	(b)	FM	—	—	99599 99600 99601 99602 99603
109	Y <sub>3</sub> (VO <sub>5</sub> )(OH) <sub>3</sub>	<i>P21/m</i> (11)	SM	—	—	FM	—	HQ	262400
110	La <sub>3</sub> (VO <sub>5</sub> )(OH) <sub>3</sub>	<i>P21/m</i> (11)	SM	—	—	AFM	—	HQ	262402
111	Na <sub>3</sub> In(PO <sub>4</sub> ) <sub>2</sub>	<i>P21/m</i> (11)	Triv.	—	(b)	NM	—	HQ	87833 90941
112	PbSO <sub>4</sub> (PbO) <sub>2</sub>	<i>P21/m</i> (11)	Triv.	—	—	NM	—	—	30711 61427 <sup>(b)</sup> 61428 <sup>(b)</sup> 63639 <sup>(b)</sup> 100681 <sup>(b)</sup>
113	TlCu(OH)SO <sub>4</sub>	<i>P21/m</i> (11)	SM	—	(b)	FM	—	HQ	36581
114	La <sub>3</sub> Os <sub>2</sub> O <sub>10</sub>	<i>C2/m</i> (12)	SM	—	—	FM	—	HQ	10104
115	MoV <sub>2</sub> O <sub>8</sub>	<i>C2/m</i> (12)	TI	Fig. 29	(b)	NM	—	—	28471
116	LiH <sub>2</sub> PO <sub>2</sub>	<i>C2/m</i> (12)	Triv.	—	—	NM	—	HQ	59823 250176
117	Sr <sub>7</sub> Re <sub>4</sub> O <sub>19</sub>	<i>C2/m</i> (12)	Triv.	—	(b,s)	FM	—	HQ	93804
118	(Sr <sub>2</sub> CoO <sub>3</sub> )	<i>C2/m</i> (12)	SM	Fig. 29	—	FM	—	—	99894
119	Cr <sub>3</sub> O <sub>8</sub>	<i>C2/m</i> (12)	TI	Fig. 29	(b)	FM	—	—	155847
120	Cr <sub>3</sub> O <sub>8</sub>	<i>C2/m</i> (12)	Triv.	—	—	FM	—	—	155848
121	LiH <sub>3</sub> As <sub>2</sub> O <sub>7</sub>	<i>C2/m</i> (12)	Triv.	—	—	NM	—	HQ	172988
122	MgBr <sub>2</sub> (H <sub>2</sub> O) <sub>6</sub>	<i>C2/m</i> (12)	Triv.	—	—	NM	—	HQ	189844
123	Br <sub>6</sub> Si <sub>2</sub>	<i>C2/m</i> (12)	Triv.	—	—	NM	—	—	239354
124	Br <sub>4</sub> Nb	<i>C2/m</i> (12)	Triv.	—	(b,s)	NM	—	—	239640
125	Li <sub>2</sub> CrCl <sub>4</sub>	<i>C2/m</i> (12)	Triv.	—	(b)	FM	—	HQ	403035
126	BaAu <sub>2</sub> (SO <sub>4</sub> ) <sub>4</sub>	<i>C2/m</i> (12)	Triv.	—	(b)	NM	—	HQ	427677
127	ReScI <sub>3</sub>	<i>C2/m</i> (12)	Triv.	—	(b,s)	—	—	—	429458
128	Li <sub>4</sub> N <sub>1</sub>	<i>C2/m</i> (12)	Triv.	—	—	—	—	—	675129
129	AgPdZr <sub>2</sub> F <sub>11</sub>	<i>C2/m</i> (12)	Triv.	—	—	FM	—	HQ	65181
130	NaPd(Zr <sub>2</sub> F <sub>11</sub> )	<i>C2/m</i> (12)	Triv.	—	—	FM	—	HQ	77241
131	NaCo(Zr <sub>2</sub> F <sub>11</sub> )	<i>C2/m</i> (12)	SM	—	—	FM	—	HQ	81221
132	NaNi(Zr <sub>2</sub> F <sub>11</sub> )	<i>C2/m</i> (12)	Triv.	—	—	FM	—	HQ	81222
133	NaZn(Zr <sub>2</sub> F <sub>11</sub> )	<i>C2/m</i> (12)	Triv.	—	—	NM	—	HQ	81223
134	CaC <sub>2</sub>	<i>C2/m</i> (12)	Triv.	—	—	NM	—	HQ	54185 54188 94385 252719 252725 252728 252731 252740 252743 252746 252749 252752 252755 252758 252761 252764 252767 252770 252773 252776 290833 411190 672970
135	Mg(CrO <sub>4</sub> )	<i>C2/m</i> (12)	Triv.	—	(b)	NM	—	—	18120
136	Ag <sub>3</sub> In(PO <sub>4</sub> ) <sub>2</sub>	<i>C2/m</i> (12)	Triv.	—	(b)	NM	—	HQ	245001
137	Ga <sub>2</sub> O <sub>3</sub>	<i>C2/m</i> (12)	Triv.	—	(b)	NM	—	HQ	34243 83645 166198 184327 603563 673058
138	Al <sub>2</sub> O <sub>3</sub>	<i>C2/m</i> (12)	Triv.	—	(b)	NM	—	HQ	82504 673079
139	La <sub>6</sub> I <sub>5</sub> Ge <sub>3</sub>	<i>C2/m</i> (12)	SM	—	(b)	—	—	HQ	414175

140	YCl(MoO <sub>4</sub> )	C2/m (12)	Triv.	—	(b)	NM	—	HQ	249647
141	K <sub>2</sub> Na(Ag(CN) <sub>2</sub> ) <sub>3</sub>	C2/m (12)	Triv.	Fig. 29	(k*,b)	NM	—	HQ	59723 59724 59725 59726
142	Pb <sub>2</sub> O(SO <sub>4</sub> )	C2/m (12)	Triv.	—	—	NM	—	HQ	14246 <sup>(b,s)</sup> 29268 <sup>(b,s)</sup> 30627 35757
143	Pb <sub>2</sub> O(WO <sub>4</sub> )	C2/m (12)	Triv.	—	—	NM	—	—	61399
144	Pb <sub>2</sub> Co(WO <sub>6</sub> )	C2/m (12)	SM	—	(b,s)	AFM	—	HQ	77912
145	TlFeS <sub>2</sub>	C2/m (12)	Triv.	—	—	NM	—	—	30011 63381
146	TlFeS <sub>2</sub>	C2/m (12)	TI	—	—	NM	—	—	600815 659748
147	Ba <sub>3</sub> Y <sub>2</sub> PtCu <sub>2</sub> O <sub>10</sub>	C2/m (12)	TI	—	(b,s)	NM	—	HQ	62390
148	Y <sub>2</sub> Ba <sub>3</sub> Cu <sub>2</sub> PtO <sub>10</sub>	C2/m (12)	TI	—	(b,s)	NM	—	HQ	65614
149	Y <sub>5</sub> Mo <sub>2</sub> O <sub>12</sub>	C2/m (12)	SM	Fig. 29	(b)	FM	—	HQ	60957 62215
150	K(H <sub>2</sub> PO <sub>4</sub> )	P2/c (13)	Triv.	Fig. 30	—	NM	—	HQ	79341
151	RbLi <sub>2</sub> Ga <sub>2</sub> (BO <sub>3</sub> ) <sub>3</sub>	P2/c (13)	Triv.	—	(b)	NM	—	HQ	280205
152	Na(CN)(H <sub>2</sub> O) <sub>2</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	—	830 2244 16765
153	Li(NH <sub>4</sub> )(PO <sub>3</sub> F)	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	—	1439
154	Li <sub>2</sub> (SO <sub>4</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	(b)	NM	—	HQ	2512 58 23723 30276
155	B <sub>2</sub> F <sub>4</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	—	27867
156	WO <sub>3</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	(b)	NM	—	—	31823 <sup>(s)</sup> 190632 647640 <sup>(s)</sup> 673316 <sup>(s)</sup> 84848 <sup>(s)</sup> 190631 <sup>(s)</sup> 14332 <sup>(s)</sup> 16080 17003 <sup>(s)</sup> 50727 80056 <sup>(s)</sup> 80057 190630 <sup>(s)</sup>
157	Cs(HSO <sub>4</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	HQ	67108 39252 91808 291375 291374
158	Mo(As <sub>2</sub> O <sub>7</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	(b,s)	NM	—	—	72518
159	Cu(HSeO <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P2 <sub>1</sub> /c (14)	SM	—	—	FM	—	—	80932
160	Cd(MoO <sub>2</sub> )(PO <sub>4</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	(b)	FM	—	—	82090
161	(HCONH <sub>2</sub> ) <sub>2</sub> (Cu(HCOO) <sub>2</sub> )	P2 <sub>1</sub> /c (14)	SM	—	—	FM	—	—	109973 194113
162	Pb <sub>2</sub> Cu(BO <sub>3</sub> ) <sub>2</sub>	P2 <sub>1</sub> /c (14)	SM	—	(b)	FM	—	HQ	155317
163	Mg(SiO <sub>3</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	—	159550 15805 <sup>(b,s)</sup> 24270 <sup>(b)</sup> 30893 <sup>(b)</sup> 30895 <sup>(b)</sup> 34163 <sup>(b)</sup> 92750 <sup>(b)</sup> 159551 <sup>(b)</sup> 159552 <sup>(b)</sup> 159553 <sup>(b)</sup> 180445 <sup>(b)</sup> 196432 <sup>(b)</sup> 201535 <sup>(b)</sup>
164	Sn <sub>2</sub> (P <sub>2</sub> O <sub>7</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	HQ	170847
165	K <sub>2</sub> (SeMoO <sub>6</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	—	412999
166	OsOF <sub>4</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	HQ	417246
167	KAgAsS <sub>2</sub>	P2 <sub>1</sub> /c (14)	Triv.	Fig. 30	—	—	—	—	431760
168	Na <sub>2</sub> TeO <sub>3</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	—	100693
169	ScOF	P2 <sub>1</sub> /c (14)	Triv.	—	(b)	NM	—	HQ	24112 100562 100563 100564
170	Ca <sub>2</sub> (SiO <sub>4</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	HQ	963 <sup>(b)</sup> 16616 <sup>(b)</sup> 24640 79550 79551 79552 79553 <sup>(b)</sup> 79554 79555 <sup>(b)</sup> 81096 <sup>(b)</sup> 196150 <sup>(b)</sup> 245074 <sup>(b)</sup> 245075 <sup>(b)</sup> 245076 <sup>(b)</sup> 245077 <sup>(b)</sup> 245078 <sup>(b)</sup> 245079 <sup>(b)</sup> 245080 <sup>(b)</sup> 421708 <sup>(b)</sup> 280995 <sup>(b)</sup>
171	Cu(HSeO <sub>3</sub> ) <sub>2</sub>	P2 <sub>1</sub> /c (14)	SM	—	—	FM	—	HQ	29538 51676 <sup>(b)</sup>
172	Cu(OH)Cl	P2 <sub>1</sub> /c (14)	TI	—	—	FM	—	HQ	38384
173	Cu(OH)Cl	P2 <sub>1</sub> /c (14)	TI	—	—	FM	—	HQ	91088
174	Cs <sub>2</sub> (As <sub>2</sub> F <sub>8</sub> O <sub>2</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	HQ	6070
175	K <sub>2</sub> (W <sub>2</sub> O <sub>7</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	(b,s)	NM	—	HQ	67284
176	KCuCl <sub>3</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	—	FM	—	HQ	15590 109325 252663
177	Cu(AlAsO <sub>5</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	(b)	NM	—	—	91551
178	VO <sub>2</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	(b)	FM	—	—	15889 34033 74705 602360 647604 647610
179	Na <sub>2</sub> (Ni(H <sub>2</sub> O) <sub>2</sub> )(V <sub>2</sub> O <sub>4</sub> F <sub>6</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	—	FM	—	—	424345
180	Na <sub>2</sub> (PdF <sub>4</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	(b)	NM	—	HQ	33889 71101
181	CuSb <sub>2</sub> O <sub>6</sub>	P2 <sub>1</sub> /c (14)	SM	—	(b)	FM	—	—	30410 71762 80576 628623 <sup>(s)</sup>
182	Y(NiO <sub>3</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	(b)	FM	—	HQ	88043 89417 92047 191790
183	K <sub>2</sub> (Pt(CN) <sub>4</sub> I <sub>2</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	HQ	413706
184	Rb <sub>2</sub> (Pt(CN) <sub>4</sub> I <sub>2</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	HQ	421673
185	XeF <sub>4</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	—	NM	—	HQ	26626 27467
186	VF <sub>4</sub>	P2 <sub>1</sub> /c (14)	SM	—	(b,s)	FM	—	—	65785
187	Ag(AuF <sub>4</sub> ) <sub>2</sub>	P2 <sub>1</sub> /c (14)	SM	—	(b,s)	FM	—	HQ	85416
188	Na <sub>4</sub> Sn <sub>3</sub> F <sub>10</sub>	C2/c (15)	Triv.	—	(b)	NM	—	—	9891
189	V <sub>2</sub> O <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub>	C2/c (15)	SM	—	—	FM	—	—	16727

190	V(S <sub>2</sub> ) <sub>2</sub>	C2/c (15)	Triv.	—	—	NM	—	—	16797 64770 428285
191	Na <sub>2</sub> (Nb <sub>4</sub> O <sub>11</sub> )	C2/c (15)	Triv.	—	(b)	—	—	—	18305
192	Li <sub>2</sub> Cu(P <sub>2</sub> O <sub>7</sub> )	C2/c (15)	SM	—	(b)	FM	—	HQ	72485 160321
193	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )(Cu(HCOO) <sub>3</sub> )	C2/c (15)	SM	—	—	FM	—	—	110500 151227
194	PbPd <sub>2</sub> O <sub>4</sub>	C2/c (15)	Triv.	Fig. 30	(b)	NM	—	HQ	263050
195	K(Cl <sub>3</sub> (MoOCl <sub>2</sub> ) <sub>2</sub> )	C2/c (15)	Triv.	—	(b)	FM	—	HQ	410954
196	Ag <sub>4</sub> CuTeO <sub>6</sub>	C2/c (15)	SM	—	(b)	FM	—	HQ	416931
197	(NH <sub>4</sub> ) <sub>2</sub> (MoO <sub>2</sub> S <sub>2</sub> )	C2/c (15)	Triv.	—	—	NM	—	HQ	41688 423990
198	BaCu(SeO <sub>3</sub> ) <sub>2</sub>	C2/c (15)	SM	—	(b,s)	FM	—	HQ	202388
199	SrCu(SeO <sub>3</sub> ) <sub>2</sub>	C2/c (15)	SM	—	(b,s)	FM	—	HQ	202389
200	Cs <sub>2</sub> MoO <sub>2</sub> S <sub>2</sub>	C2/c (15)	Triv.	—	—	NM	—	HQ	423982 423983
201	Rb <sub>2</sub> MoO <sub>2</sub> S <sub>2</sub>	C2/c (15)	Triv.	—	—	NM	—	HQ	423992
202	Cs(Sb <sub>2</sub> F <sub>7</sub> )	C2/c (15)	Triv.	—	—	NM	—	—	14119 24741
203	Cu(H <sub>2</sub> PO <sub>2</sub> ) <sub>2</sub> (CO(NH <sub>2</sub> ) <sub>2</sub> )	C2/c (15)	SM	—	—	FM	—	—	279589 <sup>(b)</sup> 279590 279591
204	Cu <sub>2</sub> (P <sub>4</sub> O <sub>12</sub> )	C2/c (15)	TI	—	(b)	FM	—	—	23756
205	(N <sub>2</sub> H <sub>5</sub> )(BF <sub>4</sub> )	C2/c (15)	Triv.	—	—	NM	—	—	9895 245055
206	Na <sub>2</sub> Cu(P <sub>2</sub> O <sub>7</sub> )	C2/c (15)	SM	—	(b)	FM	—	HQ	79868 80418
207	CaNi(BP <sub>2</sub> O <sub>7</sub> (OH) <sub>3</sub> )	C2/c (15)	Triv.	—	—	FM	—	—	409898
208	LaCu <sub>2</sub> O <sub>4</sub>	C2/c (15)	SM	—	(b,s)	—	—	HQ	83486
209	YC <sub>2</sub> O <sub>4</sub>	C2/c (15)	SM	Fig. 30	(b,s)	—	—	HQ	83493
210	NiZn(P <sub>4</sub> O <sub>12</sub> )	C2/c (15)	Triv.	—	(b)	FM	—	—	37137
211	La(MnO <sub>3</sub> )	C2/c (15)	Triv.	—	(b,s)	FM	—	HQ	150258
212	VOSb <sub>2</sub> O <sub>4</sub>	C2/c (15)	SM	—	(b)	FM	—	HQ	2292 27800
213	Sr <sub>3</sub> CuPtO <sub>6</sub>	C2/c (15)	SM	—	(b,s)	FM	—	HQ	66347 72721
214	(VO)(PO <sub>3</sub> ) <sub>2</sub>	C2/c (15)	SM	—	(b)	FM	—	HQ	39762 160942 160943 160944
215	Sc <sub>4</sub> OsCl <sub>4</sub>	C2/c (15)	Triv.	—	—	NM	—	HQ	421532
216	MgTeMoO <sub>6</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 (18)	Triv.	—	(b)	NM	—	HQ	184714
217	Zn(TeMoO <sub>6</sub> )	P2 <sub>1</sub> 2 <sub>1</sub> 2 (18)	Triv.	—	(b,s)	NM	—	HQ	250523 163981
218	As <sub>2</sub> O <sub>5</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (19)	Triv.	—	(b,s)	NM	—	HQ	987 654040
219	AsPO <sub>5</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (19)	Triv.	—	(b)	NM	—	HQ	36649
220	SbAsO <sub>5</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (19)	Triv.	—	(b)	NM	—	HQ	36650
221	NaCu(PO <sub>4</sub> )	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (19)	SM	—	(b)	FM	—	HQ	35451
222	BaVS <sub>3</sub>	C222 <sub>1</sub> (20)	SM	—	(b,s)	FM	—	HQ	63230
223	GeTiONF	Pmm2 (25)	Triv.	—	—	—	—	—	674260
224	KCu(CO <sub>3</sub> )F	Pmc <sub>2</sub> 1 (26)	SM	—	(b)	FM	—	HQ	75401
225	CsBi(Nb <sub>2</sub> O <sub>7</sub> )	Pmc <sub>2</sub> 1 (26)	Triv.	—	(b,s)	NM	—	HQ	96510 162981 162982 162983 162984
226	Bi <sub>2</sub> (MoO <sub>6</sub> )	Pca <sub>2</sub> 1 (29)	Triv.	—	—	NM	—	—	14266 47139 <sup>(b)</sup> 201685 <sup>(b)</sup>
227	InO(OH)	Pmn <sub>2</sub> 1 (31)	Triv.	—	—	NM	—	HQ	15082 166253
228	LiV <sub>2</sub> O <sub>5</sub>	Pmn <sub>2</sub> 1 (31)	SM	—	(b)	FM	—	HQ	88640
229	Cu(NH <sub>4</sub> )(PO <sub>4</sub> )(H <sub>2</sub> O)	Pmn <sub>2</sub> 1 (31)	SM	—	—	FM	—	HQ	250189
230	(NH <sub>4</sub> )(Co(PO <sub>4</sub> )(H <sub>2</sub> O))	Pmn <sub>2</sub> 1 (31)	SM	—	—	AFM	—	HQ	280044
231	(NH <sub>4</sub> )(NiPO <sub>4</sub> )(H <sub>2</sub> O)	Pmn <sub>2</sub> 1 (31)	Triv.	—	—	FM	—	HQ	424553
232	V <sub>2</sub> O <sub>5</sub>	Pmn <sub>2</sub> 1 (31)	Triv.	—	(b)	NM	—	—	15984 <sup>(s)</sup> 29140 41030 82151 <sup>(s)</sup> 157988 <sup>(s)</sup>
233	SrGaH <sub>5</sub>	Pna <sub>2</sub> 1 (33)	Triv.	—	—	NM	—	—	240697
234	FeP	Pna <sub>2</sub> 1 (33)	SM	—	—	—	—	HQ	15057
235	Rb(AlSiO <sub>4</sub> )	Pna <sub>2</sub> 1 (33)	Triv.	—	(b,s)	NM	—	—	4335 160823
236	Cs(AlSiO <sub>4</sub> )	Pna <sub>2</sub> 1 (33)	Triv.	—	(b,s)	NM	—	HQ	160822 <sup>(k)</sup> 186607 <sup>(k)</sup> 186608 186609 186610
237	TlTeVO <sub>5</sub>	Pna <sub>2</sub> 1 (33)	Triv.	—	(b)	NM	—	—	173863 173864
238	FeS <sub>2</sub>	Pnn2 (34)	Triv.	—	—	NM	—	HQ	42726
239	FeTe <sub>2</sub>	Pnn2 (34)	Triv.	—	—	—	—	HQ	42727 633870
240	Ba <sub>2</sub> Ge <sub>2</sub> TiO <sub>8</sub>	Cmm2 (35)	Triv.	—	(b,s)	—	—	HQ	39133
241	BaZnF <sub>4</sub>	Cmc <sub>2</sub> 1 (36)	Triv.	Fig. 30	(b,s)	—	—	—	672719 16925 182604 182605 182606 182607 182609 402925 402926
242	Al <sub>5</sub> (BO <sub>3</sub> )O <sub>6</sub>	Cmc <sub>2</sub> 1 (36)	Triv.	—	(b)	NM	—	HQ	20172 167307 167308 <sup>(s)</sup> 167309 167310 167311 167312 167313 167314 167315 167316 190085
243	BaNiF <sub>4</sub>	Cmc <sub>2</sub> 1 (36)	Triv.	—	(b,s)	FM	—	—	23141 261190 410708
244	BaCoF <sub>4</sub>	Cmc <sub>2</sub> 1 (36)	SM	—	(b,s)	FM	—	HQ	26067 261189
245	BaVS <sub>3</sub>	Cmc <sub>2</sub> 1 (36)	SM	—	(b,s)	FM	—	HQ	52692 63229 154182 616099
246	Rb <sub>2</sub> (PbO <sub>3</sub> )	Cmc <sub>2</sub> 1 (36)	Triv.	—	(b,s)	NM	—	—	1413

247	Na <sub>3</sub> (VOS <sub>3</sub> )	Cmc2 <sub>1</sub> (36)	Triv.	—	—	NM	—	HQ	281593(b) 415217
248	Sr <sub>2</sub> (Ta <sub>2</sub> O <sub>7</sub> )	Cmc2 <sub>1</sub> (36)	Triv.	—	(b,s)	NM	—	HQ	16388
249	Na <sub>2</sub> (W <sub>2</sub> O <sub>7</sub> )	Cmc2 <sub>1</sub> (36)	Triv.	—	(b,s)	NM	—	HQ	65780
250	CaGa(BO <sub>3</sub> )O	Ccc2 (37)	Triv.	—	(b)	NM	—	HQ	93390
251	Ba(TiO <sub>3</sub> )	Amm2 (38)	Triv.	—	(b)	NM	—	HQ	154346 161341 31155(k,s,l) 73637(k,s,l) 73638(k,s,l) 73639(k,s,l) 73640(k,s,l) 73641(k,s,l) 161419(k,s) 186460(s,l) 237106(s,l) 237109(s,l)
252	Rb <sub>4</sub> (CO <sub>4</sub> )	Amm2 (38)	Triv.	—	—	NM	—	—	245441
253	K(NbO <sub>3</sub> )	Amm2 (38)	Triv.	—	(b,s,l*)	NM	—	—	9533(k) 14363 190922(k)
254	Pb(ZrO <sub>3</sub> )	Amm2 (38)	Triv.	—	(b,s,l*)	NM	—	HQ	39607
255	Ag <sub>2</sub> (TeO <sub>2</sub> (OH)4)	Fdd2 (43)	Triv.	—	(b)	NM	—	HQ	240968
256	Rb <sub>2</sub> ((Al <sub>2</sub> Si <sub>3</sub> )O <sub>10</sub> )	Fdd2 (43)	Triv.	—	(b,s)	NM	—	—	180324
257	IrF <sub>4</sub>	Fdd2 (43)	SM	—	(b,s)	FM	—	—	23483
258	Bi <sub>2</sub> (CO <sub>3</sub> )O <sub>2</sub>	Imm2 (44)	Triv.	Fig. 30	—	NM	—	HQ	94740 252588
259	Fe(Ti <sub>3</sub> O <sub>7</sub> )	Imm2 (44)	Triv.	—	—	FM	—	—	190042
260	W <sub>6</sub> PCl <sub>17</sub>	Imm2 (44)	Triv.	—	—	AFM	—	HQ	422270
261	Ba <sub>4</sub> In <sub>6</sub> O <sub>13</sub>	Iba2 (45)	Triv.	Fig. 30	(b)	NM	—	—	72887
262	Ag(C(CN) <sub>3</sub> )	Ima2 (46)	Triv.	—	—	NM	—	HQ	43823 428560
263	Sr(TiO <sub>3</sub> )	Ima2 (46)	Triv.	—	(b,s)	NM	—	—	182248
264	Pb(TiO <sub>3</sub> )	Pmmm (47)	Triv.	—	(b,s,l*)	—	—	—	27949
265	YBaCo <sub>2</sub> O <sub>5</sub>	Pmmm (47)	SM	—	(b,s)	FM	—	—	171433 247220
266	LaBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub>	Pmmm (47)	TI	Fig. 31	(b,s)	NM	—	—	81167
267	YBa(Fe <sub>2</sub> O <sub>5</sub> )	Pmmm (47)	SM	—	(b,s)	FM	—	—	164176 281205 281206
268	SiO <sub>2</sub>	Pnnn (48)	Triv.	—	(b,s)	NM	—	—	170533
269	SiO <sub>2</sub>	Pban (50)	Triv.	—	(b,s)	NM	—	—	170535
270	La <sub>2</sub> (NiO <sub>4</sub> )	Pban (50)	Triv.	—	(b,s,l*)	FM	—	HQ	201940
271	Cu(H <sub>2</sub> PO <sub>2</sub> ) <sub>2</sub>	Pmma (51)	SM	—	—	FM	—	HQ	280921
272	CuCo <sub>2</sub> Ge <sub>2</sub>	Pmma (51)	SM	—	—	FM	—	HQ	62856
273	Cu(GeO <sub>3</sub> )	Pmma (51)	SM	—	(b)	FM	—	HQ	25754 50329 50331 56606 56607 56699 56701 78475 85325 85326 89400 89401 89402 89403 89404 89405 89406 89407 246664 411018 411019
274	Cu(SiO <sub>3</sub> )	Pmma (51)	SM	—	(b)	FM	—	HQ	89669
275	LaCoAl <sub>4</sub>	Pmma (51)	TI	—	—	NM	—	HQ	9986
276	Ga(GaCl <sub>4</sub> )	Pnna (52)	Triv.	—	(b)	NM	—	HQ	14218 62664 66548
277	In(InBr <sub>4</sub> )	Pnna (52)	Triv.	—	(b)	NM	—	HQ	60851 62240
278	CuPtO <sub>2</sub>	Pmna (53)	SM	—	—	—	—	—	670125
279	Na <sub>3</sub> Cu <sub>4</sub> S <sub>4</sub>	Pbam (55)	SM	—	—	NM	—	HQ	10004
280	Na <sub>2</sub> (TiCl <sub>4</sub> )	Pbam (55)	Triv.	—	(b)	FM	—	HQ	400264
281	Bi <sub>2</sub> Al <sub>4</sub> O <sub>9</sub>	Pbam (55)	Triv.	—	(b)	NM	—	—	20069 26807 88775 200051 236561 251938
282	Rb(VOF <sub>3</sub> )	Pbam (55)	TI	—	(b,s)	FM	—	HQ	249403 426620
283	YCrB <sub>4</sub>	Pbam (55)	Triv.	—	—	NM	—	—	16171
284	YVB <sub>4</sub>	Pbam (55)	TI	—	—	NM	—	—	615679
285	Na <sub>2</sub> (MnCl <sub>4</sub> )	Pbam (55)	SM	—	(b)	FM	—	HQ	9136
286	Sc <sub>2</sub> CrB <sub>6</sub>	Pbam (55)	TI	—	—	FM	—	—	99646
287	Sc <sub>4</sub> Cl <sub>6</sub> B	Pbam (55)	SM	—	(b)	NM	—	HQ	201977
288	Sc <sub>4</sub> Cl <sub>6</sub> N	Pbam (55)	SM	—	(b)	NM	—	HQ	201979
289	Bi <sub>3</sub> NF <sub>6</sub>	Pbcm (57)	Triv.	—	(b)	NM	—	—	79395
290	Fe <sub>2</sub> C	Pbcm (57)	TI	—	(b)	—	—	—	670573
291	Ca <sub>2</sub> (AsO <sub>4</sub> )Cl	Pbcm (57)	Triv.	—	(b)	NM	—	—	26234
292	ScFe <sub>2</sub> Si <sub>2</sub>	Pbcm (57)	SM	—	—	FM	—	HQ	402545 633456
293	(NH <sub>4</sub> )(VO <sub>3</sub> )	Pbcm (57)	Triv.	—	—	NM	—	—	1487
294	NaO <sub>2</sub>	Pnnm (58)	SM	—	—	FM	—	—	26583 87179 87180 87181 180562 673259
295	Li <sub>4</sub> Ca(BO <sub>3</sub> ) <sub>2</sub>	Pnnm (58)	Triv.	—	—	NM	—	HQ	99503 239000
296	MnB <sub>4</sub>	Pnnm (58)	SM	—	(b)	FM	—	HQ	194807
297	FeB <sub>4</sub>	Pnnm (58)	Triv.	—	—	NM	—	—	196424 425311 670854
298	Ba <sub>2</sub> CoCl <sub>2</sub> (SeO <sub>3</sub> ) <sub>2</sub>	Pnnm (58)	SM	—	(b)	AFM	—	HQ	280965

299	$\text{Al}_2(\text{SiO}_4)\text{O}$	$Pnnm$ (58)	Triv.	—	—	NM	—	—	$24275^{(b)}$ $26688^{(b)}$ $30677^{(b)}$ $30678^{(b)}$ $30679^{(b)}$ $30680^{(b)}$ $76936^{(b)}$ $84613^{(b)}$ $84614^{(b)}$ $85743^{(b)}$ $86340$ $92634^{(b)}$ $92635^{(b)}$ $100395^{(b)}$ $100396^{(b)}$ $100397^{(b)}$ $100398^{(b)}$ $100399^{(b)}$ $169412^{(b)}$ $172725^{(b)}$ $172726^{(b)}$ $172727^{(b)}$ $172728^{(b)}$ $172729^{(b)}$ $172730^{(b)}$ $172731^{(b)}$ $172732^{(b)}$
300	$\text{CuZn}(\text{AsO}_4)(\text{OH})$	$Pnnm$ (58)	Triv.	—	(b)	FM	—	—	160894
301	$\text{CrO}_2$	$Pnnm$ (58)	Triv.	—	(b)	FM	—	—	$155832$ $185886$ $290478$ $290479$ $290480$
302	$\text{FeSe}_2$	$Pnnm$ (58)	Triv.	—	—	NM	—	—	$25680$ $42041$ $42115$ $44751$ $633469$ $633479$
303	$\text{FeS}_2$	$Pnnm$ (58)	Triv.	—	—	NM	—	—	$26756$ $42415$ $42416$ $109374$ $633255$ $633275$ $633304$
304	$\text{CoAs}_2$	$Pnnm$ (58)	SM	—	—	NM	SC	—	610034
305	$\text{MnS}_2$	$Pnnm$ (58)	SM	Fig. 31	—	FM	—	—	643441
306	$\text{Fe}(\text{NCNH})_2$	$Pnnm$ (58)	Triv.	—	—	NM	—	HQ	419222 $422725$
307	$\text{CaBi}(\text{CO}_3)\text{OF}$	$Pmmn$ (59)	Triv.	—	—	NM	—	HQ	87759
308	$\text{Na}_2(\text{TiO})(\text{GeO}_4)$	$Pmmn$ (59)	Triv.	—	(b,s)	NM	—	HQ	160149
309	$\text{CoCu}_2\text{O}_3$	$Pmmn$ (59)	SM	Fig. 31	—	FM	—	HQ	33996
310	$\text{Na}(\text{V}_2\text{O}_5)$	$Pmmn$ (59)	SM	—	(b)	FM	—	HQ	$59345^{(s)}$ $88354^{(s)}$ $88861$ $88862$ $88863^{(s)}$ $88864$ $89411^{(s)}$ $89412$ $89413$ $92954^{(s)}$ $251182$ $409210^{(s)}$
311	$\text{LiV}_2\text{O}_5$	$Pmmn$ (59)	SM	—	(b,s)	—	—	HQ	88639
312	$\text{CsMgH}_3$	$Pmmn$ (59)	Triv.	—	(b)	NM	—	—	159177
313	$\text{CrOCl}$	$Pmmn$ (59)	SM	—	(b)	FM	—	HQ	4086 $28318$
314	$\text{FeOCl}$	$Pmmn$ (59)	SM	—	(b)	AFM	—	HQ	$16013$ $27136$ $40963$ $167393$
315	$\text{RuCl}_3$	$Pmmn$ (59)	Triv.	—	—	FM	—	HQ	414041
316	$\text{Sr}(\text{V}_3\text{O}_7)$	$Pmmn$ (59)	SM	—	(b)	AFM	—	HQ	$241176$ $241177$ $241178$ $241179$ $241180$ $241181$ $241182$ $241183$ $241184$ $241185$ $241186$ $241187$
317	$\text{FeNb}_2\text{O}_6$	$Pbcn$ (60)	Triv.	—	(b)	FM	—	—	$15855$ $31943$ $151720$
318	$\text{Fe}(\text{Nb}_2\text{O}_6)$	$Pbcn$ (60)	TI	—	(b)	FM	—	—	24216
319	$\text{CuNb}_2\text{O}_6$	$Pbcn$ (60)	SM	—	(b)	FM	—	—	$71606$ $74424$ $79455$ $80316^{(s)}$
320	$\text{CoNb}_2\text{O}_6$	$Pbcn$ (60)	SM	—	(b)	FM	—	—	182710 $182711$
321	$\text{Na}_2(\text{Si}_2\text{O}_5)$	$Pbcn$ (60)	Triv.	—	(b,s)	NM	—	—	34669
322	$\text{O}(\text{CN})_2$	$Pbca$ (61)	Triv.	—	—	—	—	—	670397
323	$\text{Te}(\text{CN})_2$	$Pbca$ (61)	Triv.	—	—	—	—	—	670400
324	$\text{Cu}(\text{SeO}_3)$	$Pbca$ (61)	Triv.	—	(b)	NM	—	—	29506 $61342$
325	$\text{WO}_3$	$Pnma$ (62)	Triv.	—	(b,s)	NM	—	—	836
326	$\text{Mg}_3(\text{SiO}_4)\text{F}_2$	$Pnma$ (62)	Triv.	—	(b)	NM	—	—	15203 $252073$
327	$\text{K}_2\text{ClO}_3\text{N}$	$Pnma$ (62)	Triv.	—	—	NM	—	HQ	28211
328	$\text{Li}(\text{CN})$	$Pnma$ (62)	Triv.	—	—	NM	—	—	77321
329	$\text{AgHg}_2\text{O}_2(\text{NO}_3)$	$Pnma$ (62)	Triv.	—	—	NM	—	—	89685
330	$\text{K}_2\text{Pd}(\text{P}_2\text{S}_6)$	$Pnma$ (62)	Triv.	—	—	NM	—	—	165316
331	$\text{PbPd}(\text{P}_2\text{O}_7)$	$Pnma$ (62)	Triv.	—	(b)	NM	—	—	195305 $420534$
332	$\text{WO}_3(\text{H}_2\text{O})$	$Pnma$ (62)	Triv.	—	—	NM	—	HQ	201806
333	$\text{MoO}_2$	$Pnma$ (62)	Triv.	—	(b)	—	—	—	243549
334	$\text{KYTe}_2\text{O}_6$	$Pnma$ (62)	Triv.	—	(b)	NM	—	—	291295
335	$\text{LiSr}(\text{BS}_3)$	$Pnma$ (62)	Triv.	—	(b)	NM	—	HQ	380105
336	$(\text{AgF})(\text{AuF}_6)$	$Pnma$ (62)	SM	—	(b)	NM	—	—	422686
337	$(\text{NH}_4)(\text{Co}(\text{PO}_4))(\text{H}_2\text{O})$	$Pnma$ (62)	SM	—	—	FM	—	—	424548
338	$\text{Al}_2\text{FeC}$	$Pnma$ (62)	TI	—	(b,s)	—	—	—	670820
339	$\text{Li}_2\text{C}_2$	$Pnma$ (62)	Triv.	—	—	—	—	—	$671756$ $671757$ $671758$ $671759$ $671760$ $671761$ $671762$ $671763$ $671764$ $671765$ $671766$ $671767$ $671768$ $671769$ $671770$ $671771$
340	$\text{Al}_2(\text{SiO}_4)\text{O}$	$Pnma$ (62)	Triv.	—	(b)	NM	—	—	$25711$ $31115$ $85200$ $85201$ $85202$ $85203$ $85204$ $85744$ $86342$ $92632^{(s)}$ $92633$ $96722$ $100450$ $100451$ $100452$ $100453$ $100454$ $172720$ $172721$ $172722$ $172723$ $172724$ $92636$ $92637$
341	$\text{Li}(\text{VO})(\text{AsO}_4)$	$Pnma$ (62)	SM	Fig. 31	(b)	FM	—	—	90991
342	$\text{FeOOH}$	$Pnma$ (62)	SM	—	—	AFM	—	—	$239321$ $239322$ $239323$ $239324$ $245057$

343	PbCO <sub>3</sub>	<i>Pnma</i> (62)	Triv.	—	—	NM	—	HQ	6178 36164 36554 56101 166089 190074 247490 247491 247492 247493
344	Cd <sub>2</sub> (OH) <sub>3</sub> Cl	<i>Pnma</i> (62)	Triv.	—	(b)	NM	—	—	39285 83524
345	SnSO <sub>4</sub>	<i>Pnma</i> (62)	Triv.	—	—	NM	—	—	2748 25838 245904
346	Ca(B <sub>2</sub> Si <sub>2</sub> O <sub>8</sub> )	<i>Pnma</i> (62)	Triv.	—	(b,s)	NM	—	—	6254 20590 26491 29545 29546 29547 29548 29549 29550 30296
347	PbF <sub>2</sub>	<i>Pnma</i> (62)	Triv.	—	—	NM	—	—	36275 14324 154994 154995 154996 154997 154998 161080 161391 161392 161393 161394 673364
348	Tl <sub>2</sub> BeF <sub>4</sub>	<i>Pnma</i> (62)	Triv.	—	—	NM	—	HQ	171178 171179 171180 171181 171182 171183
349	Cs <sub>2</sub> CuCl <sub>4</sub>	<i>Pnma</i> (62)	SM	—	—	FM	—	HQ	9468 15699 91186 91187 91188 169176
350	Cs <sub>2</sub> CuBr <sub>4</sub>	<i>Pnma</i> (62)	SM	—	—	FM	—	HQ	10185 26024 169179
351	Rb <sub>5</sub> (SiAs <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	—	NM	—	—	300191
352	Cu(IO <sub>3</sub> )(OH)	<i>Pnma</i> (62)	SM	—	(b)	FM	—	HQ	41804
353	In(PO <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	—	(b)	NM	—	HQ	85579
354	K <sub>2</sub> (S <sub>3</sub> O <sub>6</sub> )	<i>Pnma</i> (62)	Triv.	—	—	NM	—	—	8200
355	Tl <sub>2</sub> (SeO <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	—	—	NM	—	HQ	73411 99382 99383 419775 419776 419777
356	K <sub>2</sub> (VO <sub>2</sub> F <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	—	NM	—	—	9122 60621
357	K(P <sub>4</sub> N <sub>7</sub> )	<i>Pnma</i> (62)	Triv.	—	(b,s)	NM	—	—	410630
358	Cs(P <sub>4</sub> N <sub>7</sub> )	<i>Pnma</i> (62)	Triv.	—	(b)	NM	—	—	410632
359	CuInO(PO <sub>4</sub> )	<i>Pnma</i> (62)	SM	—	(b)	FM	—	—	89606
360	Cu(SeO <sub>3</sub> )	<i>Pnma</i> (62)	SM	—	(b)	FM	—	HQ	498 51847 97747 5418 42079 42080 42081 42082 43247 53200 53201 76028 626498 626502 626514
361	CrP	<i>Pnma</i> (62)	SM	—	—	FM	—	—	9496 16543 41759 250011 610846
362	MnAs	<i>Pnma</i> (62)	TI	—	—	FM	—	—	30412 43246 43399 60880 61136 76089 76090 76091 643200 643213 643217 643220
363	MnP	<i>Pnma</i> (62)	TI	—	—	FM	—	—	30413 34036 42447 42448 42449 42450 42451 48031 48033 48034 48035 48036 610452 610474
364	FeAs	<i>Pnma</i> (62)	SM	—	—	FM	—	—	43248 43400 62607 633046 633050
365	FeP	<i>Pnma</i> (62)	SM	—	—	FM	SC	HQ	43248 43400 62607 633046 633050
366	Na <sub>2</sub> NiInF <sub>7</sub>	<i>Pnma</i> (62)	Triv.	—	(b,s)	FM	—	—	72110
367	Na <sub>2</sub> Ni(HPO <sub>3</sub> ) <sub>2</sub>	<i>Pnma</i> (62)	Triv.	Fig. 31	(b)	FM	—	—	247564
368	LiCu <sub>2</sub> O <sub>2</sub>	<i>Pnma</i> (62)	SM	—	(b)	FM	—	HQ	71221 71683 188111
369	Li(Sb <sub>2</sub> F <sub>7</sub> )	<i>Pnma</i> (62)	Triv.	—	(b,s)	NM	—	—	428176
370	FeMg(SiO <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	—	(b)	FM	—	—	164171 164172
371	AgCu(VO <sub>4</sub> )	<i>Pnma</i> (62)	SM	—	(b)	FM	—	HQ	419201 419202
372	P <sub>2</sub> O <sub>5</sub>	<i>Pnma</i> (62)	Triv.	—	(b,s)	NM	—	—	16611 29045 79698
373	NaZn(MoO <sub>4</sub> )(OH)	<i>Pnma</i> (62)	Triv.	—	(b)	NM	—	—	9783
374	Pb(V <sub>2</sub> O <sub>6</sub> )	<i>Pnma</i> (62)	Triv.	—	—	NM	—	—	6109
375	NaTaO <sub>3</sub>	<i>Pnma</i> (62)	Triv.	—	—	NM	—	—	980 <sup>(b,s)</sup> 23319 88375 <sup>(b,s)</sup> 150430 <sup>(b,s)</sup> 173757 <sup>(b,s)</sup> 239690 <sup>(b,s)</sup> 241443 <sup>(b,s)</sup>
376	YTiO <sub>3</sub>	<i>Pnma</i> (62)	SM	—	(b)	FM	SC*	HQ	8150 84608 84609 84610 174118 9008 25533 72319
377	Na(NiF <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	Fig. 31	(b)	FM	—	—	192140 192142 192144 200062
378	La(GaO <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	—	NM	—	—	41280 50388 <sup>(b,s)</sup> 51285 <sup>(b,s)</sup> 73759 <sup>(b,s)</sup> 73760 <sup>(b,s)</sup> 73761 <sup>(b,s)</sup> 79662 <sup>(b,s,l)</sup> 88146 <sup>(b,s)</sup> 88259 <sup>(b,s)</sup> 88349 <sup>(b,s)</sup> 91786 <sup>(b,s)</sup> 94299 <sup>(b,s)</sup> 98168 <sup>(b,s)</sup> 98410 <sup>(b,s)</sup> 153307 <sup>(b,s)</sup> 160233 <sup>(b,s)</sup> 160234 <sup>(b,s)</sup> 160235 <sup>(b,s)</sup> 161782 <sup>(b,s)</sup>
379	La(VO <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	(b,s)	AFM	—	—	63520 73898 73899 185831
380	Na(ZnF <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	(b)	NM	—	HQ	69349 72320
381	La(MnO <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	(b)	FM	—	—	82226 <sup>(s)</sup> 82228 <sup>(s)</sup> 88388 <sup>(s)</sup> 90424 161928 <sup>(s)</sup> 161929 <sup>(s)</sup> 180180 <sup>(s)</sup> 185279 252946
382	Y(CoO <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	(b)	FM	—	HQ	155834 155835 155836 155837 155838
383	Ca(SiO <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	(b,s)	NM	—	—	240462 240463 240464 240465 240466 240467 240468 240469
384	Rb(Li(NH <sub>2</sub> ) <sub>2</sub> )	<i>Pnma</i> (62)	Triv.	—	—	NM	—	—	95786
385	Sr(VO <sub>3</sub> )Cl	<i>Pnma</i> (62)	Triv.	—	(b,s)	NM	—	HQ	50787

386	BaCs(VS <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	—	(b)	NM	—	HQ	430160
387	MnO <sub>2</sub>	<i>Pnma</i> (62)	SM	—	(b)	AFM	—	—	20228 24034 78331 171866
388	Ca <sub>5</sub> Sb <sub>3</sub>	<i>Pnma</i> (62)	SM	—	—	NM	—	—	2065 619564
389	Ca <sub>5</sub> Bi <sub>3</sub>	<i>Pnma</i> (62)	SM	—	—	NM	—	—	2140 616533
390	Y <sub>4</sub> Ti(SiO <sub>4</sub> ) <sub>2</sub> OF <sub>6</sub>	<i>Cmcm</i> (63)	Triv.	—	(b)	NM	—	—	20003
391	K(FeF <sub>4</sub> )	<i>Cmcm</i> (63)	SM	—	(b,s)	FM	—	—	23588 60615
392	(PbF <sub>2</sub> ) <sub>7</sub> (PbI <sub>2</sub> )	<i>Cmcm</i> (63)	Triv.	—	—	NM	—	HQ	36337 <sup>(b,s)</sup> 431846
393	(CuO <sub>2</sub> ) <sub>4</sub>	<i>Cmcm</i> (63)	SM	—	(b,s)	FM	—	HQ	54129
394	BaVS <sub>3</sub>	<i>Cmcm</i> (63)	SM	Fig. 31	(k*)	—	—	HQ	63228
395	Tl <sub>2</sub> (AlF <sub>5</sub> )	<i>Cmcm</i> (63)	Triv.	—	—	NM	—	—	109365
396	CuO <sub>2</sub>	<i>Cmcm</i> (63)	SM	—	(b,s)	FM	—	HQ	150913
397	Mg(Al <sub>2</sub> O <sub>4</sub> )	<i>Cmcm</i> (63)	Triv.	—	(b)	NM	—	—	161057
398	LiFeP	<i>Cmcm</i> (63)	TI	—	—	NM	—	—	187134
399	BaCu <sub>2</sub> (Ge <sub>3</sub> O <sub>9</sub> )(H <sub>2</sub> O)	<i>Cmcm</i> (63)	TI	—	—	FM	—	—	424818
400	AlF <sub>3</sub>	<i>Cmcm</i> (63)	Triv.	—	(k*,b,s)	NM	—	HQ	202681
401	KFe <sub>2</sub> S <sub>3</sub>	<i>Cmcm</i> (63)	SM	—	(b)	FM	—	—	632396 99507
402	Ca <sub>3</sub> (VN <sub>3</sub> )	<i>Cmcm</i> (63)	Triv.	—	(b)	NM	—	—	72118
403	NiSO <sub>4</sub>	<i>Cmcm</i> (63)	Triv.	Fig. 31	(b)	AFM	—	—	16691 16741 33737
404	Ni(SeO <sub>4</sub> )	<i>Cmcm</i> (63)	Triv.	Fig. 32	(b)	FM	—	—	25700
405	TiPO <sub>4</sub>	<i>Cmcm</i> (63)	SM	—	(b)	FM	—	HQ	36520 431885
406	Rb(Fe <sub>2</sub> Se <sub>3</sub> )	<i>Cmcm</i> (63)	SM	—	—	FM	—	HQ	81547
407	Cs(Fe <sub>2</sub> Se <sub>3</sub> )	<i>Cmcm</i> (63)	SM	—	—	FM	—	HQ	81549 187535
408	Cs(Fe <sub>2</sub> S <sub>3</sub> )	<i>Cmcm</i> (63)	SM	—	(b)	FM	—	HQ	99504
409	Tl(Fe <sub>2</sub> S <sub>3</sub> )	<i>Cmcm</i> (63)	SM	—	(b)	NM	—	HQ	166049
410	BaFe <sub>2</sub> Se <sub>3</sub>	<i>Cmcm</i> (63)	TI	—	—	FM	SC	HQ	290594 290596
411	KFe <sub>2</sub> Se <sub>3</sub>	<i>Cmcm</i> (63)	SM	—	—	FM	—	HQ	424671 424672
412	TiCu <sub>2</sub>	<i>Cmcm</i> (63)	TI	—	—	NM	—	—	629379 629386 629405
413	K <sub>2</sub> (NiP <sub>2</sub> )	<i>Cmcm</i> (63)	Triv.	—	—	NM	—	HQ	300119
414	K <sub>2</sub> (NiAs <sub>2</sub> )	<i>Cmcm</i> (63)	Triv.	—	—	NM	—	HQ	300120
415	Cs <sub>2</sub> NiP <sub>2</sub>	<i>Cmcm</i> (63)	Triv.	—	—	—	—	—	656056
416	Cs <sub>2</sub> PtSb <sub>2</sub>	<i>Cmcm</i> (63)	Triv.	—	—	NM	—	—	658700
417	Cs <sub>2</sub> PdSb <sub>2</sub>	<i>Cmcm</i> (63)	Triv.	—	—	NM	—	—	658702
418	Cs <sub>2</sub> NiBi <sub>2</sub>	<i>Cmcm</i> (63)	Triv.	—	—	—	—	—	658704
419	K <sub>3</sub> Pt <sub>2</sub> O <sub>4</sub>	<i>Cmcm</i> (63)	SM	—	(b,s)	FM	—	—	14158
420	KCuZrF <sub>7</sub>	<i>Cmcm</i> (63)	Triv.	—	(b,s)	FM	—	—	92469
421	KCuHfF <sub>7</sub>	<i>Cmcm</i> (63)	Triv.	—	(b,s)	FM	—	—	92470
422	Mg(V <sub>2</sub> O <sub>5</sub> )	<i>Cmcm</i> (63)	TI	—	(b)	FM	—	HQ	50979 50981
423	Li(V <sub>2</sub> O <sub>5</sub> )	<i>Cmcm</i> (63)	SM	—	(b,s)	FM	—	HQ	50980 50982 201974
424	LiFe(PO <sub>4</sub> )	<i>Cmcm</i> (63)	Triv.	—	(b)	AFM	—	HQ	97766
425	LiNi(PO <sub>4</sub> )	<i>Cmcm</i> (63)	Triv.	—	(b)	AFM	—	HQ	97767
426	CuMgVO <sub>4</sub>	<i>Cmcm</i> (63)	Triv.	—	(b)	NM	—	—	239746
427	Al <sub>2</sub> La <sub>2</sub> Ge	<i>Cmcm</i> (63)	TI	—	—	NM	—	HQ	423614
428	Na(NbO <sub>3</sub> )	<i>Cmcm</i> (63)	Triv.	—	(b,s)	NM	—	—	22065 <sup>(I)</sup> 23323 192404 192405 280098
429	Na(TaO <sub>3</sub> )	<i>Cmcm</i> (63)	Triv.	—	(b,s)	NM	—	HQ	23320 23321 <sup>(I)</sup> 88376 239691 241444 241445 280099
430	FeTi <sub>2</sub> O <sub>5</sub>	<i>Cmcm</i> (63)	TI	—	(b)	FM	—	—	37231
431	SrCuO <sub>2</sub>	<i>Cmcm</i> (63)	SM	—	—	NM	SC	—	16217 77291 83051 93653 202992 670129
432	CuBaO <sub>2</sub>	<i>Cmcm</i> (63)	SM	—	—	—	SC	—	670104
433	La <sub>2</sub> (CuO <sub>4</sub> )	<i>Cmce</i> (64)	SM	—	(b)	NM	—	—	1076 <sup>(s,l)</sup> 41499 50265 <sup>(s,l)</sup> 67837 <sup>(s,l)</sup> 69311 <sup>(s,l)</sup> 69312 <sup>(s,l)</sup> 72237 <sup>(s,l)</sup> 73906 <sup>(s,l)</sup> 73907 <sup>(s,l)</sup> 73908 <sup>(s,l)</sup> 73909 <sup>(s,l)</sup> 73910 <sup>(s,l)</sup> 74145 <sup>(s,l)</sup> 74150 <sup>(s,l)</sup> 75891 <sup>(s,l)</sup> 78194 <sup>(s,l)</sup> 78237 <sup>(s,l)</sup> 78287 <sup>(s,l)</sup> 78288 <sup>(s,l)</sup> 78289 <sup>(s,l)</sup> 78290 <sup>(s,l)</sup> 78291 <sup>(s,l)</sup> 78292 <sup>(s,l)</sup> 78293 <sup>(s,l)</sup> 78294 <sup>(s,l)</sup> 78295 <sup>(s,l)</sup> 78296 <sup>(s,l)</sup> 78297 <sup>(s,l)</sup> 78298 <sup>(s,l)</sup> 78299 <sup>(s,l)</sup> 78300 <sup>(s,l)</sup> 87969 <sup>(s,l)</sup> 89173 <sup>(s,l)</sup> 173891 <sup>(s,l)</sup> 173893 <sup>(s,l)</sup> 173895 <sup>(s,l)</sup> 186588 <sup>(s,l)</sup> 261661 <sup>(s,l)</sup>
434	La <sub>2</sub> (NiO <sub>4</sub> )	<i>Cmce</i> (64)	Triv.	—	(b,s)	AFM	—	HQ	50244 <sup>(I)</sup> 56318 <sup>(I)</sup> 63398 <sup>(I)</sup> 67838 <sup>(I)</sup> 69752 69754 <sup>(I)</sup> 69755 <sup>(I)</sup>
435	Rb <sub>2</sub> CuCl <sub>4</sub>	<i>Cmce</i> (64)	SM	—	(b,s)	FM	—	HQ	15145 <sup>(I)</sup> 55013

436	Rb <sub>2</sub> CuCl <sub>2</sub> Br <sub>2</sub>	<i>Cmce</i> (64)	SM	—	(b)	FM	—	HQ	15147
437	K <sub>2</sub> CuF <sub>4</sub>	<i>Cmce</i> (64)	SM	—	(b,s,l*)	FM	—	HQ	38426 174116
438	Cs <sub>2</sub> AgF <sub>4</sub>	<i>Cmce</i> (64)	SM	—	(b,s,l*)	FM	—	—	155817 155818
439	Ba <sub>5</sub> Sb <sub>4</sub>	<i>Cmce</i> (64)	Triv.	—	—	NM	—	HQ	280022
440	Na(IO <sub>3</sub> )	<i>Cmmm</i> (65)	TI	Fig. 32	(k*,b,s,l*)	NM	—	—	33664
441	Ca(TiO <sub>3</sub> )	<i>Cmmm</i> (65)	Triv.	—	(k*,b,s,l*)	NM	—	—	187294
442	Na <sub>3</sub> B <sub>20</sub>	<i>Cmmm</i> (65)	SM	—	—	NM	—	HQ	407159 410247
443	AuMgO <sub>2</sub>	<i>Cmmm</i> (65)	Triv.	—	—	—	—	—	670092
444	Mo <sub>2</sub> CuGa <sub>5</sub>	<i>Cmmm</i> (65)	TI	—	—	—	—	—	670139
445	AlFe <sub>2</sub> B <sub>2</sub>	<i>Cmmm</i> (65)	SM	—	—	FM	—	—	20322 23205 239296 241907 241908 241909 251811
446	YNi <sub>4</sub> Si	<i>Cmmm</i> (65)	SM	—	—	NM	—	—	290731
447	LaNi <sub>4</sub> Si	<i>Cmmm</i> (65)	SM	—	—	NM	—	—	290732
448	Al <sub>3</sub> Ni <sub>5</sub>	<i>Cmmm</i> (65)	SM	—	—	NM	—	—	58041 191113 608803
449	Ga <sub>3</sub> Ni <sub>5</sub>	<i>Cmmm</i> (65)	SM	—	—	NM	—	—	103861 634860 634865
450	KSc <sub>2</sub> F <sub>7</sub>	<i>Cmmm</i> (65)	Triv.	—	—	NM	—	HQ	47227
451	Li <sub>2</sub> (MnBr <sub>4</sub> )	<i>Cmmm</i> (65)	SM	—	(b)	FM	—	HQ	33865
452	MnPt <sub>3</sub> O <sub>6</sub>	<i>Cmmm</i> (65)	SM	—	(b)	FM	—	HQ	35337
453	ZnPt <sub>3</sub> O <sub>6</sub>	<i>Cmmm</i> (65)	Triv.	—	(b)	NM	—	HQ	35339
454	CdPt <sub>3</sub> O <sub>6</sub>	<i>Cmmm</i> (65)	Triv.	—	(b)	NM	—	HQ	35407
455	K <sub>2</sub> Na(FeO <sub>3</sub> )	<i>Cmme</i> (67)	SM	—	(b)	AFM	—	—	36380
456	FeSe	<i>Cmme</i> (67)	Triv.	—	—	FM	—	—	182545 169283
457	Pb <sub>2</sub> OFCl	<i>Cmme</i> (67)	Triv.	—	—	NM	—	HQ	200211 200212 200213
458	LiFeAs	<i>Cmme</i> (67)	TI	—	—	FM	—	—	168206
459	FeSe	<i>Cmme</i> (67)	TI	—	—	NM	—	HQ	166441 169295 169299 169303 169306 169309 169311 169313 169315
460	FeSe	<i>Cmme</i> (67)	TI	—	—	NM	—	HQ	169285
461	SiO <sub>2</sub>	<i>Ccce</i> (68)	Triv.	—	(b,s)	NM	—	—	170527
462	Cs <sub>2</sub> Pd <sub>3</sub> Se <sub>4</sub>	<i>Fmmm</i> (69)	Triv.	—	(k*,b)	NM	—	HQ	33892
463	Cs <sub>2</sub> Ni <sub>3</sub> S <sub>4</sub>	<i>Fmmm</i> (69)	Triv.	—	(k*,b)	NM	—	—	627055
464	Rb <sub>2</sub> Pb(Cu(NO <sub>2</sub> ) <sub>6</sub> )	<i>Fmmm</i> (69)	SM	—	—	FM	—	HQ	372
465	PbK <sub>2</sub> (Cu(NO <sub>2</sub> ) <sub>6</sub> )	<i>Fmmm</i> (69)	SM	—	—	FM	—	HQ	1274
466	K <sub>2</sub> Ba(Cu(NO <sub>2</sub> ) <sub>6</sub> )	<i>Fmmm</i> (69)	SM	—	—	FM	—	HQ	1830
467	K <sub>2</sub> Ca(Cu(NO <sub>2</sub> ) <sub>6</sub> )	<i>Fmmm</i> (69)	SM	—	—	FM	—	HQ	6183
468	Cs <sub>2</sub> PbCu(NO <sub>2</sub> ) <sub>6</sub>	<i>Fmmm</i> (69)	SM	—	—	—	—	HQ	8284 8285 56252 56253
469	Cu <sub>2</sub> Cl <sub>2</sub> O	<i>Fddd</i> (70)	TI	—	(b)	FM	—	—	1055 96610
470	K <sub>4</sub> P <sub>6</sub>	<i>Fddd</i> (70)	Triv.	—	—	NM	—	HQ	33260
471	Cu <sub>16</sub> O <sub>8</sub> Cl <sub>16</sub>	<i>Fddd</i> (70)	TI	—	(b)	—	—	—	430861
472	RbVSe <sub>2</sub>	<i>Fddd</i> (70)	Triv.	—	(b,s)	NM	—	HQ	415479
473	CaBi <sub>2</sub> (CO <sub>3</sub> ) <sub>2</sub> O <sub>2</sub>	<i>Immm</i> (71)	TI	—	—	NM	—	HQ	94741
474	K <sub>3</sub> Ir	<i>Immm</i> (71)	TI	—	—	—	—	—	674660
475	Sr <sub>2</sub> FeO <sub>3</sub>	<i>Immm</i> (71)	Triv.	—	—	AFM	—	HQ	251018 251019 251020
476	Sr <sub>3</sub> (Fe <sub>2</sub> O <sub>5</sub> )	<i>Immm</i> (71)	Triv.	—	(b,s)	FM	—	HQ	420234
477	Cs(FeS <sub>2</sub> )	<i>Immm</i> (71)	TI	—	(b,s)	FM	—	—	25697 53234 201112
478	RbFeS <sub>2</sub>	<i>Immm</i> (71)	TI	—	(b,s)	FM	—	—	633207
479	Li <sub>2</sub> NiO <sub>2</sub>	<i>Immm</i> (71)	Triv.	—	(b)	FM	—	—	25000
480	Li <sub>2</sub> (CuO <sub>2</sub> )	<i>Immm</i> (71)	SM	—	(b)	FM	—	—	25001 67204 67205 202996 238945 47106 67150 67151 291072
481	Na <sub>2</sub> PtO <sub>2</sub>	<i>Immm</i> (71)	Triv.	—	(b)	NM	—	—	25018
482	VOCl <sub>2</sub>	<i>Immm</i> (71)	SM	—	(b,s)	FM	—	—	24380
483	VOBr <sub>2</sub>	<i>Immm</i> (71)	SM	—	(b,s)	FM	—	—	24381
484	PtSO <sub>4</sub>	<i>Ibam</i> (72)	Triv.	—	(b)	—	—	—	671488
485	K <sub>2</sub> (MnS <sub>2</sub> )	<i>Ibam</i> (72)	SM	Fig. 32	(b,s)	FM	—	HQ	65453
486	Rb <sub>2</sub> (MnS <sub>2</sub> )	<i>Ibam</i> (72)	SM	Fig. 32	(b,s)	AFM	—	HQ	65454
487	Cs <sub>2</sub> (MnS <sub>2</sub> )	<i>Ibam</i> (72)	SM	Fig. 32	(b,s)	FM	—	HQ	65455
488	K <sub>2</sub> (MnSe <sub>2</sub> )	<i>Ibam</i> (72)	SM	Fig. 32	(b,s)	FM	—	HQ	65456
489	Rb <sub>2</sub> (MnSe <sub>2</sub> )	<i>Ibam</i> (72)	SM	Fig. 32	(b,s)	FM	—	HQ	65457
490	Cs <sub>2</sub> (MnSe <sub>2</sub> )	<i>Ibam</i> (72)	SM	Fig. 33	(b,s)	FM	—	HQ	65458
491	Rb <sub>2</sub> (MnTe <sub>2</sub> )	<i>Ibam</i> (72)	SM	Fig. 33	(b,s)	FM	—	HQ	65460
492	Cs <sub>2</sub> (MnTe <sub>2</sub> )	<i>Ibam</i> (72)	SM	Fig. 33	(b,s)	FM	—	HQ	65461
493	K <sub>2</sub> CoS <sub>2</sub>	<i>Ibam</i> (72)	SM	—	(b,s)	FM	—	HQ	67387 623958 623960

494	Rb <sub>2</sub> CoS <sub>2</sub>	<i>Ibam</i> (72)	SM	—	(b,s)	FM	—	HQ	67388
495	Cs <sub>2</sub> CoS <sub>2</sub>	<i>Ibam</i> (72)	SM	—	(b,s)	FM	—	HQ	67389
496	K <sub>2</sub> CoSe <sub>2</sub>	<i>Ibam</i> (72)	SM	—	(b,s)	FM	—	HQ	67390
497	Rb <sub>2</sub> CoSe <sub>2</sub>	<i>Ibam</i> (72)	SM	—	(b,s)	FM	—	HQ	67391
498	Cs <sub>2</sub> CoSe <sub>2</sub>	<i>Ibam</i> (72)	SM	—	(b,s)	FM	—	HQ	67392
499	Na <sub>2</sub> CoSe <sub>2</sub>	<i>Ibam</i> (72)	SM	—	(b,s)	FM	—	—	624264
500	Na <sub>3</sub> (AlAs <sub>2</sub> )	<i>Ibam</i> (72)	Triv.	—	(b)	NM	—	HQ	63149
501	Na <sub>3</sub> (AlP <sub>2</sub> )	<i>Ibam</i> (72)	Triv.	—	(b)	NM	—	HQ	73278 402081
502	K <sub>3</sub> (InP <sub>2</sub> )	<i>Ibam</i> (72)	Triv.	—	(b,s)	NM	—	HQ	73281 300141
503	KAg(CO <sub>3</sub> )	<i>Ibca</i> (73)	Triv.	—	—	NM	—	HQ	26632 31021 242236 242239 409484
504	CsMoO <sub>2</sub> F <sub>3</sub>	<i>Imma</i> (74)	Triv.	—	—	NM	—	HQ	9710
505	Na <sub>4</sub> Ni(P <sub>2</sub> O <sub>7</sub> )F <sub>2</sub>	<i>Imma</i> (74)	Triv.	—	(b)	AFM	—	—	251665 251666
506	MgAlBO <sub>4</sub>	<i>Imma</i> (74)	Triv.	—	(b)	—	—	—	670206
507	Na <sub>2</sub> NiGaF <sub>7</sub>	<i>Imma</i> (74)	Triv.	—	(k*,b,s)	FM	—	HQ	408111
508	Cs(Pd <sub>2</sub> F <sub>5</sub> )	<i>Imma</i> (74)	Triv.	—	(b,s)	FM	—	—	35284
509	RbPd <sub>2</sub> F <sub>5</sub>	<i>Imma</i> (74)	Triv.	—	(b,s)	FM	—	HQ	72299
510	Zn(AlF <sub>5</sub> )(H <sub>2</sub> O) <sub>2</sub>	<i>Imma</i> (74)	Triv.	—	—	NM	—	HQ	245171
511	LiCuVO <sub>4</sub>	<i>Imma</i> (74)	SM	—	—	FM	—	HQ	15836 <sup>(b)</sup> 26992 <sup>(b)</sup> 65677 <sup>(b)</sup> 72846 <sup>(b)</sup> 261517 <sup>(b)</sup> 290738 290739 291437 <sup>(b)</sup> 291440 <sup>(b)</sup> 291441 <sup>(b)</sup>
512	Mg <sub>2</sub> (SiO <sub>4</sub> )	<i>Imma</i> (74)	Triv.	—	—	NM	—	HQ	6311 <sup>(b)</sup> 23597 <sup>(b)</sup> 27530 <sup>(b)</sup> 83784 83785 83786 83787 63178 <sup>(b)</sup> 66490 <sup>(b)</sup> 100725 <sup>(b)</sup> 159955 <sup>(b)</sup> 171064 <sup>(b)</sup> 171065 <sup>(b)</sup> 171066 <sup>(b)</sup> 290205 <sup>(b)</sup> 290206 <sup>(b)</sup> 290207 <sup>(b)</sup> 290208 <sup>(b)</sup> 670570 <sup>(b)</sup>
513	Ca(SiO <sub>3</sub> )	<i>Imma</i> (74)	Triv.	—	(b,s)	NM	—	—	240422 240423 240424 240425 240426 240427 240428 240429
514	K <sub>4</sub> (CuV <sub>5</sub> O <sub>15</sub> Cl)	<i>P4</i> (75)	SM	—	(b,s)	FM	—	HQ	401042
515	WOCl <sub>4</sub>	<i>I4</i> (79)	Triv.	—	—	NM	—	HQ	255119 426524
516	(NH <sub>4</sub> )(WAgS <sub>4</sub> )	<i>I</i> 4̄ (82)	Triv.	—	—	NM	—	HQ	84370
517	Cs(As <sub>4</sub> F <sub>13</sub> )	<i>I</i> 4̄ (82)	Triv.	—	—	NM	—	HQ	281641
518	RbLa(Si(CN <sub>2</sub> ) <sub>4</sub> )	<i>I</i> 4̄ (82)	Triv.	—	—	NM	—	HQ	419337
519	ZrF <sub>4</sub>	<i>P4</i> <sub>2</sub> /m (84)	Triv.	—	—	NM	—	—	35100
520	Cs <sub>2</sub> (V <sub>4</sub> O <sub>9</sub> )	<i>P4</i> <sub>2</sub> /m (84)	Triv.	—	(b)	FM	—	HQ	79408
521	CuCl(B(OH) <sub>4</sub> )	<i>P4</i> /n (85)	SM	—	—	FM	—	HQ	56963
522	(AgF)(BF <sub>4</sub> )	<i>P4</i> /n (85)	SM	—	—	NM	—	HQ	80645 80646
523	(VO)(PO <sub>4</sub> )	<i>P4</i> /n (85)	Triv.	—	(b)	NM	—	HQ	425536 77598 108983
524	Ca(V <sub>4</sub> O <sub>9</sub> )	<i>P4</i> /n (85)	TI	—	(b)	FM	—	HQ	2556 90927
525	Sr(V <sub>4</sub> O <sub>9</sub> )	<i>P4</i> /n (85)	TI	—	(b)	FM	—	HQ	90926
526	(VO)MoO <sub>4</sub>	<i>P4</i> /n (85)	SM	—	(b,s)	AFM	—	HQ	27315
527	As <sub>2</sub> O <sub>3</sub>	<i>P4</i> <sub>2</sub> /n (86)	Triv.	—	(b,s)	NM	—	—	183096
528	N <sub>4</sub> P <sub>4</sub> Br <sub>8</sub>	<i>P4</i> <sub>2</sub> /n (86)	Triv.	—	—	NM	—	—	2716
529	BaFe <sub>2</sub> S <sub>4</sub>	<i>I4</i> /m (87)	SM	—	—	FM	—	HQ	23081
530	Rb <sub>2</sub> (TeBr <sub>6</sub> )	<i>I4</i> /m (87)	Triv.	—	—	NM	—	HQ	49520
531	Bi <sub>4</sub> RuI <sub>2</sub>	<i>I4</i> /m (87)	Triv.	—	—	NM	—	HQ	406949
532	(NH <sub>3</sub> ) <sub>4</sub> Pd(N <sub>3</sub> ) <sub>4</sub> Pd	<i>I4</i> /m (87)	Triv.	—	—	—	—	HQ	410384
533	VAu <sub>4</sub>	<i>I4</i> /m (87)	SM	—	—	FM	—	—	612460
534	Ni(VO(PO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub>	<i>I4</i> /m (87)	TI	—	—	FM	—	HQ	85597
535	(Co(H <sub>2</sub> O) <sub>4</sub> )(VO(PO <sub>4</sub> ) <sub>2</sub> )	<i>I4</i> /m (87)	SM	—	—	FM	—	HQ	281336
536	Sr <sub>2</sub> Cu(WO <sub>6</sub> )	<i>I4</i> /m (87)	SM	—	(b,s)	FM	—	—	33571 72812 88701 99303 186027 190594 193614 291133 291134 291135
537	Sr <sub>2</sub> CuTeO <sub>6</sub>	<i>I4</i> /m (87)	SM	—	(b,s)	FM	—	—	33573 88702
538	Ba <sub>2</sub> Cu(WO <sub>6</sub> )	<i>I4</i> /m (87)	SM	—	(b,s)	FM	—	HQ	72813
539	Sr <sub>2</sub> Fe(WO <sub>6</sub> )	<i>I4</i> /m (87)	Triv.	—	(k*,b,s)	AFM	—	—	78677
540	Ba <sub>2</sub> Cu(TeO <sub>6</sub> )	<i>I4</i> /m (87)	SM	—	(b,s)	FM	—	—	88703
541	Sr <sub>2</sub> Ni(WO <sub>6</sub> )	<i>I4</i> /m (87)	Triv.	Fig. 34	(b,s)	AFM	—	HQ	91791 153327 190591
542	Ba <sub>2</sub> (FeWO <sub>6</sub> )	<i>I4</i> /m (87)	Triv.	Fig. 34	(k*,b,s)	AFM	—	HQ	95518 95520 95521 95522 95523
543	Sr <sub>2</sub> NiMoO <sub>6</sub>	<i>I4</i> /m (87)	Triv.	—	(b,s)	AFM	—	HQ	98191 155273 155274 155732 157020 157021 157022 157023 157025

544	$\text{Sr}_2(\text{FeMoO}_6)$	$I4/m$ (87)	Triv.	Fig. 34	(b,s)	FM	—	HQ	150701 153426 155482 157600 157601 157602 166816 172212 193690 247539 248460 <sup>(k)</sup> 248461 248462 248463 248464
545	$\text{Sr}_2(\text{FeReO}_6)$	$I4/m$ (87)	SM	Fig. 33	(b,s)	FM	—	HQ	150702
546	$\text{Sr}_2\text{Mg}(\text{WO}_6)$	$I4/m$ (87)	Triv.	Fig. 34	(b,s)	NM	—	HQ	151703 152574 155306 155307 155308 155309 155310 168463
547	$\text{Sr}_2(\text{NiOsO}_6)$	$I4/m$ (87)	Triv.	—	(b,s)	FM	—	HQ	152440 152441 152442 152443
548	$\text{Sr}_2(\text{CoMoO}_6)$	$I4/m$ (87)	SM	Fig. 33	(b,s)	FM	—	HQ	153544 153545 153546
549	$\text{Sr}_2(\text{NiMoO}_6)$	$I4/m$ (87)	TI	—	(b,s)	AFM	—	HQ	157024 157026
550	$\text{Sr}_2\text{GaTaO}_6$	$I4/m$ (87)	Triv.	—	(b,s)	NM	—	HQ	172330
551	$\text{Sr}_2\text{NiReO}_6$	$I4/m$ (87)	SM	—	(b,s)	FM	—	HQ	173487 173490
552	$\text{Sr}_2\text{CoReO}_6$	$I4/m$ (87)	TI	Fig. 33	(b,s)	AFM	—	HQ	173488
553	$\text{Sr}_2\text{Cu}(\text{MoO}_6)$	$I4/m$ (87)	SM	—	(b,s)	FM	—	HQ	186038
554	$\text{Sr}_2\text{MgMoO}_6$	$I4/m$ (87)	Triv.	Fig. 34	(b,s)	NM	—	HQ	187662
555	$\text{Sr}_2\text{MnMoO}_6$	$I4/m$ (87)	SM	Fig. 33	(b,s)	FM	—	HQ	187669
556	$\text{Sr}_2\text{CoWO}_6$	$I4/m$ (87)	SM	Fig. 33	(b,s)	AFM	—	—	190593 245470
557	$\text{Sr}_2\text{CoNbO}_6$	$I4/m$ (87)	Triv.	Fig. 34	(b,s)	—	—	—	192327
558	$\text{Sr}_2\text{CoOsO}_6$	$I4/m$ (87)	SM	—	(b,s)	FM	—	HQ	236435 236436
559	$\text{Sr}_2\text{Li}(\text{ReO}_6)$	$I4/m$ (87)	Triv.	—	(b,s)	NM	—	—	246730 418991 <sup>(k)</sup>
560	$\text{InK}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_4$	$I4_1/a$ (88)	Triv.	—	—	NM	—	—	99956
561	$\text{Y}(\text{Pd}_2\text{O}_4)$	$I4_1/a$ (88)	SM	—	(b)	NM	—	HQ	78846
562	$\text{PbPd}_2\text{O}_4$	$I4_1/a$ (88)	Triv.	Fig. 34	(b)	NM	—	HQ	263049
563	$\text{TiTiCl}_4$	$I4_1/a$ (88)	Triv.	—	(b)	NM	—	HQ	4031
564	$\text{Ca}(\text{WO}_4)$	$I4_1/a$ (88)	Triv.	—	—	NM	—	HQ	15586 <sup>(b)</sup> 15869 <sup>(b)</sup> 18135 <sup>(b)</sup> 60547 <sup>(b)</sup> 60548 <sup>(b)</sup> 60549 <sup>(b)</sup> 60550 <sup>(b)</sup> 60551 <sup>(b)</sup> 77335 155423 <sup>(b)</sup> 155791 <sup>(b)</sup> 157428 <sup>(b)</sup> 193047 <sup>(b)</sup> 193491 <sup>(b)</sup> 291535 <sup>(b)</sup> 671942 <sup>(b)</sup>
565	$\text{Ca}(\text{MoO}_4)$	$I4_1/a$ (88)	Triv.	—	—	NM	—	—	22351 <sup>(b)</sup> 23699 <sup>(b)</sup> 60552 <sup>(b)</sup> 60553 <sup>(b)</sup> 60554 <sup>(b)</sup> 60555 <sup>(b)</sup> 60556 <sup>(b)</sup> 60557 <sup>(b)</sup> 60558 <sup>(b)</sup> 62219 <sup>(b)</sup> 77334 183446 183447 <sup>(b)</sup> 193793 <sup>(b)</sup> 194078 <sup>(b)</sup> 194079 <sup>(b)</sup> 417513 <sup>(b)</sup>
566	$\text{Zr}(\text{GeO}_4)$	$I4_1/a$ (88)	Triv.	—	(b)	NM	—	HQ	29262
567	$\text{Hf}(\text{GeO}_4)$	$I4_1/a$ (88)	Triv.	—	(b,s)	NM	—	HQ	202080
568	$\text{YNbO}_4$	$I4_1/a$ (88)	Triv.	—	—	NM	—	—	239208 239209 430917 430918 430919 430920 430921 430922
569	$\text{Bi}_2\text{ZnTiO}_6$	$P4mm$ (99)	Triv.	—	(b,s)	NM	—	—	162766 162767 162768 186801
570	$\text{BiFeO}_3$	$P4mm$ (99)	SM	—	(b,s)	AFM	—	—	188467 188466
571	$\text{LaCoO}_3$	$P4mm$ (99)	SM	—	(b,s)	—	—	—	673191
572	$\text{La}_1\text{Fe}_1\text{O}_3$	$P4mm$ (99)	SM	—	(b,s)	—	—	—	673196
573	$\text{BaSiO}_3$	$P4mm$ (99)	Triv.	—	(b,s)	—	—	—	674089
574	$\text{BiAlO}_3$	$P4mm$ (99)	Triv.	—	(b,s)	—	—	—	674105 673462
575	$\text{RbWNO}_2$	$P4mm$ (99)	Triv.	—	(b,s)	—	—	—	674128
576	$\text{Sb}_2\text{N}_2\text{O}$	$P4mm$ (99)	Triv.	—	—	—	—	—	674157
577	$\text{YTIO}_2\text{S}$	$P4mm$ (99)	Triv.	—	—	—	—	—	674170
578	$\text{CaSnO}_2\text{S}$	$P4mm$ (99)	Triv.	—	—	—	—	—	674175
579	$\text{HfMgO}_2\text{S}$	$P4mm$ (99)	Triv.	—	—	—	—	—	674184
580	$\text{YAlO}_2\text{S}$	$P4mm$ (99)	Triv.	—	(b,s)	—	—	—	674195
581	$\text{GeAlO}_2\text{F}$	$P4mm$ (99)	Triv.	—	(b,s)	—	—	—	674205
582	$\text{KSiO}_2\text{F}$	$P4mm$ (99)	Triv.	—	(b,s)	—	—	—	674212
583	$\text{GeGaO}_2\text{F}$	$P4mm$ (99)	Triv.	—	—	—	—	—	674223
584	$\text{RbSiO}_2\text{F}$	$P4mm$ (99)	Triv.	—	(b,s)	—	—	—	674238
585	$\text{SrZrO}_3$	$P4mm$ (99)	Triv.	—	(b,s)	—	—	—	674926 188449
586	$\text{YBaCuFeO}_5$	$P4mm$ (99)	SM	—	(b,s)	FM	—	—	67978 <sup>(I)</sup> 71355 87466 241398 <sup>(I)</sup>
587	$\text{Pb}(\text{TiO}_3)$	$P4mm$ (99)	Triv.	—	(b,s)	NM	—	—	1610 1611 1612 16621 31152 51838 <sup>(k)</sup> 51839 <sup>(k,l)</sup> 51840 51841 <sup>(k,l)</sup> 55054 55055 55056 55057 55058 55059 55060 55061 60188 61168 61169 <sup>(k)</sup> 90693 93553 161709 162044 <sup>(k)</sup> 162045 162046 <sup>(k)</sup> 162048 165498 <sup>(k)</sup> 186727 236933
588	$\text{K}(\text{NbO}_3)$	$P4mm$ (99)	Triv.	—	( $k^*$ , $b$ , $s$ , $l^*$ )	NM	—	—	9532 9535 190921

589	Ba(TiO <sub>3</sub> )	<i>P4mm</i> (99)	Triv.	—	(b,s)	NM	—	—	 15453 <sup>(l)</sup> 23758 <sup>(k,l)</sup> 23759 <sup>(k,l)</sup> 30617 <sup>(k,l)</sup> 31153 <sup>(k,l)</sup> 34637 <sup>(k,l)</sup> 67520 <sup>(k,l)</sup> 73642 <sup>(k)</sup> 73643 <sup>(k)</sup> 73644 <sup>(k)</sup> 73645 <sup>(k,l)</sup> 73646 <sup>(k,l)</sup> 95436 99737 100799 <sup>(k,l)</sup> 100800 <sup>(k,l)</sup> 100801 <sup>(k,l)</sup> 100802 <sup>(k,l)</sup> 100803 <sup>(k,l)</sup> 100804 <sup>(k,l)</sup> 130020 <sup>(k)</sup> 154343 <sup>(k,l)</sup> 154345 <sup>(k,l)</sup> 157806 <sup>(k,l)</sup> 161340 <sup>(l)</sup> 161418 <sup>(l)</sup> 168763 183932 <sup>(k,l)</sup> 185407 <sup>(k,l)</sup> 186457 <sup>(k,l)</sup> 186458 186459 188644 189381 190835 192889 <sup>(l)</sup> 237105 <sup>(k)</sup> 237107 <sup>(k)</sup> 237108 <sup>(k)</sup> 245944 <sup>(k,l)</sup> 245945 <sup>(k,l)</sup> 245946 <sup>(k,l)</sup> 248395 252558 <sup>(l)</sup> 253030 <sup>(k,l)</sup> 253245 <sup>(k,l)</sup> 290023 <sup>(k,l)</sup> 671606 <sup>(k,l)</sup> 673334 <sup>(k)</sup>
590	Sr(HfO <sub>3</sub> )	<i>P4mm</i> (99)	Triv.	—	(b,s,l*)	NM	—	—	161594
591	La <sub>1</sub> Mn <sub>1</sub> O <sub>3</sub>	<i>P4mm</i> (99)	Triv.	Fig. 34	(k*,b,s,l*)	—	—	—	673198
592	CaHfO <sub>3</sub>	<i>P4mm</i> (99)	Triv.	—	(b,s)	—	—	—	674068
593	CaTiO <sub>3</sub>	<i>P4mm</i> (99)	Triv.	—	(b,s)	—	—	—	674096
594	KWNO <sub>2</sub>	<i>P4mm</i> (99)	Triv.	—	(b,s)	—	—	—	674127
595	ZnAlO <sub>2</sub> F	<i>P4mm</i> (99)	Triv.	—	(b)	—	—	—	674207
596	KSnO <sub>2</sub> F	<i>P4mm</i> (99)	Triv.	—	(b,s)	—	—	—	674215
597	(VO) <sub>3</sub> (AsO <sub>3</sub> ) <sub>2</sub>	<i>P4bm</i> (100)	SM	Fig. 35	(b)	FM	—	HQ	424067
598	Ba <sub>2</sub> (TiO)(Si <sub>2</sub> O <sub>7</sub> )	<i>P4bm</i> (100)	Triv.	—	(b)	NM	—	—	4451 15715 34453 66628 <sup>(s)</sup> 66629 <sup>(s)</sup> 155316 201844 201845 672977
599	Ba <sub>2</sub> (VO)(Si <sub>2</sub> O <sub>7</sub> )	<i>P4bm</i> (100)	SM	—	(b)	FM	—	HQ	51479 98722
600	K <sub>2</sub> (Zn <sub>6</sub> O <sub>7</sub> )	<i>P4<sub>2</sub>nm</i> (102)	Triv.	—	(b)	NM	—	—	1120 2496
601	LiSr <sub>4</sub> Si <sub>4</sub> N <sub>8</sub> F	<i>P4nc</i> (104)	Triv.	—	(b,s)	—	—	—	432269
602	Cu(Sb <sub>2</sub> O <sub>4</sub> )	<i>P4<sub>2</sub>bc</i> (106)	SM	—	(b)	FM	—	HQ	190731
603	Sr <sub>2</sub> SbMnO <sub>6</sub>	<i>I4mm</i> (107)	Triv.	—	(b,s)	—	—	HQ	39351 190647
604	SrCu <sub>2</sub> (BO <sub>3</sub> ) <sub>2</sub>	<i>I4cm</i> (108)	Triv.	—	(b)	FM	—	HQ	247206
605	Ca <sub>5</sub> Ge <sub>3</sub>	<i>I4cm</i> (108)	SM	—	—	NM	—	—	181076
606	Li <sub>8</sub> SeN <sub>2</sub>	<i>I4<sub>1</sub>md</i> (109)	Triv.	—	—	NM	—	HQ	247255 247256 421252
607	ZnGa <sub>2</sub> S <sub>4</sub>	<i>P4̄2m</i> (111)	Triv.	—	(b)	NM	—	—	635300
608	CdTeMoO <sub>6</sub>	<i>P4̄2<sub>1</sub>m</i> (113)	Triv.	—	(b)	NM	—	HQ	93794 188038
609	Ca(FeO <sub>2</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	Triv.	—	—	FM	—	HQ	246244 674880
610	Ca(FeO <sub>2</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	TI	—	(b,s)	AFM	—	HQ	246245
611	Ca <sub>2</sub> Zn(Si <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	Triv.	—	(b)	NM	—	HQ	18114 30262 <sup>(s)</sup> 186944 <sup>(s)</sup>
612	Ca <sub>2</sub> Be(Si <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	Triv.	—	(b,s)	NM	—	HQ	31234 94063
613	Sr <sub>2</sub> Zn(Ge <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	Triv.	—	(b,s)	NM	—	HQ	39159 251824 420521 670006
614	Ba <sub>2</sub> Cu(Ge <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	SM	—	(b,s)	FM	—	—	77132
615	Sr <sub>2</sub> Mn(Ge <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	SM	—	(b,s)	AFM	—	HQ	84033
616	Ca <sub>2</sub> Co(Si <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	SM	—	(b)	AFM	—	HQ	94132 94135 <sup>(s)</sup> 94137 <sup>(s)</sup> 94139
617	Ba <sub>2</sub> Cu(Si <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	SM	—	(b,s)	FM	—	HQ	97762
618	K <sub>2</sub> Fe(P <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	Triv.	—	—	—	—	HQ	191281
619	K <sub>2</sub> Cu(P <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	SM	—	(b)	FM	—	HQ	191282
620	Sr <sub>2</sub> Co(Ge <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	SM	—	(b,s)	AFM	—	HQ	262398 262399
621	Ba <sub>2</sub> Co(Si <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	SM	—	(b,s)	AFM	—	HQ	281293
622	Ba <sub>2</sub> Co(Ge <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	SM	—	(b,s)	AFM	—	HQ	290483 290484 423350 423351
623	Ba <sub>2</sub> Zn(Ge <sub>2</sub> O <sub>7</sub> )	<i>P4̄2<sub>1</sub>m</i> (113)	Triv.	—	(b,s)	NM	—	HQ	420550
624	YBa <sub>2</sub> CuCu <sub>2</sub> O <sub>6</sub>	<i>P4̄m2</i> (115)	TI	—	(b,s)	—	—	—	63423
625	Pb <sub>2</sub> OF <sub>2</sub>	<i>P4̄m2</i> (115)	Triv.	—	(b)	NM	—	—	76964
626	Mo <sub>2</sub> CuGa <sub>5</sub>	<i>P4̄m2</i> (115)	Triv.	—	—	—	—	—	670138
627	SiO <sub>2</sub>	<i>P4̄c2</i> (116)	Triv.	—	(b,s)	NM	—	—	170532
628	K(NbF <sub>6</sub> )	<i>P4̄c2</i> (116)	Triv.	—	(b,s)	NM	—	—	16729
629	K(BiF <sub>6</sub> )	<i>P4̄c2</i> (116)	Triv.	—	(b,s)	NM	—	—	25025
630	SiO <sub>2</sub>	<i>P4̄n2</i> (118)	Triv.	—	(b,s)	NM	—	—	170511
631	RbMnSe <sub>2</sub>	<i>I4̄m2</i> (119)	Triv.	—	(b,s)	FM	—	HQ	50819
632	BaCu(Si <sub>2</sub> O <sub>6</sub> )	<i>I4̄m2</i> (119)	Triv.	—	(b)	—	—	HQ	74633
633	KMnS <sub>2</sub>	<i>I4̄m2</i> (119)	Triv.	—	(b,s)	—	—	—	672264
634	KMnSe <sub>2</sub>	<i>I4̄m2</i> (119)	Triv.	—	(b,s)	—	—	—	672265
635	KMnTe <sub>2</sub>	<i>I4̄m2</i> (119)	Triv.	—	(b,s)	—	—	—	672266 87983
636	RbMnTe <sub>2</sub>	<i>I4̄m2</i> (119)	Triv.	—	(b,s)	FM	—	HQ	87984

637	KAgO	$I\bar{4}m2$ (119)	Triv.	—	(b)	—	—	HQ	24818 37324 188525
638	KCuO	$I\bar{4}m2$ (119)	Triv.	—	—	NM	—	HQ	37325 188522
639	NaAgO	$I\bar{4}m2$ (119)	Triv.	—	(b)	NM	—	HQ	49752 188524
640	NaCuO	$I\bar{4}m2$ (119)	Triv.	—	(b)	NM	—	HQ	49756 188521
641	SrCu <sub>2</sub> (BO <sub>3</sub> ) <sub>2</sub>	$I\bar{4}c2$ (120)	Triv.	—	(b)	—	—	HQ	247205
642	(Ag(XeF <sub>2</sub> ) <sub>2</sub> )(PF <sub>6</sub> )	$I\bar{4}c2$ (120)	Triv.	—	(b,s)	—	—	HQ	412662
643	SrCu <sub>2</sub> (BO <sub>3</sub> ) <sub>2</sub>	$I\bar{4}2m$ (121)	Triv.	—	(b)	FM	—	HQ	247061 247200 247201 247202 247204
644	AgFe <sub>2</sub> GaTe <sub>4</sub>	$I\bar{4}2m$ (121)	Triv.	—	—	FM	—	HQ	192470
645	K(H <sub>2</sub> PO <sub>4</sub> )	$I\bar{4}2d$ (122)	Triv.	—	(b)	NM	—	HQ	66079 30257 76195 87895
646	Cs <sub>2</sub> (V <sub>4</sub> O <sub>9</sub> )	$I\bar{4}2d$ (122)	Triv.	—	(b)	AFM	—	HQ	79409
647	CO <sub>2</sub>	$I\bar{4}2d$ (122)	Triv.	—	(b,s)	NM	—	—	188890 29053 674668
648	AgAlS <sub>2</sub>	$I\bar{4}2d$ (122)	Triv.	—	—	NM	—	—	28744 604692 604694 604698
649	KCoO <sub>2</sub>	$I\bar{4}2d$ (122)	SM	—	(b,s)	FM	—	—	4199
650	SiS <sub>2</sub>	$I\bar{4}2d$ (122)	Triv.	—	(b,s)	NM	—	HQ	16952 291214 291215 291216 291217
651	CaF <sub>2</sub>	$P4/mmm$ (123)	Triv.	—	—	NM	—	—	51237
652	CsLaNb <sub>2</sub> O <sub>7</sub>	$P4/mmm$ (123)	Triv.	—	(b,s)	NM	—	HQ	82378
653	Ba(TiO <sub>3</sub> )	$P4/mmm$ (123)	SM	—	(b)	NM	—	—	109327
654	MgNiH	$P4/mmm$ (123)	SM	—	(b)	NM	—	—	187257
655	CsV <sub>2</sub> OS <sub>2</sub>	$P4/mmm$ (123)	SM	—	(b,s,l)	FM	—	—	430299
656	CaFeO <sub>2</sub>	$P4/mmm$ (123)	SM	—	(b,s,l)	—	—	—	674881 173438
657	AlMn	$P4/mmm$ (123)	SM	—	—	FM	—	—	57969 608456
658	CdPt	$P4/mmm$ (123)	SM	—	—	NM	—	—	102052 102053 620293 620295 620296
659	HgPt	$P4/mmm$ (123)	SM	—	—	NM	—	—	104337
660	HgBa <sub>2</sub> CuO <sub>4</sub>	$P4/mmm$ (123)	SM	—	(b,s,l)	NM	SC	—	75720 75721 75722 75723 75724
661	Bi <sub>2</sub> YO <sub>4</sub> Cl	$P4/mmm$ (123)	Triv.	—	(b)	NM	—	HQ	92405
662	Bi <sub>2</sub> YO <sub>4</sub> Br	$P4/mmm$ (123)	Triv.	—	(b)	NM	—	HQ	92418
663	LaCr <sub>2</sub> Si <sub>2</sub> C	$P4/mmm$ (123)	SM	—	(b,s,l)	FM	—	—	160691
664	BaPd <sub>2</sub> As <sub>2</sub>	$P4/mmm$ (123)	SM	—	—	NM	—	—	36376 190705
665	Cs <sub>2</sub> (MnF <sub>5</sub> )	$P4/mmm$ (123)	Triv.	—	—	FM	—	HQ	69675
666	K <sub>2</sub> (AlF <sub>5</sub> )	$P4/mmm$ (123)	Triv.	—	—	NM	—	—	81864
667	Rb <sub>2</sub> (MnF <sub>5</sub> )	$P4/mmm$ (123)	Triv.	—	—	FM	—	HQ	82218
668	KCu <sub>4</sub> S <sub>3</sub>	$P4/mmm$ (123)	SM	—	—	NM	SC	HQ	23336 602356 602358(b,s)
669	(CuCl)LaTa <sub>2</sub> O <sub>7</sub>	$P4/mmm$ (123)	SM	—	(b,s)	FM	—	HQ	51261
670	InPd <sub>3</sub>	$P4/mmm$ (123)	SM	—	—	NM	—	—	59476
671	MnRh <sub>2</sub> Sb	$P4/mmm$ (123)	SM	Fig. 35	—	FM	—	—	76202
672	Cu <sub>2</sub> NiZn	$P4/mmm$ (123)	TI	—	—	NM	—	—	103079
673	AlNi <sub>3</sub>	$P4/mmm$ (123)	SM	—	—	—	—	—	107862
674	Pd <sub>3</sub> Tl	$P4/mmm$ (123)	SM	—	—	—	—	—	108675
675	Pd <sub>3</sub> V	$P4/mmm$ (123)	SM	—	(k*)	FM	—	—	108677
676	Pt <sub>3</sub> Al	$P4/mmm$ (123)	SM	—	(k*)	NM	—	—	109235 191186
677	Pt <sub>3</sub> In	$P4/mmm$ (123)	SM	—	(k*)	NM	—	—	109236
678	FeNiN	$P4/mmm$ (123)	SM	—	(b)	FM	—	—	53505
679	PdO	$P4/mmm$ (123)	TI	—	—	NM	—	—	28837
680	FeSe	$P4/mmm$ (123)	SM	—	—	FM	—	—	53543 633467
681	FeSi <sub>2</sub>	$P4/mmm$ (123)	TI	—	—	FM	—	HQ	5257 24360 633533 633544 633550
682	FeSi <sub>2</sub>	$P4/mmm$ (123)	TI	—	—	FM	—	—	5258
683	Hg <sub>2</sub> Rh	$P4/mmm$ (123)	SM	—	—	NM	—	—	106786
684	HgMn	$P4/mmm$ (123)	SM	—	—	FM	—	—	104323
685	HgNi	$P4/mmm$ (123)	SM	—	—	NM	—	—	104332 639119
686	NbRu	$P4/mmm$ (123)	SM	—	—	NM	—	—	105222 645296
687	NiZn	$P4/mmm$ (123)	SM	—	—	NM	—	—	105469 647134 647137
688	RuTa	$P4/mmm$ (123)	SM	—	—	NM	—	—	105995 105996 650691 650692
689	AuMn	$P4/mmm$ (123)	SM	—	—	FM	—	—	109349
690	SrSi	$P4/mmm$ (123)	SM	—	—	—	—	—	160108
691	MgNi	$P4/mmm$ (123)	TI	—	—	NM	—	—	187255
692	K <sub>2</sub> (PdBr <sub>4</sub> )	$P4/mmm$ (123)	Triv.	—	—	NM	—	HQ	1982
693	K <sub>2</sub> PtCl <sub>4</sub>	$P4/mmm$ (123)	Triv.	—	—	NM	—	HQ	2722 <sup>(b)</sup> 23998 <sup>(b)</sup> 37014 <sup>(b)</sup> 37015 <sup>(b)</sup> 60110 68767 <sup>(b)</sup> 68768 <sup>(b)</sup>

694	K <sub>2</sub> PdCl <sub>4</sub>	<i>P4/mmm</i> (123)	Triv.	—	—	NM	—	HQ	2723 23997 27522 <sup>(b)</sup> 39852 65034 <sup>(b)</sup> 65035 <sup>(b)</sup> 65036 68769 73505 73506
695	K <sub>2</sub> PtBr <sub>4</sub>	<i>P4/mmm</i> (123)	Triv.	—	—	NM	—	HQ	6063
696	Cs <sub>2</sub> (PdCl <sub>4</sub> )	<i>P4/mmm</i> (123)	Triv.	—	—	NM	—	HQ	95813
697	NaAlF <sub>4</sub>	<i>P4/mmm</i> (123)	Triv.	—	(b,s,l)	NM	—	—	20572
698	Rb(FeF <sub>4</sub> )	<i>P4/mmm</i> (123)	SM	—	(b,s,l)	FM	—	—	21072
699	Tl(AlF <sub>4</sub> )	<i>P4/mmm</i> (123)	Triv.	—	(b,s,l)	NM	—	—	25615 200637 202453 202454
700	LaNiO <sub>2</sub>	<i>P4/mmm</i> (123)	SM	—	(b,s,l)	FM	—	—	47123 153058
701	SrFeO <sub>2</sub>	<i>P4/mmm</i> (123)	SM	—	(b,s,l)	AFM	—	HQ	173434 418603 418605 418606
702	KCuF <sub>3</sub>	<i>P4/mmm</i> (123)	SM	—	(k*,b,s,l)	—	—	—	27689
703	K(CrF <sub>3</sub> )	<i>P4/mmm</i> (123)	Triv.	—	(b,s,l)	FM	—	—	27690
704	Ba(TiO <sub>3</sub> )	<i>P4/mmm</i> (123)	Triv.	—	(k*,b,s,l)	NM	—	—	27965 27966 27967 27968 27969 27974 28620 29146 29148 29280 31884 31885 31886 31887 31888 31889 31890 67519 187295 674386
705	Na(NbO <sub>3</sub> )	<i>P4/mmm</i> (123)	Triv.	—	(k*,b,s,l)	NM	—	—	28584 28585 28586 28587
706	Pb(TiO <sub>3</sub> )	<i>P4/mmm</i> (123)	Triv.	—	(b,s,l)	—	—	—	28624 29117 <sup>(k)</sup>
707	Tl(CuF <sub>3</sub> )	<i>P4/mmm</i> (123)	SM	—	(b,s,l)	—	—	—	43457
708	Rb(CuF <sub>3</sub> )	<i>P4/mmm</i> (123)	SM	—	(b,s,l)	—	—	—	109293
709	CsAuCl <sub>3</sub>	<i>P4/mmm</i> (123)	SM	—	(k*,b,s,l)	NM	—	HQ	417373
710	SrGaO <sub>2</sub> F	<i>P4/mmm</i> (123)	Triv.	—	(b,s)	—	—	—	674208
711	BaAlO <sub>2</sub> F	<i>P4/mmm</i> (123)	Triv.	—	(b,s)	—	—	—	674211
712	RbHfO <sub>2</sub> F	<i>P4/mmm</i> (123)	Triv.	—	(b,s)	—	—	—	674219
713	YBaMn <sub>2</sub> O <sub>5</sub>	<i>P4/mmm</i> (123)	SM	—	(b,s)	AFM	—	HQ	83690
714	LaBaMn <sub>2</sub> O <sub>6</sub>	<i>P4/mmm</i> (123)	SM	—	(k*,b,s,l*)	FM	—	HQ	150703
715	LaRu <sub>2</sub> Al <sub>2</sub> B	<i>P4/mmm</i> (123)	TI	—	(b,s,l)	NM	—	HQ	174342
716	CsCa <sub>2</sub> (Ta <sub>3</sub> O <sub>10</sub> )	<i>P4/mmm</i> (123)	Triv.	—	(b,s,l)	NM	—	HQ	89011
717	RbSr <sub>2</sub> (Nb <sub>3</sub> O <sub>10</sub> )	<i>P4/mmm</i> (123)	Triv.	—	(b,s,l)	NM	SC*	HQ	93674
718	CsSr <sub>2</sub> (Nb <sub>3</sub> O <sub>10</sub> )	<i>P4/mmm</i> (123)	Triv.	—	(b,s,l)	NM	SC	HQ	93675
719	CsBa <sub>2</sub> (Nb <sub>3</sub> O <sub>10</sub> )	<i>P4/mmm</i> (123)	Triv.	—	(b,s,l)	NM	SC*	HQ	93676 671284
720	CsSr <sub>2</sub> (Ta <sub>3</sub> O <sub>10</sub> )	<i>P4/mmm</i> (123)	Triv.	—	(b,s,l)	NM	—	HQ	93677
721	RbCa <sub>2</sub> (Nb <sub>3</sub> O <sub>10</sub> )	<i>P4/mmm</i> (123)	Triv.	—	(b,s,l)	NM	SC*	HQ	260289
722	CsBa <sub>2</sub> Ta <sub>3</sub> O <sub>10</sub>	<i>P4/mmm</i> (123)	Triv.	—	(b,s,l)	—	—	—	671285
723	RbLa(Ta <sub>2</sub> O <sub>7</sub> )	<i>P4/mmm</i> (123)	Triv.	—	(b,s)	NM	—	HQ	81870
724	TlYBa <sub>2</sub> Cu <sub>2</sub> O <sub>7</sub>	<i>P4/mmm</i> (123)	TI	—	(b,s,l*)	NM	SC*	HQ	74163
725	Ba <sub>2</sub> YCu <sub>3</sub> O <sub>6</sub>	<i>P4/mmm</i> (123)	TI	—	(b,s)	NM	SC*	HQ	63269 63424 66903 67016 68008 68046 68290 72254 84739 203116
726	HgBa <sub>2</sub> CaCu <sub>2</sub> O <sub>6</sub>	<i>P4/mmm</i> (123)	TI	—	(b,s,l*)	NM	SC	—	75725 75726 75727 75728 75729 83087
727	SiO <sub>2</sub>	<i>P4/nbm</i> (125)	SM	—	—	NM	—	—	170502
728	SiO <sub>2</sub>	<i>P4/nbm</i> (125)	TI	Fig. 35	(b,s)	NM	—	—	170538
729	RbAg <sub>5</sub> Se <sub>3</sub>	<i>P4/nbm</i> (125)	SM	—	—	NM	—	HQ	50738
730	K <sub>8</sub> (Tl <sub>10</sub> Zn)	<i>P4/nnc</i> (126)	SM	—	—	NM	—	—	165614
731	SiO <sub>2</sub>	<i>P4/nnc</i> (126)	SM	—	—	NM	—	—	170503
732	SiO <sub>2</sub>	<i>P4/nnc</i> (126)	Triv.	—	—	NM	—	—	170537
733	Rb <sub>2</sub> IN <sub>3</sub>	<i>P4/mbm</i> (127)	Triv.	—	—	NM	—	HQ	202077
734	Cs <sub>2</sub> V <sub>3</sub> O <sub>8</sub>	<i>P4/mbm</i> (127)	SM	—	(b,s)	—	—	—	239713
735	Mn <sub>2</sub> Hg <sub>5</sub>	<i>P4/mbm</i> (127)	SM	—	—	—	SC	—	670164 104324
736	NaO <sub>2</sub>	<i>P4/mbm</i> (127)	SM	—	—	—	—	—	673261
737	Ti <sub>3</sub> Co <sub>5</sub> B <sub>2</sub>	<i>P4/mbm</i> (127)	SM	—	—	NM	—	—	20140
738	Mn <sub>2</sub> Ga <sub>5</sub>	<i>P4/mbm</i> (127)	SM	—	—	FM	SC*	HQ	249632 634613 634639
739	Cs <sub>3</sub> (GeF <sub>7</sub> )	<i>P4/mbm</i> (127)	Triv.	Fig. 35	—	NM	—	HQ	202917
740	K(AlF <sub>4</sub> )	<i>P4/mbm</i> (127)	Triv.	—	(b,s)	NM	—	HQ	16413 60524 201947 201948 201949
741	Rb(AlF <sub>4</sub> )	<i>P4/mbm</i> (127)	Triv.	—	(b,s)	NM	—	HQ	54120 54121 200638 <sup>(1)</sup>
742	Rb(FeF <sub>4</sub> )	<i>P4/mbm</i> (127)	SM	—	(b,s)	FM	—	HQ	85499
743	(PbCl <sub>2</sub> )(Pb(CO <sub>3</sub> ))	<i>P4/mbm</i> (127)	TI	—	—	—	—	—	38358
744	KCuF <sub>3</sub>	<i>P4/mbm</i> (127)	SM	—	(b)	FM	—	HQ	21110 <sup>(s,l)</sup> 21111
745	Na(TaO <sub>3</sub> )	<i>P4/mbm</i> (127)	Triv.	—	(b,s)	NM	—	HQ	23322 <sup>(1)</sup> 88377 239692 280101 <sup>(1)</sup>
746	Na(NbO <sub>3</sub> )	<i>P4/mbm</i> (127)	Triv.	—	(b,s)	NM	—	—	23563 <sup>(1)</sup> 192406 <sup>(1)</sup> 236892 280100

747	NaMgF <sub>3</sub>	<i>P4/mbm</i> (127)	Triv.	—	(b,s,l*)	NM	—	HQ	193088
748	BaPtLa <sub>2</sub> O <sub>5</sub>	<i>P4/mbm</i> (127)	Triv.	—	(b,s)	NM	—	HQ	68794 670385
749	FeMo <sub>2</sub> B <sub>2</sub>	<i>P4/mbm</i> (127)	SM	—	—	FM	—	—	5431 44292
750	W <sub>2</sub> FeB <sub>2</sub>	<i>P4/mbm</i> (127)	SM	—	—	FM	—	—	43016
751	InNi <sub>2</sub> Sc <sub>2</sub>	<i>P4/mbm</i> (127)	SM	—	—	NM	—	HQ	107333
752	FeNb <sub>2</sub> B <sub>2</sub>	<i>P4/mbm</i> (127)	SM	—	—	FM	—	—	614047
753	Li <sub>2</sub> Sr <sub>4</sub> N <sub>8</sub> Si <sub>4</sub> O	<i>P4/mnc</i> (128)	Triv.	—	(b,s)	NM	—	—	420677
754	Na <sub>3</sub> ScF <sub>6</sub>	<i>P4/mnc</i> (128)	Triv.	—	(b,s)	—	—	—	671947
755	K <sub>2</sub> (TeBr <sub>6</sub> )	<i>P4/mnc</i> (128)	Triv.	—	—	NM	—	—	37270 65117
756	Tl <sub>2</sub> (TeBr <sub>6</sub> )	<i>P4/mnc</i> (128)	Triv.	—	—	NM	—	HQ	99127
757	WO <sub>3</sub>	<i>P4/nmm</i> (129)	Triv.	Fig. 35	(b,s)	NM	—	—	89092 27961 <sup>(l)</sup> 27962 <sup>(l)</sup> 88367 <sup>(k)</sup> 673313 <sup>(k)</sup>
758	VSe	<i>P4/nmm</i> (129)	SM	—	—	NM	—	—	162898
759	CrSe	<i>P4/nmm</i> (129)	Triv.	—	—	FM	—	—	162899
760	WH <sub>4</sub>	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	247601 247602
761	HfCd	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	619964
762	AgLa(TiO <sub>4</sub> )	<i>P4/nmm</i> (129)	Triv.	—	(b,s)	NM	—	—	78719
763	Sr <sub>2</sub> NiO <sub>3</sub> Cl	<i>P4/nmm</i> (129)	SM	—	(b,s)	AFM	—	—	237581
764	Ba <sub>2</sub> Pb <sub>4</sub> Br <sub>2</sub> F <sub>10</sub>	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	411087
765	Ba <sub>2</sub> Pb <sub>4</sub> I <sub>2</sub> F <sub>10</sub>	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	411088
766	BaNiS <sub>2</sub>	<i>P4/nmm</i> (129)	TI	—	—	NM	—	—	15289 246945
767	K(CoO <sub>2</sub> )	<i>P4/nmm</i> (129)	TI	—	—	FM	—	—	15770
768	CsLiBr <sub>2</sub>	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	40479 245979
769	BaHfN <sub>2</sub>	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	50994 184052 184053 184054 184055 184056 184057
770	Ba(ZrN <sub>2</sub> )	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	74904 74905
771	BaCoS <sub>2</sub>	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	82639
772	CsAgCl <sub>2</sub>	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	150300
773	CsAgBr <sub>2</sub>	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	150302
774	SrNiS <sub>2</sub>	<i>P4/nmm</i> (129)	TI	—	—	—	—	—	673416
775	Ir <sub>2</sub> YSi <sub>2</sub>	<i>P4/nmm</i> (129)	SM	—	—	NM	—	—	44668 181770 188325 641031 641036
776	Sr <sub>2</sub> Sb <sub>2</sub> Se <sub>4</sub> F <sub>2</sub>	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	171430
777	Bi <sub>2</sub> OS <sub>2</sub>	<i>P4/nmm</i> (129)	Triv.	—	—	NM	SC	—	196230
778	Ca <sub>2</sub> Ge <sub>2</sub> Ni <sub>2</sub> H <sub>2</sub>	<i>P4/nmm</i> (129)	SM	—	—	NM	—	—	263028
779	CsMnF <sub>4</sub>	<i>P4/nmm</i> (129)	Triv.	—	(b,s)	FM	—	—	14104
780	Fe <sub>2</sub> As	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	16844 415628 610464 610470 610472
781	KNaO	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	32743
782	FeLiP	<i>P4/nmm</i> (129)	SM	—	—	NM	SC	—	42327 247089 632441 247248
783	MnAlGe	<i>P4/nmm</i> (129)	TI	—	—	FM	—	—	42750 607972 607974 657172
784	MnVAs	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	44009
785	NiRhAs	<i>P4/nmm</i> (129)	SM	—	—	NM	—	—	44030 187596 601484
786	MgMnGe	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	66948 66952 <sup>(b)</sup> 66953 87116 <sup>(b)</sup> 87117 <sup>(b)</sup>
787	CaMnSn	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	66958 <sup>(b)</sup> 66950 66959 <sup>(b)</sup>
788	MnFeAs	<i>P4/nmm</i> (129)	TI	—	—	FM	—	—	93237 93238 610492
789	CoLiAs	<i>P4/nmm</i> (129)	SM	—	—	NM	—	—	107932
790	LiFeAs	<i>P4/nmm</i> (129)	SM	—	—	FM	SC	—	162056 162250 163870 166457 290700 610480 169175
791	LiFeP	<i>P4/nmm</i> (129)	TI	—	—	NM	—	—	166456
792	CoMnSb	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	248374 248375 248376 248377
793	MgCoGe	<i>P4/nmm</i> (129)	SM	—	—	NM	—	—	418853
794	MnCuAs	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	423230
795	GaMnGe	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	634253 634255
796	Fe(MoO <sub>4</sub> )Cl	<i>P4/nmm</i> (129)	SM	—	(b,s)	AFM	—	—	49516 202186 202187 202188
797	FeWO <sub>4</sub> Cl	<i>P4/nmm</i> (129)	SM	—	(b,s)	AFM	—	—	80798
798	FeSe	<i>P4/nmm</i> (129)	SM	—	—	NM	SC*	—	26889 162901 163559 163560 163561 163562 165958 165959 165960 169970 182544 185464 196297 196298 977901 977903
799	FeS	<i>P4/nmm</i> (129)	Triv.	—	—	NM	SC	—	42977 43391 81087 182249 182250 238590 633302 182251
800	FeTe	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	44753 169974

801	MnSe	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	162900
802	CoSe	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	162902
803	FeSe	<i>P4/nmm</i> (129)	TI	—	—	NM	—	—	169253 169255 169257 169259 169261 169263 169265 169267 169269 169271 290701
804	FeTe	<i>P4/nmm</i> (129)	TI	—	—	FM	SC*	—	180602 633877
805	FeSe	<i>P4/nmm</i> (129)	Triv.	—	—	FM	—	—	633480
806	K(MoO(PO <sub>4</sub> )Cl)	<i>P4/nmm</i> (129)	SM	—	(b)	FM	—	—	50988
807	Na <sub>2</sub> (TiO)(GeO <sub>4</sub> )	<i>P4/nmm</i> (129)	Triv.	—	(b,s)	NM	—	—	20129 91546 160148 59359 417276 417277 <sup>(s)</sup> 417278 <sup>(s)</sup> 417279 417280 <sup>(s)</sup> 417281 417282 417283 417284 417285 417286
808	Li <sub>2</sub> (VO)(SiO <sub>4</sub> )	<i>P4/nmm</i> (129)	SM	—	(b)	AFM	—	—	
809	Ag <sub>3</sub> Cl(CrO <sub>4</sub> )	<i>P4/nmm</i> (129)	Triv.	—	(b)	NM	—	—	409541
810	LiMnP	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	26458
811	LiMnAs	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	26459 60739 60740 60741 60742 192817 192818 192819 192820 192821 192822 192823
812	LiMnSb	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	642150
813	TiSe	<i>P4/nmm</i> (129)	SM	—	—	NM	—	—	162897
814	SnO	<i>P4/nmm</i> (129)	SM	—	—	NM	—	—	185350
815	BaBrF	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	1129 2294 35393 155005
816	PbFCl	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	5037 30287 31132 39165 82884 155010
817	PbFBr	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	5038 30288 155011
818	BiOF	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	24096 201620
819	BiOCl	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	24608 29143 74502 195115 185970
820	CaHCl	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	25601 37199
821	SrHCl	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	25602 37200
822	BaHCl	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	25603 37201
823	NaMnP	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	26460 60726 60727 60728 60729 601595
824	NaMnAs	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	26461 60730 60731 60732 610878
825	NaMnSb	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	26462 60733 60734 60735 601596
826	BiOI	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	29145 5036 24610 185972 391354
827	YOCl	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	31667 60586
828	KMgSb	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	41709
829	RbMnSb	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	41868 643395 643396
830	CsMnSb	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	41869 627027 627028
831	KMnP	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	41882 89592 89593
832	KMnAs	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	41883 60743 60744 60745
833	MnBaGe	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	42370 66964 66965 615891
834	CaMnGe	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	52758 66956 66957(b)
835	MnSrGe	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	53707 66960 66961
836	NaMnBi	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	60736 60737 60738 601587 616814
837	CaMnSi	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	66949 66954 66955
838	SrMnSn	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	66951 66962 66963
839	LaMnSi	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	75046 75047 85849 641449
840	MnYSi	<i>P4/nmm</i> (129)	TI	—	—	FM	—	—	76235 643705
841	LaMnGe	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	80007 80008 85857
842	LaFeSi	<i>P4/nmm</i> (129)	SM	—	—	NM	—	—	85853 632432 656907
843	LaCoGe	<i>P4/nmm</i> (129)	Triv.	—	—	FM	—	—	85860
844	KMnSb	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	89590 89591 602269
845	RbMnP	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	89594 89595 643229
846	RbMnAs	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	89596 89597 610910
847	CoGeLa	<i>P4/nmm</i> (129)	TI	—	—	FM	—	—	106471
848	PbFI	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	150194 150195 56667 150193 155012 279599
849	NaFeAs	<i>P4/nmm</i> (129)	SM	—	—	FM	SC	—	163143 163144
850	KMnBi	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	601586
851	KMgAs	<i>P4/nmm</i> (129)	Triv.	—	—	NM	—	—	610753
852	CsMnBi	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	616575
853	RbMnBi	<i>P4/nmm</i> (129)	SM	—	—	FM	—	—	616824
854	CoLaSi	<i>P4/nmm</i> (129)	Triv.	—	—	FM	—	—	624027
855	CoPdP	<i>P4/nmm</i> (129)	TI	—	(b)	NM	—	—	624599

856	CoLaSi	$P4/nmm$ (129)	SM	—	—	FM	—	—	658265
857	BaSnF <sub>4</sub>	$P4/nmm$ (129)	Triv.	—	(b,s)	NM	—	—	166207 673273
858	CsMnAs	$P4/nmm$ (129)	SM	—	—	FM	—	—	40572 40573 610293
859	CsMnP	$P4/nmm$ (129)	SM	—	—	FM	—	—	89598 89599 627022
860	SrFI	$P4/nmm$ (129)	Triv.	—	—	NM	—	—	155009 159280
861	$(\text{Fe}_2\text{As}_2)(\text{Sr}_4\text{Sc}_2\text{O}_6)$	$P4/nmm$ (129)	Triv.	—	(b,s)	FM	SC	—	180528
862	$(\text{Co}_2\text{As}_2)(\text{Sr}_4\text{Sc}_2\text{O}_6)$	$P4/nmm$ (129)	SM	—	(b,s)	—	—	—	262356
863	$(\text{Co}_2\text{P}_2)(\text{Sr}_4\text{Sc}_2\text{O}_6)$	$P4/nmm$ (129)	SM	—	(b,s)	FM	—	—	262357
864	NaKLaNbO <sub>5</sub>	$P4/nmm$ (129)	Triv.	—	(b)	NM	—	—	94743
865	LaKNaTaO <sub>5</sub>	$P4/nmm$ (129)	Triv.	—	(b)	NM	—	—	419855
866	YOF	$P4/nmm$ (129)	Triv.	—	—	NM	—	—	76426
867	LaOF	$P4/nmm$ (129)	Triv.	—	—	NM	—	—	76427 430270 <sup>(b)</sup>
868	BiCuSeO	$P4/nmm$ (129)	Triv.	—	—	NM	—	—	74475 75128 189174 262598 674374
869	LaCoPO	$P4/nmm$ (129)	SM	—	—	FM	—	—	80203 161910 161911
870	LaAgSb <sub>2</sub>	$P4/nmm$ (129)	TI	—	—	NM	—	—	95220 95221 95222 95223
871	SrCuFS	$P4/nmm$ (129)	Triv.	—	—	NM	—	—	157433
872	LaFePO	$P4/nmm$ (129)	Triv.	—	—	FM	—	—	162724 391428 420381
873	SrFeAsF	$P4/nmm$ (129)	Triv.	—	—	FM	SC	—	162808 163915 168775 163496 163497 163835 163868 173432 180438 180439 180440 184645 192739 421998 602489
874	LaFeAsO	$P4/nmm$ (129)	Triv.	—	—	AFM	—	—	237385 237387
875	SrCuFS	$P4/nmm$ (129)	TI	—	—	NM	—	—	172796
876	BaFCuS	$P4/nmm$ (129)	Triv.	—	—	NM	—	—	183712
877	SrFMnP	$P4/nmm$ (129)	SM	—	—	FM	—	—	189939
878	SrFMnAs	$P4/nmm$ (129)	SM	—	—	—	—	—	189940
879	SrFMnSb	$P4/nmm$ (129)	SM	—	—	FM	—	—	189941
880	CrLaAsO	$P4/nmm$ (129)	Triv.	—	—	AFM	—	—	237385 237387
881	CrLaAsO	$P4/nmm$ (129)	TI	—	—	AFM	—	—	237386
882	BaMnSbF	$P4/nmm$ (129)	SM	—	—	FM	—	—	248364 248366
883	BaMnAsF	$P4/nmm$ (129)	SM	—	—	—	—	—	248365
884	LaMnSbO	$P4/nmm$ (129)	SM	—	—	FM	—	—	419355
885	BaMnBiF	$P4/nmm$ (129)	SM	—	—	—	—	—	426033
886	LaFeSb <sub>2</sub>	$P4/nmm$ (129)	SM	—	—	FM	—	—	657914 657985
887	LaCoSb <sub>2</sub>	$P4/nmm$ (129)	SM	—	—	FM	—	—	657919 657990
888	VZrSi	$P4/nmm$ (129)	SM	—	—	NM	—	—	42337 652544
889	LaTiGe	$P4/nmm$ (129)	SM	—	—	NM	—	—	107617
890	HfVGe	$P4/nmm$ (129)	SM	—	—	NM	—	—	636594
891	HfVSi	$P4/nmm$ (129)	SM	—	—	NM	—	—	638931
892	WO <sub>3</sub>	$P4/ncc$ (130)	Triv.	—	(b,s)	—	—	—	673314 50732 50733 88366
893	Ca <sub>5</sub> Ge <sub>3</sub>	$P4/ncc$ (130)	TI	—	—	NM	—	—	181075
894	CuBi <sub>2</sub> O <sub>4</sub>	$P4/ncc$ (130)	SM	—	(b)	FM	SC	HQ	15865 56390 67018 <sup>(s)</sup> 68812 <sup>(s)</sup> 68813 <sup>(s)</sup> 68814 <sup>(s)</sup> 68815 <sup>(s)</sup> 69307 <sup>(s)</sup> 69308 <sup>(s)</sup> 69746 69747 71313 <sup>(s)</sup> 202994 <sup>(s)</sup>
895	PdBi <sub>2</sub> O <sub>4</sub>	$P4/ncc$ (130)	Triv.	—	(b)	NM	—	HQ	200145
896	Na <sub>2</sub> PdCl <sub>4</sub>	$P4/ncc$ (130)	Triv.	—	(b)	NM	—	HQ	202971
897	Sr <sub>3</sub> (SiO <sub>4</sub> )O	$P4/ncc$ (130)	Triv.	—	—	NM	—	—	18151 28534 418933 <sup>(b)</sup>
898	CaNiN	$P4_2/mmc$ (131)	SM	—	(b)	NM	—	—	69044 656846
899	KCuC <sub>2</sub>	$P4_2/mmc$ (131)	Triv.	—	—	NM	—	HQ	412037 412038
900	RbCuC <sub>2</sub>	$P4_2/mmc$ (131)	Triv.	—	—	NM	—	HQ	412039 412040
901	IrN	$P4_2/mmc$ (131)	Triv.	—	—	NM	—	—	187717
902	SiO <sub>2</sub>	$P4_2/mcm$ (132)	Triv.	—	(b,s)	NM	—	—	170500
903	Pb <sub>3</sub> O <sub>4</sub>	$P4_2/mpc$ (135)	Triv.	—	(b)	NM	—	—	4106 22325 36253 42484 647270
904	Cu(As <sub>2</sub> O <sub>4</sub> )	$P4_2/mpc$ (135)	SM	Fig. 35	(b)	FM	—	HQ	4287 16829 4459 61466 61467 61468 61469 61470 61471 61472 61473 155151 182798
905	FeO(Sb <sub>2</sub> O <sub>3</sub> )	$P4_2/mpc$ (135)	Triv.	—	(b)	FM	—	HQ	30350 158916
906	FeSb <sub>2</sub> O <sub>4</sub>	$P4_2/mpc$ (135)	SM	—	(b)	FM	—	—	647261
907	Pb <sub>3</sub> O <sub>4</sub>	$P4_2/mpc$ (135)	SM	—	(b,s)	NM	—	—	72387
908	LiSr <sub>2</sub> (CoN <sub>2</sub> )	$P4_2/mnm$ (136)	SM	—	(b)	FM	—	HQ	670200 99714 644069
909	MoO <sub>2</sub>	$P4_2/mnm$ (136)	Triv.	—	(b)	—	—	—	671853
910	Li <sub>2</sub> S <sub>2</sub>	$P4_2/mnm$ (136)	Triv.	—	—	—	—	—	—

911	VF <sub>2</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	—	(b)	—	—	—	673336 32552 38069 62768 62769 201245
912	CoF <sub>2</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	—	(b)	—	—	—	674847 9167 14144 26604 53987 73460 98785 98786 280604
913	Hf <sub>2</sub> Cu <sub>2</sub> In	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	—	—	—	—	—	130032
914	IrIn <sub>3</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	—	—	NM	—	HQ	407548 639819
915	RhIn <sub>3</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	—	—	NM	SC	HQ	407549 640336
916	RhGa <sub>3</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	—	—	NM	—	—	635208
917	ZrNi <sub>4</sub> P <sub>2</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	—	—	—	SC	HQ	40435 76681
918	KPd(PS <sub>4</sub> )	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	Triv.	—	(b,s)	NM	—	HQ	165315
919	Li <sub>3</sub> (BN <sub>2</sub> )	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	Triv.	—	(b)	NM	—	—	71085
920	WOI <sub>3</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	Triv.	—	(b,s)	FM	—	HQ	65183
921	WOCl <sub>3</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	Triv.	—	(b,s)	FM	—	HQ	416393
922	K <sub>2</sub> Na <sub>4</sub> (Be <sub>2</sub> O <sub>5</sub> )	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	Triv.	—	(b)	NM	—	HQ	33849
923	MnO <sub>2</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	Fig. 35	(b)	AFM	—	HQ	393 20229 56006 73713 246888 643186 643187 643197 670198 670366
924	VO <sub>2</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	—	(b)	FM	—	HQ	1504 4110 10141 2492 27482 34418 34420 34421 56003 66665 237337 647613 647637
925	ZnF <sub>2</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	Triv.	—	(b)	NM	—	HQ	9169 14146 26606 53981 76270 184219 280605
926	CrO <sub>2</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	Triv.	—	—	FM	—	HQ	9423 <sup>(b)</sup> 28711 <sup>(b)</sup> 35327 43461 <sup>(b)</sup> 43739 <sup>(b)</sup> 155831 <sup>(b)</sup> 166021 <sup>(b)</sup> 166022 <sup>(b)</sup> 166023 <sup>(b)</sup> 166024 <sup>(b)</sup> 166025 <sup>(b)</sup> 166026 <sup>(b)</sup> 166027 <sup>(b)</sup> 166028 <sup>(b)</sup> 166485 <sup>(b)</sup> 167237 <sup>(b)</sup> 185885 <sup>(b)</sup> 186836 <sup>(b)</sup> 202835 <sup>(b)</sup> 202836 <sup>(b)</sup> 202837 <sup>(b)</sup> 202838 <sup>(b)</sup> 246898 <sup>(b)</sup> 246899 <sup>(b)</sup> 246900 <sup>(b)</sup> 246901 <sup>(b)</sup> 246902 <sup>(b)</sup> 626487 <sup>(b)</sup> 670197 <sup>(b)</sup>
927	RuO <sub>2</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	Triv.	—	(b)	NM	—	HQ	15071 23961 51159 56007 84575 84618 108861 172178 236962 236963 290496 647373 647376 647377 670201 670735 671872
928	Mg <sub>2</sub> C	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	TI	—	(b)	—	—	—	671332
929	Zn(Sb <sub>2</sub> O <sub>6</sub> )	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	Triv.	—	(b)	NM	—	—	30409 96612
930	Fe(Sb <sub>2</sub> O <sub>6</sub> )	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	—	(b)	AFM	—	—	40344
931	Ni(Ta <sub>2</sub> O <sub>6</sub> )	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	Triv.	Fig. 36	(b)	FM	—	HQ	61198 247807
932	NiSb <sub>2</sub> O <sub>6</sub>	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	Triv.	—	(b)	AFM	—	—	80802 426852
933	Cu(Ta <sub>2</sub> O <sub>6</sub> )	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	Fig. 36	(b)	FM	—	—	83367
934	Cu(Sb <sub>2</sub> O <sub>6</sub> )	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	—	(b)	FM	—	HQ	84789
935	Co(Ta <sub>2</sub> O <sub>6</sub> )	<i>P</i> 4 <sub>2</sub> / <i>mnm</i> (136)	SM	—	(b)	AFM	—	—	166673 166674 203095 247812
936	Pb <sub>2</sub> F <sub>2</sub> O	<i>P</i> 4 <sub>2</sub> / <i>nmc</i> (137)	Triv.	—	(b)	NM	—	HQ	10416
937	Pb <sub>2</sub> (ZnF <sub>6</sub> )	<i>P</i> 4 <sub>2</sub> / <i>ncm</i> (138)	Triv.	—	(b,s)	NM	—	—	162073 162074
938	Ba <sub>2</sub> CuWO <sub>6</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	(b,s)	FM	—	—	33569
939	Cs <sub>2</sub> CuO <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	(b,s,l)	FM	—	HQ	39535
940	K <sub>4</sub> Al <sub>2</sub> Nb <sub>11</sub> O <sub>20</sub> F	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	(b)	NM	—	—	65738
941	Ba <sub>2</sub> Cu <sub>2</sub> (Si <sub>4</sub> O <sub>12</sub> )	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	(b)	FM	—	HQ	71535
942	CsFe <sub>2</sub> As <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	FM	SC	—	74877
943	CrNbF <sub>6</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	(b,s)	FM	—	HQ	75384
944	Sr <sub>2</sub> Cu <sub>2</sub> MnO <sub>2</sub> S <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	(b,s,l)	AFM	SC	HQ	84734
945	V <sub>4</sub> Zn <sub>5</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	—	—	106213 653404
946	LaF <sub>3</sub>	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	—	NM	—	—	167555 155554 164056 96133 96134
947	C	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	—	NM	—	—	190717 190718 190719 182761 190716
948	CaO <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	—	—	—	—	671324 619462 20275
949	Cu <sub>3</sub> Ti <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	FM	—	—	103132 629380 629398
950	Al <sub>3</sub> Nb	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	SC	—	58015 107857 186000 608658 608663 608670 608672 608682 608686 608690 607056 670759
951	Al <sub>3</sub> V	<i>I</i> 4/ <i>mmm</i> (139)	SM	Fig. 36	—	NM	SC	—	58201 151104 167811 609613 609617 670975
952	InPd <sub>3</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	—	NM	—	—	247188 247189 420251
953	TlPd <sub>3</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	—	NM	—	HQ	247272 649056 649063
954	CrSi <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	—	—	71499
955	Ag <sub>2</sub> Sc	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	—	—	605791 605793
956	Au <sub>2</sub> Hf	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	—	—	611956

957	Ba <sub>2</sub> Cu <sub>3</sub> O <sub>4</sub> Br <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	(b)	NM	—	—	36128 75576
958	Ba <sub>2</sub> (ZnF <sub>6</sub> )	<i>I4/mmm</i> (139)	Triv.	—	(b,s,l)	NM	—	—	21054
959	TlCo <sub>2</sub> Se <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	—	FM	—	—	67362 95138 95139 95140 95141 625007 674509
960	KCo <sub>2</sub> Se <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	—	FM	—	—	67370 182837 182838 623961
961	BaCu <sub>2</sub> S <sub>2</sub>	<i>I4/mmm</i> (139)	Triv.	—	—	NM	—	HQ	89575 203088 615832 615834 615837 670743
962	TlCo <sub>2</sub> S <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	—	FM	—	HQ	100438 624879
963	KFe <sub>2</sub> S <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	—	NM	SC*	—	186572
964	KNi <sub>2</sub> Se <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	—	FM	SC	HQ	424686 641276
965	KNi <sub>2</sub> S <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	—	—	SC	—	431754 641273
966	Co <sub>2</sub> KS <sub>2</sub>	<i>I4/mmm</i> (139)	SM	Fig. 36	—	FM	—	—	623956
967	Co <sub>2</sub> RbS <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	—	FM	—	—	624795
968	Sr <sub>2</sub> CoO <sub>2</sub> Cl <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	(b,s,l)	AFM	—	HQ	59697 151787 151788
969	Sr <sub>2</sub> CoO <sub>2</sub> Br <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	(b,s,l)	AFM	—	HQ	59698 151789 151790
970	Sr <sub>3</sub> (Co <sub>2</sub> O <sub>5</sub> Cl <sub>2</sub> )	<i>I4/mmm</i> (139)	TI	Fig. 36	(b,s)	FM	—	HQ	90123 91749
971	KO <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	—	FM	—	HQ	38245 180563 196755 38138
972	CsO <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	—	FM	—	—	38247 627060 627062
973	BaC <sub>2</sub>	<i>I4/mmm</i> (139)	Triv.	—	—	NM	—	—	56160 88098 88101 168410 186575 615792 615794
974	RbO <sub>2</sub>	<i>I4/mmm</i> (139)	SM	—	—	FM	—	—	180564 196756 647338
975	CoO	<i>I4/mmm</i> (139)	SM	—	—	AFM	—	—	53059 174027
976	MnN	<i>I4/mmm</i> (139)	SM	—	—	FM	—	—	106932
977	Sr <sub>2</sub> FeMoO <sub>6</sub>	<i>I4/mmm</i> (139)	Triv.	Fig. 37	(b,s)	—	—	—	94079 151617 169377 <sup>(k)</sup> 184911
978	Ba <sub>2</sub> (FeReO <sub>6</sub> )	<i>I4/mmm</i> (139)	SM	Fig. 36	(k*,b,s)	FM	—	HQ	155174
979	Sr <sub>2</sub> VZrO <sub>6</sub>	<i>I4/mmm</i> (139)	SM	Fig. 36	(k*,b,s)	FM	—	—	191359
980	Sr <sub>2</sub> VHfO <sub>6</sub>	<i>I4/mmm</i> (139)	SM	Fig. 36	(k*,b,s)	FM	—	—	191360
981	Sr <sub>2</sub> CoHfO <sub>6</sub>	<i>I4/mmm</i> (139)	SM	—	(k*,b,s)	FM	—	—	191364
982	Sr <sub>2</sub> FeZrO <sub>6</sub>	<i>I4/mmm</i> (139)	Triv.	—	—	—	—	—	191365
983	Sr <sub>2</sub> FeHfO <sub>6</sub>	<i>I4/mmm</i> (139)	Triv.	—	(k*,b,s)	AFM	—	—	191366
984	Ba <sub>2</sub> Fe(MoO <sub>6</sub> )	<i>I4/mmm</i> (139)	Triv.	Fig. 37	(k*,b,s)	FM	—	HQ	246541 246542 246543 246544
985	Pb <sub>2</sub> Co(TeO <sub>6</sub> )	<i>I4/mmm</i> (139)	SM	—	(k*,b,s)	FM	—	HQ	405782
986	BaBi <sub>2</sub> Zn	<i>I4/mmm</i> (139)	Triv.	—	—	NM	—	—	58638
987	Bi <sub>2</sub> CdSr	<i>I4/mmm</i> (139)	Triv.	—	—	NM	—	HQ	58764
988	K <sub>2</sub> CuF <sub>4</sub>	<i>I4/mmm</i> (139)	SM	—	(b,s,l)	FM	—	HQ	15372 31688
989	Cs <sub>2</sub> AgF <sub>4</sub>	<i>I4/mmm</i> (139)	SM	Fig. 37	(b,s,l)	FM	—	—	16254
990	Cs <sub>2</sub> CdCl <sub>4</sub>	<i>I4/mmm</i> (139)	Triv.	—	(b,s,l)	—	—	—	16576
991	(SrO) <sub>2</sub> TiO <sub>2</sub>	<i>I4/mmm</i> (139)	Triv.	—	(b,s,l)	NM	SC*	—	20293 157402 194713 194714 194715 194716 194717 194718 194719
992	K <sub>2</sub> MnF <sub>4</sub>	<i>I4/mmm</i> (139)	SM	—	(b,s,l)	FM	—	—	23183 23184 33521
993	Sr <sub>2</sub> (MnO <sub>4</sub> )	<i>I4/mmm</i> (139)	SM	—	(b,s,l)	FM	—	—	26560 26561 50794
994	Sr <sub>2</sub> SnO <sub>4</sub>	<i>I4/mmm</i> (139)	Triv.	—	(b,s,l)	NM	—	—	27114 84245 150387 150388 150389 150390
995	Sr <sub>4</sub> P <sub>2</sub> O	<i>I4/mmm</i> (139)	Triv.	—	(b,s,l)	NM	—	HQ	33903
996	Rb <sub>2</sub> CaH <sub>4</sub>	<i>I4/mmm</i> (139)	Triv.	Fig. 37	(b,s,l)	NM	—	—	65196
997	K <sub>2</sub> MgH <sub>4</sub>	<i>I4/mmm</i> (139)	Triv.	Fig. 37	(b,s,l)	NM	—	—	68358
998	K <sub>4</sub> OB <sub>2</sub>	<i>I4/mmm</i> (139)	Triv.	—	(b,s,l)	NM	—	HQ	68505
999	Ba <sub>2</sub> (ZrS <sub>4</sub> )	<i>I4/mmm</i> (139)	Triv.	—	(b,s,l)	NM	—	HQ	69853 80651
1000	Cs <sub>2</sub> HgF <sub>4</sub>	<i>I4/mmm</i> (139)	Triv.	—	(b,s,l)	NM	—	—	72353
1001	Cs <sub>2</sub> MgH <sub>4</sub>	<i>I4/mmm</i> (139)	Triv.	Fig. 37	(b,s,l)	NM	—	—	162261
1002	Sr <sub>2</sub> (CrO <sub>4</sub> )	<i>I4/mmm</i> (139)	TI	—	(b,s,l)	FM	—	HQ	245595
1003	Sr <sub>2</sub> (CoO <sub>4</sub> )	<i>I4/mmm</i> (139)	SM	—	(b,s,l)	AFM	—	HQ	246483
1004	Rb <sub>4</sub> Br <sub>2</sub> O	<i>I4/mmm</i> (139)	Triv.	—	(b,s,l)	NM	—	HQ	411954
1005	K <sub>4</sub> (Ru <sub>2</sub> Cl <sub>10</sub> O)	<i>I4/mmm</i> (139)	Triv.	—	—	NM	—	HQ	8054
1006	ScLaSb	<i>I4/mmm</i> (139)	TI	—	—	NM	—	HQ	427126
1007	YNi <sub>2</sub> B <sub>2</sub> C	<i>I4/mmm</i> (139)	SM	—	(b)	NM	SC	—	41549 75816 79574 83231 89142
1008	Li <sub>2</sub> Sr(Ta <sub>2</sub> O <sub>7</sub> )	<i>I4/mmm</i> (139)	Triv.	—	(b)	NM	—	HQ	88464 154175 246278
1009	KCuO	<i>I4/mmm</i> (139)	Triv.	—	—	NM	—	HQ	40158
1010	RbCuO	<i>I4/mmm</i> (139)	Triv.	—	—	NM	—	HQ	40159
1011	Cs(AuO)	<i>I4/mmm</i> (139)	Triv.	—	—	NM	—	HQ	409553
1012	Pd <sub>3</sub> Tl	<i>I4/mmm</i> (139)	SM	Fig. 37	—	NM	—	—	105729
1013	InPd <sub>3</sub>	<i>I4/mmm</i> (139)	SM	Fig. 37	—	NM	—	—	247194 247195 420250

1014	K <sub>2</sub> NiO <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	(b)	FM	—	—	21069 201891
1015	Na <sub>2</sub> (HgO <sub>2</sub> )	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	(b)	NM	—	—	25511 27409
1016	Rb <sub>2</sub> (NiO <sub>2</sub> )	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	(b)	AFM	—	HQ	66277
1017	Sr <sub>2</sub> (ZnN <sub>2</sub> )	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	(b)	NM	—	HQ	80376 670402
1018	La <sub>2</sub> PdO <sub>4</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	(b,s,l)	NM	—	—	40262
1019	Cs <sub>2</sub> (PdCl <sub>4</sub> )I <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	—	HQ	240484
1020	Rb <sub>3</sub> (TlF <sub>6</sub> )	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	—	NM	—	—	19075
1021	Cs <sub>3</sub> TlF <sub>6</sub>	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	—	NM	—	—	19076
1022	Rb <sub>3</sub> YF <sub>6</sub>	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	Fig. 38	—	NM	—	—	19077
1023	Cs <sub>3</sub> YF <sub>6</sub>	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	—	NM	—	—	19078
1024	RbNa <sub>2</sub> NiO <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	(b)	FM	—	HQ	73209
1025	CsK <sub>2</sub> (CoO <sub>2</sub> )	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	(b)	AFM	—	HQ	74889
1026	Co	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	—	—	—	671035
1027	PbF <sub>4</sub>	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	(b,s,l)	NM	—	—	16795 78895
1028	(Cu <sub>2</sub> S <sub>2</sub> )(Sr <sub>2</sub> NiO <sub>2</sub> )	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	(b,s,l)	FM	—	HQ	88424
1029	K <sub>3</sub> Zn <sub>2</sub> F <sub>7</sub>	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	(b,s,l*)	NM	—	—	9925 100299
1030	K <sub>3</sub> Cu <sub>2</sub> F <sub>7</sub>	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	(b,s,l*)	FM	—	HQ	15373
1031	(SrO) <sub>3</sub> (TiO <sub>2</sub> ) <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	Fig. 38	(b,s,l*)	NM	—	—	20294 34629 63704
1032	Sr <sub>3</sub> V <sub>2</sub> O <sub>7</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	(b,s,l*)	FM	—	HQ	71320 71451
1033	K <sub>2</sub> Sr(Ta <sub>2</sub> O <sub>7</sub> )	<i>I</i> 4/ <i>mmm</i> (139)	Triv.	—	(b,s)	NM	—	HQ	93492
1034	CaCo <sub>2</sub> Ge <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	—	NM	—	—	406 81751
1035	CaCo <sub>2</sub> P <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	—	FM	SC*	HQ	10462 85890 85891 85892 619210
1036	Co <sub>2</sub> YB <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	SC	HQ	23653 55298 602345 613409 613423
1037	LaCo <sub>2</sub> B <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	Fig. 38	—	NM	—	HQ	41787 55297 181185 182572 182573 423045 613135
1038	Ir <sub>2</sub> YSi <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	SC	—	44667 181768 181769 188326 600299 641030
1039	CaRh <sub>2</sub> P <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	Fig. 38	—	NM	SC	HQ	50185
1040	SrRh <sub>2</sub> P <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	—	NM	—	HQ	50186
1041	LaCo <sub>2</sub> Si <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	Fig. 38	—	NM	—	—	52999 90777
1042	Co <sub>2</sub> YSi <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	—	—	53088 427109 625128
1043	LaRh <sub>2</sub> Ge <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	Fig. 38	—	NM	—	—	55926 81759 636847
1044	YCo <sub>2</sub> Ge <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	SC	HQ	81748 623662
1045	LaCo <sub>2</sub> Ge <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	FM	—	HQ	81750 291377 623460
1046	LaCo <sub>2</sub> P <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	FM	—	—	87581 87582 87583 624010
1047	SrRh <sub>2</sub> As <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	—	NM	—	—	165120
1048	CaFe <sub>2</sub> As <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	—	AFM	—	—	166016 182277 182278 182279
1049	CaFe <sub>2</sub> As <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	—	AFM	SC	—	182276 192309 192310 192311
1050	SrRh <sub>2</sub> As <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	—	NM	—	HQ	417002
1051	CaCo <sub>2</sub> Si <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	—	NM	—	HQ	420974
1052	CaFe <sub>2</sub> Si <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	FM	—	HQ	425467
1053	LaRh <sub>2</sub> Si <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	—	—	601417 601614 603880 604623 641747 641750 641752
1054	CaCo <sub>2</sub> As <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	TI	—	—	FM	—	—	609899
1055	Co <sub>2</sub> LaAs <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	FM	—	—	610073
1056	CsCo <sub>2</sub> S <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	FM	—	—	622529
1057	CsCo <sub>2</sub> Se <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	FM	—	—	622533
1058	Co <sub>2</sub> RbSe <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	FM	—	—	624798
1059	Co <sub>2</sub> ScSi <sub>2</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	—	—	624957 624959
1060	Al <sub>8</sub> Fe <sub>4</sub> Y	<i>I</i> 4/ <i>mmm</i> (139)	SM	Fig. 39	—	FM	—	—	57842 240140 240141 607728 607735
1061	Be <sub>12</sub> Pd	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	NM	SC	—	109314
1062	ScFe <sub>4</sub> Al <sub>8</sub>	<i>I</i> 4/ <i>mmm</i> (139)	SM	—	—	FM	—	HQ	240138 240139 607626
1063	Al <sub>8</sub> Fe <sub>4</sub> Hf	<i>I</i> 4/ <i>mmm</i> (139)	TI	Fig. 38	—	FM	—	—	607535
1064	Al <sub>8</sub> Fe <sub>4</sub> Zr	<i>I</i> 4/ <i>mmm</i> (139)	TI	Fig. 38	—	FM	—	—	607756
1065	K(BrF <sub>4</sub> )	<i>I</i> 4/ <i>mcm</i> (140)	Triv.	—	—	FM	—	—	16633 10326 16700
1066	(K(HF <sub>2</sub> ))(IF <sub>5</sub> ) <sub>2</sub>	<i>I</i> 4/ <i>mcm</i> (140)	Triv.	—	—	NM	—	—	71583
1067	Li <sub>5</sub> (VO)(PO <sub>4</sub> ) <sub>2</sub>	<i>I</i> 4/ <i>mcm</i> (140)	TI	—	(b)	FM	—	—	245847
1068	Hf <sub>2</sub> Ge	<i>I</i> 4/ <i>mcm</i> (140)	SM	—	—	NM	—	—	636554
1069	FeSn <sub>2</sub>	<i>I</i> 4/ <i>mcm</i> (140)	SM	Fig. 39	—	FM	SC	—	24570 102800 103636 247483 409909 604017 633753 633760 633761
1070	MnSn <sub>2</sub>	<i>I</i> 4/ <i>mcm</i> (140)	SM	—	—	FM	SC	—	24571 102799 171198 247482 643736 643742

1071	Zr <sub>2</sub> Si	<i>I4/mcm</i> (140)	TI	—	—	NM	SC	—	24717 42522 652618
1072	FeGe <sub>2</sub>	<i>I4/mcm</i> (140)	SM	Fig. 39	—	FM	SC	—	42519 77313 195131 631984 631999 632023 632024
1073	SiHf <sub>2</sub>	<i>I4/mcm</i> (140)	TI	—	—	NM	SC	—	42523 638912
1074	Hf <sub>2</sub> Ge	<i>I4/mcm</i> (140)	TI	—	—	NM	SC	—	42524 636547 636548
1075	CoSn <sub>2</sub>	<i>I4/mcm</i> (140)	SM	—	—	NM	SC	—	102672 108319 247484 409910 625260 625263 625269
1076	RuSn <sub>2</sub>	<i>I4/mcm</i> (140)	SM	—	—	NM	—	—	105993
1077	FeSb <sub>2</sub>	<i>I4/mcm</i> (140)	TI	—	—	FM	—	—	186636 186638 186639 186640 186641 186642
1078	Zr <sub>2</sub> Si	<i>I4/mcm</i> (140)	SM	—	—	NM	—	—	652615
1079	Ca <sub>5</sub> Ge <sub>3</sub>	<i>I4/mcm</i> (140)	SM	Fig. 39	—	NM	—	—	42139 93704 181074
1080	Ca <sub>5</sub> Si <sub>3</sub>	<i>I4/mcm</i> (140)	SM	Fig. 39	—	NM	—	HQ	93699
1081	Ba <sub>3</sub> O(SiO <sub>4</sub> )	<i>I4/mcm</i> (140)	Triv.	—	—	NM	—	HQ	1449
1082	Tl <sub>3</sub> CoCl <sub>5</sub>	<i>I4/mcm</i> (140)	SM	—	(b,s)	FM	—	—	10137
1083	Sr <sub>3</sub> (AlO <sub>4</sub> )F	<i>I4/mcm</i> (140)	Triv.	—	(b)	NM	—	HQ	50736 195183 195184
1084	CsSn <sub>2</sub> Br <sub>5</sub>	<i>I4/mcm</i> (140)	Triv.	—	(b)	NM	—	HQ	93792 151987
1085	AgTlI <sub>2</sub>	<i>I4/mcm</i> (140)	Triv.	—	(b,s)	NM	—	—	26318
1086	RbAuF <sub>4</sub>	<i>I4/mcm</i> (140)	Triv.	—	—	NM	—	—	9907 33952
1087	CaPdF <sub>4</sub>	<i>I4/mcm</i> (140)	Triv.	—	(b)	NM	—	—	32674
1088	CdCuF <sub>4</sub>	<i>I4/mcm</i> (140)	SM	—	(b)	FM	—	HQ	73478
1089	BaPdF <sub>4</sub>	<i>I4/mcm</i> (140)	Triv.	—	—	NM	—	—	108991
1090	PbPdF <sub>4</sub>	<i>I4/mcm</i> (140)	Triv.	—	—	NM	—	—	108992
1091	Sr(ZrO <sub>3</sub> )	<i>I4/mcm</i> (140)	Triv.	Fig. 39	(b,s)	NM	—	HQ	1522 89356 89357 89358 89359 89360 89361 89362 <sup>(1)</sup> 89363 <sup>(1)</sup> 89364 <sup>(1)</sup> 188451 290620 674924
1092	Sr(TiO <sub>3</sub> )	<i>I4/mcm</i> (140)	Triv.	—	(b,s)	NM	—	—	56718 <sup>(1)</sup> 182247 182762 <sup>(1)</sup> 182763 <sup>(1)</sup> 182764 <sup>(1)</sup> 248380 <sup>(1)</sup> 290619 <sup>(1)</sup> 673335
1093	Ca(TiO <sub>3</sub> )	<i>I4/mcm</i> (140)	Triv.	—	(b,s)	NM	—	HQ	153173 <sup>(1)</sup> 162919 162920 162921 162922 162923
1094	Sr(TcO <sub>3</sub> )	<i>I4/mcm</i> (140)	SM	—	(b,s,l*)	NM	—	HQ	183452
1095	Ca(SiO <sub>3</sub> )	<i>I4/mcm</i> (140)	Triv.	—	(b,s)	NM	—	—	240414 240415 240416 240417 240418 240419 240420 240421
1096	Ca <sub>5</sub> Sn <sub>3</sub> H	<i>I4/mcm</i> (140)	SM	—	—	NM	—	HQ	165190
1097	SrCu <sub>2</sub> (BO <sub>3</sub> ) <sub>2</sub>	<i>I4/mcm</i> (140)	TI	—	(b)	FM	—	—	92953 247207 247208
1098	PbSe <sub>2</sub>	<i>I4/mcm</i> (140)	Triv.	—	—	NM	—	HQ	174577
1099	Cl <sub>2</sub> O	<i>I4<sub>1</sub>/amd</i> (141)	Triv.	—	—	NM	—	HQ	407768
1100	TiO <sub>2</sub>	<i>I4<sub>1</sub>/amd</i> (141)	Triv.	—	—	NM	—	HQ	9852 <sup>(b)</sup> 9853 <sup>(b)</sup> 9854 <sup>(b)</sup> 9855 <sup>(b)</sup> 24276 <sup>(b)</sup> 31064 <sup>(b)</sup> 44882 <sup>(b)</sup> 63711 <sup>(b)</sup> 76173 <sup>(b)</sup> 92363 <sup>(b)</sup> 93098 <sup>(b)</sup> 94566 <sup>(b)</sup> 96946 <sup>(b)</sup> 154601 <sup>(b)</sup> 154602 <sup>(b)</sup> 154603 <sup>(b)</sup> 154604 <sup>(b)</sup> 154607 <sup>(b)</sup> 154608 <sup>(b)</sup> 154609 <sup>(b)</sup> 154610 <sup>(b)</sup> 156838 <sup>(b)</sup> 159910 <sup>(b)</sup> 161908 <sup>(b)</sup> 172914 <sup>(b)</sup> 172916 <sup>(b)</sup> 183767 <sup>(b)</sup> 184368 <sup>(b)</sup> 189318 <sup>(b)</sup> 190785 <sup>(b)</sup> 193265 <sup>(b)</sup> 193267 <sup>(b)</sup> 193269 <sup>(b)</sup> 193271 <sup>(b)</sup> 200392 <sup>(b)</sup> 202242 <sup>(b)</sup> 202243 <sup>(b)</sup> 237000 <sup>(b)</sup> 242104 <sup>(b)</sup> 242105 <sup>(b)</sup> 242106 <sup>(b)</sup> 671957 <sup>(b)</sup> 673140 674666 <sup>(b)</sup>
1101	Rb <sub>4</sub> (SbBr <sub>6</sub> ) <sub>2</sub>	<i>I4<sub>1</sub>/amd</i> (141)	Triv.	—	—	NM	—	—	26058
1102	Cs <sub>2</sub> (SbCl <sub>6</sub> )	<i>I4<sub>1</sub>/amd</i> (141)	Triv.	—	—	NM	—	—	49706 49707 <sup>(b)</sup> 49708 <sup>(b)</sup>
1103	Fe <sub>2</sub> (PO <sub>4</sub> )O	<i>I4<sub>1</sub>/amd</i> (141)	SM	—	(b)	FM	—	HQ	80554 80555 108812 108813
1104	Li <sub>3</sub> (BN <sub>2</sub> )	<i>I4<sub>1</sub>/amd</i> (141)	Triv.	Fig. 39	(b,s)	NM	—	HQ	155126 155127
1105	YCrO <sub>4</sub>	<i>I4<sub>1</sub>/amd</i> (141)	SM	—	(b)	FM	—	—	26989 95971 157933
1106	BaGeGe <sub>3</sub> O <sub>9</sub>	<i>P3</i> (143)	Triv.	—	(b,s)	NM	—	—	15674
1107	Ba <sub>3</sub> Si <sub>6</sub> O <sub>9</sub> N <sub>4</sub>	<i>P3</i> (143)	Triv.	—	(b)	NM	—	HQ	415918
1108	Na <sub>3</sub> (ReO <sub>5</sub> )	<i>P3<sub>1</sub></i> (144)	Triv.	—	—	—	—	HQ	36637
1109	CsCd(NO <sub>2</sub> ) <sub>3</sub>	<i>R3</i> (146)	Triv.	—	—	NM	—	HQ	95536
1110	RbCd(NO <sub>2</sub> ) <sub>3</sub>	<i>R3</i> (146)	Triv.	—	—	NM	—	HQ	95537
1111	KCd(NO <sub>2</sub> ) <sub>3</sub>	<i>R3</i> (146)	Triv.	—	—	NM	—	HQ	95538
1112	TlCd(NO <sub>2</sub> ) <sub>3</sub>	<i>R3</i> (146)	Triv.	—	—	NM	—	HQ	95539
1113	K <sub>2</sub> Pb <sub>2</sub> Ge <sub>2</sub> O <sub>7</sub>	<i>P3</i> (147)	Triv.	—	(b,s)	NM	—	—	30247
1114	Zr <sub>3</sub> O <sub>5</sub> (SO <sub>4</sub> )	<i>P3</i> (147)	Triv.	—	(b)	NM	—	—	68335
1115	Zr(HPO <sub>3</sub> ) <sub>2</sub>	<i>P3</i> (147)	Triv.	—	(b)	NM	—	HQ	74463

1116	Ba(CoPO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ (147)	Triv.	—	(b)	FM	—	HQ	250709
1117	Ba(Al <sub>2</sub> Si <sub>2</sub> O <sub>8</sub> )	P $\bar{3}$ (147)	Triv.	—	—	NM	—	HQ	188056 191252(b,s)
1118	CsFe(MoO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ (147)	SM	Fig. 40	(b,s)	FM	—	—	191592
1119	CsFe(SO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ (147)	SM	—	(b)	AFM	—	—	245667
1120	RbAg <sub>2</sub> Fe(VO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ (147)	SM	Fig. 40	(b,s)	AFM	—	HQ	194588 194589
1121	Na <sub>2</sub> BaMgP <sub>2</sub> O <sub>8</sub>	P $\bar{3}$ (147)	Triv.	—	(b)	NM	—	HQ	262716
1122	Zn(ReO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ (147)	Triv.	Fig. 40	(b,s)	NM	—	—	51017
1123	Li <sub>14</sub> Cr <sub>2</sub> N <sub>8</sub> O	P $\bar{3}$ (147)	Triv.	—	(b)	NM	—	HQ	66098 151435
1124	Li <sub>14</sub> (PON <sub>3</sub> ) <sub>2</sub> O	P $\bar{3}$ (147)	Triv.	—	—	NM	—	HQ	428737
1125	Na <sub>2</sub> (SO <sub>3</sub> )	P $\bar{3}$ (147)	Triv.	—	—	—	—	—	4432 31816
1126	Mn(TiO <sub>3</sub> )	R $\bar{3}$ (148)	TI	Fig. 40	(b)	AFM	—	HQ	60006 171579 184649
1127	NiPbF <sub>6</sub>	R $\bar{3}$ (148)	Triv.	—	(b,s)	FM	—	—	15108
1128	LiMgAlF <sub>6</sub>	P321 (150)	Triv.	—	(b)	NM	—	—	5007
1129	AlF <sub>3</sub>	P321 (150)	Triv.	—	(k*,b,s)	NM	—	—	29131
1130	Sr <sub>3</sub> (NbGa <sub>3</sub> Si <sub>2</sub> O <sub>14</sub> )	P321 (150)	Triv.	—	(b,s)	NM	—	—	181650
1131	Pb <sub>3</sub> Ga <sub>2</sub> Ge <sub>4</sub> O <sub>14</sub>	P321 (150)	Triv.	Fig. 40	(b,s)	NM	—	HQ	250123
1132	Ba <sub>3</sub> Ga <sub>2</sub> Ge <sub>4</sub> O <sub>14</sub>	P321 (150)	Triv.	—	(b,s)	NM	—	HQ	250124
1133	Sr <sub>3</sub> Zn <sub>3</sub> TeP <sub>2</sub> O <sub>14</sub>	P321 (150)	Triv.	—	(b)	NM	—	—	252309
1134	Ba <sub>3</sub> Zn <sub>3</sub> TeP <sub>2</sub> O <sub>14</sub>	P321 (150)	Triv.	—	(b)	NM	—	—	252310
1135	SiO <sub>2</sub>	P3 <sub>1</sub> 21 (152)	Triv.	—	—	NM	—	HQ	27745(b,s) 29122(b,s) 31048(b,s) 40009(b,s) 67117(b,s) 67121(b,s) 67122(b,s) 67123(b,s) 67124(b,s) 67125(b,s) 67126(b,s) 74529(b,s) 79634(b,s) 79635(b,s) 79636(b,s) 79637(b,s) 89658(b,s) 89659(b,s) 89660(b,s) 89661(b,s) 90145(b,s) 93974(b,s) 153453(b,s) 153454(b,s) 154289(b,s) 200721(b,s) 200722(b,s) 200723(b,s) 200724(b,s) 200725(b,s) 200726(b,s) 200727(b,s) 200728(b,s) 200729(b,s) 201352(b,s) 201353(b,s) 201354(b,s) 247141(b,s) 670929
1136	GeO <sub>2</sub>	P3 <sub>1</sub> 21 (152)	Triv.	—	(b,s)	NM	—	—	53869 53870 59624 59625 59626 59627 59626 59629 59630 59631 59632 59633 59634 59635 59636 59637 59639 79638 79639 79640 79641 79642 79643 79644 200730 200731 200732 200733 200734 200735 200736
1137	Tl(NO <sub>2</sub> )	P3 <sub>1</sub> 21 (152)	Triv.	—	—	NM	—	—	50325 50326
1138	KBe <sub>2</sub> (BO <sub>3</sub> )F <sub>2</sub>	R32 (155)	Triv.	—	—	NM	—	HQ	77277 155156
1139	CsBe <sub>2</sub> BO <sub>3</sub> F <sub>2</sub>	R32 (155)	Triv.	—	—	NM	—	HQ	247622 260440
1140	Na <sub>2</sub> Ca <sub>3</sub> Ta <sub>2</sub> O <sub>9</sub>	R32 (155)	Triv.	—	(b)	NM	—	HQ	280154
1141	YAl <sub>3</sub> (BO <sub>3</sub> ) <sub>4</sub>	R32 (155)	Triv.	—	(b)	NM	—	HQ	20223 91962 187082 674788
1142	NaK(BH <sub>4</sub> ) <sub>2</sub>	P3m1 (156)	Triv.	—	—	NM	—	—	163376
1143	NiO(OH)	P3m1 (156)	SM	—	(b)	FM	—	—	169980
1144	LiInMo <sub>3</sub> O <sub>8</sub>	P3m1 (156)	Triv.	—	(b)	NM	—	—	30579
1145	Cs <sub>3</sub> (As <sub>5</sub> O <sub>9</sub> )	P31m (157)	Triv.	—	(b,s)	NM	—	HQ	413151
1146	K <sub>3</sub> (V <sub>5</sub> O <sub>14</sub> )	P31m (157)	Triv.	—	(b,s)	NM	—	HQ	24068 248227
1147	Rb <sub>3</sub> (V <sub>5</sub> O <sub>14</sub> )	P31m (157)	Triv.	—	(b,s)	NM	—	HQ	248228 420851
1148	Mg <sub>3</sub> (Si <sub>2</sub> O <sub>5</sub> )(OH) <sub>4</sub>	P31m (157)	Triv.	—	(b,s)	NM	—	HQ	17046 67332 67333 75933 75934 87436 87438(k) 163889 163890 202358(k) 245887(k)
1149	Si <sub>3</sub> N <sub>4</sub>	P31c (159)	Triv.	—	—	NM	—	—	16752 26191(b) 34096(b) 35560(b) 35561(b) 35562(b) 35563(b) 35564(b) 35565(b) 77811(b) 79797(b) 90146(b) 92156(b) 239369(b) 644683(b)
1150	Rb <sub>2</sub> (TeW <sub>3</sub> O <sub>12</sub> )	P31c (159)	Triv.	—	(k*,b)	NM	—	—	97507
1151	Tl <sub>2</sub> (MoO <sub>3</sub> ) <sub>3</sub> (SeO <sub>3</sub> )	P31c (159)	Triv.	—	(k*,b,s)	NM	—	—	167531
1152	KAl(SiO <sub>4</sub> )	P31c (159)	Triv.	—	(b,s)	NM	—	HQ	83449
1153	Si <sub>3</sub> N <sub>4</sub>	P31c (159)	SM	—	(b)	FM	—	—	159207 187735
1154	K <sub>3</sub> MnO <sub>4</sub> CrO <sub>4</sub>	R3m (160)	Triv.	—	(k*,b)	NM	—	HQ	26803
1155	Cd(CN <sub>2</sub> )	R3m (160)	Triv.	—	—	—	—	HQ	95265
1156	Bi <sub>2</sub> O <sub>3</sub>	R3m (160)	Triv.	—	(b,s)	NM	—	—	168810
1157	C <sub>3</sub> N <sub>4</sub>	R3m (160)	Triv.	—	(k*,b)	NM	—	—	246660 673898 674277 674292
1158	CrO(OH)	R3m (160)	SM	—	—	AFM	—	HQ	1372 64754 88574

1159	NaVS <sub>2</sub>	R3m (160)	Triv.	—	(b)	FM	—	—	644994
1160	FeAl <sub>2</sub> S <sub>4</sub>	R3m (160)	Triv.	—	(b)	—	—	—	607619
1161	Y(HCOO) <sub>3</sub>	R3m (160)	Triv.	—	—	NM	—	—	109739
1162	K <sub>2</sub> Na(Ag(CN) <sub>2</sub> ) <sub>3</sub>	P $\bar{3}$ 1m (162)	Triv.	Fig. 40	(k,b)	NM	—	HQ	65699
1163	SiO <sub>2</sub>	P $\bar{3}$ 1m (162)	TI	—	(k*,b,s)	NM	—	—	170552
1164	Hg <sub>2</sub> (As <sub>2</sub> O <sub>6</sub> )	P $\bar{3}$ 1m (162)	Triv.	—	(b,s)	—	—	HQ	411230
1165	Ag <sub>3</sub> (Co(CN) <sub>6</sub> )	P $\bar{3}$ 1m (162)	Triv.	—	(k,b)	NM	—	—	16959 28501
1166	Ag <sub>3</sub> (Fe(CN) <sub>6</sub> )	P $\bar{3}$ 1m (162)	SM	—	(k,b)	FM	—	—	173552 173553
1167	Cd(Sb <sub>2</sub> O <sub>6</sub> )	P $\bar{3}$ 1m (162)	Triv.	Fig. 40	(b)	NM	—	HQ	71028
1168	Ca(Sb <sub>2</sub> O <sub>6</sub> )	P $\bar{3}$ 1m (162)	Triv.	—	(b,s)	NM	—	HQ	74539
1169	Sr(Sb <sub>2</sub> O <sub>6</sub> )	P $\bar{3}$ 1m (162)	Triv.	—	(b,s)	NM	—	HQ	74540
1170	Co(AsO <sub>3</sub> ) <sub>2</sub>	P $\bar{3}$ 1m (162)	SM	—	(b)	AFM	—	HQ	80350
1171	SrRu <sub>2</sub> O <sub>6</sub>	P $\bar{3}$ 1m (162)	Triv.	—	(b,s)	AFM	—	HQ	248351
1172	Cd(As <sub>2</sub> O <sub>6</sub> )	P $\bar{3}$ 1m (162)	Triv.	—	(b,s)	NM	—	HQ	280576
1173	K(Ag(CN) <sub>2</sub> )	P $\bar{3}$ 1c (163)	Triv.	Fig. 40	(k*,b)	NM	—	—	30275
1174	SiO <sub>2</sub>	P $\bar{3}$ 1c (163)	SM	—	—	NM	—	—	170495
1175	CdZn <sub>2</sub> KB <sub>2</sub> O <sub>6</sub> F	P $\bar{3}$ 1c (163)	Triv.	—	(b)	NM	—	HQ	248025
1176	(Ag <sub>3</sub> (H <sub>2</sub> O) <sub>3</sub> )(K(CN) <sub>2</sub> ) <sub>3</sub>	P $\bar{3}$ 1c (163)	Triv.	—	(k*)	—	—	—	248371
1177	Na <sub>2</sub> Al <sub>2</sub> (B <sub>2</sub> O <sub>7</sub> )	P $\bar{3}$ 1c (163)	Triv.	—	(b)	NM	—	HQ	93389 <sup>(s)</sup> 237154 237155 237156 237157
1178	Ti <sub>3</sub> O	P $\bar{3}$ 1c (163)	SM	Fig. 41	(b,s)	—	—	—	20041 24082
1179	Cu <sub>3</sub> Zn(OH) <sub>6</sub> Cl <sub>2</sub>	P $\bar{3}$ m1 (164)	SM	—	(k,b)	—	—	HQ	162099
1180	Ba <sub>2</sub> (BO <sub>3</sub> )Br	P $\bar{3}$ m1 (164)	Triv.	—	—	—	—	HQ	190941
1181	Cu <sub>3</sub> MgCl <sub>2</sub> (OH) <sub>6</sub>	P $\bar{3}$ m1 (164)	SM	—	(k,b)	—	—	HQ	240663
1182	POF <sub>3</sub>	P $\bar{3}$ m1 (164)	Triv.	Fig. 41	—	—	—	HQ	250498
1183	Zn(B(CN) <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ m1 (164)	Triv.	—	(b)	NM	—	HQ	415547
1184	Ba <sub>3</sub> MnNb <sub>2</sub> O <sub>9</sub>	P $\bar{3}$ m1 (164)	SM	—	(k,b,s)	AFM	—	HQ	171479 239731
1185	Sr <sub>3</sub> MgTa <sub>2</sub> O <sub>9</sub>	P $\bar{3}$ m1 (164)	Triv.	—	(k,b,s)	NM	—	—	194992
1186	Ba <sub>6</sub> IrNb <sub>2</sub> O <sub>12</sub> Cl <sub>2</sub>	P $\bar{3}$ m1 (164)	SM	—	(k*,b,s)	FM	—	HQ	40693
1187	Ba <sub>5</sub> (Nb <sub>4</sub> O <sub>15</sub> )	P $\bar{3}$ m1 (164)	Triv.	—	(k,b,s)	NM	—	HQ	95192 157477 674451
1188	Mn(OH) <sub>2</sub>	P $\bar{3}$ m1 (164)	SM	—	—	AFM	—	—	23591
1189	ReTi <sub>2</sub>	P $\bar{3}$ m1 (164)	SM	—	—	NM	—	—	168953
1190	TiS <sub>2</sub>	P $\bar{3}$ m1 (164)	Triv.	—	(b)	NM	SC*	—	26861 41663 52195 91579 174489 181500 601182 601315 603788 604416 651178 651186 651201 651203 651207 651212 651214 651217
1191	MnI <sub>2</sub>	P $\bar{3}$ m1 (164)	SM	—	(b)	FM	—	—	33673
1192	MnBr <sub>2</sub>	P $\bar{3}$ m1 (164)	SM	—	(b)	FM	—	—	60250
1193	NbS <sub>2</sub>	P $\bar{3}$ m1 (164)	SM	—	(b)	NM	—	—	237032 250594
1194	CrSe <sub>2</sub>	P $\bar{3}$ m1 (164)	TI	—	(b)	FM	—	—	626718
1195	Cs(Cu <sub>3</sub> O <sub>2</sub> )	P $\bar{3}$ m1 (164)	Triv.	—	(k,b,s)	NM	—	HQ	413342
1196	Fe <sub>2</sub> Si	P $\bar{3}$ m1 (164)	TI	—	—	FM	—	—	161133
1197	FeGa <sub>2</sub> S <sub>4</sub>	P $\bar{3}$ m1 (164)	Triv.	—	(b)	FM	—	HQ	100706 602041
1198	K <sub>2</sub> RhF <sub>6</sub>	P $\bar{3}$ m1 (164)	SM	—	(k*)	FM	—	—	28779
1199	Rb <sub>2</sub> (RhF <sub>6</sub> )	P $\bar{3}$ m1 (164)	SM	—	(k*)	FM	—	—	28780
1200	Tl <sub>2</sub> (SnF <sub>6</sub> )	P $\bar{3}$ m1 (164)	Triv.	—	(k*)	NM	—	HQ	410801
1201	Na <sub>2</sub> Tl <sub>3</sub> (SO <sub>3</sub> ) <sub>2</sub>	P $\bar{3}$ m1 (164)	Triv.	—	—	NM	—	HQ	1626
1202	Tl <sub>2</sub> (WO <sub>4</sub> )	P $\bar{3}$ m1 (164)	Triv.	—	(k*,b)	NM	—	HQ	8212
1203	Na <sub>2</sub> (SO <sub>4</sub> )	P $\bar{3}$ m1 (164)	SM	Fig. 41	—	FM	—	—	27955
1204	KNa(SO <sub>4</sub> )	P $\bar{3}$ m1 (164)	Triv.	—	—	NM	—	—	77343
1205	K <sub>3</sub> V(VO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ m1 (164)	Triv.	—	(k*,b,s)	AFM	—	HQ	100782
1206	Ca <sub>2</sub> (GeO <sub>4</sub> )	P $\bar{3}$ m1 (164)	Triv.	Fig. 41	(k*,b)	NM	—	—	182051
1207	Ca <sub>2</sub> (SiO <sub>4</sub> )	P $\bar{3}$ m1 (164)	Triv.	Fig. 41	(k*,b)	NM	—	—	182052
1208	Tl <sub>2</sub> (MoO <sub>4</sub> )	P $\bar{3}$ m1 (164)	Triv.	—	—	NM	—	HQ	280056
1209	RbIn(WO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ m1 (164)	Triv.	Fig. 42	(k*,b)	NM	—	—	24859
1210	KAl(MoO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ m1 (164)	Triv.	—	(k*,b,s)	NM	—	HQ	28018
1211	KSc(MoO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ m1 (164)	Triv.	—	(k*,b,s)	NM	—	HQ	28019
1212	KFe(MoO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ m1 (164)	SM	Fig. 41	(k*,b,s)	AFM	—	HQ	153864
1213	BaZr(PO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ m1 (164)	Triv.	—	(k*,b)	NM	—	HQ	173842
1214	CsV(MoO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ m1 (164)	Triv.	—	(k*,b,s)	AFM	—	HQ	202907
1215	RbFe(MoO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ m1 (164)	SM	Fig. 41	(k*,b,s)	FM	—	—	245665 250409
1216	CsFe(MoO <sub>4</sub> ) <sub>2</sub>	P $\bar{3}$ m1 (164)	SM	Fig. 41	(k*,b,s)	FM	—	HQ	260887

1217	Li <sub>2</sub> MnO <sub>2</sub>	$P\bar{3}m1$ (164)	SM	—	—	FM	—	HQ	37327
1218	CaMn <sub>2</sub> As <sub>2</sub>	$P\bar{3}m1$ (164)	TI	—	—	FM	—	HQ	41792 609906
1219	CaMn <sub>2</sub> P <sub>2</sub>	$P\bar{3}m1$ (164)	TI	—	—	FM	—	HQ	49017
1220	SrMn <sub>2</sub> P <sub>2</sub>	$P\bar{3}m1$ (164)	TI	—	—	FM	—	HQ	49019 77669 77670
1221	LiCrS <sub>2</sub>	$P\bar{3}m1$ (164)	SM	—	—	FM	—	—	150674
1222	LiTiS <sub>2</sub>	$P\bar{3}m1$ (164)	SM	—	—	FM	—	HQ	200709 642322
1223	LiCrSe <sub>2</sub>	$P\bar{3}m1$ (164)	SM	—	—	—	—	—	252879
1224	Rb <sub>2</sub> PdC <sub>2</sub>	$P\bar{3}m1$ (164)	Triv.	—	—	NM	—	HQ	94394 421493 421494
1225	Rb <sub>2</sub> PtC <sub>2</sub>	$P\bar{3}m1$ (164)	Triv.	—	—	NM	—	HQ	94395
1226	Cs <sub>2</sub> PdC <sub>2</sub>	$P\bar{3}m1$ (164)	Triv.	—	—	NM	—	HQ	94396
1227	Cs <sub>2</sub> PtC <sub>2</sub>	$P\bar{3}m1$ (164)	Triv.	—	—	NM	—	HQ	94397
1228	K <sub>2</sub> PdC <sub>2</sub>	$P\bar{3}m1$ (164)	Triv.	—	—	NM	—	HQ	421489 421490
1229	K <sub>2</sub> PtC <sub>2</sub>	$P\bar{3}m1$ (164)	Triv.	—	—	NM	—	HQ	421491 421492
1230	Pd <sub>3</sub> (PS <sub>4</sub> ) <sub>2</sub>	$P\bar{3}m1$ (164)	Triv.	—	(k,b)	NM	—	—	16296 35361
1231	Rb <sub>2</sub> (Sb <sub>2</sub> Al <sub>2</sub> O <sub>7</sub> )	$P\bar{3}m1$ (164)	Triv.	—	(k*,b,s)	NM	—	HQ	154360
1232	NaFe <sub>2</sub> O <sub>3</sub>	$P\bar{3}m1$ (164)	SM	—	—	FM	—	—	200009 424349
1233	Cs <sub>2</sub> Mn(TeS <sub>3</sub> ) <sub>2</sub>	$P\bar{3}c1$ (165)	SM	—	(b,s)	FM	—	HQ	165378
1234	KFe(MoO <sub>4</sub> ) <sub>2</sub>	$P\bar{3}c1$ (165)	SM	—	(b,s)	AFM	—	HQ	28020
1235	K <sub>5</sub> CuSb <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	(b)	NM	—	HQ	32032
1236	K <sub>2</sub> Pt <sub>3</sub> PtS <sub>6</sub>	$R\bar{3}m$ (166)	Triv.	Fig. 42	(k*,b)	NM	—	—	40062
1237	Li <sub>4</sub> NCl	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	HQ	84649
1238	Li <sub>5</sub> NCl <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	HQ	84763
1239	C <sub>60</sub>	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	—	95370
1240	KPd <sub>2</sub> O <sub>3</sub>	$R\bar{3}m$ (166)	Triv.	—	(b)	NM	—	HQ	248051
1241	K <sub>2</sub> Hf <sub>3</sub> OF <sub>12</sub>	$R\bar{3}m$ (166)	Triv.	—	—	—	—	—	251076
1242	ScAlOC	$R\bar{3}m$ (166)	Triv.	—	(b)	NM	—	HQ	419683
1243	CLi <sub>6</sub>	$R\bar{3}m$ (166)	Triv.	—	(b)	—	—	—	670920
1244	Li <sub>3</sub> In <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	—	NM	—	HQ	10051 659829
1245	(B <sub>12</sub> C)C <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	—	612562
1246	Ba <sub>2</sub> NiTeO <sub>6</sub>	$R\bar{3}m$ (166)	TI	Fig. 42	(k*,b,s)	AFM	—	—	25005
1247	K <sub>2</sub> Li(AlF <sub>6</sub> )	$R\bar{3}m$ (166)	Triv.	—	(b,s)	NM	—	HQ	408552 37250(k)
1248	Cs <sub>9</sub> Ni <sub>9</sub> F <sub>27</sub>	$R\bar{3}m$ (166)	TI	Fig. 42	(k,b,s)	FM	—	HQ	410393
1249	In <sub>2</sub> Se <sub>3</sub>	$R\bar{3}m$ (166)	SM	—	(b)	NM	—	—	17007 640489 640492 640498 640512
1250	MnCl <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	(b)	FM	—	HQ	33752
1251	MnBr <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	(b)	FM	—	HQ	67500
1252	Ni <sub>7</sub> Y <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	(k)	FM	—	—	108650 647051 647060 647076
1253	Cs <sub>2</sub> Cu <sub>3</sub> ZrF <sub>12</sub>	$R\bar{3}m$ (166)	SM	—	(k,b,s)	FM	—	HQ	79114 182755
1254	Cs <sub>2</sub> SnCu <sub>3</sub> F <sub>12</sub>	$R\bar{3}m$ (166)	SM	—	(k,b,s)	FM	—	HQ	291388 291391
1255	Cu <sub>3</sub> Zn(OH) <sub>6</sub> Cl <sub>2</sub>	$R\bar{3}m$ (166)	SM	Fig. 42	(k,b)	FM	—	HQ	425834
1256	LiVO <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	—	AFM	—	—	24594 202540 202541
1257	KCrS <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	(b)	FM	—	—	25723 42406 42407
1258	NaTiS <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	(b)	FM	—	—	26305
1259	Cu(CrO <sub>2</sub> )	$R\bar{3}m$ (166)	SM	—	—	AFM	SC*	—	26676 157800 163253 163254 163255 184467 189047 194151 194152 402290 670110
1260	Ba <sub>2</sub> PCl	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	—	28134
1261	LiGaO <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	—	28388
1262	RbScO <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	(b)	NM	—	—	31959
1263	NaTiO <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	(b)	FM	—	—	43439
1264	LiFeO <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	—	FM	—	HQ	51207 51759 78712
1265	Ca <sub>2</sub> NCl	$R\bar{3}m$ (166)	Triv.	Fig. 42	(b)	NM	—	HQ	62555 153101
1266	Ca <sub>2</sub> NBr	$R\bar{3}m$ (166)	Triv.	Fig. 42	(b)	NM	—	HQ	62556 153105
1267	Na(RhO <sub>2</sub> )	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	HQ	66280
1268	NaTaN <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	HQ	67346 67347 76382 190937 657406
1269	NaNbN <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	HQ	72557 657407
1270	Na(FeO <sub>2</sub> )	$R\bar{3}m$ (166)	SM	—	—	AFM	—	HQ	75588 167376 167377 187705
1271	NaVSe <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	—	FM	—	—	77597
1272	Sr <sub>2</sub> NCl	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	HQ	172595 172596 410769
1273	Sr <sub>2</sub> NBr	$R\bar{3}m$ (166)	Triv.	—	(b)	NM	—	HQ	172600 172601
1274	LiTiS <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	—	FM	—	HQ	189825 189826
1275	Sr <sub>2</sub> NI	$R\bar{3}m$ (166)	Triv.	—	(b)	NM	—	HQ	240899

1276	NaYO <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	—	—	—	—	—	291907
1277	Na(VO <sub>2</sub> )	$R\bar{3}m$ (166)	Triv.	—	—	AFM	—	HQ	—	420137
1278	KZrS <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	(b)	NM	—	—	—	641350
1279	NaYSe <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	—	—	645037
1280	Mg <sub>2</sub> Ni <sub>3</sub> Si	$R\bar{3}m$ (166)	TI	Fig. 42	(k)	NM	—	—	—	44926
1281	Fe <sub>3</sub> S <sub>4</sub>	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	HQ	—	42537
1282	Mg <sub>2</sub> Ni <sub>3</sub> P	$R\bar{3}m$ (166)	SM	Fig. 43	(k)	NM	—	HQ	—	72409
1283	K <sub>2</sub> Zr(BO <sub>3</sub> ) <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	(b)	—	—	HQ	—	67982
1284	K <sub>2</sub> Co(SeO <sub>3</sub> ) <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	(k*,b)	AFM	—	HQ	—	71536
1285	Ba <sub>3</sub> Mn <sub>2</sub> O <sub>8</sub>	$R\bar{3}m$ (166)	TI	—	(k*)	AFM	—	HQ	—	280045
1286	K <sub>2</sub> Pt <sub>4</sub> Se <sub>6</sub>	$R\bar{3}m$ (166)	Triv.	—	(k*,b)	NM	—	HQ	—	69438
1287	Rb <sub>2</sub> Pt <sub>3</sub> PtSe <sub>6</sub>	$R\bar{3}m$ (166)	Triv.	—	(k*,b)	NM	—	HQ	—	69439
1288	Na <sub>4</sub> HgP <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	HQ	—	67260
1289	K <sub>4</sub> ZnP <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	Fig. 43	—	NM	—	HQ	—	67261
1290	K <sub>4</sub> HgP <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	Fig. 43	(b)	NM	—	HQ	—	67263
1291	K <sub>4</sub> (BeP <sub>2</sub> )	$R\bar{3}m$ (166)	Triv.	Fig. 43	(b)	NM	—	HQ	—	300110
1292	K <sub>4</sub> (BeAs <sub>2</sub> )	$R\bar{3}m$ (166)	Triv.	Fig. 43	—	NM	—	HQ	—	300111
1293	K <sub>4</sub> (CdAs <sub>2</sub> )	$R\bar{3}m$ (166)	Triv.	Fig. 43	(b)	NM	—	HQ	—	300190
1294	K <sub>4</sub> (HgAs <sub>2</sub> )	$R\bar{3}m$ (166)	Triv.	Fig. 43	—	NM	—	HQ	—	402573
1295	K <sub>4</sub> ZnAs <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	Fig. 43	—	NM	—	HQ	—	409919
1296	Na <sub>2</sub> (Ti <sub>3</sub> Cl <sub>8</sub> )	$R\bar{3}m$ (166)	TI	Fig. 44	(k,b)	FM	—	HQ	—	401026
1297	NaN <sub>3</sub>	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	—	—	1144 34267 34674
1298	Cd(CN <sub>2</sub> )	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	HQ	—	95264
1299	Nb <sub>2</sub> S <sub>2</sub> C	$R\bar{3}m$ (166)	TI	—	(b)	NM	—	HQ	—	95110 95112
1300	Nb <sub>3</sub> Br <sub>8</sub>	$R\bar{3}m$ (166)	Triv.	Fig. 44	—	NM	—	HQ	—	25766 421609
1301	Nb <sub>3</sub> I <sub>8</sub>	$R\bar{3}m$ (166)	Triv.	Fig. 44	—	NM	—	HQ	—	25767
1302	Co <sub>3</sub> Sn <sub>2</sub> S <sub>2</sub>	$R\bar{3}m$ (166)	SM	Fig. 44	(k,b,s)	FM	—	—	—	5435 173760 173761 173762 173763 173764 195422 196310 426752 426753 624867
1303	Co <sub>3</sub> In <sub>2</sub> S <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	(k,b,s)	FM	—	—	—	5436 195432 423459
1304	Co <sub>3</sub> InSnS <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	Fig. 44	(k,b,s)	NM	—	—	—	5437 425136
1305	Rh <sub>3</sub> In <sub>2</sub> S <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	(k,b,s)	NM	—	—	—	5439 420726 640339
1306	Rh <sub>3</sub> InPbS <sub>2</sub>	$R\bar{3}m$ (166)	SM	Fig. 44	(k,b,s)	NM	—	—	—	5440 640213
1307	Rh <sub>3</sub> Pb <sub>2</sub> Se <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	(k,b,s)	NM	—	—	—	5441 648427
1308	Ni <sub>3</sub> Sn <sub>2</sub> S <sub>2</sub>	$R\bar{3}m$ (166)	TI	—	(k,b,s)	NM	—	HQ	—	402458 674419
1309	In <sub>2</sub> Ni <sub>3</sub> S <sub>2</sub>	$R\bar{3}m$ (166)	TI	—	(k,b,s)	NM	—	HQ	—	415258
1310	Rh <sub>3</sub> Sn <sub>2</sub> S <sub>2</sub>	$R\bar{3}m$ (166)	SM	Fig. 44	(k,b,s)	NM	—	HQ	—	420728
1311	Tl <sub>2</sub> Ni <sub>3</sub> S <sub>2</sub>	$R\bar{3}m$ (166)	TI	—	(k,b,s)	NM	—	HQ	—	422328
1312	InSnCo <sub>3</sub> S <sub>2</sub>	$R\bar{3}m$ (166)	SM	Fig. 44	(k,b,s)	—	—	HQ	—	425137
1313	Ni <sub>3</sub> In <sub>2</sub> S <sub>2</sub>	$R\bar{3}m$ (166)	TI	—	(k,b,s)	NM	—	—	—	640134
1314	Ni <sub>3</sub> Sn <sub>2</sub> S <sub>2</sub>	$R\bar{3}m$ (166)	TI	—	(k,b,s)	NM	—	—	—	646379 654948
1315	Ni <sub>3</sub> Tl <sub>2</sub> S <sub>2</sub>	$R\bar{3}m$ (166)	TI	—	(k,b,s)	NM	—	—	—	646398
1316	Rh <sub>3</sub> Tl <sub>2</sub> S <sub>2</sub>	$R\bar{3}m$ (166)	SM	—	(k,b,s)	NM	—	—	—	650236
1317	B <sub>12</sub> P <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	Fig. 45	—	NM	—	HQ	—	62748
1318	B <sub>12</sub> As <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	Fig. 45	—	NM	—	—	—	62749
1319	B <sub>6</sub> As	$R\bar{3}m$ (166)	Triv.	Fig. 45	—	NM	—	HQ	—	68151 107916
1320	B <sub>6</sub> P	$R\bar{3}m$ (166)	Triv.	Fig. 45	—	NM	—	—	—	615156 615157
1321	Sr <sub>2</sub> N	$R\bar{3}m$ (166)	SM	—	(b)	NM	—	HQ	—	69016 410315 411612 414330 644701
1322	Ca <sub>2</sub> N	$R\bar{3}m$ (166)	SM	—	(b)	NM	—	HQ	—	90630 90631 90632 280526 410312 411417 414329
1323	Rb <sub>2</sub> (OF <sub>3</sub> (HfF <sub>3</sub> ) <sub>3</sub> )	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	—	—	95847
1324	Rb <sub>2</sub> (OF <sub>3</sub> (ZrF <sub>3</sub> ) <sub>3</sub> )	$R\bar{3}m$ (166)	Triv.	—	—	NM	—	—	—	95848
1325	TlGaO <sub>2</sub>	$R\bar{3}m$ (166)	Triv.	Fig. 45	(k,b,s)	—	—	—	—	33579
1326	ZrCl	$R\bar{3}m$ (166)	TI	—	—	NM	—	HQ	—	869 20145
1327	YCl	$R\bar{3}m$ (166)	Triv.	—	—	FM	—	HQ	—	30708 61107
1328	SiO <sub>2</sub>	$R\bar{3}c$ (167)	Triv.	—	(b,s)	NM	—	—	—	170492 170514 170539
1329	SiO <sub>2</sub>	$R\bar{3}c$ (167)	SM	—	(b,s)	—	—	—	—	170515
1330	AlH <sub>3</sub>	$R\bar{3}c$ (167)	Triv.	—	(b,s)	NM	—	—	—	15225 165294 168162 182533
1331	TiF <sub>3</sub>	$R\bar{3}c$ (167)	SM	—	(b,s)	FM	—	—	—	52159 52162 52165 67148
1332	CrF <sub>3</sub>	$R\bar{3}c$ (167)	SM	—	(b,s)	AFM	—	HQ	—	59966 59968 59969 59972 59973
1333	VF <sub>3</sub>	$R\bar{3}c$ (167)	SM	—	(b,s)	FM	—	HQ	—	69167

1334	CoF <sub>3</sub>	<i>R</i> 3 <i>c</i> (167)	Triv.	—	(b,s)	FM	—	HQ	77618
1335	Cs <sub>4</sub> (PbBr <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	—	(b,s)	NM	—	—	25124 162158
1336	NaCa <sub>3</sub> (IrO <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	—	(b,s)	—	—	HQ	50169
1337	Rb <sub>4</sub> PbBr <sub>6</sub>	<i>R</i> 3 <i>c</i> (167)	Triv.	—	(b)	NM	—	HQ	65300
1338	Sr <sub>4</sub> IrO <sub>6</sub>	<i>R</i> 3 <i>c</i> (167)	SM	—	(b,s)	FM	—	HQ	72926
1339	Sr <sub>3</sub> ZnPtO <sub>6</sub>	<i>R</i> 3 <i>c</i> (167)	Triv.	—	(b,s)	NM	—	HQ	81467 280519
1340	Ca <sub>4</sub> (IrO <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	SM	—	(b)	FM	—	HQ	81902 <sup>(s)</sup> 280873
1341	Sr <sub>3</sub> Zn(IrO <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	SM	—	(b,s)	FM	—	HQ	81903 82658 82659 82660
1342	Sr <sub>3</sub> Cd(IrO <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	SM	—	(b,s)	FM	—	HQ	81904
1343	Sr <sub>3</sub> Mg(PtO <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	—	(b,s)	NM	—	HQ	84736 281299
1344	Sr <sub>3</sub> Mg(IrO <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	SM	—	(b,s)	FM	—	HQ	84737
1345	Sr <sub>3</sub> (PbNiO <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	Fig. 45	(b)	AFM	—	HQ	152588 152589 <sup>(s)</sup> 152590 <sup>(s)</sup> 152591 <sup>(s)</sup> 152592 <sup>(s)</sup> 152593 <sup>(s)</sup>
1346	Sr <sub>3</sub> Cd(PtO <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	—	(b,s)	NM	—	HQ	280518
1347	NaBa <sub>3</sub> IrO <sub>6</sub>	<i>R</i> 3 <i>c</i> (167)	Triv.	—	(b)	FM	—	HQ	405134
1348	Li <sub>4</sub> Osh <sub>6</sub>	<i>R</i> 3 <i>c</i> (167)	Triv.	—	(b,s)	NM	—	—	638269
1349	K <sub>8</sub> Tl <sub>11</sub>	<i>R</i> 3 <i>c</i> (167)	SM	—	—	NM	—	—	370009
1350	Rb <sub>8</sub> Tl <sub>11</sub>	<i>R</i> 3 <i>c</i> (167)	SM	—	—	NM	—	—	370035
1351	K <sub>3</sub> (B <sub>3</sub> O <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	—	—	NM	—	—	16005
1352	NaSn <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub>	<i>R</i> 3 <i>c</i> (167)	Triv.	—	(b)	NM	—	—	72217 72218 <sup>(s)</sup>
1353	LiZr <sub>2</sub> (AsO <sub>4</sub> ) <sub>3</sub>	<i>R</i> 3 <i>c</i> (167)	Triv.	—	(b,s)	NM	—	—	190656
1354	Si <sub>3</sub> N <sub>4</sub>	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	—	NM	—	—	67241 74741 <sup>(b)</sup> 74742 <sup>(b)</sup> 74743 <sup>(b)</sup> 74744 <sup>(b)</sup> 74745 <sup>(b)</sup> 74746 <sup>(b)</sup> 74747 <sup>(b)</sup> 74748 <sup>(b)</sup> 74749 <sup>(b)</sup> 74750 <sup>(b)</sup> 74751 <sup>(b)</sup> 74752 <sup>(b)</sup> 74753 <sup>(b)</sup> 74754 <sup>(b)</sup> 74755 <sup>(b)</sup> 77812
1355	Cs <sub>2</sub> (I <sub>4</sub> O <sub>11</sub> )	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	(b)	—	—	—	413942 420352
1356	Ca(Al <sub>2</sub> O <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	(b)	NM	—	—	157457
1357	Cs <sub>2</sub> (MoO <sub>3</sub> ) <sub>3</sub> (SeO <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	(k*,b)	NM	—	—	75473
1358	(Cs <sub>2</sub> (SeO <sub>3</sub> ))(WO <sub>3</sub> ) <sub>3</sub>	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	(k*,b,s)	NM	—	—	80392
1359	Rb <sub>2</sub> (MoO <sub>3</sub> ) <sub>3</sub> (SeO <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	(k*,b)	NM	—	—	167530
1360	Cs <sub>2</sub> TeW <sub>3</sub> O <sub>12</sub>	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	(k*,b,s)	—	—	—	429738
1361	K(VO <sub>2</sub> ) <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub>	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	(b,s)	NM	—	—	81231
1362	Rb(Se <sub>2</sub> V <sub>3</sub> O <sub>12</sub> )	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	(b,s)	NM	—	—	163600
1363	Tl(Se <sub>2</sub> V <sub>3</sub> O <sub>12</sub> )	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	(k*,b,s)	NM	—	—	163601
1364	Cs(VO <sub>2</sub> ) <sub>3</sub> (TeO <sub>3</sub> ) <sub>2</sub>	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	(k*,b,s)	NM	—	—	411111
1365	La <sub>3</sub> AlTiS <sub>7</sub>	<i>P</i> 6 <sub>3</sub> (173)	SM	Fig. 45	(b)	FM	—	—	608322
1366	La <sub>3</sub> AlVS <sub>7</sub>	<i>P</i> 6 <sub>3</sub> (173)	SM	Fig. 45	(b)	FM	—	—	608323
1367	La <sub>3</sub> BeTiS <sub>7</sub>	<i>P</i> 6 <sub>3</sub> (173)	SM	—	—	FM	—	—	616310
1368	KAl(SiO <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> (173)	Triv.	Fig. 46	(b,s)	NM	—	HQ	34350
1369	Ga <sub>9</sub> Tl <sub>3</sub> O <sub>2</sub> S <sub>13</sub>	<i>P</i> 6̄ (174)	Triv.	—	(b)	NM	—	HQ	61256
1370	BaZn(BO <sub>3</sub> )F	<i>P</i> 6̄ (174)	Triv.	Fig. 46	(b)	NM	—	HQ	248042 429814
1371	BaAl(BO <sub>3</sub> )F <sub>2</sub>	<i>P</i> 6̄ (174)	Triv.	—	(b)	—	—	—	291434 409663
1372	Pb <sub>7</sub> F <sub>12</sub> Br <sub>2</sub>	<i>P</i> 6̄ (174)	Triv.	—	—	NM	—	HQ	92293
1373	Ca <sub>7</sub> H <sub>12</sub> Cl <sub>2</sub>	<i>P</i> 6̄ (174)	Triv.	—	—	NM	—	HQ	420927
1374	La <sub>2</sub> ClB <sub>3</sub>	<i>P</i> 6̄ (174)	SM	—	—	NM	—	HQ	417604
1375	LiCd(BO <sub>3</sub> )	<i>P</i> 6̄ (174)	Triv.	—	(b)	NM	—	HQ	20191 20835
1376	Mg <sub>3</sub> F <sub>3</sub> (BO <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> /m (176)	Triv.	Fig. 46	(b)	—	—	HQ	4226
1377	Bi <sub>3</sub>	<i>P</i> 6 <sub>3</sub> /m (176)	Triv.	—	—	NM	SC	HQ	173375 28328 411463
1378	NaCs <sub>2</sub> (C <sub>2</sub> N <sub>3</sub> ) <sub>3</sub>	<i>P</i> 6 <sub>3</sub> /m (176)	Triv.	Fig. 46	—	NM	—	—	407809
1379	Pb <sub>3</sub> Cd <sub>3</sub> (BO <sub>3</sub> ) <sub>4</sub>	<i>P</i> 6 <sub>3</sub> /m (176)	Triv.	—	(k)	NM	—	—	422862
1380	Cu <sub>2</sub> Bi <sub>2</sub> S <sub>3</sub> (AlCl <sub>4</sub> ) <sub>2</sub>	<i>P</i> 6 <sub>3</sub> /m (176)	Triv.	—	(b,s)	NM	—	—	428727
1381	LiCa(AIH <sub>4</sub> ) <sub>3</sub>	<i>P</i> 6 <sub>3</sub> /m (176)	Triv.	—	(b)	—	—	—	670844
1382	Li <sub>2</sub> RbCd(CO <sub>3</sub> ) <sub>2</sub> F	<i>P</i> 6 <sub>3</sub> /m (176)	Triv.	—	(b)	NM	—	HQ	710094
1383	AgCd <sub>3</sub> Hf <sub>3</sub> F <sub>20</sub>	<i>P</i> 6 <sub>3</sub> /m (176)	SM	—	—	NM	—	—	78893
1384	Sc <sub>2</sub> (HPO <sub>3</sub> ) <sub>3</sub>	<i>P</i> 6 <sub>3</sub> /m (176)	Triv.	—	(b)	NM	—	—	409724
1385	Pb <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> F	<i>P</i> 6 <sub>3</sub> /m (176)	Triv.	—	—	NM	—	—	20500
1386	Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> F	<i>P</i> 6 <sub>3</sub> /m (176)	Triv.	—	—	NM	—	—	24236 <sup>(b)</sup> 30261 <sup>(b)</sup> 38118 <sup>(b)</sup> 52385 <sup>(b)</sup> 56313 56314 84227 94081 94082 94083 99581 180314 19352 670544
1387	Sr <sub>3</sub> MnN <sub>3</sub>	<i>P</i> 6 <sub>3</sub> /m (176)	TI	—	(b)	FM	—	HQ	80772
1388	Ba <sub>3</sub> (CrN <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> /m (176)	SM	—	(b)	NM	—	HQ	154802

1389	Sr <sub>3</sub> (CrN <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	(b)	NM	—	HQ	154803
1390	Ba <sub>4</sub> Nb <sub>2</sub> O <sub>9</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	TI	—	—	NM	—	HQ	251133
1391	BCl <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	Triv.	—	—	NM	—	—	24526 27869
1392	BBr <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	Triv.	—	—	NM	—	—	24527 173374
1393	Fe <sub>2</sub> (BP <sub>3</sub> O <sub>12</sub> )	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	Triv.	—	(b)	FM	—	—	260895 420638
1394	KMo <sub>3</sub> S <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	—	HQ	30752 603631 641249
1395	RbMo <sub>3</sub> S <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	—	HQ	30753 603622 644175
1396	CsMo <sub>3</sub> S <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	—	HQ	30754 603614 627033
1397	InMo <sub>3</sub> Te <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	SC	HQ	53100 603669 604497 640025
1398	TlMo <sub>3</sub> Te <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	SC	HQ	90811 603670 644485
1399	BaMo <sub>3</sub> Se <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	—	—	603615 615982
1400	NaMo <sub>3</sub> Se <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	SC	—	603625 603827 604518 643974
1401	KMo <sub>3</sub> Se <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	SC	—	603628 604517 641256
1402	RbMo <sub>3</sub> Se <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	SC	—	603629 604516 644181
1403	NaMo <sub>3</sub> Te <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	—	—	603641 604501 643979
1404	CsMo <sub>3</sub> Se <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	SC	—	603651 603826 604515
1405	KMo <sub>3</sub> Te <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	—	—	603671 604500
1406	RbMo <sub>3</sub> Te <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	—	—	603672 604499
1407	CsMo <sub>3</sub> Te <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	—	NM	—	—	603673 604498
1408	La <sub>3</sub> FeWS <sub>3</sub> O <sub>6</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	(b,s)	AFM	—	HQ	380402
1409	La <sub>3</sub> NiWS <sub>3</sub> O <sub>6</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	(b,s)	FM	—	HQ	380403
1410	La <sub>3</sub> CoWS <sub>3</sub> O <sub>6</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	Triv.	—	(b,s)	NM	—	HQ	380405
1411	La <sub>3</sub> MnWS <sub>3</sub> O <sub>6</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	(b,s)	FM	—	HQ	380406
1412	V <sub>3</sub> S <sub>4</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	(b)	NM	SC	HQ	72920 72921 72922
1413	Ti <sub>3</sub> Se <sub>4</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	(b)	NM	—	HQ	79629
1414	TlSbO <sub>3</sub>	<i>P</i> 6 <sub>3</sub> 22 (182)	Triv.	Fig. 46	(b,s)	NM	—	—	10142
1415	SiO <sub>2</sub>	<i>P</i> 6 <sub>3</sub> 22 (182)	Triv.	Fig. 46	(b,s)	NM	—	—	29343
1416	BaAl <sub>2</sub> O <sub>4</sub>	<i>P</i> 6 <sub>3</sub> 22 (182)	Triv.	—	(b,s)	NM	—	—	75427 16845 21080
1417	Ta <sub>3</sub> CrS <sub>6</sub>	<i>P</i> 6 <sub>3</sub> 22 (182)	SM	—	(b)	FM	—	—	626633
1418	RbSn( IO <sub>6</sub> )	<i>P</i> 6 <sub>3</sub> 22 (182)	Triv.	—	(b,s)	NM	—	—	73614
1419	Ba <sub>3</sub> CrS <sub>5</sub>	<i>P</i> 6 <sub>3</sub> cm (185)	SM	—	(b,s)	FM	—	HQ	97539
1420	Li <sub>2</sub> Ba(SiO <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> cm (185)	Triv.	—	(b)	NM	—	—	180289 260259
1421	C <sub>3</sub> N <sub>4</sub>	<i>P</i> 6 <sub>3</sub> cm (185)	Triv.	—	(b)	—	—	—	674271 674285
1422	Na <sub>3</sub> N	<i>P</i> 6 <sub>3</sub> cm (185)	Triv.	—	—	NM	—	—	165992 165993
1423	Li <sub>8</sub> O <sub>2</sub> (GeO <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> cm (185)	Triv.	—	(b)	NM	—	HQ	65175
1424	Li <sub>8</sub> O <sub>2</sub> (SiO <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> cm (185)	Triv.	—	(b)	NM	—	HQ	65176
1425	Mg <sub>3</sub> (Si <sub>2</sub> O <sub>5</sub> (OH) <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> cm (185)	Triv.	—	(b,s)	NM	—	—	87439 202359
1426	Sn <sub>6</sub> O <sub>4</sub> (SiO <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	(k*,b,s)	NM	—	HQ	156236
1427	Zn(OH)(N <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	—	—	—	—	196345
1428	Li <sub>2</sub> InMo <sub>3</sub> O <sub>8</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	SM	—	(b)	—	—	HQ	426618
1429	(Al <sub>2</sub> O <sub>3</sub> ) <sub>5</sub> (H <sub>2</sub> O)	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	(k*)	NM	—	—	23651
1430	Ba <sub>3</sub> (NiSb <sub>2</sub> O <sub>9</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	(k*,b,s)	AFM	—	HQ	1177
1431	Ba <sub>3</sub> Cu(Sb <sub>2</sub> O <sub>9</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	SM	Fig. 46	(k*,b,s)	FM	—	HQ	2279
1432	La <sub>4</sub> NS <sub>3</sub> Cl <sub>3</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	(b)	NM	—	HQ	74902
1433	CsCuCl <sub>3</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	SM	—	(k*,b,s)	FM	—	HQ	2064
1434	Cs(CrBr <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	SM	—	(k*,b,s)	FM	—	HQ	2590
1435	CsCrI <sub>3</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	SM	—	(k*,b,s)	—	—	HQ	8105
1436	CsCrCl <sub>3</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	SM	—	(k*,b,s)	FM	—	HQ	10206
1437	(Hg <sub>3</sub> S)(AsS <sub>3</sub> )Cl	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	(k*,b)	—	—	HQ	280329
1438	K <sub>6</sub> (HgS <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	(b)	NM	—	HQ	266 47218
1439	Na <sub>6</sub> (MnS <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	SM	—	(b)	FM	—	HQ	65447 95065 95066 642996
1440	LaNi <sub>5</sub> H <sub>7</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	(k*,b)	NM	—	—	96245 236996 236997
1441	LiBH <sub>4</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	—	NM	—	HQ	95208 (k) 186262 245569
1442	Al(PO <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	(k*,b,s)	NM	—	HQ	279582
1443	Li(BrO <sub>4</sub> )(H <sub>2</sub> O) <sub>3</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	—	NM	—	HQ	73706
1444	Li(TcO <sub>4</sub> )(H <sub>2</sub> O) <sub>3</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	—	NM	—	HQ	422191
1445	LaAuGe	<i>P</i> 6 <sub>3</sub> mc (186)	SM	—	—	NM	—	HQ	405322 656867
1446	K <sub>3</sub> TaF <sub>8</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	(k*)	NM	—	HQ	248063
1447	Mg <sub>3</sub> BeAl <sub>8</sub> O <sub>16</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	(k*,b)	NM	—	—	31227 31256
1448	MnLa <sub>4</sub> OSe <sub>6</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	SM	—	(b,s)	AFM	—	HQ	391303

1449	MnLa <sub>4</sub> OS <sub>6</sub>	<i>P</i> 6 <sub>3</sub> <i>mc</i> (186)	SM	—	(b,s)	FM	—	HQ	391305
1450	Na <sub>2</sub> (MnO <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> <i>mc</i> (186)	SM	—	—	FM	—	HQ	39504
1451	Ca <sub>2</sub> (SiO <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> <i>mc</i> (186)	Triv.	—	(k*,b)	NM	—	—	182053 182054
1452	Na(Be <sub>4</sub> SbO <sub>7</sub> )	<i>P</i> 6 <sub>3</sub> <i>mc</i> (186)	Triv.	Fig. 46	(k*,b)	NM	—	—	27599
1453	YBaZn <sub>3</sub> GaO <sub>7</sub>	<i>P</i> 6 <sub>3</sub> <i>mc</i> (186)	Triv.	—	(k*,b)	NM	—	—	252148
1454	GaN	<i>P</i> 6 <sub>3</sub> <i>mc</i> (186)	Triv.	—	—	NM	SC	—	159250 25676 34476 41481 41483 41543 42000 54698 67769 87830 153887 153888 153889 153890 153891 156259 157398 157512 181358 184926 190424 191773 634715 671112 672115 672140 672569 672724 672741 673190 673464
1455	Zn <sub>2</sub> Mo <sub>3</sub> O <sub>8</sub>	<i>P</i> 6 <sub>3</sub> <i>mc</i> (186)	Triv.	—	(b)	—	—	HQ	14321 36174 248083 260410 280130
1456	ScZn(Mo <sub>3</sub> O <sub>8</sub> )	<i>P</i> 6 <sub>3</sub> <i>mc</i> (186)	SM	—	(b)	FM	—	HQ	40534
1457	C <sub>3</sub> N <sub>4</sub>	<i>P</i> 6̄ <i>m</i> 2 (187)	Triv.	—	(k*,b)	NM	—	—	83265
1458	Ba(CoO <sub>3</sub> )	<i>P</i> 6̄ <i>m</i> 2 (187)	SM	—	(b,s)	FM	—	—	88670
1459	Ca <sub>3</sub> SiBr <sub>2</sub>	<i>P</i> 6̄ <i>m</i> 2 (187)	TI	—	—	FM	—	—	89543
1460	La <sub>2</sub> Ni <sub>2</sub> I	<i>P</i> 6̄ <i>m</i> 2 (187)	SM	—	—	NM	—	HQ	165262
1461	KCdCO <sub>3</sub> F	<i>P</i> 6̄ <i>m</i> 2 (187)	Triv.	—	—	—	—	—	239110
1462	CaKF(CO <sub>3</sub> )	<i>P</i> 6̄ <i>m</i> 2 (187)	Triv.	—	—	—	—	HQ	262230 59878 154681 154682 154683 154685
1463	LiAuC <sub>2</sub>	<i>P</i> 6̄ <i>m</i> 2 (187)	Triv.	—	—	NM	—	HQ	411253
1464	InNbS <sub>2</sub>	<i>P</i> 6̄ <i>m</i> 2 (187)	TI	—	(b)	NM	—	—	74702
1465	IrLi	<i>P</i> 6̄ <i>m</i> 2 (187)	TI	—	—	NM	—	—	104487 659856
1466	LiPd	<i>P</i> 6̄ <i>m</i> 2 (187)	SM	—	—	NM	—	—	104770 104771 659883
1467	TlTaGe <sub>3</sub> O <sub>9</sub>	<i>P</i> 6̄ <i>c</i> 2 (188)	Triv.	—	(b,s)	NM	—	—	10383
1468	LaSiO <sub>2</sub> N	<i>P</i> 6̄ <i>c</i> 2 (188)	SM	Fig. 47	(b)	NM	—	—	9752
1469	Sr(GeO <sub>3</sub> )	<i>P</i> 6̄2 <i>m</i> (189)	Triv.	Fig. 47	—	NM	—	—	28603
1470	Ag <sub>2</sub> Te(VS <sub>2</sub> ) <sub>3</sub>	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	FM	—	—	251064
1471	Ba <sub>3</sub> Nb <sub>6</sub> Si <sub>4</sub> O <sub>26</sub>	<i>P</i> 6̄2 <i>m</i> (189)	Triv.	—	(b)	NM	—	—	15934 16029
1472	Ba <sub>3</sub> Ta <sub>6</sub> Si <sub>4</sub> O <sub>26</sub>	<i>P</i> 6̄2 <i>m</i> (189)	Triv.	—	(b)	NM	—	—	15935 18317
1473	Sr <sub>3</sub> Ta <sub>6</sub> Si <sub>4</sub> O <sub>26</sub>	<i>P</i> 6̄2 <i>m</i> (189)	Triv.	—	(b)	NM	—	—	15936
1474	Rb <sub>6</sub> (Si <sub>10</sub> O <sub>23</sub> )	<i>P</i> 6̄2 <i>m</i> (189)	Triv.	—	(b,s)	NM	—	—	250379
1475	GaNiTi	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	NM	—	—	103885
1476	K <sub>3</sub> Ta <sub>3</sub> B <sub>2</sub> O <sub>12</sub>	<i>P</i> 6̄2 <i>m</i> (189)	Triv.	—	(b)	NM	—	HQ	201143
1477	K <sub>2</sub> Te <sub>2</sub>	<i>P</i> 6̄2 <i>m</i> (189)	Triv.	—	—	NM	—	HQ	73178
1478	Rb <sub>2</sub> Te <sub>2</sub>	<i>P</i> 6̄2 <i>m</i> (189)	Triv.	—	—	NM	—	HQ	73179
1479	Ti <sub>3</sub> Rh <sub>2</sub> In <sub>3</sub>	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	NM	—	HQ	410967
1480	NbMnSi	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	FM	—	—	24185
1481	NbCrGe	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	FM	—	—	42061
1482	TiCoSi	<i>P</i> 6̄2 <i>m</i> (189)	SM	Fig. 47	—	FM	—	—	42735
1483	NbMnGe	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	FM	—	—	42911 637001
1484	Al(ZrNi)	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	NM	—	—	58080 152131 186404 410399 608967 608978
1485	ScRuGe	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	NM	—	HQ	79595
1486	TiFeP	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	FM	—	HQ	290889
1487	CrTiAs	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	FM	—	—	610275
1488	FeTiAs	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	FM	—	—	610530
1489	FeNbB	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	FM	—	—	614046
1490	FeTaB	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	NM	—	—	614205
1491	GeMnTa	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	FM	—	—	637098
1492	MnTaSi	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	FM	—	—	643653
1493	NbReSi	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	NM	SC	—	645257
1494	ReSiTa	<i>P</i> 6̄2 <i>m</i> (189)	SM	—	—	NM	—	—	650119
1495	Ba <sub>3</sub> (Cr <sub>2</sub> WO <sub>9</sub> )	<i>P</i> 6̄2 <i>c</i> (190)	TI	—	(b,s)	—	—	HQ	81072
1496	K <sub>3</sub> (Nb <sub>3</sub> O <sub>6</sub> )(Si <sub>2</sub> O <sub>7</sub> )	<i>P</i> 6̄2 <i>c</i> (190)	Triv.	—	(b)	NM	—	—	79734
1497	HfCoSn	<i>P</i> 6̄2 <i>c</i> (190)	SM	—	—	NM	—	HQ	107472 408899
1498	ScPdSn	<i>P</i> 6̄2 <i>c</i> (190)	SM	—	—	NM	—	HQ	418976
1499	TaON	<i>P</i> 6/mmm (191)	SM	—	(k,b,s)	NM	—	—	20321
1500	CaRh <sub>3</sub> B <sub>2</sub>	<i>P</i> 6/mmm (191)	SM	—	(k,b)	NM	—	—	66767
1501	LaFe <sub>5</sub> H <sub>12</sub>	<i>P</i> 6/mmm (191)	SM	—	(k,b)	FM	—	—	160914
1502	RhN <sub>2</sub>	<i>P</i> 6/mmm (191)	SM	—	—	—	—	—	671729

										54245 104675 104676 104750 155045 155913 159117 161600 162124 182513 183383 189352 193881 196601 200240 242016 242017 242018 242019 242020 242026 242027 242028 242029 242030 600409 601621 602015 603845 641488 641507 641513 641518 641519 641520 641521 641522 641523 641524 641526 641529 641532 641535 641540 641542 641543 641545 641549 657601 658150 670633
1503	LaNi <sub>5</sub>	<i>P6/mmm</i> (191)	SM	Fig. 47	(k)	FM	—	HQ	54422 105462 105463 603868 647059 647075 647084 647089 647093 647101 659941 673580	
1504	YNi <sub>5</sub>	<i>P6/mmm</i> (191)	SM	Fig. 48	(k)	FM	—	—	54474 58916 619438 619442 619446 619447 619449 619452	
1505	CaNi <sub>5</sub>	<i>P6/mmm</i> (191)	SM	Fig. 47	(k)	FM	—	HQ	58672 616030	
1506	BaPd <sub>5</sub>	<i>P6/mmm</i> (191)	SM	Fig. 47	(k)	NM	—	—	102731 102732 106506 107253 1996872 196875 600442 625573 625577 625579 625587 625591 625597 625603 625616 625623 625630 625634 625642 656885 659057 659669	
1507	Co <sub>5</sub> Y	<i>P6/mmm</i> (191)	SM	—	(k)	FM	—	—	103699 107256 184905	
1508	Fe <sub>5</sub> Y	<i>P6/mmm</i> (191)	SM	—	(k)	FM	—	—	105336 646468	
1509	Ni <sub>5</sub> Sc	<i>P6/mmm</i> (191)	SM	Fig. 48	(k)	FM	—	—	105707 648964	
1510	Pd <sub>5</sub> Sr	<i>P6/mmm</i> (191)	TI	Fig. 47	(k)	NM	—	—	106357 673956	
1511	CaPd <sub>5</sub>	<i>P6/mmm</i> (191)	TI	Fig. 47	(k)	NM	—	—	183385	
1512	LaNi <sub>3</sub> Rh <sub>2</sub>	<i>P6/mmm</i> (191)	SM	—	(k)	FM	—	—	53459 631998 632006 632016 632022	
1513	FeGe	<i>P6/mmm</i> (191)	SM	—	(k)	FM	—	—	55564 102671 151390 161110 161113 161115 161116 161117 161118 625264 670158	
1514	CoSn	<i>P6/mmm</i> (191)	SM	—	(k)	NM	—	HQ	59435 161111 161114 161123 161124 161125 161126 185625 640117	
1515	InNi	<i>P6/mmm</i> (191)	SM	Fig. 48	(k)	NM	—	—	103634 103635 152339 161109 161112 161119 161120 161121 161122 633740 633747	
1516	FeSn	<i>P6/mmm</i> (191)	SM	—	(k)	FM	—	—	105819	
1517	PtTl	<i>P6/mmm</i> (191)	SM	—	(k)	NM	—	—	626107	
1518	ScCr <sub>6</sub> Ge <sub>6</sub>	<i>P6/mmm</i> (191)	SM	—	(k)	FM	—	—	658018	
1519	YCr <sub>6</sub> Ge <sub>6</sub>	<i>P6/mmm</i> (191)	SM	Fig. 48	(k)	NM	—	—	92308	
1520	Li <sub>2</sub> NaN	<i>P6/mmm</i> (191)	SM	—	—	NM	—	—	92310	
1521	LiNa <sub>2</sub> N	<i>P6/mmm</i> (191)	SM	—	—	NM	—	—	165989	
1522	Na <sub>3</sub> N	<i>P6/mmm</i> (191)	SM	—	—	NM	—	—	182352	
1523	Ta <sub>2</sub> N <sub>3</sub> O	<i>P6/mmm</i> (191)	SM	—	(k,b)	FM	—	—	182353	
1524	Ta <sub>2</sub> N <sub>3</sub> F	<i>P6/mmm</i> (191)	TI	—	(k,b)	NM	—	—	168592	
1525	La <sub>6</sub> Mn <sub>2</sub> S <sub>10</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	(b)	FM	—	—	33796	
1526	Ca <sub>6</sub> FeN <sub>5</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	(b,s)	FM	—	HQ	80184	
1527	Ca <sub>6</sub> (MnN <sub>3</sub> )N <sub>2</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	(b,s)	FM	—	HQ	50725	
1528	La <sub>5</sub> Sb <sub>3</sub> Br	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	NM	—	HQ	95238	
1529	La <sub>5</sub> Sn <sub>3</sub> Cl	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	NM	—	HQ	95239	
1530	La <sub>5</sub> Sn <sub>3</sub> Br	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	NM	—	HQ	95241	
1531	La <sub>5</sub> Bi <sub>3</sub> Br	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	NM	—	HQ	44361 636545	
1532	La <sub>5</sub> Pb <sub>3</sub> I	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	FM	—	HQ	23932 602016 651814	
1533	Sc <sub>5</sub> Si <sub>3</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	NM	—	—	56028 637960	
1534	Hf <sub>5</sub> Ge <sub>3</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	TI	—	—	NM	—	—	62591 168415 652424 671881	
1535	Ta <sub>5</sub> Ge <sub>3</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	NM	—	—	104273 183487 638947	
1536	Ti <sub>5</sub> Si <sub>3</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	TI	—	—	NM	SC	—	109292 169008 652783 652785 670883	
1537	Ta <sub>5</sub> Si <sub>3</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	NM	—	—	76159 652324 652335	
1538	Hf <sub>5</sub> Sn <sub>3</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	NM	—	—	652605 652612 652616 652621 656924	
1539	Ti <sub>5</sub> Sn <sub>3</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	TI	—	—	NM	—	—	99999	
1540	Ca <sub>5</sub> Sb <sub>3</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	NM	—	HQ	173026 619563	
1541	Hf <sub>5</sub> Ge <sub>3</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	NM	—	—	636541	
1542	Ti <sub>5</sub> Si <sub>3</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	NM	—	—	652420	
1543	Zr <sub>5</sub> Si <sub>3</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	SM	—	—	NM	SC	—	109145	
1544	K <sub>3</sub> N	<i>P6<sub>3</sub>/mcm</i> (193)	TI	Fig. 48	(b,s)	NM	—	—	—	
1545	NbI <sub>3</sub>	<i>P6<sub>3</sub>/mcm</i> (193)	SM	Fig. 48	—	FM	—	—	—	

1546	SiO <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(k,b,s)	NM	—	—	170481 170496 38126 40902 40903 44270 162623 162624 200478
1547	LiFeAs	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	FM	—	—	187133
1548	KV <sub>3</sub> Ge <sub>2</sub> O <sub>9</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(k,b,s)	FM	—	HQ	187490
1549	ZnO	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	—	—	—	670354 670355
1550	SnNi <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k)	—	—	—	670879 105357 150926 411928 646749 646751
1551	Cr <sub>2</sub> AlC	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(b)	NM	SC	—	42918 606181
1552	Sc <sub>2</sub> AlC	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(b)	NM	—	—	160378
1553	Sc <sub>2</sub> InC	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(b)	NM	—	—	160380 163503 163510 163511
1554	Ti <sub>2</sub> SnC	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	TI	—	(b)	NM	—	—	161063 161064 252840 618806
1555	Ba <sub>5</sub> IrIn <sub>2</sub> Al <sub>2</sub> O <sub>13</sub> Cl	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(k*,b,s)	FM	—	—	71602
1556	RbNiF <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	FM	—	—	15090 22127 91834
1557	Rb(ZnF <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(k*,b,s)	NM	—	—	41618 91835 91836
1558	K <sub>3</sub> Na(Re <sub>2</sub> O <sub>9</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(b,s)	NM	—	—	73300
1559	K <sub>3</sub> La(Te <sub>2</sub> O <sub>9</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(k*,b,s)	—	—	HQ	195647
1560	Ba <sub>3</sub> Sb <sub>2</sub> NiO <sub>9</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	AFM	—	—	200299
1561	Rb <sub>6</sub> Ni <sub>6</sub> F <sub>18</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	Fig. 48	(k*,b,s)	FM	—	—	410390 410391
1562	Ba(MnO <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(k,b,s)	AFM	—	—	23874
1563	BaNiO <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	175(b,s) 30661(k)
1564	BaCoO <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	FM	—	—	922(b,s) 26586(k) 173504(b,s)
1565	Cs(MnBr <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	FM	—	—	2782 9703
1566	BaVS <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	Fig. 48	(k*)	FM	SC	—	8193 8194 15537 23194 62711 154181 616097 616098
1567	Rb(MnBr <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	FM	—	—	9704(b,s) 14077
1568	CsMnI <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	FM	—	—	10042 15949 15950 15951 15952
1569	BaMnO <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(b,s)	AFM	—	—	10331(k) 10332
1570	CsScCl <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	NM	—	—	10474
1571	Ba(VSe <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	Fig. 49	(k*)	FM	—	—	10486
1572	RbNiCl <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	FM	—	—	15010
1573	RbNiBr <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	FM	—	—	15011
1574	CsVCl <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	FM	—	—	15932 201828 201832
1575	BaTaS <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	NM	—	—	16083 616077 659541
1576	CsVI <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	FM	—	—	26453 26454
1577	CsCoCl <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	FM	—	—	27511
1578	CsCrCl <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	TI	—	(k*)	FM	—	—	36132
1579	CsTiBr <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	FM	—	—	41320 400053
1580	Rb(TiCl <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	FM	—	—	49747
1581	Cs(TiCl <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	FM	—	—	49748
1582	CsNiCl <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	FM	—	—	59371 60262 423828
1583	Rb(CuCl <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	FM	—	—	84212
1584	Rb(TiBr <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	FM	—	HQ	154257
1585	Cs(TiI <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	FM	—	HQ	154258
1586	LaCrGe <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	FM	—	HQ	158976 290669 290670 290671 290672
1587	CsFeBr <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(k*)	FM	—	—	174041
1588	CsVBr <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	FM	—	—	201829 201833
1589	RbVCl <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	FM	—	—	201830 201834
1590	RbVBr <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	FM	—	—	201831
1591	Cs(FeCl <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(k*,b,s)	NM	—	—	300249
1592	CsNiBr <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	FM	—	HQ	423829
1593	CsNiI <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*,b,s)	—	—	HQ	423830
1594	BaTaSe <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	NM	SC*	—	616129 659547
1595	BaNbS <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	NM	SC	—	659538
1596	Y(MnO <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	TI	—	(b)	FM	—	—	73361 182284 422982 422990
1597	Cs <sub>3</sub> Ru <sub>2</sub> Cl <sub>9</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(k*)	NM	—	—	201057
1598	Cs <sub>3</sub> (Nb <sub>2</sub> I <sub>9</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(k*)	FM	—	HQ	421295
1599	CuAlO <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	31368 60845 95661
1600	CuScO <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	Fig. 49	—	NM	—	—	60847 95667 151929 670128
1601	AgAlO <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	95662 300020
1602	CuGaO <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	95664
1603	AgGaO <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	95665

1604	AgScO <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	95668 670073
1605	CuInO <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	95670 186620
1606	AuInO <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	95672
1607	AgYO <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	95674 670075
1608	AuYO <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	95675 670100
1609	Ni	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	FM	—	—	76668 671412
1610	NiMnGe	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	Fig. 49	—	FM	—	—	41921 637011 637019 637029
1611	AlAuTi	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	FM	—	—	57506
1612	InNi <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	NM	—	—	59436 59437 185624 640098 640107 670969
1613	CoNiSn	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	Fig. 49	—	FM	—	—	102582 196627
1614	Co <sub>2</sub> Sn	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	TI	—	—	FM	—	—	102673 625262
1615	CoFeGe	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	—	—	—	196628
1616	Co <sub>2</sub> Ge	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	TI	—	—	FM	—	—	623418 623430
1617	GaNi <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	NM	—	—	634869 670968
1618	Ni <sub>1</sub> Sb <sub>1</sub> V <sub>1</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	—	—	—	671080 671081
1619	K <sub>5</sub> (AuAs <sub>2</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(b)	NM	—	—	40698
1620	K <sub>5</sub> (AuP <sub>2</sub> )	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(b)	NM	—	—	40700
1621	Co <sub>2</sub> Ge	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	FM	—	—	108289
1622	LaI	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	TI	—	—	NM	—	—	83678 171451
1623	Co <sub>3</sub> Nb <sub>2</sub> Si	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	NM	—	—	53018
1624	ZrAl <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	TI	—	(k*)	NM	—	—	55594 191009 603593 609703 609713 609721 609743
1625	ZrAl <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	TI	—	(k*)	NM	SC	—	150527
1626	Na <sub>2</sub> Cs	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	NM	—	—	246932 627052
1627	Ni <sub>3</sub> Sc <sub>2</sub> Si	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	—	—	—	646484
1628	TiNb <sub>4</sub> S <sub>8</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(b)	NM	—	—	645332
1629	VNb <sub>4</sub> S <sub>8</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(b)	FM	—	—	645339
1630	K <sub>3</sub> P	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	25550
1631	K <sub>3</sub> Bi	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	NM	—	—	26885
1632	K <sub>3</sub> Sb	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	26886 656327
1633	Rb <sub>3</sub> Sb	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	—	NM	—	—	77991 650044
1634	Na <sub>2</sub> MgPb	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	NM	—	HQ	238202
1635	Na <sub>2</sub> MgSn	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	NM	—	HQ	262676
1636	BiRb <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	NM	—	—	616995 616997
1637	Na <sub>2</sub> O(Al <sub>2</sub> O <sub>3</sub> ) <sub>11</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	Triv.	—	(b)	NM	—	—	15970 16933 606335
1638	AlTi <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	NM	—	—	58188 99779 181338 609523 609538
1639	Co <sub>3</sub> Mo	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	Fig. 49	(k*)	FM	—	—	102542 624214 624216 671172
1640	Co <sub>3</sub> W	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	Fig. 49	(k*)	FM	—	—	102722 187993 625553 671174
1641	GaTi <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	NM	SC	—	103991 182429 635554
1642	Ni <sub>3</sub> In	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	Fig. 49	(k*)	FM	—	—	151196 185623 185627 640100
1643	Co <sub>3</sub> Ta	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	NM	—	—	187991 671178
1644	La <sub>3</sub> Al	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	NM	—	—	603210 608280
1645	Ti <sub>3</sub> In	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	NM	—	—	640656
1646	Co <sub>3</sub> Nb	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	(k*)	—	—	—	671176
1647	FeSe	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	FM	—	—	29308 53541 53542 166442 166443 166444 169252 169254 169256 169258 169261 169262 169264 169261 169268 169270 169272 169284 169286 169288 169290 169292 169294 169296 169298 169300 169302 169307 290407 290410 633482 633490
1648	FeSb	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	Fig. 49	—	FM	SC	—	53535 53971 633396
1649	MnSb	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	TI	—	—	FM	SC	—	53970 54266 76212 76258 76620 163322 191176 191783 601839 603577 643511 643513 643514 643515 643517 643519 643522 643523 643527 643529 643530 643532 643533 643535
1650	BiMn	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	SM	—	—	FM	SC	—	58805 192873 192874 192875 192876 192877 192878 192879 192880 192881 616808 616811 616812 672818
1651	CoSb	<i>P</i> 6 <sub>3</sub> / <i>mmc</i> (194)	TI	—	—	NM	SC	—	76118 169166 169167 169168 169169 189946 624893 624900 624901 624909 657491

1652	IrSn	$P6_3/mmc$ (194)	SM	—	—	NM	—	—	104561 641051
1653	$Sr_3P(BO_3)$	$P6_3/mmc$ (194)	Triv.	—	—	NM	—	—	401207
1654	AgBaBi	$P6_3/mmc$ (194)	SM	—	—	NM	—	—	56978
1655	BaBiCu	$P6_3/mmc$ (194)	SM	—	—	NM	—	—	106303
1656	LaPdSb	$P6_3/mmc$ (194)	SM	—	—	NM	—	—	641676
1657	InO(OH)	$P2_13$ (198)	Triv.	—	—	NM	—	—	166255 166256
1658	$Hg_3(AsO_4)Cl$	$P2_13$ (198)	Triv.	—	(b)	NM	—	—	89687 92963 411757
1659	$Na_3(AsS_3)$	$P2_13$ (198)	Triv.	—	—	NM	—	HQ	645 1036
1660	$K_3(SbO_3)$	$P2_13$ (198)	Triv.	—	(b)	NM	—	HQ	279579
1661	$Cs_3(SbO_3)$	$P2_13$ (198)	Triv.	—	(b)	NM	—	HQ	279580
1662	$Cs_3(BiO_3)$	$P2_13$ (198)	Triv.	—	—	NM	—	HQ	406563
1663	$Rb_3(BiO_3)$	$P2_13$ (198)	Triv.	—	(b)	NM	—	HQ	407294
1664	$Cs_3SbS_3$	$P2_13$ (198)	Triv.	—	—	NM	—	HQ	426551
1665	$K_3SbS_3$	$P2_13$ (198)	Triv.	—	—	NM	—	HQ	426552 641323
1666	$Rb_3SbS_3$	$P2_13$ (198)	Triv.	—	(b)	NM	—	HQ	426554
1667	$Na(ClO_3)$	$P2_13$ (198)	SM	—	—	NM	—	—	31056
1668	$SiO_2$	$P2_13$ (198)	Triv.	—	(b,s)	NM	—	—	24587 44269 162616 162617
1669	$Tl_2Pb(Cu(NO_2)_6)$	$Fm\bar{3}$ (202)	SM	—	—	NM	—	HQ	16
1670	$K_2Sr(Ni(NO_2)_6)$	$Fm\bar{3}$ (202)	SM	—	—	AFM	—	HQ	179
1671	$CaCu_3Ru_4O_{12}$	$Im\bar{3}$ (204)	SM	—	(k,b)	FM	—	HQ	51894 95715 183110
1672	$LaCu_3Ir_4O_{12}$	$Im\bar{3}$ (204)	SM	—	(k,b)	—	—	HQ	251657
1673	$CoN_3$	$Im\bar{3}$ (204)	TI	—	—	NM	—	—	162105
1674	$CoN_3$	$Im\bar{3}$ (204)	SM	—	—	NM	—	—	162106
1675	$RhN_3$	$Im\bar{3}$ (204)	Triv.	—	—	NM	—	—	162107
1676	$RhN_3$	$Im\bar{3}$ (204)	SM	—	—	NM	—	—	162108
1677	$Ge(SeO_3)_2$	$Pa\bar{3}$ (205)	Triv.	—	(b,s)	NM	—	—	422884
1678	$MgSe_2$	$Pa\bar{3}$ (205)	Triv.	—	—	NM	—	—	642815
1679	$Ca(NO_3)_2$	$Pa\bar{3}$ (205)	Triv.	—	—	NM	—	—	52351 56089
1680	$Sn(SeO_3)_2$	$Pa\bar{3}$ (205)	Triv.	—	(b)	NM	—	—	154716
1681	$Si(P_2O_7)$	$Pa\bar{3}$ (205)	Triv.	—	(b,s)	NM	—	—	19047
1682	$SiO_2$	$Ia\bar{3}$ (206)	Triv.	—	(b,s)	NM	—	—	170545
1683	$SiO_2$	$F4_132$ (210)	SM	—	(b,s)	NM	—	—	170504
1684	$SiO_2$	$I4_32$ (211)	SM	—	(b,s)	NM	—	—	170506
1685	$Na(BH_4)$	$P\bar{4}3m$ (215)	Triv.	—	—	NM	—	—	182734
1686	$Cs_4(CO_4)$	$P\bar{4}3m$ (215)	Triv.	—	—	NM	—	—	245445
1687	$Cd(CN)_2$	$P\bar{4}3m$ (215)	Triv.	—	—	NM	—	—	20748 66938
1688	$Zn(CN)_2$	$P\bar{4}3m$ (215)	Triv.	—	—	NM	—	—	22392 670038
1689	$Be_4O(TeO_6)$	$F\bar{4}3m$ (216)	Triv.	—	(k*,p*,b)	NM	—	HQ	1322
1690	$CsLi(MoO_4)$	$F\bar{4}3m$ (216)	Triv.	Fig. 50	(k*,p*,b,s)	NM	—	HQ	20805
1691	$IrIn_7GeO_8$	$F\bar{4}3m$ (216)	Triv.	—	(k*,b)	NM	—	—	417829
1692	$Ni_5Zr$	$F\bar{4}3m$ (216)	SM	Fig. 50	(k*)	FM	—	—	54985 150648 150939 189201 647156
1693	$Ni_4ZnZr$	$F\bar{4}3m$ (216)	SM	Fig. 50	(k*,p*)	NM	—	—	105477
1694	$MgYNi_4$	$F\bar{4}3m$ (216)	SM	Fig. 51	(k*,p*)	NM	—	—	107033 107424 183095 191556
1695	$CaMgNi_4$	$F\bar{4}3m$ (216)	TI	Fig. 50	(k*,p*)	FM	—	—	107419
1696	$LaMgNi_4$	$F\bar{4}3m$ (216)	SM	Fig. 51	(k*,p*)	FM	—	—	107420 162119 184164 242011 242012 242013 242014 242015 242021 242022 242023 242024 242025
1697	$ScNi_4Cd$	$F\bar{4}3m$ (216)	SM	Fig. 51	(k*,p*)	NM	—	—	185106
1698	$YNi_4Cd$	$F\bar{4}3m$ (216)	SM	Fig. 51	(k*,p*)	—	—	HQ	423939
1699	$ZrNi_5$	$F\bar{4}3m$ (216)	TI	Fig. 50	(k*)	FM	—	—	601018
1700	$ScAuNi_4$	$F\bar{4}3m$ (216)	TI	Fig. 50	(k*,p*)	NM	—	—	612227
1701	$YAuNi_4$	$F\bar{4}3m$ (216)	TI	Fig. 50	(k*,p*)	—	—	—	612233
1702	$Be_5Fe$	$F\bar{4}3m$ (216)	SM	—	(k*)	FM	—	—	616267
1703	$YNi_4Mn$	$F\bar{4}3m$ (216)	SM	—	(k*,p*)	FM	—	—	643173
1704	$HfNi_5$	$F\bar{4}3m$ (216)	SM	Fig. 50	(k*)	—	—	—	672665
1705	$CsMn(Cr(CN)_6)$	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	56602
1706	$Li_2IrGa$	$F\bar{4}3m$ (216)	TI	—	—	NM	—	—	107085
1707	$Li_2IrIn$	$F\bar{4}3m$ (216)	TI	—	—	NM	—	—	107089
1708	$Mn_2CoIn$	$F\bar{4}3m$ (216)	Triv.	—	—	FM	—	—	160705
1709	$Mn_2CoSi$	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	160706

1710	Mn <sub>2</sub> CoGe	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	160707
1711	Mn <sub>2</sub> CoSn	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	160708 183043
1712	Mn <sub>2</sub> CoSb	$F\bar{4}3m$ (216)	Triv.	—	—	FM	—	—	160709
1713	RuMn <sub>2</sub> Sn	$F\bar{4}3m$ (216)	TI	—	—	FM	—	—	182829
1714	RuMn <sub>2</sub> Si	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	182830
1715	Ti <sub>2</sub> CoIn	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	185664
1716	Ti <sub>2</sub> ZnAl	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	185882
1717	CoFeMnGa	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	186830
1718	CoFeMnGe	$F\bar{4}3m$ (216)	Triv.	—	—	FM	—	—	186831
1719	Mn <sub>2</sub> CoAs	$F\bar{4}3m$ (216)	SM	Fig. 51	—	FM	—	—	191648
1720	CoFeTiAl	$F\bar{4}3m$ (216)	Triv.	Fig. 52	—	NM	—	—	191657 673236
1721	CoFeTiGa	$F\bar{4}3m$ (216)	SM	Fig. 51	—	NM	—	—	191658
1722	CoFeTiSi	$F\bar{4}3m$ (216)	SM	Fig. 51	—	FM	—	—	191659
1723	CoFeTiGe	$F\bar{4}3m$ (216)	SM	Fig. 52	—	FM	—	—	191660
1724	CoFeTiAs	$F\bar{4}3m$ (216)	SM	Fig. 52	—	FM	—	—	191661
1725	CoFeTiSb	$F\bar{4}3m$ (216)	SM	Fig. 52	—	FM	—	—	191662
1726	CoFeV <sub>2</sub> Ga	$F\bar{4}3m$ (216)	SM	Fig. 52	—	FM	—	—	191664
1727	CoFeVAs	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	191667
1728	CoFeVSb	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	191668
1729	CoRhMnAl	$F\bar{4}3m$ (216)	TI	—	—	—	—	—	670591
1730	CoRhMnGa	$F\bar{4}3m$ (216)	TI	—	—	—	—	—	670592
1731	CoRhMnGe	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	670593
1732	CoRhMnSi	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	670594
1733	CoFeSiZr	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	670706
1734	CoFeGeZr	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	670707
1735	CrVScSi	$F\bar{4}3m$ (216)	Triv.	—	—	—	—	—	670792
1736	Zr <sub>2</sub> CoAl	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	671654
1737	Fe <sub>2</sub> MnGe	$F\bar{4}3m$ (216)	SM	Fig. 52	—	—	—	—	671982
1738	Fe <sub>2</sub> MnAl	$F\bar{4}3m$ (216)	TI	Fig. 51	—	—	—	—	672261
1739	CoRuFeSi	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	672893 672894 672895
1740	CoRuFeGe	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	672896 672897 672898
1741	CoRuFeSn	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	672899 672900 672901
1742	Co <sub>2</sub> MnSi	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	672941 672942 675078
1743	VCoHfGa	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	674822
1744	Co <sub>2</sub> MnAl	$F\bar{4}3m$ (216)	Triv.	—	—	—	—	—	675066
1745	Co <sub>2</sub> MnGa	$F\bar{4}3m$ (216)	Triv.	—	—	—	—	—	675070
1746	Co <sub>2</sub> MnGe	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	675074
1747	CoMnCrSb	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	675083 675084 675085 675086 675087 675088
1748	GaMo <sub>4</sub> S <sub>8</sub>	$F\bar{4}3m$ (216)	SM	—	—	FM	—	HQ	33994 <sup>(b)</sup> 41935 <sup>(b)</sup> 49566 <sup>(b)</sup> 158198 <sup>(b)</sup> 634707
1749	Ge <sub>4</sub> Se <sub>8</sub>	$F\bar{4}3m$ (216)	Triv.	—	—	FM	—	HQ	50503 <sup>(b)</sup> 195256
1750	GaV <sub>4</sub> S <sub>8</sub>	$F\bar{4}3m$ (216)	SM	—	(b)	FM	—	HQ	89980 158194 603133
1751	Al(V <sub>4</sub> S <sub>8</sub> )	$F\bar{4}3m$ (216)	SM	—	(b)	FM	—	HQ	195251
1752	PdMnTe	$F\bar{4}3m$ (216)	SM	—	—	FM	—	HQ	40908 44996
1753	CuMnSb	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	42978 53311 76251 628385 628386 628393
1754	LiZnP	$F\bar{4}3m$ (216)	Triv.	—	—	NM	—	—	44824 642242 670561
1755	AuMnSb	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	52673 612166 612167 612171
1756	CdLiP	$F\bar{4}3m$ (216)	Triv.	—	—	NM	—	—	52813 670566
1757	CoMnSb	$F\bar{4}3m$ (216)	SM	Fig. 52	—	FM	—	—	53001 624126 624133
1758	CoVSb	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	53071 107117 624925
1759	NiMnSb	$F\bar{4}3m$ (216)	SM	Fig. 52	—	FM	—	—	54255 76078 182485 643105 643108 643111 643121
1760	RhMnSb	$F\bar{4}3m$ (216)	SM	Fig. 53	—	FM	—	—	54343 76199 76201 643415
1761	AuMnSn	$F\bar{4}3m$ (216)	SM	—	—	FM	—	HQ	54465 240860
1762	CoNbSn	$F\bar{4}3m$ (216)	Triv.	Fig. 53	—	FM	—	—	102552 102553
1763	IrMnSn	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	104498
1764	MnPtSn	$F\bar{4}3m$ (216)	SM	Fig. 53	—	FM	—	—	104955 104956 643383 643387
1765	CoHfSb	$F\bar{4}3m$ (216)	Triv.	—	—	NM	—	—	108294
1766	GaMnPt	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	108482
1767	NiCrSb	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	182484
1768	RbCsN	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	191639

1769	RbCsP	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	191640
1770	RbCsAs	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	191641
1771	FeVTe	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	191683
1772	CoCrTe	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	191684
1773	LiMnAs	$F\bar{4}3m$ (216)	SM	—	—	FM	—	HQ	192816
1774	LiCdAs	$F\bar{4}3m$ (216)	SM	—	—	NM	—	—	609965 609966 670567
1775	MnNiSb	$F\bar{4}3m$ (216)	Triv.	—	—	FM	—	—	643109 643120
1776	MnPtSb	$F\bar{4}3m$ (216)	Triv.	—	—	FM	—	—	643377
1777	PtMnBi	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	671364 671368 671372
1778	PtFeBi	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	671365 671369 671373
1779	PtCoBi	$F\bar{4}3m$ (216)	Triv.	—	—	—	—	—	671366 671374
1780	PtCoBi	$F\bar{4}3m$ (216)	TI	—	—	—	—	—	671370
1781	MnTiTe	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	671981
1782	LiCaC	$F\bar{4}3m$ (216)	SM	Fig. 53	—	—	—	—	672030
1783	NaCaC	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	672032
1784	PtCoSb	$F\bar{4}3m$ (216)	Triv.	—	—	—	—	—	672160
1785	PtCrSb	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	672161
1786	PtMnSb	$F\bar{4}3m$ (216)	TI	—	—	—	—	—	672162
1787	CrTiGe	$F\bar{4}3m$ (216)	Triv.	—	—	—	—	—	675079
1788	CrTiSi	$F\bar{4}3m$ (216)	Triv.	—	—	—	—	—	675081
1789	Mn <sub>2</sub> Te	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	675105
1790	Li <sub>6</sub> PO <sub>5</sub> Cl	$F\bar{4}3m$ (216)	Triv.	—	(k*,b)	NM	—	HQ	421479
1791	Li <sub>6</sub> PO <sub>5</sub> Br	$F\bar{4}3m$ (216)	Triv.	—	(k*,b)	NM	—	HQ	421480 421481
1792	MnSe	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	24252 41526 670505 671667
1793	FeN	$F\bar{4}3m$ (216)	SM	—	—	NM	—	—	41258 184376 236789 236790 670506
1794	MnS	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	76205 670482
1795	CoN	$F\bar{4}3m$ (216)	SM	—	—	NM	—	—	79936 161754 184378 236791 236792 670475
1796	YN	$F\bar{4}3m$ (216)	Triv.	—	—	NM	—	—	161077 183180 190624 670502
1797	CaSe	$F\bar{4}3m$ (216)	Triv.	—	—	NM	—	—	167834 670485
1798	ScC	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	169407 189086 670497
1799	CrTe	$F\bar{4}3m$ (216)	TI	—	—	FM	—	—	169766 181056 670501 671345
1800	MnTe	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	181324
1801	YC	$F\bar{4}3m$ (216)	SM	—	—	NM	—	—	183160
1802	ZrC	$F\bar{4}3m$ (216)	Triv.	—	—	NM	—	—	183162
1803	MnAs	$F\bar{4}3m$ (216)	Triv.	—	—	FM	—	—	184925 191787
1804	MnSn	$F\bar{4}3m$ (216)	SM	Fig. 53	—	FM	—	—	191171
1805	MnSb	$F\bar{4}3m$ (216)	Triv.	—	—	FM	—	—	191175 191786
1806	RbSb	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	191491
1807	RbTe	$F\bar{4}3m$ (216)	SM	—	—	FM	—	—	191493
1808	MnP	$F\bar{4}3m$ (216)	Triv.	—	—	FM	—	—	191788
1809	ScN	$F\bar{4}3m$ (216)	Triv.	—	—	NM	—	—	236779 236780
1810	CaO	$F\bar{4}3m$ (216)	Triv.	—	—	—	—	—	670280
1811	SrO	$F\bar{4}3m$ (216)	Triv.	—	—	—	—	—	670287
1812	CrSe	$F\bar{4}3m$ (216)	TI	—	—	—	—	—	671343
1813	CaN	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	672205 672206
1814	TiBi	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	674898
1815	KSe	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	675036
1816	KTe	$F\bar{4}3m$ (216)	SM	—	—	—	—	—	675040
1817	GaMo <sub>4</sub> CS <sub>8</sub>	$F\bar{4}3m$ (216)	SM	Fig. 53	(b,s)	NM	—	—	76848
1818	MgV <sub>2</sub> O <sub>4</sub>	$F\bar{4}3m$ (216)	SM	Fig. 53	(k*,p*,b)	—	—	—	674693
1819	Cu <sub>2</sub> Al <sub>4</sub> O <sub>7</sub>	$F\bar{4}3m$ (216)	SM	Fig. 53	(k*,p*,b)	FM	—	—	100355
1820	SiO <sub>2</sub>	$I\bar{4}3m$ (217)	Triv.	Fig. 54	(b,s)	NM	—	HQ	183701
1821	Ni <sub>3</sub> Sb <sub>4</sub> O <sub>6</sub> F <sub>6</sub>	$I\bar{4}3m$ (217)	TI	—	(k,b)	FM	—	HQ	427047 427048
1822	Ca <sub>3</sub> Ir <sub>4</sub> Ge <sub>4</sub>	$I\bar{4}3m$ (217)	SM	—	(k)	NM	SC	HQ	195500 429727
1823	Sr <sub>3</sub> Ir <sub>4</sub> Sn <sub>4</sub>	$I\bar{4}3m$ (217)	SM	—	(k)	NM	—	HQ	410992
1824	Sr <sub>3</sub> Ir <sub>4</sub> Ge <sub>4</sub>	$I\bar{4}3m$ (217)	SM	—	(k)	—	—	HQ	429725
1825	Na <sub>3</sub> BiO <sub>3</sub>	$I\bar{4}3m$ (217)	Triv.	—	(b)	NM	—	—	23347
1826	Zn <sub>4</sub> O(BO <sub>2</sub> ) <sub>6</sub>	$I\bar{4}3m$ (217)	Triv.	—	(b)	NM	—	—	15800 <sup>(s)</sup> 16826 27357 34085 <sup>(s)</sup> 100290 <sup>(s)</sup> 261810 <sup>(s)</sup>
1827	Mg <sub>4</sub> P <sub>6</sub> (SN <sub>12</sub> )	$I\bar{4}3m$ (217)	Triv.	—	(b)	NM	—	HQ	65838 <sup>(s)</sup> 642665

1828	Cd <sub>4</sub> P <sub>6</sub> N <sub>12</sub> S	<i>I</i> 43 <i>m</i> (217)	Triv.	—	(b,s)	NM	—	HQ	71019
1829	Zn <sub>8</sub> (P <sub>12</sub> N <sub>24</sub> )O <sub>2</sub>	<i>I</i> 43 <i>m</i> (217)	Triv.	—	(b)	NM	—	—	417324
1830	Na <sub>8</sub> (Al <sub>6</sub> Si <sub>6</sub> O <sub>24</sub> )Cl <sub>2</sub>	<i>P</i> 43 <i>n</i> (218)	Triv.	—	(b,s)	NM	—	—	15336 29443 30263 40129 41188 41189 41190 68426 71432 83323 83324 83325 83326 98807 98808 98809 98810 98811 98812 98813 98814 98815 98816 98817 98818 98819 98820 162491 166827 402574 417689 673830
1831	Na <sub>8</sub> (Al <sub>6</sub> Si <sub>6</sub> O <sub>24</sub> )	<i>P</i> 43 <i>n</i> (218)	SM	—	(b,s)	NM	—	—	56710
1832	Na <sub>4</sub> Cl(Al <sub>3</sub> Si <sub>3</sub> O <sub>12</sub> )	<i>P</i> 43 <i>n</i> (218)	Triv.	—	(b,s)	NM	—	—	65004 74537
1833	Cd <sub>8</sub> (BeSiO <sub>4</sub> ) <sub>6</sub> S <sub>2</sub>	<i>P</i> 43 <i>n</i> (218)	Triv.	—	(b,s)	NM	—	—	81485
1834	K <sub>8</sub> (AlSiO <sub>4</sub> ) <sub>6</sub>	<i>P</i> 43 <i>n</i> (218)	SM	—	(b,s)	NM	—	—	237001
1835	Si <sub>3</sub> N <sub>4</sub>	<i>I</i> 43 <i>d</i> (220)	Triv.	—	(b)	NM	—	—	97567
1836	Ge <sub>3</sub> N <sub>4</sub>	<i>I</i> 43 <i>d</i> (220)	Triv.	—	(b)	NM	—	—	97569
1837	PbPd <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 54	(k)	NM	SC	—	42600 648357
1838	Ni <sub>3</sub> Ge	<i>Pm</i> 3 <i>m</i> (221)	TI	Fig. 54	(k)	NM	—	—	53745 104162 600112 637356 637358 637362 637364
1839	AlNi <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 54	(k)	FM	—	—	58038 58039 105529 151385 185893 187989 196567 196568 604410 608781 608782 608790 608797 608799 608811 608814 671563 671564 672104 672243 673108
1840	InNi <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 54	(k)	FM	—	—	59438 59439
1841	Ni <sub>3</sub> Si	<i>Pm</i> 3 <i>m</i> (221)	TI	Fig. 54	(k)	NM	—	—	76413 77960 105343 105344 163353 600224 646572 646573 646579 646584
1842	Co <sub>3</sub> Ti	<i>Pm</i> 3 <i>m</i> (221)	SM	—	(k)	FM	—	—	97992 97993 102708 187964 187984 625462 625468 625481 625484
1843	Co <sub>3</sub> Ta	<i>Pm</i> 3 <i>m</i> (221)	SM	—	(k)	FM	—	—	102689 187967 187985
1844	FePd <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	—	(k)	FM	—	—	103582 103583 181720 633132 633134 633135 633140 633141 675019
1845	GaNi <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 55	(k)	FM	—	—	103856 103857 634857 634864
1846	MnNi <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	—	(k)	FM	—	—	104920
1847	MnZn <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 55	(k)	FM	—	—	105020
1848	Ni <sub>3</sub> Sn	<i>Pm</i> 3 <i>m</i> (221)	TI	Fig. 54	(k)	NM	—	—	105353 671094
1849	Pd <sub>3</sub> Sc	<i>Pm</i> 3 <i>m</i> (221)	SM	—	(k)	NM	—	—	105673 105674 648807 659956
1850	Pd <sub>3</sub> Sn	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 55	(k)	NM	—	—	105689 105690 648912 648916 648921 672133
1851	Pd <sub>3</sub> Ti	<i>Pm</i> 3 <i>m</i> (221)	SM	—	(k)	NM	—	—	105724 167655 185637
1852	GeNb <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	—	(k)	NM	—	—	108521 672135
1853	Nb <sub>3</sub> Si	<i>Pm</i> 3 <i>m</i> (221)	SM	—	(k)	NM	SC	—	108629 645435
1854	MgPd <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	—	(k)	NM	—	—	153055
1855	Co <sub>3</sub> W	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 55	(k)	FM	—	—	187963 187987 671175
1856	Co <sub>3</sub> V	<i>Pm</i> 3 <i>m</i> (221)	TI	—	(k)	NM	—	—	187965 187988
1857	Co <sub>3</sub> Nb	<i>Pm</i> 3 <i>m</i> (221)	TI	—	(k)	NM	—	—	187966 671177
1858	Co <sub>3</sub> Mo	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 55	(k)	FM	—	—	187969 671173
1859	MgNi <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 54	(k)	FM	SC*	—	193569
1860	InPd <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 55	(k)	NM	—	—	247193 247197
1861	Cu <sub>3</sub> Ni	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 55	(k)	—	—	—	670622
1862	CuNi <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 55	(k)	—	—	—	670623
1863	Ni <sub>3</sub> Pd	<i>Pm</i> 3 <i>m</i> (221)	SM	—	(k)	—	—	—	670625
1864	CuPd <sub>3</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	Fig. 56	(k)	—	—	—	670626 675018
1865	Ni <sub>3</sub> Zr <sub>1</sub>	<i>Pm</i> 3 <i>m</i> (221)	SM	—	(k)	—	—	—	671414
1866	KCl	<i>Pm</i> 3 <i>m</i> (221)	Triv.	—	—	NM	—	—	31232 60402 61557 290513 290514 290515 290516 290517 290518 290519 290520 290521 290522 290523 290524 290525 290526 290527 290528 290529 290530 290531 290532 290533 290534 290535 290536 290537 290538 290539 290540 290541 290542 290543 290544 290545 290546 290547 290548 671476 674957
1867	RhSi	<i>Pm</i> 3 <i>m</i> (221)	SM	—	—	NM	—	—	44385 182507
1868	RbI	<i>Pm</i> 3 <i>m</i> (221)	Triv.	—	—	NM	—	—	44619 61523 61559 674967

1869	FeAl	$Pm\bar{3}m$ (221)	SM	—	—	FM	—	—	55601 57791 165164 165165 169548 169549 607481 607487 658488 671099
1870	CoFe	$Pm\bar{3}m$ (221)	SM	—	—	FM	—	—	56273 155839 187982 622884
1871	AlCo	$Pm\bar{3}m$ (221)	TI	—	—	NM	—	—	57596 187973 606532 606533 606535 657493
1872	BeCo	$Pm\bar{3}m$ (221)	SM	—	—	FM	—	—	58693 150619 616204 616206
1873	BeNi	$Pm\bar{3}m$ (221)	TI	—	—	FM	—	—	58726 616363 616367
1874	CaCd	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	—	58874 619188
1875	InRh	$Pm\bar{3}m$ (221)	SM	—	—	NM	SC	—	59515 59516
1876	RbBr	$Pm\bar{3}m$ (221)	Triv.	—	—	NM	—	—	61522 61560 674964 61556 290554 290555 290556 290557 290558 290559 290561 290561 290562 290563 290564 290565 290566 290567 290568 290569 290570 290571 290572 290573 290574 290575 290576 290577 290578 290579 290580 290581 290582 674956
1877	KBr	$Pm\bar{3}m$ (221)	Triv.	—	—	NM	—	—	77865 96139 150938 189111 189112
1878	PbS	$Pm\bar{3}m$ (221)	TI	—	—	NM	—	—	100533 103660 103661 190972 633925 633930 633937 633945 633950
1879	TiFe	$Pm\bar{3}m$ (221)	TI	—	—	NM	—	—	102061 620407 670253 102423 603022 623049 623050 623053 623057 657494
1880	FeTi	$Pm\bar{3}m$ (221)	TI	—	—	NM	SC	HQ	102705 108322 150937 187975 189225 625473 625477 625485 670727
1881	CdSc	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	—	102737 102738 189944 625667 625675 625704 670613 670728
1882	CoGa	$Pm\bar{3}m$ (221)	SM	—	—	FM	—	—	103142 163697 185944 629426 629433 629435 672101
1883	CoSc	$Pm\bar{3}m$ (221)	TI	—	—	FM	SC	—	102642 624932
1884	CoTi	$Pm\bar{3}m$ (221)	SM	—	—	FM	SC	—	102737 102738 189944 625667 625675 625704 670613 670728
1885	CoZr	$Pm\bar{3}m$ (221)	SM	—	—	FM	SC	—	103681 103682 634034 670598 670599 670600 670601 670602
1886	CuY	$Pm\bar{3}m$ (221)	SM	—	—	NM	SC	—	103948 657338
1887	FeV	$Pm\bar{3}m$ (221)	SM	—	—	FM	—	—	103950
1888	GaRh	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	—	104305 639065 670252
1889	GaRu	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	—	104557 640974 657998 670271
1890	HgLa	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	—	104769 642255 642257
1891	IrSc	$Pm\bar{3}m$ (221)	TI	—	—	NM	SC	—	104847 104848 163195 642749
1892	LiPd	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	—	104855 656818
1893	MgPd	$Pm\bar{3}m$ (221)	TI	—	—	NM	—	—	104960 643391
1894	MgRh	$Pm\bar{3}m$ (221)	SM	Fig. 56	—	NM	—	—	105017
1895	MnRh	$Pm\bar{3}m$ (221)	TI	—	—	FM	—	—	105470 647135
1896	MnZn	$Pm\bar{3}m$ (221)	SM	—	—	FM	—	—	105972 105973 650527 650530 650535 650536 650541
1897	NiZn	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	—	106004 106005 650737 650738
1898	RhY	$Pm\bar{3}m$ (221)	TI	—	—	NM	SC	—	106022 650789
1899	RuTi	$Pm\bar{3}m$ (221)	TI	—	—	NM	SC	—	106195
1900	RuZr	$Pm\bar{3}m$ (221)	TI	—	—	NM	SC	—	106225 106226 653454 653455 653460 653464 653468
1901	TlY	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	—	106298 670610 672131
1902	YZn	$Pm\bar{3}m$ (221)	SM	—	—	NM	SC	—	163382 182360 670357
1903	RhZn	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	HQ	169396 191243
1904	MgSc	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	—	181289 672519
1905	AuMn	$Pm\bar{3}m$ (221)	SM	—	—	FM	—	—	183242
1906	TiRu	$Pm\bar{3}m$ (221)	TI	—	—	NM	—	—	187256
1907	CoSi	$Pm\bar{3}m$ (221)	SM	—	—	FM	—	—	187981
1908	ZnO	$Pm\bar{3}m$ (221)	Triv.	—	—	NM	—	—	187983
1909	PdN	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	—	191170
1910	ZrRu	$Pm\bar{3}m$ (221)	TI	—	—	NM	—	—	236829 236830
1911	PbS	$Pm\bar{3}m$ (221)	Triv.	—	—	NM	—	—	236829 236830
1912	MgNi	$Pm\bar{3}m$ (221)	TI	—	—	NM	—	—	236829 236830
1913	CoMn	$Pm\bar{3}m$ (221)	TI	—	—	FM	—	—	236829 236830
1914	CoNi	$Pm\bar{3}m$ (221)	SM	—	—	FM	—	—	236829 236830
1915	MnSn	$Pm\bar{3}m$ (221)	SM	Fig. 56	—	FM	—	—	236829 236830
1916	FeN	$Pm\bar{3}m$ (221)	SM	—	—	FM	—	—	236829 236830

1917	CoN	$Pm\bar{3}m$ (221)	SM	—	—	FM	—	—	236831 236832
1918	CuN	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	—	236835 236836
1919	ZnN	$Pm\bar{3}m$ (221)	SM	—	—	NM	—	—	236837 236838 670709
1920	RuTa	$Pm\bar{3}m$ (221)	SM	—	—	FM	—	—	650690
1921	CoAl	$Pm\bar{3}m$ (221)	TI	—	—	—	—	—	670160 671171
1922	PdCu	$Pm\bar{3}m$ (221)	SM	—	—	—	—	—	670618 670621
1923	KSe	$Pm\bar{3}m$ (221)	SM	—	—	—	—	—	675033
1924	Rb(HgF <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	15169
1925	K(CoF <sub>3</sub> )	$Pm\bar{3}m$ (221)	SM	—	(k,b,s,l)	FM	—	HQ	15246 15425 44785 189368
1926	KMnF <sub>3</sub>	$Pm\bar{3}m$ (221)	SM	Fig. 56	(k,b,s,l)	FM	—	—	15423 37254 43721 44783 75409 75410 75411 189367 201254 201255
1927	KFeF <sub>3</sub>	$Pm\bar{3}m$ (221)	Triv.	Fig. 59	(k,b,s,l)	FM	—	—	15424 37262 44784 107514
1928	Sr(TiO <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	SC	HQ	23076 27045 56902 56717 65088 65089 65090 76186 80871 80872 80873 80874 91899 94573 184455 184921 186725 186895 187296 187480 187619 191828 192314 201256 248379 262269 290370 290617 671735 672571 673179 673390 673418 673419 673892 674457 675010
1929	Tl(MnCl <sub>3</sub> )	$Pm\bar{3}m$ (221)	SM	—	(k,b,s,l)	FM	—	—	23167
1930	GaMn <sub>3</sub> C	$Pm\bar{3}m$ (221)	SM	—	(k,b,s,l)	AFM	—	—	23586 76845 617912 617913 617914
1931	Cs(HgBr <sub>3</sub> )	$Pm\bar{3}m$ (221)	SM	Fig. 56	(k,b,s,l)	NM	—	—	24479
1932	Cs(HgCl <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	24482
1933	Sr(ZrO <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	27046 29153 89365 89366 187481 188448 191829 290618 671952
1934	Sr(SnO <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	27047 181089 674084
1935	Ba(ZrO <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	27048 43136 90049 97459 97460 97461 97462 290002 671502 672709 672997 673866 674065 674771
1936	Ba(SnO <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	27049 43138 180138 181091 184338 185615 186899 188149 190601 239582 424820 670659 672199 674074 674772
1937	Ca(SnO <sub>3</sub> )	$Pm\bar{3}m$ (221)	SM	—	(k,b,s,l)	FM	—	—	27777
1938	BaTiO <sub>3</sub>	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	27970 27971 27972 27973 27975 27976 27977 28848 28849 28850 28851 28852 28853 28854 29147 43125 56093 67518 95437 99736 154344 166225 185374 186437 187291 190924 252562 290019 670888 670895 670904 671088 671604 672744 673178 674385
1939	KVF <sub>3</sub>	$Pm\bar{3}m$ (221)	SM	Fig. 56	(k,b,s,l)	FM	—	—	28145
1940	RbVF <sub>3</sub>	$Pm\bar{3}m$ (221)	SM	Fig. 56	(k,b,s,l)	FM	—	—	28146
1941	Na(NbO <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	28588 28589 28590 31867 192407 192408 236890 252485
1942	Na(TaO <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	28617 28618 28619 88378 239693
1943	La(CrO <sub>3</sub> )	$Pm\bar{3}m$ (221)	SM	Fig. 56	(k,b,s,l)	FM	—	—	28930 29120 41061 673194
1944	KMgF <sub>3</sub>	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	28949 40476 40477 56096 94089 192409 674545
1945	AgZnF <sub>3</sub>	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	28950 673278
1946	Ca(ZrO <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	29003 56094
1947	BaFeO <sub>3</sub>	$Pm\bar{3}m$ (221)	SM	—	(k,b,s,l)	FM	—	—	29096 262131 262132 672484
1948	La(FeO <sub>3</sub> )	$Pm\bar{3}m$ (221)	SM	—	(k,b,s,l)	FM	—	—	29118 673197 674500
1949	La(MnO <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	Fig. 59	(k,b,s,l)	FM	—	—	29119 188401 673199 674501 674623 674779
1950	Sr(HfO <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	—	29154 89386 161593 164620 184791 673486
1951	Ca(TiO <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	SC	—	31865 77060 153174 162924 162925 162926 165076 187293
1952	Sr(ZrO <sub>3</sub> )	$Pm\bar{3}m$ (221)	SM	—	(k,b,s,l)	NM	—	—	33666
1953	K <sub>3</sub> OB <sub>r</sub>	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	HQ	33920
1954	K <sub>3</sub> OI	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	—	HQ	36512
1955	K(TaO <sub>3</sub> )	$Pm\bar{3}m$ (221)	Triv.	—	(k,b,s,l)	NM	SC*	HQ	39673 39905 56439 56440 184922 280424 674515

1956	Rb(MnF <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 57	(k,b,s,l)	FM	—	—	43722
1957	AlCo <sub>3</sub> C	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	NM	—	—	43847
1958	AlFe <sub>3</sub> C	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	FM	—	—	43853 656541 672402
1959	Mn <sub>3</sub> GeC	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	FM	—	—	44351
1960	Rh <sub>3</sub> YB	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 57	(k,b,s,l)	NM	—	—	44568 615341
1961	K(CdF <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	44788
1962	CsCdF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	49582 290343 290344 290345 674681
1963	CsFeF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	FM	—	—	49583
1964	RbMgF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	49585
1965	RbFeF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	FM	—	—	49586 671396
1966	RbCdF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	49587
1967	Ca(SnO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	56095 181086 181087
1968	NaVF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 57	(k,b,s,l)	FM	—	—	60611
1969	Sr(RuO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 57	(k,b,s,l)	FM	—	HQ	69360 82981 82982 82983 82984 162777 187484
1970	Rb <sub>3</sub> AuO	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	HQ	75499 79087
1971	Mn <sub>3</sub> NiN	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	FM	—	—	76056
1972	Mn <sub>3</sub> ZnN	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	FM	—	—	76070 237710
1973	Fe <sub>3</sub> ZnC	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 57	(k,b,s,l)	FM	—	—	76763
1974	Co <sub>3</sub> MgC	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 57	(k,b,s,l)	FM	—	—	76790
1975	Co <sub>3</sub> ScC	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	NM	—	—	76793
1976	Co <sub>3</sub> ZnC	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 57	(k,b,s,l)	FM	—	—	76797
1977	Fe <sub>3</sub> SnC	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	NM	—	—	76842
1978	Sr(CoO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	FM	—	—	77142 184078
1979	Mn <sub>3</sub> SnC	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	FM	—	—	77153 194052 618271 618272
1980	Mn <sub>3</sub> ZnC	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	FM	—	—	77154 150829 618284
1981	Rb <sub>3</sub> BrO	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	77196
1982	CsCaBr <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	77242
1983	YRh <sub>3</sub> C	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 57	(k,b,s,l)	NM	—	—	77389
1984	K <sub>3</sub> AuO	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	HQ	79086
1985	Sr(VO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 58	(k,b,s,l)	FM	—	HQ	88982 96291 108826 672730 673312
1986	La(AlO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	90550 90551 90552 90553 90554 90555 90556 92561 92562 153831 153832 153833 153834 153835 153836 170772 191414 191415 191416 191417 191424 191425 191426 191427 191428 191429 191464 672200 673133 673339 674095
1987	SrFeO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	FM	—	HQ	91062 92335 163228
1988	CaPd <sub>3</sub> C	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	NM	—	—	108128
1989	Co <sub>3</sub> SnC	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	FM	—	—	108129
1990	Sr(CrO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	FM	—	—	108903 245834
1991	Sr(TcO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 58	(k,b,s,l)	NM	—	—	109076 183453 671084 671085
1992	Pb(TiO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	HQ	153406 162043 162047 187295 187505 262090 672655 673003
1993	KCaF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	154073 154074 670413
1994	BiAlO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	157549 158756
1995	BiGaO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	157550 158757
1996	Bi(InO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	158758
1997	Bi(ScO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	158759 181115 181116 181117 181118 181119 181120
1998	Pb(CrO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	FM	—	HQ	160196 194155
1999	Pb(HfO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	HQ	161702
2000	Ca(MnO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 58	(k,b,s,l)	FM	—	—	168902 168903 168905 181782 673449
2001	NaMgF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	HQ	171813 193089
2002	Pb(GeO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	185693 185694 185695 185696 185697 185698 185699 185700 185701
2003	Pb(VO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 58	(k,b,s,l)	FM	—	—	187637
2004	Sr(MnO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 58	(k,b,s,l)	AFM	—	—	188415 236949
2005	K(NbO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	HQ	190920 673080
2006	Ba(VO <sub>3</sub> )	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 58	(k,b,s,l)	FM	—	HQ	191203 673477
2007	SrGeO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	HQ	195084 672202 674088

2008	RbCaF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	201252 201253 670414
2009	CaLiF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	—	236756 236757
2010	InNiCo <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 58	(k,b,s,l)	FM	—	HQ	247066
2011	TlPd <sub>3</sub> H	<i>Pm</i>  <i>m</i> (221)	TI	—	(k,b,s,l)	NM	—	HQ	247273
2012	PbZrO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	HQ	262104 262105 290872 290873 290874 290875 290876 290877 290878 290879 672047 673004
2013	CdCo <sub>3</sub> N	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 58	(k,b,s,l)	FM	—	HQ	422858
2014	YPd <sub>3</sub> H	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	—	—	—	670902
2015	CaTcO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 59	(k,b,s,l)	—	—	—	671082 671083
2016	BaTcO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 59	(k,b,s,l)	—	—	—	671086 671087
2017	YBiO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	—	—	—	672990
2018	ZnSnO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 59	(k,b,s,l)	—	—	—	673496
2019	BaRuO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	—	—	—	673893
2020	BaHfO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	—	—	—	674059
2021	KSbO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	Fig. 59	(k,b,s,l)	—	—	—	674060
2022	LiSrF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	—	—	—	674527
2023	ReO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	NM	—	—	16810 77679 105546 647350 647352 671107
2024	NbF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	SM	—	(k,b,s,l)	FM	—	—	25596 60246
2025	MoF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 59	(k,b,s,l)	FM	—	—	30612
2026	ScF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	Fig. 60	(k,b,s,l)	NM	—	—	77071 194248 194249 194250 194273 261067 261068 261069 261070 261071 261072 261073 261074 261075 261076 261077 261078 261079 261080 261081 261082 261083 261084 261085 261086 261087 261088 261089 261090 261091 261092 261093 261094 261095 261108 673424 673425 673426 673427 673428 673429 673430 673431 673432 673433 673434 673435 673436
2027	WO <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	Fig. 60	(k,b,s,l)	NM	SC*	—	108651 183408 674843
2028	AlF <sub>3</sub>	<i>Pm</i>  <i>m</i> (221)	Triv.	—	(k,b,s,l)	NM	—	HQ	130021
2029	Na <sub>3</sub> N	<i>Pm</i>  <i>m</i> (221)	SM	Fig. 59	(k,b,s,l)	NM	—	—	165988 249566 412313 421109 421110 421111 421112 421113 421115 421116 421117 421118
2030	MgO	<i>Pm</i>  <i>n</i> (223)	Triv.	Fig. 60	—	NM	—	—	181465
2031	AuTa <sub>3</sub>	<i>Pm</i>  <i>n</i> (223)	SM	—	—	NM	—	—	58599
2032	AuV <sub>3</sub>	<i>Pm</i>  <i>n</i> (223)	SM	—	—	FM	SC	—	58612 612451 612456 612459
2033	PdV <sub>3</sub>	<i>Pm</i>  <i>n</i> (223)	SM	—	—	NM	SC	—	105739 649092
2034	Al <sub>3</sub> Mo	<i>Pm</i>  <i>n</i> (223)	SM	—	—	—	—	—	672120
2035	SiC <sub>2</sub> N <sub>4</sub>	<i>Pn</i>  <i>m</i> (224)	Triv.	Fig. 60	(b)	NM	—	—	93543
2036	MoZn <sub>7</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k)	NM	—	—	130003 644500
2037	LiPd <sub>7</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k)	NM	—	—	642266
2038	Co <sub>9</sub> S <sub>8</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	NM	—	HQ	23929 31753 40046 600664 624834 657415 660368
2039	Cs <sub>2</sub> Mn(Mn(CN) <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	FM	—	HQ	248046
2040	Cs <sub>2</sub> NaBiCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	2738 59195
2041	Ba <sub>2</sub> Mn(ReO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 61	(k*,b,s)	FM	—	—	4169 109256
2042	K <sub>2</sub> Na(AlF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 61	—	NM	—	HQ	6027 22109 <sup>(b)</sup> 40886 <sup>(b)</sup>
2043	KTl <sub>2</sub> MoF <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 60	(b)	FM	—	—	15775
2044	NaTl <sub>2</sub> MoF <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 60	(k*,b,s)	FM	—	—	15776
2045	K <sub>2</sub> NaCuF <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(b)	FM	—	—	22111
2046	K <sub>2</sub> NaScF <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	—	22112 65730
2047	K <sub>2</sub> NaInF <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	—	22113 23430
2048	K <sub>2</sub> NaTlF <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 61	(k*,b,s)	NM	—	—	22114
2049	Cs <sub>2</sub> NaTlF <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 62	(k*,b,s)	NM	—	—	22118
2050	Ba <sub>2</sub> MgWO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	—	24982 152572 152573 183771 262318 423033
2051	Ba <sub>2</sub> ZnWO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(b)	NM	—	—	24983 185847 243794 <sup>(k,s)</sup> 423034 <sup>(k,s)</sup>
2052	Ba <sub>2</sub> NiWO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	AFM	—	—	24984 27426 28342 243798
2053	Ba <sub>2</sub> CaWO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(b)	NM	—	—	24985 60499 <sup>(k,s)</sup> 76436 <sup>(k,s)</sup> 195954 245599 <sup>(k,s)</sup> 246111 <sup>(k,s)</sup>
2054	Ba <sub>2</sub> LaReO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	—	25392
2055	Sr <sub>2</sub> YReO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	—	25404

2056	Ba <sub>2</sub> CoWO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 60	(k*,b,s)	FM	—	—	27425 97029 195130 672551
2057	Sr <sub>2</sub> Ni(WO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	—	AFM	—	—	28597(k,b,s) 109165
2058	Sr <sub>2</sub> Co(WO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 60	(k*,b,s)	FM	—	—	28598
2059	Sr <sub>2</sub> Ni(MoO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	—	28600 155733 157027
2060	Sr <sub>2</sub> Co(MoO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 61	(k*,b,s)	AFM	—	—	28601 153543
2061	Sr <sub>2</sub> Ca(WO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	—	36459
2062	Rb <sub>2</sub> K(CoF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(b)	NM	—	—	42147
2063	Rb <sub>2</sub> Na(CoF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(b)	NM	—	—	42148
2064	Rb <sub>2</sub> Na(NiF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(b)	FM	—	—	42150
2065	K <sub>2</sub> Na(NiF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	—	42151
2066	K <sub>3</sub> WF <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	HQ	51264
2067	Ba <sub>2</sub> MnWO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	AFM	—	HQ	51607 51608 51609 51610 51611 51612 51613
2068	Cs <sub>2</sub> KScCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	59196
2069	Cs <sub>2</sub> LiYCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	65731
2070	Cs <sub>2</sub> NaYCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	65732 245353 245354
2071	Pb <sub>2</sub> Mg(WO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	67880
2072	Sr <sub>2</sub> Ca(MoO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	72815
2073	Ba <sub>2</sub> Ca(IrO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	HQ	74029
2074	Pb <sub>2</sub> (ScTaO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	—	77739
2075	(NH <sub>4</sub> ) <sub>2</sub> NaInF <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	79099
2076	Ca <sub>2</sub> Fe(WO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	FM	—	—	81203
2077	Ca <sub>2</sub> TiSiO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	83455
2078	Ba <sub>2</sub> (YSbO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	84650 155253 155346 163373
2079	YBa <sub>2</sub> (ReO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(b)	FM	—	HQ	94215(k,s) 94216(k,s) 168215(k,s) 168216
2080	Ba <sub>2</sub> FeMoO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 62	(k*,b,s)	FM	—	—	96688 99063 184909 190613 190614 191681 246545 246546
2081	Ba <sub>2</sub> (CoMoO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 61	(k*,b,s)	AFM	—	HQ	97028 184910 672550
2082	Ba <sub>2</sub> NiMoO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	AFM	—	HQ	98192
2083	Ba <sub>2</sub> (MnMoO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	AFM	—	HQ	98739 99090
2084	Ba <sub>2</sub> (FeWO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 62	(k*,b,s)	AFM	—	HQ	99061 672159
2085	Ba <sub>2</sub> (InNbO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(b)	NM	—	—	99698(k,s) 109162 172166(k,s)
2086	Ba <sub>2</sub> Ni(ReO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	—	109251
2087	Ba <sub>2</sub> Fe(ReO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 61	(k*,b,s)	FM	—	—	109252 155175
2088	Ba <sub>2</sub> Co(ReO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	—	109254 672552 674903
2089	Ba <sub>2</sub> Zn(ReO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	—	109255
2090	Ba <sub>2</sub> Li(ReO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	—	109259 418994
2091	Ba <sub>2</sub> Na(ReO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(b)	NM	—	—	109260(k,s) 200876 418993
2092	Sr <sub>2</sub> Mg(WO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	152575 152576
2093	Ba <sub>2</sub> YIrO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	FM	—	HQ	152679 427064
2094	Sr <sub>2</sub> (GaSbO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 62	(k*,b,s)	NM	—	HQ	157016 157017 157018 157019
2095	Sr <sub>2</sub> (FeMoO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 62	(k*,b,s)	AFM	—	HQ	157603 181752 248459
2096	Sr <sub>2</sub> Y(SbO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 62	(k*,b,s)	NM	—	—	157886 157887
2097	Ba <sub>2</sub> YTaO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	160172 171172 171173 171174 171175 261453
2098	Ba <sub>2</sub> CaOsO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	HQ	171988 171989 192844 192845
2099	Ba <sub>2</sub> BiIrO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(b)	FM	—	HQ	174289
2100	Sr <sub>2</sub> CrZrO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	AFM	—	—	181750
2101	Sr <sub>2</sub> MnNbO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	FM	—	—	181751
2102	Pb <sub>2</sub> MnReO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	FM	—	HQ	182001
2103	Ba <sub>2</sub> MgTeO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	—	—	HQ	191563
2104	Pb <sub>2</sub> MnWO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	AFM	—	—	239438
2105	Ba <sub>2</sub> CaTeO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 62	(k*,b,s)	NM	—	HQ	246112
2106	Sr <sub>2</sub> Li(ReO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	—	246731 418992
2107	(NH <sub>4</sub> ) <sub>2</sub> Na(AlF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	HQ	249157
2108	Sr <sub>2</sub> FeOsO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 61	(k*,b,s)	AFM	—	—	251068
2109	Cs <sub>2</sub> InAgCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 62	(k*,b,s)	—	—	—	257115
2110	K <sub>3</sub> AlF <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(b)	NM	—	HQ	262078
2111	Rb <sub>2</sub> Na(AlF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(b)	NM	—	HQ	290318
2112	K <sub>2</sub> Li(AlF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	408553
2113	Ba <sub>2</sub> Li(OsO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	HQ	412142

2114	Ba <sub>2</sub> Na(OsO <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(b)	FM	—	HQ	412143
2115	Rb <sub>2</sub> K(GaF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(b)	NM	—	HQ	416605
2116	(NH <sub>4</sub> ) <sub>2</sub> Na(GaF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	HQ	418737
2117	Pb <sub>2</sub> NaIO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 61	(k*,b,s)	NM	—	HQ	427115 5270 5271 20597 24523 53984 60013 60014 60372 76420 180950 180951 180952 180953 181557 201113 201114 201115
2118	PbF <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	—	26735 60439 183837 641321 55115 55116 55117 55131 55132 55133 55134 55135 55136 182743
2119	K <sub>2</sub> S	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 63	—	NM	—	—	26735 60439 183837 641321
2120	Rb <sub>2</sub> Te	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	—	55115 55116 55117 55131 55132 55133 55134 55135 55136 182743
2121	Na <sub>2</sub> O	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	—	60435 180570 644917
2122	K <sub>2</sub> Se	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 63	—	NM	—	—	60440 168448 196758
2123	K <sub>2</sub> Te	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 63	—	NM	—	—	60441 96739 182742 631721 641376
2124	CrO <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	186838
2125	Ca <sub>2</sub> Pb	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	—	191749
2126	LiCo <sub>2</sub> Ge	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 64	—	NM	—	—	25324
2127	LiPd <sub>2</sub> Ge	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	42130
2128	K <sub>3</sub> Sb	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	—	44677 246648
2129	LiNi <sub>2</sub> Si	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	44819
2130	InMgNi <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	51982
2131	InMnNi <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	51984 51985 639954 639955 639956 639958
2132	InMnPd <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	51988
2133	CoFe <sub>2</sub> Ge	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 64	—	FM	—	—	52954
2134	Co <sub>2</sub> FeSi	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	52958 247649 622985 672918 675045
2135	Co <sub>2</sub> MnGe	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	52971 623489 623490 623496 672229 674762 675071 675072 675073
2136	Co <sub>2</sub> ZnGe	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 64	—	FM	—	—	52994
2137	Co <sub>2</sub> MnSb	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	53002 624129
2138	Co <sub>2</sub> MnSi	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	53007 624141 624143 624144 624157 659021 672228 672940 673044 675047 675075 675076 675077
2139	Co <sub>2</sub> TiSi	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 64	—	FM	—	—	53080 53081 185969 189222 625083
2140	Co <sub>2</sub> VSi	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 64	—	FM	—	—	53086 659022
2141	CsK <sub>2</sub> Sb	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	—	53237
2142	Fe <sub>3</sub> Ge	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	FM	—	—	53462 672765
2143	FeRu <sub>2</sub> Si	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 67	—	FM	—	—	53525 633245 633246
2144	Fe <sub>3</sub> Si	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	53545 56281 157941 412838 600519 633528 633531 633534 633535 633537 633545 633552 658523 672766
2145	Fe <sub>2</sub> VSi	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 64	—	FM	—	—	53555 633623 659019
2146	MnNi <sub>2</sub> Ge	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	53687 192566
2147	MnPd <sub>2</sub> Ge	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	53705
2148	MnRh <sub>2</sub> Ge	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	53706 637070 637071
2149	ZrNi <sub>2</sub> In	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 64	—	NM	—	HQ	54546 59460
2150	HfNi <sub>2</sub> In	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 65	—	NM	—	—	54595
2151	TiNi <sub>2</sub> In	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	SC	—	54596 59451 59452
2152	AlCo <sub>2</sub> Cr	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	57600 291940 672915 675041
2153	Co <sub>2</sub> HfAl	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	57611 110809 606590
2154	AlCo <sub>2</sub> Mn	<i>Fm</i>  <i>m</i> (225)	TI	—	—	FM	—	—	57612 606611 606614 672231 675063 675064 675065
2155	AlCo <sub>2</sub> Nb	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	57620 606622
2156	AlCo <sub>2</sub> Ta	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	57634 606667
2157	AlCo <sub>2</sub> V	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	57643 188397 606704 606705 674449
2158	AlCo <sub>2</sub> Zr	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	57648 606733 606737 606738
2159	AlCrFe <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 65	—	FM	—	—	57654 184446
2160	AlFe <sub>3</sub>	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 65	—	FM	—	—	57793 607482 607484 607485 672764
2161	AlFe <sub>2</sub> Mo	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 65	—	FM	—	—	57807
2162	AlFe <sub>2</sub> V	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	—	57832 57833 107814
2163	AlMnPt <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	57985
2164	AlMnRh <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	TI	—	—	FM	—	—	57986

2165	AlNi <sub>2</sub> Sc	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	58050
2166	AlNi <sub>2</sub> Ti	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	SC	—	58063 165902
2167	BiK <sub>3</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	SC	—	58793
2168	BiRb <sub>3</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	58849
2169	InNi <sub>2</sub> Sc	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	59446
2170	MnNi <sub>2</sub> Sb	<i>Fm</i>  <i>m</i> (225)	TI	—	—	FM	—	—	76080 643107 643114
2171	Pd <sub>2</sub> MnSb	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	76100 643311 643312 643318
2172	Mn <sub>3</sub> Si	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 65	—	FM	SC	—	76227 643616 643621 643647
2173	Co <sub>2</sub> CrGa	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	102318 675042
2174	CoFe <sub>2</sub> Ga	<i>Fm</i>  <i>m</i> (225)	TI	Fig. 63	—	FM	—	—	102385
2175	Co <sub>2</sub> FeGa	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	102386 247653
2176	Co <sub>2</sub> HfGa	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 65	—	FM	—	—	102433 623080
2177	Co <sub>2</sub> MnGa	<i>Fm</i>  <i>m</i> (225)	TI	—	—	FM	—	—	102438 623116 623118 623121 672230 675067 675068 675069
2178	Co <sub>2</sub> GaNb	<i>Fm</i>  <i>m</i> (225)	TI	—	—	FM	—	—	102441 623126
2179	Co <sub>2</sub> GaTa	<i>Fm</i>  <i>m</i> (225)	TI	—	—	FM	—	—	102451
2180	Co <sub>2</sub> GaTi	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	102453 102454 623206 623207 623209 623211
2181	Co <sub>2</sub> GaV	<i>Fm</i>  <i>m</i> (225)	TI	—	—	FM	—	—	102456 623228 623230 674450
2182	Co <sub>2</sub> HfSn	<i>Fm</i>  <i>m</i> (225)	TI	Fig. 63	—	FM	—	—	102483 108295 291934 623806 659656
2183	Co <sub>2</sub> MnSn	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	102554 102555 190615 624326 624333
2184	Co <sub>2</sub> NbSn	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	102646
2185	Co <sub>2</sub> ScSn	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	102682 102683 625282 625285 625286 625289 625291 625292 672408
2186	Co <sub>2</sub> SnTi	<i>Fm</i>  <i>m</i> (225)	TI	Fig. 63	—	FM	—	—	102684 102685 625303 625306
2187	Co <sub>2</sub> SnV	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	102687 108321 190131 625312 625314 625318
2188	Co <sub>2</sub> SnZr	<i>Fm</i>  <i>m</i> (225)	TI	Fig. 63	—	FM	—	—	102755 184448
2189	CrFe <sub>2</sub> Ga	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 65	—	FM	—	—	102996 102997 628019
2190	Cu <sub>2</sub> MnIn	<i>Fm</i>  <i>m</i> (225)	TI	Fig. 63	—	FM	—	—	103092
2191	CuRh <sub>2</sub> Sn	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	103473 103474 631850
2192	Fe <sub>2</sub> GaV	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 67	—	NM	—	—	103641 103642 186058 633766
2193	Fe <sub>2</sub> SnTi	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 65	—	NM	—	—	103644 291933
2194	Fe <sub>2</sub> SnV	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 66	—	FM	—	—	103734 634320
2195	GaHfNi <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	SC	—	103874
2196	GaNi <sub>2</sub> Sc	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	103886
2197	GaNi <sub>2</sub> Ti	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	104926 104927 191631 291935 643152 643153 643156 643157 643158 643159 643161 674344
2198	MnNi <sub>2</sub> Sn	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 66	—	FM	—	—	104945 104946 643324 643325 643327
2199	MnPbRh <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	104964 104965 643424 643427 643428
2200	MnPd <sub>2</sub> Sn	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	104980
2201	MnRh <sub>2</sub> Sn	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	105327
2202	Mn <sub>2</sub> WSn	<i>Fm</i>  <i>m</i> (225)	TI	—	—	NM	—	—	105339 657254
2203	NiRh <sub>2</sub> Sn	<i>Fm</i>  <i>m</i> (225)	TI	Fig. 64	—	FM	—	—	105354 671093 671334
2204	Ni <sub>2</sub> ScSn	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 66	—	NM	—	HQ	105376 105377 646810
2205	Ni <sub>3</sub> Sn	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	105376 105377 646810
2206	Ni <sub>2</sub> SnV	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	SC	—	105933
2207	Rh <sub>2</sub> SnV	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	107955
2208	AsMnPd <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	108436 672763
2209	Fe <sub>3</sub> Ga	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 66	—	FM	—	—	151207
2210	Cu <sub>2</sub> CoSn	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	169468 169469 623633 623637
2211	Co <sub>2</sub> TiGe	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 66	—	FM	—	—	185936 622905
2212	Co <sub>2</sub> NiGa	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	185966 606679 606680 606682 606685
2213	Co <sub>2</sub> FeGe	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	185999
2214	Co <sub>2</sub> TiAl	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 66	—	FM	—	—	186056
2215	Fe <sub>2</sub> CrSn	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 66	—	FM	—	—	186057
2216	Fe <sub>2</sub> TiIn	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	186059
2217	Fe <sub>2</sub> TiGe	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 67	—	NM	—	—	186060
2218	Fe <sub>2</sub> TiAs	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 66	—	FM	—	—	186060
2219	Fe <sub>2</sub> TiSb	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 67	—	FM	—	—	186060

2220	Ni <sub>2</sub> FeGa	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	187492 672424
2221	Sc <sub>2</sub> MnSi	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	190996
2222	Sc <sub>2</sub> MnGe	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	190998
2223	Pd <sub>3</sub> N	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	191232
2224	Co <sub>2</sub> CrIn	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	416260
2225	Ru <sub>2</sub> VGe	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 67	—	—	—	—	671340
2226	Co <sub>2</sub> CrSi	<i>Fm</i>  <i>m</i> (225)	TI	—	—	—	—	—	672916 675044
2227	Ti <sub>2</sub> CoAl	<i>Fm</i>  <i>m</i> (225)	SM	—	—	—	—	—	674767
2228	Ru <sub>2</sub> ZrSb	<i>Fm</i>  <i>m</i> (225)	SM	—	—	—	—	—	675061
2229	Fe <sub>2</sub> ZrP	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 67	—	—	—	—	675102
2230	Co <sub>2</sub> TiIn	<i>Fm</i>  <i>m</i> (225)	SM	—	—	—	—	—	675103
2231	Co <sub>2</sub> VIn	<i>Fm</i>  <i>m</i> (225)	TI	—	—	—	—	—	675104
2232	K <sub>2</sub> (SnCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 68	(k*)	NM	—	HQ	604 1668 6058 23991 26111
2233	(NH <sub>4</sub> ) <sub>2</sub> (SnCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 68	(k*)	NM	—	HQ	605 9021 163660
2234	K <sub>2</sub> PtCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	HQ	2582 2583 31114 36304 48137 52033 52034 52035 52036 52037 52038 52039 68765 68766 82375 82376 280458 280459 280460 280461 280462 280463 280464 280465 280466 280467 280468
2235	(NH <sub>4</sub> ) <sub>2</sub> ReCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	HQ	8044
2236	Rb <sub>2</sub> SnCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 68	(k*)	NM	—	HQ	9022 26698 29026 65059 65060
2237	Cs <sub>2</sub> SnCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	Fig. 68	(k*)	NM	—	HQ	9023 26699 29030
2238	Rb <sub>2</sub> TeCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	9315 26703 29027
2239	Rb <sub>2</sub> MnCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 67	(k*)	FM	—	HQ	9347
2240	K <sub>2</sub> MnCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	—	9679
2241	K <sub>2</sub> TcCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	HQ	22096
2242	K <sub>2</sub> ReCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	HQ	23769 26755 68763
2243	K <sub>2</sub> (ReBr <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	HQ	23770 26623
2244	K <sub>2</sub> (PtBr <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	HQ	23771
2245	Cs <sub>2</sub> TeBr <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	HQ	24151 27695 65057 65058
2246	K <sub>2</sub> (MoCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	—	26643
2247	Rb <sub>2</sub> (TiCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26689
2248	Cs <sub>2</sub> (TiCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26690
2249	Rb <sub>2</sub> (SeCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26692
2250	Cs <sub>2</sub> (SeCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26693
2251	Rb <sub>2</sub> (ZrCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26694
2252	Cs <sub>2</sub> (ZrCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26695
2253	Tl <sub>2</sub> (SnCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26700
2254	Cs <sub>2</sub> (TeCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26704 29031
2255	Tl <sub>2</sub> (TeCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26705
2256	Rb <sub>2</sub> (PtCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26708 29028
2257	Tl <sub>2</sub> (PtCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26710
2258	Rb <sub>2</sub> (PbCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26712 29029
2259	Cs <sub>2</sub> (PbCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26713 29033
2260	K <sub>2</sub> TiCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	26934
2261	Cs <sub>2</sub> PoBr <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	—	—	—	27694
2262	Cs <sub>2</sub> (GeCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	28892
2263	K <sub>2</sub> PdCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	33709 65037 65038 65039 73723
2264	K <sub>2</sub> (SeBr <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	36228 69441
2265	PdBr <sub>6</sub> Rb <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	36305
2266	K <sub>2</sub> (TeBr <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	HQ	38346 65118
2267	Tl <sub>2</sub> (SiF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	—	38549 52292(k)
2268	K <sub>2</sub> (HfF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	47244
2269	Rb <sub>2</sub> (TeBr <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	HQ	49521 49522
2270	K <sub>2</sub> TaCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 68	(k*)	FM	—	HQ	59894
2271	Cs <sub>2</sub> ReCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	HQ	64613
2272	(NH <sub>4</sub> ) <sub>2</sub> (PtCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	HQ	97927
2273	Mg <sub>2</sub> FeH <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	107500 238723
2274	K <sub>2</sub> (SnBr <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	158955
2275	Cs <sub>2</sub> PdBr <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	—	—	—	243749

2276	Rb <sub>2</sub> (NbCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 68	(k*)	FM	—	HQ	245747
2277	Rb <sub>2</sub> (WBr <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	HQ	402439
2278	Cs <sub>2</sub> (WBr <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	HQ	402441
2279	Rb <sub>2</sub> (WCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	HQ	409632
2280	Cs <sub>2</sub> (WCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	HQ	409674
2281	Cs <sub>2</sub> (MoCl <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	HQ	409808
2282	K <sub>2</sub> WCl <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	HQ	409840
2283	(NH <sub>4</sub> ) <sub>2</sub> (ReBr <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*)	FM	—	HQ	412159
2284	Sr <sub>2</sub> FeH <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	—	632211
2285	Y <sub>2</sub> Ni <sub>6</sub> C	<i>Fm</i>  <i>m</i> (225)	SM	Fig. 67	(k*)	—	—	—	673582
2286	K <sub>2</sub> (B <sub>6</sub> H <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	HQ	65507
2287	Mg <sub>6</sub> MnO <sub>8</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k,b)	AFM	—	HQ	24710 27874 76174 82182
2288	Mg <sub>7</sub> VH <sub>16</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k)	FM	—	—	169051
2289	Mg <sub>7</sub> NbH <sub>16</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k)	FM	—	—	169052
2290	MoZn <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k)	NM	—	—	260686
2291	Na <sub>6</sub> ClF(SO <sub>4</sub> ) <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	HQ	26914 29330 52291
2292	(PtIn <sub>6</sub> )(GaO <sub>4</sub> ) <sub>2</sub>	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*)	NM	—	HQ	411505
2293	CoO	<i>Fm</i>  <i>m</i> (225)	SM	—	—	AFM	—	HQ	9865 28505 28506 29049 29081 29226 53057 53058 53929 61326 76638 191776 245319 245320 245321 245322 245323 245324 624575 624580 671734 673072 674028 675002
2294	NiO	<i>Fm</i>  <i>m</i> (225)	SM	—	—	AFM	—	HQ	9866 24014 24018 28834 28910 53930 53931 61318 61324 61544 76669 182948 184626 184918 241420 646096 646098 646099 671425 671943 674029 674434 674638 675004
2295	MnS	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	18007 41331 76204 158647 158648 158649 158650 158651 158652 603118 643434 643435 643436 643437 643438 643439 643443 643444 643445 643450 643451 643453 643456
2296	FeO	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	FM	—	—	27856 31081 53519 60683 76639 82233 180972 180973 180974 633029 633030 633038 670891 674027
2297	ZnTe	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	31840 52512 653197
2298	AgN	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	167858 183195 185555
2299	CrTe	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	169767
2300	NiC	<i>Fm</i>  <i>m</i> (225)	TI	—	—	NM	—	—	180457
2301	FeN	<i>Fm</i>  <i>m</i> (225)	SM	—	—	FM	—	—	184375 236810
2302	ZnTe	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	—	184497 248454
2303	MnSb	<i>Fm</i>  <i>m</i> (225)	TI	—	—	FM	—	—	191173
2304	CuN	<i>Fm</i>  <i>m</i> (225)	SM	—	—	NM	—	—	236815 236816
2305	CsSe	<i>Fm</i>  <i>m</i> (225)	SM	—	—	—	—	—	670583
2306	Ba <sub>2</sub> YSbO <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k,b,s,l)	NM	—	—	33624
2307	Na(SbF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	—	NM	—	HQ	16640 56251 (b) 77919
2308	Ca(PbF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	—	25522
2309	Ca(SnF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	NM	—	HQ	35713
2310	Fe(ZrF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	FM	—	HQ	35716 100301
2311	Cr(ZrF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	Triv.	—	(k*,b,s)	FM	—	HQ	35719
2312	VZrF <sub>6</sub>	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	—	73354 94454
2313	Co(ZrF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	HQ	83724
2314	V(HfF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	HQ	94455
2315	Ti(ZrF <sub>6</sub> )	<i>Fm</i>  <i>m</i> (225)	SM	—	(k*,b,s)	FM	—	HQ	94456
2316	K(SbO <sub>3</sub> )	<i>Fd</i>  <i>m</i> (227)	Triv.	—	(k,p,b,s)	NM	—	—	77333
2317	As <sub>2</sub> O <sub>3</sub>	<i>Fd</i>  <i>m</i> (227)	Triv.	—	(b,s)	NM	—	—	2114 16850 24227 183098 409611
2318	As <sub>4</sub> O <sub>6</sub>	<i>Fd</i>  <i>m</i> (227)	Triv.	—	(b,s)	NM	—	—	36144 238612 238613 238614 238615 238616 238617 238618 238619 238620 238621 238622 238623 238624 238625 238626 238627 238628 238629 238630 238631 238632 238633 238634 238635 238636 238637
2319	Ca <sub>2</sub> NH	<i>Fd</i>  <i>m</i> (227)	Triv.	Fig. 68	(k,p)	NM	—	—	292

2320	Hf <sub>3</sub> Zn <sub>3</sub> C	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p,b,s)	NM	—	—	42936 618069
2321	CsAlO <sub>2</sub>	<i>Fd</i> $\bar{3}m$ (227)	Triv.	—	(k,p,b,s)	NM	—	—	28372
2322	RbAlO <sub>2</sub>	<i>Fd</i> $\bar{3}m$ (227)	Triv.	—	(k,p,b,s)	NM	—	—	28373
2323	CsNbN <sub>2</sub>	<i>Fd</i> $\bar{3}m$ (227)	Triv.	Fig. 68	(k,p,b,s)	NM	—	HQ	72546
2324	KAlO <sub>2</sub>	<i>Fd</i> $\bar{3}m$ (227)	Triv.	—	(k,p,b,s)	NM	—	HQ	262975
2325	YS <sub>2</sub>	<i>Fd</i> $\bar{3}m$ (227)	SM	Fig. 69	(k,p)	NM	—	—	52216
2326	Mn <sub>2</sub> Y	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p)	FM	—	HQ	54375 105001 105002 150743 603250 643875 643894 643895 643896 643902 643910 643915
2327	YFe <sub>2</sub>	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p)	FM	—	—	57792 103697 103698 106699 150744 601992 603459 634075 634079 634083 634084 634085 634088 634091 634096 634097 634099 634100 634102 634103 634105 634106 634107 634108 634117 634122 672932
2328	BaPt <sub>2</sub>	<i>Fd</i> $\bar{3}m$ (227)	TI	Fig. 69	(k,p)	NM	SC	—	58675 616039 616040
2329	Be <sub>2</sub> Nb	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p)	NM	SC	—	58721 616354
2330	CaNi <sub>2</sub>	<i>Fd</i> $\bar{3}m$ (227)	SM	Fig. 69	(k,p)	NM	—	—	58915 619440 619441
2331	Fe <sub>2</sub> Sc	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p)	FM	—	—	103618 103619 633420 633429 633433
2332	Ir <sub>2</sub> Sc	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p)	NM	SC	—	104558 104559 640973 657997
2333	Ir <sub>2</sub> Sr	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p)	NM	SC	—	104564 641065
2334	Ir <sub>2</sub> Y	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p)	NM	SC	—	104601 104602 641175 641180 641183
2335	Ni <sub>2</sub> Sc	<i>Fd</i> $\bar{3}m$ (227)	SM	Fig. 69	(k,p)	NM	—	—	105334 105335 646466
2336	Ni <sub>2</sub> Y	<i>Fd</i> $\bar{3}m$ (227)	SM	Fig. 69	(k,p)	NM	SC	—	105458 105459 150746 183094 196784 647056 647057 647058 647072 647082 647083 647086 647087 647088 647090 647099 647108 657906 670873
2337	Zn <sub>2</sub> Zr	<i>Fd</i> $\bar{3}m$ (227)	Triv.	Fig. 69	(k,p)	FM	SC	—	106236 106237 653507 653508 653510 653517 653523
2338	CaIr <sub>2</sub>	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p)	NM	SC	—	108146
2339	Nb <sub>2</sub> Fe	<i>Fd</i> $\bar{3}m$ (227)	TI	—	(k,p)	FM	—	—	188269
2340	Ni <sub>2</sub> Cr	<i>Fd</i> $\bar{3}m$ (227)	TI	—	(k,p)	FM	—	—	188273
2341	CaLi <sub>2</sub>	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p)	NM	—	HQ	413207
2342	Sc <sub>2</sub> (Si <sub>2</sub> O <sub>7</sub> )	<i>Fd</i> $\bar{3}m$ (227)	Triv.	—	(k,p,b,s)	NM	—	HQ	1457
2343	La <sub>2</sub> (Zr <sub>2</sub> O <sub>7</sub> )	<i>Fd</i> $\bar{3}m$ (227)	Triv.	—	(k,p,b,s)	NM	—	—	15165 51573 150206 153222 153814 154752 159321 248878 253061 253063 671158 671161 672848
2344	Ca <sub>2</sub> (Nb <sub>2</sub> O <sub>7</sub> )	<i>Fd</i> $\bar{3}m$ (227)	Triv.	—	(k,p,b,s)	NM	—	—	22411 72206
2345	Pb <sub>2</sub> Sb <sub>2</sub> O <sub>7</sub>	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p)	NM	—	—	24246
2346	Sn <sub>2</sub> (Ta <sub>2</sub> O <sub>7</sub> )	<i>Fd</i> $\bar{3}m$ (227)	Triv.	Fig. 70	(k,p,b,s)	NM	—	—	27119 163818
2347	Pb <sub>2</sub> Sb <sub>2</sub> O <sub>7</sub>	<i>Fd</i> $\bar{3}m$ (227)	SM	Fig. 69	(k,p,b,s)	NM	—	—	27120
2348	Ca <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	<i>Fd</i> $\bar{3}m$ (227)	Triv.	Fig. 70	(k,p,b,s)	NM	—	—	27121
2349	Hg <sub>2</sub> Cu <sub>2</sub> F <sub>6</sub> S	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p,b,s)	FM	—	HQ	27327
2350	Hg <sub>2</sub> Zn <sub>2</sub> F <sub>6</sub> O	<i>Fd</i> $\bar{3}m$ (227)	Triv.	Fig. 70	(k,p,b,s)	NM	—	HQ	27330
2351	Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	<i>Fd</i> $\bar{3}m$ (227)	SM	Fig. 69	(k,p)	NM	—	—	33672
2352	Bi <sub>2</sub> (Ru <sub>2</sub> O <sub>7</sub> )	<i>Fd</i> $\bar{3}m$ (227)	Triv.	—	(k,p,b,s)	NM	—	HQ	73787 78114 161102 163387 166566 166567
2353	Hg <sub>2</sub> Cu <sub>2</sub> F <sub>6</sub> S	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p,b,s)	FM	—	HQ	156366 156367 156368
2354	Bi <sub>2</sub> (Rh <sub>2</sub> O <sub>7</sub> )	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p,b,s)	NM	—	—	161099
2355	Bi <sub>2</sub> (Ti <sub>2</sub> O <sub>7</sub> )	<i>Fd</i> $\bar{3}m$ (227)	Triv.	—	(k,p,b,s)	NM	—	—	161100 180394
2356	Bi <sub>2</sub> (Ir <sub>2</sub> O <sub>7</sub> )	<i>Fd</i> $\bar{3}m$ (227)	SM	—	(k,p,b,s)	NM	—	—	161103 237820 252134 252135
2357	Bi <sub>2</sub> (Pt <sub>2</sub> O <sub>7</sub> )	<i>Fd</i> $\bar{3}m$ (227)	Triv.	—	(k,p,b)	NM	—	—	161104 <sup>(s)</sup> 202346
2358	Sn <sub>2</sub> (Nb <sub>2</sub> O <sub>7</sub> )	<i>Fd</i> $\bar{3}m$ (227)	Triv.	Fig. 70	(k,p,b,s)	NM	—	—	163817
2359	La <sub>2</sub> (Zr <sub>2</sub> O <sub>7</sub> )	<i>Fd</i> $\bar{3}m$ (227)	TI	—	(k,p,b,s)	NM	—	—	173795 184089 184090 184091 184092 184093 184094 184095 184096 184097 184098 184099 184100 184101 184102
2360	Y <sub>2</sub> (Ir <sub>2</sub> O <sub>7</sub> )	<i>Fd</i> $\bar{3}m$ (227)	SM	Fig. 70	(k,p,b,s)	FM	—	HQ	187534
2361	In <sub>2</sub> Ge <sub>2</sub> O <sub>7</sub>	<i>Fd</i> $\bar{3}m$ (227)	Triv.	—	(k,p,b,s)	NM	—	—	239593
2362	La <sub>2</sub> Ge <sub>2</sub> O <sub>7</sub>	<i>Fd</i> $\bar{3}m$ (227)	Triv.	—	(k,p,b,s)	—	—	—	672851
2363	Co <sub>2</sub> (SiO <sub>4</sub> )	<i>Fd</i> $\bar{3}m$ (227)	TI	—	(k,p,b)	FM	—	HQ	859
2364	Ni <sub>2</sub> SiO <sub>4</sub>	<i>Fd</i> $\bar{3}m$ (227)	Triv.	—	(k,p,b)	FM	—	HQ	2136 40992 40993 40994 40995 100544 100545 100546 100547 100548 100549 100550 100551 200129 200130 200131

2365	Mg <sub>2</sub> (SiO <sub>4</sub> )	<i>Fd</i> 3̄ <i>m</i> (227)	Triv.	—	(k,p,b)	NM	—	—	27531 74535 83779 83780 83781 83782 83783 86504 161023 162347 162348 162406 191506 671941
2366	LiMn <sub>2</sub> O <sub>4</sub>	<i>Fd</i> 3̄ <i>m</i> (227)	SM	—	(k,p,b)	FM	—	—	40485 50415 50427 53603 85341 85345 88644 89459 89985 93591 94339 94340 151907 155282 155665 165871 165872 182717 192369 193444 195840 242133 261557
2367	Fe <sub>2</sub> (SiO <sub>4</sub> )	<i>Fd</i> 3̄ <i>m</i> (227)	Triv.	—	(k,p,b)	AFM	—	HQ	41002 41003 41004 41005 41006 87462 100552 185517 185518 185519 185520 185521 185522 185523 200133 200134 238745 238746 238747 238748 238749 238751 238752 238753 238754 238755 238756 238757
2368	CuRh <sub>2</sub> S <sub>4</sub>	<i>Fd</i> 3̄ <i>m</i> (227)	SM	—	(k,p,b)	NM	SC*	—	41900 291917 628767
2369	CuRh <sub>2</sub> Se <sub>4</sub>	<i>Fd</i> 3̄ <i>m</i> (227)	SM	—	(k,p,b)	NM	SC*	—	41903 602898 628775 628777
2370	CuTi <sub>2</sub> S <sub>4</sub>	<i>Fd</i> 3̄ <i>m</i> (227)	SM	—	(k,p,b)	FM	SC	—	44609 53336 170227 628916
2371	FeAl <sub>2</sub> O <sub>4</sub>	<i>Fd</i> 3 <i>m</i> (227)	SM	—	(k,p,b)	AFM	—	—	56117 185610 187920 252227
2372	Mg <sub>2</sub> VO <sub>4</sub>	<i>Fd</i> 3̄ <i>m</i> (227)	SM	Fig. 70	(k,p,b)	FM	—	—	76980
2373	Ge <sub>3</sub> N <sub>4</sub>	<i>Fd</i> 3̄ <i>m</i> (227)	Triv.	—	(k,b)	NM	SC	HQ	87767 97568 156338
2374	Sn <sub>3</sub> N <sub>4</sub>	<i>Fd</i> 3̄ <i>m</i> (227)	Triv.	—	(k,b)	NM	—	HQ	89525
2375	SnZn <sub>2</sub> O <sub>4</sub>	<i>Fd</i> 3̄ <i>m</i> (227)	Triv.	—	(k,p,b)	NM	—	—	187039
2376	SnCd <sub>2</sub> O <sub>4</sub>	<i>Fd</i> 3̄ <i>m</i> (227)	Triv.	—	(k,p,b)	NM	—	—	187040
2377	CoAl <sub>2</sub> O <sub>4</sub>	<i>Fd</i> 3̄ <i>m</i> (227)	SM	Fig. 70	(k,p,b)	AFM	—	HQ	290133
2378	Al <sub>2</sub> NiO <sub>4</sub>	<i>Fd</i> 3̄ <i>m</i> (227)	SM	Fig. 71	(k,p,b)	AFM	—	—	608815
2379	MoF <sub>6</sub>	<i>Im</i> 3̄ <i>m</i> (229)	Triv.	—	—	NM	—	HQ	1879

## 2. List of curated materials with flat atomic bands

We have also searched for materials with flat atomic bands defined in Appendix B 1 and which are excluded in Appendix H 1. Since we cannot probe directly the absence of coupling between orbitals of neighboring atoms, we rely on a series of indicators that are easier to access using the database described in Appendix C. Our search criteria are:

- The bands should be extremely flat along all the directions in the BZ.
- The flat bands should be the first set of conduction bands or the last set of valence bands near the Fermi level.
- The DOS peak associated to the set of flat bands should have its center at a maximum distance of 1eV from the Fermi energy and its gaussian width lower than 1eV (see Appendix C 2 b).
- The BRs of the flat bands should be classified by the symmetry eigenvalues as topologically trivial and non-fragile (*i.e.*, LCEBR) [29,43–49,53,54](#).

For flat atomic bands, the electronic states are (exponentially) localized on one occupied Wyckoff position. In addition we could have *flat molecular bands* where the electronic states are (exponentially) localized on several occupied Wyckoff positions. In some cases, these flat molecular bands could be identified by properties such as bonding within molecular unit, such as poly-atomic ions, coordination-complexes and their ions, or neutral molecules. The rigorous distinction between flat atomic bands and flat molecular bands requires a systematic evaluation of the Wannier states which is beyond the scope of this article. For that reason, we include the compounds with flat molecular bands in the list of flat atomic band compounds.

Based on these criteria, we have obtained 1,102 unique materials (1,830 ICSD entries) exhibiting flat atomic bands near the Fermi level. These materials are listed in Table XIII.

Table XIII: Manually curated list of materials with atomic flat bands. We provide in this table the list of the 1,102 entries of atomic flat-band materials, indexed by the first column. The second column gives the chemical formula, the third column the space group symbol (and number in parentheses). The fourth column indicates the topological classification at the Fermi level: topological insulator (TI), topological semi-metal (SM) or trivial insulator (Triv.). The fifth column details the sublattices found for each material and common to every ICSD entries of this material. Here 'k' stands for Kagome, 'p' for pyrochlore, 'b' for bipartite, 's' for split lattice and 'l' for Lieb sublattice. A star superscript after 'k' ('l') indicates that only approximate Kagome (Lieb) sublattices were found (as defined in Appendix D). The sixth column gives the magnetic properties as obtained from [Materials Project](#) (NM for non-magnetic, FM for ferromagnetic, AFM for anti-ferromagnetic, FIM for ferrimagnetic, '—' when the information is not available). The seventh column indicates if the material is known to be superconductor according to the [NIMS Materials Database](#). SC stands for superconductor while SC\* means that alloys based on this material are superconductors. The eighth column tells which material are "high-quality" as defined in Appendix H 1. The last column gives all the ICSD entries related to each material. If a given ICSD has additional sublattices compared to those common to all ICSD entries, a superscript label provides the list of these additional sublattices.

Num.	chem. formula	space group	Topo. at $E_f$	sublat.	magn.	super- conduct.	high quality	ICSDs
1	B <sub>3</sub> H <sub>7</sub> (CO)	P1 (1)	Triv.	—	NM	—	HQ	<a href="#">101171</a>
2	Re <sub>2</sub> Cl <sub>5</sub> O <sub>4</sub>	P1 (1)	SM	—	FM	—	HQ	<a href="#">121111</a>
3	Bi <sub>2</sub> Pb <sub>2</sub> V <sub>2</sub> O <sub>10</sub>	P1 (1)	Triv.	(b)	NM	—	HQ	<a href="#">60577</a>
4	NaBi <sub>3</sub> V <sub>2</sub> O <sub>10</sub>	P1 (1)	Triv.	—	NM	—	HQ	<a href="#">88455</a>
5	SiO <sub>2</sub>	P1 (1)	Triv.	—	NM	—	—	<a href="#">170536</a> <a href="#">39830</a> <sup>(b,s)</sup> <a href="#">56608</a> <sup>(b,s)</sup> <a href="#">75656</a> <sup>(b,s)</sup> <a href="#">75660</a> <sup>(b,s)</sup> <a href="#">75661</a> <sup>(b,s)</sup> <a href="#">75663</a> <a href="#">75666</a> <sup>(b,s)</sup> <a href="#">75667</a> <sup>(b,s)</sup> <a href="#">75670</a> <sup>(b,s)</sup>
6	S <sub>3</sub> N <sub>2</sub> NH <sub>2</sub> BF <sub>4</sub>	P1 (1)	Triv.	—	NM	—	HQ	<a href="#">201705</a>
7	NbCl <sub>3</sub> OS <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> (C <sub>2</sub> H <sub>4</sub> )	P1 (1)	Triv.	—	—	—	—	<a href="#">241969</a>
8	Li <sub>6</sub> Cu(B <sub>4</sub> O <sub>10</sub> )	P1 (1)	SM	—	FM	—	HQ	<a href="#">249215</a>
9	CsB <sub>3</sub> O <sub>5</sub>	P1 (1)	Triv.	(b,s)	—	—	—	<a href="#">673574</a>
10	Ca(HPO <sub>4</sub> )	P1 (1)	Triv.	—	NM	—	HQ	<a href="#">918</a> <a href="#">10504</a> <a href="#">87196</a>
11	Ca((VO)(PO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub>	P1 (1)	Triv.	—	FM	—	HQ	<a href="#">43608</a> <a href="#">67660</a>
12	LiH(C <sub>2</sub> O <sub>4</sub> )(H <sub>2</sub> O)	P1 (1)	Triv.	—	NM	—	HQ	<a href="#">246786</a>
13	(Cu(NH <sub>3</sub> ) <sub>2</sub> )(Sn(OH) <sub>6</sub> )	P <bar>1</bar> (2)	SM	—	FM	—	—	<a href="#">103</a>
14	(F <sub>2</sub> (ZrF <sub>3</sub> (H <sub>2</sub> O) <sub>3</sub> ) <sub>2</sub> )	P <bar>1</bar> (2)	Triv.	—	NM	—	—	<a href="#">1309</a>
15	Tl <sub>2</sub> (Cu(SO <sub>3</sub> ) <sub>2</sub> )	P <bar>1</bar> (2)	SM	(b)	FM	—	—	<a href="#">2896</a>
16	K <sub>3</sub> N(SO <sub>3</sub> ) <sub>2</sub> H <sub>2</sub> O	P <bar>1</bar> (2)	Triv.	—	NM	—	—	<a href="#">8001</a> <a href="#">201190</a>
17	(S <sub>4</sub> N <sub>3</sub> )BiCl <sub>4</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	—	<a href="#">9460</a>
18	(Re <sub>2</sub> O <sub>3</sub> Cl <sub>6</sub> )(ReO <sub>3</sub> Cl) <sub>2</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	—	<a href="#">10302</a>
19	K <sub>3</sub> (ReO <sub>2</sub> (CN) <sub>4</sub> )	P <bar>1</bar> (2)	Triv.	—	NM	—	—	<a href="#">16121</a> <a href="#">26223</a> <a href="#">30430</a>
20	CsKNi(CN) <sub>4</sub>	P <bar>1</bar> (2)	Triv.	—	—	—	—	<a href="#">16399</a>
21	K <sub>4</sub> ((SO <sub>3</sub> ) <sub>2</sub> (NO)) <sub>2</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	—	<a href="#">16879</a>
22	Al <sub>2</sub> (Si <sub>4</sub> O <sub>10</sub> )O	P <bar>1</bar> (2)	Triv.	(k*,b)	NM	—	—	<a href="#">30119</a>
23	Na <sub>2</sub> (B <sub>2</sub> (O <sub>2</sub> ) <sub>2</sub> (OH) <sub>4</sub> )(H <sub>2</sub> O) <sub>6</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	—	<a href="#">30532</a>
24	S <sub>3</sub> N <sub>2</sub> AsF <sub>6</sub>	P <bar>1</bar> (2)	TI	—	FM	—	HQ	<a href="#">31787</a>
25	H <sub>3</sub> OH <sub>3</sub> F <sub>4</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	—	<a href="#">32569</a>
26	(I <sub>3</sub> Cl <sub>2</sub> )(SbCl <sub>6</sub> )	P <bar>1</bar> (2)	Triv.	—	NM	—	HQ	<a href="#">32662</a> <a href="#">26402</a>
27	((CO) <sub>4</sub> MnPH <sub>2</sub> ) <sub>2</sub>	P <bar>1</bar> (2)	Triv.	—	—	—	HQ	<a href="#">33267</a>
28	Na <sub>2</sub> Mg(SO <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	HQ	<a href="#">35767</a>
29	CsH <sub>3</sub> P <sub>2</sub> O <sub>7</sub> (H <sub>2</sub> O)	P <bar>1</bar> (2)	Triv.	(b)	NM	—	—	<a href="#">38033</a>
30	(PtCl <sub>2</sub> (NH <sub>3</sub> ) <sub>4</sub> )(NO <sub>3</sub> ) <sub>2</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	HQ	<a href="#">38066</a>
31	(PdCl <sub>2</sub> (SCl <sub>2</sub> ) <sub>2</sub> )	P <bar>1</bar> (2)	Triv.	—	NM	—	—	<a href="#">39434</a>
32	(ClF <sub>2</sub> )(BiF <sub>6</sub> )	P <bar>1</bar> (2)	Triv.	—	NM	—	HQ	<a href="#">39555</a>
33	MgF <sub>2</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	—	<a href="#">51243</a>
34	MgCl <sub>2</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	—	<a href="#">51247</a>
35	SbF <sub>4</sub> (PO <sub>2</sub> F <sub>2</sub> )	P <bar>1</bar> (2)	Triv.	—	NM	—	HQ	<a href="#">51535</a>
36	PbCuAsO <sub>4</sub>	P <bar>1</bar> (2)	Triv.	(b)	NM	—	HQ	<a href="#">61677</a>
37	Na <sub>4</sub> Cu(AsO <sub>4</sub> ) <sub>2</sub>	P <bar>1</bar> (2)	SM	(b,s)	FM	—	HQ	<a href="#">63058</a>
38	I <sub>4</sub> (SbF <sub>6</sub> ) <sub>2</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	HQ	<a href="#">63301</a>
39	((SCl <sub>2</sub> ) <sub>2</sub> Pt)Cl <sub>2</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	HQ	<a href="#">66013</a>
40	(CN <sub>4</sub> H <sub>8</sub> )(SO <sub>4</sub> )	P <bar>1</bar> (2)	Triv.	—	NM	—	—	<a href="#">74825</a>
41	Na <sub>7</sub> AlH <sub>2</sub> (CO <sub>3</sub> ) <sub>4</sub> F <sub>4</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	HQ	<a href="#">77052</a>
42	K((CH <sub>3</sub> )CO <sub>3</sub> )	P <bar>1</bar> (2)	Triv.	—	NM	—	HQ	<a href="#">77115</a>
43	ReF <sub>7</sub>	P <bar>1</bar> (2)	Triv.	—	NM	—	HQ	<a href="#">78311</a>
44	Ca((HSO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> SO <sub>4</sub> ) <sub>2</sub> )	P <bar>1</bar> (2)	Triv.	—	NM	—	HQ	<a href="#">85073</a>
45	(Mg(H <sub>2</sub> O) <sub>6</sub> )(CoCl <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub> )	P <bar>1</bar> (2)	SM	—	AFM	—	HQ	<a href="#">96559</a>

46	Na <sub>2</sub> (HPO <sub>4</sub> )(H <sub>2</sub> O)	P̄I (2)	Triv.	—	NM	—	HQ	108838
47	(CH <sub>3</sub> ) <sub>2</sub> NOSiH <sub>2</sub> Cl	P̄I (2)	Triv.	—	NM	—	—	110528
48	C <sub>3</sub> F <sub>6</sub>	P̄I (2)	Triv.	—	NM	—	HQ	151184
49	AgSc(CrO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P̄I (2)	Triv.	—	NM	—	HQ	156676
50	Cu(O <sub>2</sub> N <sub>2</sub> CN) <sub>2</sub> (N <sub>2</sub> C <sub>4</sub> H <sub>4</sub> )	P̄I (2)	SM	—	—	—	HQ	168724
51	Cu(NH <sub>3</sub> ) <sub>4</sub> (ReO <sub>4</sub> ) <sub>2</sub>	P̄I (2)	SM	—	—	—	HQ	169583
52	Ca <sub>2</sub> CuTe <sub>4</sub> O <sub>10</sub> Cl <sub>2</sub>	P̄I (2)	SM	(b,s)	FM	—	HQ	171007
53	(NH <sub>4</sub> )(HSeO <sub>3</sub> )	P̄I (2)	Triv.	—	NM	—	HQ	171372
54	Na <sub>2</sub> S <sub>2</sub> O <sub>8</sub>	P̄I (2)	Triv.	—	NM	—	HQ	171374
55	Cu(SO <sub>3</sub> CF <sub>3</sub> ) <sub>2</sub>	P̄I (2)	SM	(b)	FM	—	HQ	172335
56	((C <sub>2</sub> (NH <sub>2</sub> ) <sub>2</sub> )(NH)N <sub>2</sub> ) <sub>2</sub> (SiF <sub>6</sub> )	P̄I (2)	Triv.	—	NM	—	—	180801
57	(Cd(NCS) <sub>2</sub> (CS(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub>	P̄I (2)	Triv.	—	—	—	HQ	187240
58	Tl <sub>4</sub> Cu(TeO <sub>6</sub> )	P̄I (2)	TI	(b)	FM	—	HQ	187561
59	Y <sub>2</sub> Cu(TeO <sub>3</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub>	P̄I (2)	SM	(b,s)	FM	—	HQ	194348
60	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )(H(C <sub>2</sub> O <sub>4</sub> ))(H <sub>2</sub> C <sub>2</sub> O <sub>4</sub> ) <sub>0.5</sub>	P̄I (2)	Triv.	—	NM	—	—	195083
61	(XeF <sub>3</sub> )(BiF <sub>6</sub> )	P̄I (2)	Triv.	—	NM	—	—	200043
62	Al <sub>4</sub> Si <sub>8</sub> O <sub>22</sub>	P̄I (2)	Triv.	(k*,b)	NM	—	—	201706
63	Ca <sub>2</sub> Cu(OH) <sub>4</sub> (B(OH) <sub>4</sub> ) <sub>2</sub>	P̄I (2)	SM	—	FM	—	HQ	202148
64	Fe(H <sub>2</sub> O) <sub>2</sub> (C <sub>4</sub> S <sub>4</sub> )(H <sub>2</sub> O) <sub>4</sub>	P̄I (2)	Triv.	—	—	—	HQ	203234
65	Li <sub>3</sub> CuB <sub>3</sub> O <sub>7</sub>	P̄I (2)	Triv.	—	NM	—	HQ	237524
66	K <sub>3</sub> Zn <sub>2</sub> Cl <sub>7</sub>	P̄I (2)	Triv.	—	NM	—	—	239665
67	Sn(SO <sub>4</sub> )	P̄I (2)	Triv.	—	NM	—	—	245906 245907
68	Tl <sub>4</sub> (IO <sub>3</sub> ) <sub>6</sub>	P̄I (2)	Triv.	—	NM	—	HQ	247060
69	(In <sub>2</sub> (SeO <sub>3</sub> ) <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> )(H <sub>2</sub> O) <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub>	P̄I (2)	Triv.	—	NM	—	HQ	249780
70	Fe(NCS) <sub>2</sub> (OC(CH <sub>3</sub> ) <sub>2</sub> ) <sub>2</sub>	P̄I (2)	Triv.	—	FM	—	HQ	250699
71	Hg(CH <sub>3</sub> SO <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P̄I (2)	Triv.	—	NM	—	HQ	251311
72	(C <sub>2</sub> H <sub>10</sub> N <sub>2</sub> )Cu(H <sub>2</sub> O) <sub>2</sub> (V <sub>2</sub> O <sub>2</sub> F <sub>8</sub> )	P̄I (2)	SM	—	FM	—	—	251432
73	Na <sub>4</sub> NiTeO <sub>6</sub>	P̄I (2)	Triv.	(b)	—	—	—	253698
74	K <sub>3</sub> (TcO <sub>2</sub> (CN) <sub>4</sub> )	P̄I (2)	Triv.	—	NM	—	HQ	260824
75	(C <sub>2</sub> H <sub>8</sub> N) <sub>2</sub> (Sn(CH <sub>3</sub> ) <sub>2</sub> Cl <sub>4</sub> )	P̄I (2)	Triv.	—	NM	—	—	261582
76	((Cu(H <sub>2</sub> O) <sub>2</sub> )Cl <sub>2</sub> (CdCl <sub>2</sub> ))(H <sub>2</sub> O) <sub>2</sub>	P̄I (2)	SM	—	FM	—	HQ	280299
77	((N <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ((N <sub>4</sub> C) <sub>2</sub> N <sub>2</sub> ))(N <sub>2</sub> H <sub>4</sub> ) <sub>2</sub>	P̄I (2)	Triv.	—	NM	—	—	280661
78	Te <sub>4</sub> (HfCl <sub>6</sub> )	P̄I (2)	Triv.	—	NM	—	HQ	401589
79	(CF <sub>3</sub> ) <sub>2</sub> O <sub>3</sub>	P̄I (2)	Triv.	—	NM	—	HQ	401780
80	(Li(NH <sub>3</sub> ) <sub>4</sub> ) <sub>2</sub> Te <sub>2</sub>	P̄I (2)	Triv.	—	NM	—	—	409556
81	(SeCl <sub>3</sub> )(MoOCl <sub>4</sub> )	P̄I (2)	TI	(b)	FM	—	HQ	410101
82	Ni(NH <sub>2</sub> )(SO <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub>	P̄I (2)	Triv.	—	AFM	—	—	410198
83	(Cu(C <sub>2</sub> N <sub>2</sub> H <sub>8</sub> ) <sub>2</sub> )(Ni(CN) <sub>4</sub> )	P̄I (2)	SM	—	FM	—	—	411632
84	PbF(AsF <sub>6</sub> )	P̄I (2)	Triv.	—	NM	—	HQ	411788
85	AuXe <sub>2</sub> (SbF <sub>6</sub> ) <sub>2</sub>	P̄I (2)	SM	—	FM	—	HQ	412106
86	Au <sub>2</sub> Xe <sub>2</sub> F(SbF <sub>6</sub> ) <sub>3</sub>	P̄I (2)	Triv.	—	NM	—	HQ	412107
87	(Cu(NH <sub>3</sub> ) <sub>4</sub> )(N(NO <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub>	P̄I (2)	SM	—	FM	—	—	412606
88	(Pd(NH <sub>3</sub> ) <sub>4</sub> )(N(NO <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub>	P̄I (2)	Triv.	—	NM	—	—	412607
89	KNaS <sub>2</sub> O <sub>7</sub>	P̄I (2)	Triv.	—	NM	—	HQ	413050
90	(F <sub>5</sub> S)(NCS)	P̄I (2)	Triv.	—	NM	—	HQ	413754
91	Li <sub>4</sub> (PO <sub>2</sub> NH) <sub>4</sub> (H <sub>2</sub> O) <sub>4</sub>	P̄I (2)	Triv.	—	NM	—	—	415548
92	(ReO <sub>3</sub> Cl)(ReOCl <sub>4</sub> )	P̄I (2)	Triv.	—	FM	—	HQ	416429
93	(Cs <sub>2</sub> (H <sub>6</sub> Te <sub>2</sub> O <sub>10</sub> ))(Te(OH) <sub>6</sub> )	P̄I (2)	Triv.	—	—	—	—	417437
94	Ir(PO <sub>3</sub> ) <sub>3</sub>	P̄I (2)	Triv.	(b)	NM	—	HQ	419717
95	Pd(NH <sub>3</sub> ) <sub>2</sub> (NO <sub>2</sub> ) <sub>2</sub>	P̄I (2)	Triv.	—	NM	—	HQ	420291
96	Pt(H <sub>2</sub> O) <sub>4</sub> (SbF <sub>6</sub> ) <sub>2</sub>	P̄I (2)	Triv.	—	NM	—	HQ	421861
97	Rb <sub>3</sub> In( IO <sub>3</sub> ) <sub>6</sub>	P̄I (2)	Triv.	(b)	NM	—	HQ	422058
98	Ag <sub>2</sub> BaCu(VO <sub>4</sub> ) <sub>2</sub>	P̄I (2)	TI	(b,s)	FM	—	HQ	422132
99	H <sub>6</sub> O <sub>12</sub> P <sub>4</sub> Rb <sub>2</sub>	P̄I (2)	Triv.	(b)	NM	—	HQ	423682
100	H <sub>6</sub> Cs <sub>2</sub> O <sub>12</sub> P <sub>4</sub>	P̄I (2)	Triv.	(b)	NM	—	HQ	423683
101	Ba <sub>2</sub> (Pd(HS <sub>2</sub> O <sub>7</sub> ) <sub>2</sub> (S <sub>3</sub> O <sub>10</sub> ) <sub>2</sub> )	P̄I (2)	Triv.	—	NM	—	—	425466
102	NaClO <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub>	P̄I (2)	Triv.	—	NM	—	HQ	425697
103	CuSb <sub>6</sub> O <sub>8</sub> (SO <sub>4</sub> ) <sub>2</sub>	P̄I (2)	SM	(b)	FM	—	—	428356
104	Cs(HS <sub>2</sub> O <sub>7</sub> )	P̄I (2)	Triv.	—	NM	—	HQ	428724
105	PbF(SbF <sub>6</sub> )	P̄I (2)	Triv.	—	NM	—	HQ	429016
106	(PCl <sub>4</sub> ) <sub>2</sub> (Re <sub>2</sub> Cl <sub>10</sub> )	P̄I (2)	Triv.	—	FM	—	HQ	410188

107	Ag(TaF <sub>6</sub> ) <sub>2</sub>	P $\bar{I}$ (2)	SM	(b,s)	FM	—	HQ	62543
108	Ag(BiF <sub>6</sub> ) <sub>2</sub>	P $\bar{I}$ (2)	SM	(b,s)	FM	—	HQ	79879
109	Na(AgZr <sub>2</sub> F <sub>11</sub> )	P $\bar{I}$ (2)	SM	—	FM	—	HQ	65179
110	NaCu(Zr <sub>2</sub> F <sub>11</sub> )	P $\bar{I}$ (2)	SM	—	FM	—	HQ	78869
111	(InCl <sub>2</sub> (NH <sub>3</sub> ) <sub>4</sub> )(In(NH <sub>3</sub> ) <sub>2</sub> Cl <sub>4</sub> )	P $\bar{I}$ (2)	Triv.	—	NM	—	—	281343
112	(CH <sub>3</sub> )NSOF <sub>2</sub>	P $\bar{I}$ (2)	Triv.	—	NM	—	HQ	237988
113	Ba <sub>6</sub> Mg <sub>11</sub> F <sub>34</sub>	P $\bar{I}$ (2)	Triv.	(b)	NM	—	—	413125
114	BaCoP <sub>2</sub> O <sub>7</sub>	P $\bar{I}$ (2)	Triv.	(b)	FM	—	HQ	202853
115	((C <sub>2</sub> H <sub>4</sub> (OH))NH <sub>3</sub> )(CuBr <sub>3</sub> )	P $\bar{I}$ (2)	Triv.	—	FM	—	—	110471
116	Ca(H <sub>2</sub> PO <sub>4</sub> ) <sub>2</sub>	P $\bar{I}$ (2)	Triv.	—	NM	—	—	2632 2633 <sup>(b)</sup>
117	Ca(C <sub>2</sub> O <sub>4</sub> )(H <sub>2</sub> O) <sub>3</sub>	P $\bar{I}$ (2)	Triv.	—	NM	—	—	77096 159351
118	(Co(H <sub>2</sub> O) <sub>6</sub> )(SnF <sub>3</sub> ) <sub>2</sub>	P $\bar{I}$ (2)	SM	—	AFM	—	—	27799
119	(Ni(H <sub>2</sub> O) <sub>6</sub> )(SnF <sub>3</sub> ) <sub>2</sub>	P $\bar{I}$ (2)	Triv.	—	AFM	—	HQ	79718
120	(Cd(H <sub>2</sub> O) <sub>6</sub> )(SnF <sub>3</sub> ) <sub>2</sub>	P $\bar{I}$ (2)	Triv.	—	—	—	HQ	166590
121	Cu(ReO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub>	P $\bar{I}$ (2)	SM	—	—	—	HQ	402669
122	(Ni(H <sub>2</sub> O) <sub>4</sub> )(ReO <sub>4</sub> ) <sub>2</sub>	P $\bar{I}$ (2)	Triv.	—	FM	—	HQ	402773
123	Co(H <sub>2</sub> O) <sub>4</sub> (ReO <sub>4</sub> ) <sub>2</sub>	P $\bar{I}$ (2)	SM	—	FM	—	HQ	402964
124	Cs <sub>4</sub> Cu(Si <sub>2</sub> O <sub>7</sub> )	P $\bar{I}$ (2)	SM	(b)	FM	—	HQ	50444
125	Rb <sub>4</sub> (CuSi <sub>2</sub> O <sub>7</sub> )	P $\bar{I}$ (2)	SM	(b,s)	FM	—	HQ	85405
126	CuZn <sub>2</sub> (AsO <sub>4</sub> ) <sub>2</sub>	P $\bar{I}$ (2)	SM	(b)	FM	—	—	18115 26839 100249
127	Cd <sub>2</sub> Cu(PO <sub>4</sub> ) <sub>2</sub>	P $\bar{I}$ (2)	SM	(b)	FM	—	HQ	249777
128	CuH <sub>10</sub> (AsO <sub>4</sub> ) <sub>4</sub>	P $\bar{I}$ (2)	SM	—	FM	—	—	59158
129	Na <sub>2</sub> Co(SeO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P $\bar{I}$ (2)	SM	—	—	—	HQ	98683
130	Na <sub>2</sub> Ni(SeO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P $\bar{I}$ (2)	Triv.	—	FM	—	HQ	98684
131	(Co(O <sub>2</sub> N <sub>2</sub> CN) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> (N <sub>2</sub> C <sub>4</sub> H <sub>4</sub> ))(H <sub>2</sub> O) <sub>2</sub>	P $\bar{I}$ (2)	SM	—	—	—	—	168723
132	Fe(SC(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> (NCS) <sub>2</sub>	P $\bar{I}$ (2)	Triv.	—	FM	—	—	10452
133	H <sub>3</sub> BO <sub>3</sub>	P $\bar{I}$ (2)	Triv.	—	NM	—	—	24711 52290 <sup>(b)</sup> 61354 <sup>(b)</sup> 61365 <sup>(b)</sup>
134	H <sub>3</sub> OB $\bar{F}$ <sub>4</sub>	P $\bar{I}$ (2)	Triv.	—	NM	—	HQ	15591
135	Hg(Mn(CO) <sub>5</sub> ) <sub>2</sub>	P $\bar{I}$ (2)	Triv.	—	NM	—	—	16124
136	(Br <sub>3</sub> )(AsF <sub>6</sub> )	P $\bar{I}$ (2)	Triv.	—	NM	—	HQ	33811
137	K <sub>2</sub> (O <sub>2</sub> (SO <sub>3</sub> ) <sub>2</sub> )	P $\bar{I}$ (2)	Triv.	—	NM	—	—	16972 54024
138	Cs <sub>2</sub> Cu(Cr <sub>2</sub> O <sub>7</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P $\bar{I}$ (2)	SM	—	FM	—	HQ	156678
139	K <sub>6</sub> (CuSi <sub>2</sub> O <sub>8</sub> )	P $\bar{I}$ (2)	SM	(b,s)	FM	—	HQ	85404
140	Cs <sub>6</sub> (NiSi <sub>2</sub> O <sub>8</sub> )	P $\bar{I}$ (2)	Triv.	(b,s)	NM	—	HQ	409506
141	K(HCO <sub>3</sub> )	P $\bar{I}$ (2)	Triv.	—	NM	—	—	157166
142	K(HSeO <sub>3</sub> )	P $\bar{I}$ (2)	Triv.	—	NM	—	HQ	20862
143	KMgH(CO <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub>	P $\bar{I}$ (2)	Triv.	—	NM	—	HQ	63137 63138
144	KNi(H(CO <sub>3</sub> ) <sub>2</sub> )(H <sub>2</sub> O) <sub>4</sub>	P $\bar{I}$ (2)	Triv.	—	AFM	—	HQ	68710
145	NaLa(SO <sub>4</sub> ) <sub>2</sub>	P $\bar{I}$ (2)	Triv.	—	NM	—	—	20354
146	Al <sub>2</sub> O(SiO <sub>4</sub> )	P $\bar{I}$ (2)	Triv.	—	NM	—	—	16970 <sup>(b)</sup> 16976 <sup>(b)</sup> 27771 <sup>(b)</sup> 27985 28272 77538 <sup>(b)</sup> 77539 <sup>(b)</sup> 77540 <sup>(b)</sup> 77541 <sup>(b)</sup> 77542 <sup>(b)</sup> 83450 <sup>(b)</sup> 83451 <sup>(b)</sup> 83452 <sup>(b)</sup> 83453 <sup>(b)</sup> 83454 <sup>(b)</sup> 85742 <sup>(b)</sup> 86341 <sup>(b)</sup> 100455 <sup>(b)</sup> 100456 <sup>(b)</sup> 100457 <sup>(b)</sup> 167293 <sup>(b)</sup> 167294 <sup>(b)</sup> 167295 <sup>(b)</sup>
147	Li <sub>6</sub> Ga <sub>2</sub> (BO <sub>3</sub> ) <sub>4</sub>	P $\bar{I}$ (2)	Triv.	—	NM	—	—	9987
148	Li <sub>4</sub> (P <sub>2</sub> O <sub>7</sub> )	P $\bar{I}$ (2)	Triv.	—	NM	—	HQ	59243 <sup>(b)</sup> 246859 248414 <sup>(b)</sup>
149	LiAl(PO <sub>4</sub> )(OH)	P $\bar{I}$ (2)	Triv.	(b)	NM	—	HQ	68921
150	(Mg(H <sub>2</sub> O) <sub>6</sub> )(S <sub>2</sub> O <sub>6</sub> )	P $\bar{I}$ (2)	Triv.	—	FM	—	—	1834
151	(Zn(H <sub>2</sub> O) <sub>6</sub> )(S <sub>2</sub> O <sub>6</sub> )	P $\bar{I}$ (2)	Triv.	—	NM	—	—	1836
152	(((Mn(CO) <sub>5</sub> ) <sub>2</sub> In) <sub>2</sub> Cl <sub>2</sub> )	P $\bar{I}$ (2)	Triv.	—	NM	—	—	889
153	Li <sub>6</sub> CuB <sub>4</sub> O <sub>10</sub>	P $\bar{I}$ (2)	SM	(b)	FM	—	HQ	237526
154	Na <sub>2</sub> Ca(P <sub>2</sub> O <sub>7</sub> )	P $\bar{I}$ (2)	Triv.	—	NM	—	HQ	89468
155	Na <sub>4</sub> (WO <sub>2</sub> N <sub>2</sub> )	P $\bar{I}$ (2)	Triv.	(b)	NM	—	HQ	73101
156	K(C(CN) <sub>3</sub> )	P $\bar{I}$ (2)	Triv.	—	NM	—	—	77046 428779
157	Na(ClO <sub>2</sub> )(H <sub>2</sub> O) <sub>3</sub>	P $\bar{I}$ (2)	Triv.	—	NM	—	—	1858 1954
158	Na(BrO <sub>2</sub> )(H <sub>2</sub> O) <sub>3</sub>	P $\bar{I}$ (2)	Triv.	—	NM	—	HQ	74654
159	Os <sub>3</sub> (CO) <sub>9</sub> Se <sub>2</sub>	P $\bar{I}$ (2)	Triv.	(b)	NM	—	—	30552
160	Ru <sub>3</sub> Se <sub>2</sub> (CO) <sub>9</sub>	P $\bar{I}$ (2)	Triv.	(b)	NM	—	—	72764
161	Pb <sub>4</sub> Cu(SO <sub>4</sub> ) <sub>2</sub> (OH) <sub>6</sub>	P $\bar{I}$ (2)	SM	(b)	FM	—	HQ	380382
162	PbBi <sub>6</sub> O <sub>4</sub> (PO <sub>4</sub> ) <sub>4</sub>	P $\bar{I}$ (2)	Triv.	—	NM	—	—	91258

163	Mg(SO <sub>4</sub> )(H <sub>2</sub> O) <sub>5</sub>	P $\bar{1}$ (2)	Triv.	—	NM	—	—	2776
164	((SCl <sub>2</sub> )S(SCl))(AsF <sub>6</sub> )	P $\bar{1}$ (2)	Triv.	—	NM	—	HQ	75451 154804
165	Ca <sub>2</sub> Ba(Si <sub>3</sub> O <sub>9</sub> )	P $\bar{1}$ (2)	Triv.	—	NM	—	—	24426
166	K <sub>2</sub> Co(H <sub>2</sub> P <sub>2</sub> O <sub>7</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P $\bar{1}$ (2)	SM	—	AFM	—	—	261585
167	Tl <sub>2</sub> Co(H <sub>2</sub> P <sub>2</sub> O <sub>7</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P $\bar{1}$ (2)	SM	(b)	AFM	—	—	416650
168	Tl <sub>2</sub> Ni(H <sub>2</sub> P <sub>2</sub> O <sub>7</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P $\bar{1}$ (2)	Triv.	(b)	FM	—	—	416651
169	Rb <sub>2</sub> Cu(H <sub>2</sub> PO <sub>4</sub> ) <sub>4</sub>	P $\bar{1}$ (2)	SM	(b)	FM	—	—	421806
170	Rb <sub>2</sub> Co(H <sub>2</sub> PO <sub>4</sub> ) <sub>4</sub>	P $\bar{1}$ (2)	SM	(b)	AFM	—	—	421807
171	Rb <sub>2</sub> Ni(H <sub>2</sub> PO <sub>4</sub> ) <sub>4</sub>	P $\bar{1}$ (2)	Triv.	(b)	FM	—	—	421808
172	Y <sub>2</sub> (SiO <sub>4</sub> )(CO <sub>3</sub> )	P $\bar{1}$ (2)	Triv.	—	NM	—	HQ	88878
173	Y <sub>6</sub> OsI <sub>10</sub>	P $\bar{1}$ (2)	Triv.	(b)	NM	—	HQ	74649
174	Y <sub>6</sub> IrI <sub>10</sub>	P $\bar{1}$ (2)	SM	(b)	NM	—	HQ	74650
175	(PtY <sub>6</sub> )I <sub>10</sub>	P $\bar{1}$ (2)	Triv.	(b)	NM	—	HQ	424468
176	NH <sub>4</sub> (POS(NH <sub>2</sub> ) <sub>2</sub> )	P2 <sub>1</sub> (4)	Triv.	—	NM	—	HQ	25702
177	Na <sub>3</sub> Sr(PO <sub>4</sub> )(CO <sub>3</sub> )	P2 <sub>1</sub> (4)	Triv.	—	NM	—	HQ	39559
178	(BrF <sub>3</sub> )(AuF <sub>3</sub> )	P2 <sub>1</sub> (4)	Triv.	—	NM	—	HQ	93481
179	((CH <sub>3</sub> ) <sub>3</sub> NH)(ClO <sub>4</sub> )	P2 <sub>1</sub> (4)	Triv.	—	NM	—	—	110284
180	F <sub>5</sub> TeNH <sub>2</sub>	P2 <sub>1</sub> (4)	Triv.	—	NM	—	HQ	171449
181	(Li(BH <sub>4</sub> )) <sub>3</sub> (NH <sub>2</sub> NH <sub>2</sub> )	P2 <sub>1</sub> (4)	Triv.	—	NM	—	—	189247
182	KTeOF <sub>3</sub>	P2 <sub>1</sub> (4)	Triv.	—	NM	—	HQ	201155
183	Rb <sub>4</sub> (CO <sub>4</sub> )	P2 <sub>1</sub> (4)	Triv.	—	NM	—	—	245442
184	Na(HCO <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub>	P2 <sub>1</sub> (4)	Triv.	—	NM	—	HQ	250496
185	(Zn(NH <sub>3</sub> ) <sub>2</sub> Se <sub>4</sub> )	P2 <sub>1</sub> (4)	Triv.	—	NM	—	HQ	425783
186	Cs <sub>2</sub> (S <sub>5</sub> O <sub>16</sub> )	P2 <sub>1</sub> (4)	Triv.	—	—	—	—	428769
187	Na <sub>3</sub> (FeF <sub>6</sub> )	P2 <sub>1</sub> (4)	SM	(b)	—	—	HQ	20157
188	CaBa(CO <sub>3</sub> ) <sub>2</sub>	P2 <sub>1</sub> (4)	Triv.	—	NM	—	—	24442 36201 157982
189	Cs(AsF <sub>4</sub> )	P2 <sub>1</sub> (4)	Triv.	—	NM	—	HQ	54852 413041
190	Hg(C <sub>2</sub> O <sub>4</sub> )	P2 <sub>1</sub> (4)	Triv.	—	NM	—	HQ	56458 56459 151138 151139
191	La(OH) <sub>2</sub> NO <sub>3</sub>	P2 <sub>1</sub> (4)	Triv.	—	—	—	—	243495
192	Rb(SO <sub>3</sub> (CF <sub>3</sub> ))	P2 <sub>1</sub> (4)	Triv.	—	NM	—	HQ	171662 415817
193	Cs(SO <sub>3</sub> (CF <sub>3</sub> ))	P2 <sub>1</sub> (4)	Triv.	—	NM	—	HQ	415056
194	I <sub>2</sub> Sb <sub>2</sub> F <sub>11</sub>	C2 (5)	SM	—	FM	—	HQ	6031
195	As(CN) <sub>3</sub>	C2 (5)	Triv.	—	NM	—	HQ	18199 35330
196	Sr <sub>3</sub> (Si <sub>3</sub> O <sub>9</sub> )	C2 (5)	Triv.	—	—	—	HQ	32542
197	Na <sub>2</sub> (S <sub>4</sub> O <sub>6</sub> )(H <sub>2</sub> O) <sub>2</sub>	C2 (5)	Triv.	—	NM	—	HQ	40833
198	K <sub>2</sub> LiBO <sub>3</sub>	C2 (5)	Triv.	—	NM	—	HQ	60949
199	BaCu(B <sub>2</sub> O <sub>5</sub> )	C2 (5)	SM	(b)	FM	—	HQ	84683
200	Cs <sub>4</sub> (CO <sub>4</sub> )	C2 (5)	Triv.	—	—	—	—	245453 245450 245452
201	Ca(NH <sub>2</sub> BH <sub>3</sub> ) <sub>2</sub>	C2 (5)	Triv.	—	NM	—	HQ	246139 246140
202	(NO <sub>2</sub> )(Ga(NO <sub>3</sub> ) <sub>4</sub> )	C2 (5)	Triv.	—	NM	—	HQ	280269 280270
203	Ba <sub>2</sub> (VO)(PO <sub>4</sub> ) <sub>2</sub>	C2 (5)	Triv.	(b)	—	—	HQ	405256
204	Pt(NH <sub>3</sub> ) <sub>2</sub> (NO <sub>2</sub> ) <sub>2</sub>	C2 (5)	Triv.	—	NM	—	HQ	420292
205	CsMn(HP <sub>3</sub> O <sub>10</sub> )	C2 (5)	Triv.	(b)	FM	—	HQ	39871 51089
206	CsGa(HP <sub>3</sub> O <sub>10</sub> )	C2 (5)	Triv.	(b)	NM	—	HQ	409692
207	Li <sub>4</sub> (CO <sub>4</sub> )	C2 (5)	Triv.	—	NM	—	—	245393 <sup>(b)</sup> 245395 245397 245404 245405
208	Ca <sub>3</sub> ZnGeO <sub>2</sub> (Ge <sub>4</sub> O <sub>12</sub> )	C2 (5)	Triv.	(b,s)	NM	—	—	252464
209	F <sub>6</sub> O <sub>4</sub> Os <sub>2</sub>	Pc (7)	Triv.	—	NM	—	HQ	240330
210	(NH <sub>4</sub> )Na(PO <sub>3</sub> F)(H <sub>2</sub> O)	Pc (7)	Triv.	—	NM	—	HQ	240974
211	CuCO <sub>3</sub>	Cm (8)	SM	—	FM	—	—	6179
212	K(NO <sub>2</sub> )	Cm (8)	Triv.	—	NM	—	—	26764 36202
213	(C(NH <sub>2</sub> ) <sub>3</sub> ) <sub>2</sub> (TiF <sub>6</sub> )	Cm (8)	Triv.	—	NM	—	HQ	36529
214	K <sub>3</sub> (VO(O <sub>2</sub> ) <sub>2</sub> (CO <sub>3</sub> ))	Cm (8)	Triv.	—	NM	—	HQ	60813
215	(C(NH <sub>2</sub> ) <sub>3</sub> )(NO <sub>3</sub> )	Cm (8)	Triv.	—	NM	—	HQ	75221
216	LiCsSO <sub>3</sub> (H <sub>2</sub> O) <sub>2</sub>	Cm (8)	Triv.	—	NM	—	HQ	200780
217	SrBO <sub>2</sub> F	Cm (8)	Triv.	—	—	—	—	674232
218	Ca <sub>4</sub> LaO(BO <sub>3</sub> ) <sub>3</sub>	Cm (8)	Triv.	—	NM	—	HQ	93152 180596
219	In(PO <sub>3</sub> ) <sub>3</sub>	Cc (9)	Triv.	(b)	NM	—	HQ	39710 421261
220	Ca(C <sub>2</sub> O <sub>4</sub> )	P2/m (10)	Triv.	—	NM	—	HQ	246004 246005
221	AsSbF <sub>8</sub>	P2 <sub>1</sub> /m (11)	Triv.	—	NM	—	HQ	9920
222	S <sub>4</sub> N <sub>4</sub> AsF <sub>5</sub>	P2 <sub>1</sub> /m (11)	Triv.	—	NM	—	HQ	14083

223	Cs(HSO <sub>4</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	HQ	24377
224	(C(NH <sub>2</sub> ) <sub>3</sub> ) <sub>2</sub> (MoO <sub>4</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	—	49910
225	Cu(NH <sub>3</sub> ) <sub>4</sub> (MnO <sub>4</sub> ) <sub>2</sub>	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	SM	—	FM	—	—	61243
226	(Ag(H <sub>2</sub> O) <sub>2</sub> )(MnF <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	FM	—	—	74965
227	Na <sub>3</sub> OsO <sub>4</sub> (OH) <sub>2</sub>	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	SM	(b)	FM	—	HQ	172060
228	K <sub>2</sub> (HCO <sub>3</sub> )F(H <sub>2</sub> O)	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	HQ	188659
229	Cs((CF <sub>3</sub> ) <sub>2</sub> BF <sub>2</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	HQ	200869
230	((CH <sub>3</sub> ) <sub>3</sub> (CH <sub>2</sub> Br)N)(BF <sub>4</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	—	249155
231	((CO) <sub>2</sub> (CF <sub>2</sub> )(Fe(CO) <sub>3</sub> ) <sub>2</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	—	279643
232	((ClCH <sub>2</sub> )(CH <sub>3</sub> ) <sub>3</sub> N)(BF <sub>4</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	—	320194
233	(C <sub>2</sub> H <sub>6</sub> N) <sub>3</sub> PO	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	—	409222
234	(PBr <sub>3</sub> H)(As <sub>2</sub> F <sub>11</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	—	412035
235	((CH <sub>3</sub> ) <sub>3</sub> NH)(ClO <sub>4</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	—	110285
236	((CH <sub>3</sub> ) <sub>3</sub> NH)(BF <sub>4</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	—	171202
237	PbFeGe <sub>3</sub> O <sub>10</sub> H <sub>4</sub>	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	FM	—	—	5326 290250
238	Co <sub>2</sub> (CO) <sub>8</sub>	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	—	16567 37252 37253
239	Cs(H <sub>2</sub> PO <sub>4</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	(b)	NM	—	—	79608 79609 200895
240	K <sub>2</sub> (AlF <sub>5</sub> )(H <sub>2</sub> O)	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	HQ	81863
241	K <sub>2</sub> (S <sub>2</sub> O <sub>5</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	HQ	16701 31817 60025
242	KTi(SO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O)	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	SM	—	FM	—	HQ	159479
243	KLi <sub>2</sub> (OH) <sub>3</sub>	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	NM	—	HQ	65148
244	Ag(Mo <sub>3</sub> P <sub>2</sub> O <sub>14</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	SM	(b)	FM	—	—	74937
245	K(Mo <sub>3</sub> P <sub>2</sub> O <sub>14</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	SM	(b)	FM	—	—	78069
246	K(Os(NO)F <sub>5</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	SM	—	FM	—	—	166586
247	Cs(Os(NO)F <sub>5</sub> )	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	SM	—	—	—	—	166587
248	NaFe(SO <sub>4</sub> )F(H <sub>2</sub> O) <sub>2</sub>	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	AFM	—	—	169110
249	NaNi(SO <sub>4</sub> )F(H <sub>2</sub> O) <sub>2</sub>	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	Triv.	—	FM	—	—	169112
250	La <sub>2</sub> Br <sub>5</sub>	<i>P</i> 2 <sub>1</sub> / <i>m</i> (11)	SM	(b)	FM	—	HQ	65480
251	NbCl <sub>4</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	(b,s)	NM	—	HQ	1010
252	(Cu(NH <sub>3</sub> ) <sub>4</sub> )(I <sub>2</sub> ) <sub>2</sub>	<i>C</i> 2/ <i>m</i> (12)	SM	—	FM	—	HQ	4072
253	AgCo(CO) <sub>4</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	—	31388
254	(I <sub>4</sub> )(AsF <sub>6</sub> ) <sub>2</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	HQ	37001
255	K <sub>2</sub> (Pd(NO <sub>2</sub> ) <sub>2</sub> Cl <sub>2</sub> )	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	HQ	39851
256	O <sub>2</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	FM	—	—	43074 18311 173932 173933
257	(I <sub>2</sub> (IO <sub>3</sub> CO) <sub>3</sub> ) <sub>2</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	HQ	68901
258	Li <sub>8</sub> Bi <sub>2</sub> PdO <sub>10</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	(b)	NM	—	HQ	73000
259	(NH <sub>4</sub> ) <sub>2</sub> (Cu(H <sub>2</sub> O) <sub>2</sub> (PO <sub>3</sub> F) <sub>2</sub> )	<i>C</i> 2/ <i>m</i> (12)	SM	—	FM	—	HQ	74551
260	(Ni(N(CN) <sub>2</sub> ) <sub>2</sub> )(HCON(CH <sub>3</sub> ) <sub>2</sub> ) <sub>2</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	FM	—	—	109784
261	(Co(C <sub>2</sub> N <sub>3</sub> ) <sub>2</sub> )(HCON(CH <sub>3</sub> ) <sub>2</sub> ) <sub>2</sub>	<i>C</i> 2/ <i>m</i> (12)	SM	—	FM	—	—	109797
262	Cs <sub>2</sub> (Pt(C <sub>2</sub> O <sub>4</sub> )F <sub>4</sub> )	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	—	109890
263	((CH <sub>3</sub> ) <sub>3</sub> NH) <sub>2</sub> (SnF <sub>6</sub> )(H <sub>2</sub> O) <sub>2</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	—	110229
264	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )I	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	HQ	110536 110537
265	Rb <sub>4</sub> (Cl <sub>12</sub> C(ZrCl) <sub>6</sub> )	<i>C</i> 2/ <i>m</i> (12)	Triv.	(b)	NM	—	HQ	165401
266	(N(CH <sub>3</sub> ) <sub>4</sub> ) <sub>2</sub> Cs(Co(CN) <sub>6</sub> )	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	—	168575
267	(NH <sub>4</sub> ) <sub>2</sub> C <sub>4</sub> O <sub>4</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	HQ	172053 172054
268	(NH <sub>4</sub> ) <sub>2</sub> S <sub>8</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	—	187244
269	Mg(ClO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	HQ	261132
270	C <sub>22</sub> F <sub>14</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	—	411879 411880
271	NaBa(PO <sub>2</sub> NH) <sub>3</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	—	415259
272	Na <sub>2</sub> (CrF <sub>6</sub> )(HF) <sub>2</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	FM	—	HQ	418677
273	Rb <sub>2</sub> (C <sub>2</sub> )(NH <sub>3</sub> ) <sub>2</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	—	—	HQ	425117
274	NaMn(Zr <sub>2</sub> F <sub>11</sub> )	<i>C</i> 2/ <i>m</i> (12)	SM	—	FM	—	HQ	81219
275	Na(VHf <sub>2</sub> F <sub>11</sub> )	<i>C</i> 2/ <i>m</i> (12)	SM	—	FM	—	HQ	94460
276	Li(SO <sub>3</sub> F)	<i>C</i> 2/ <i>m</i> (12)	Triv.	(b)	NM	—	HQ	1384
277	AlWO <sub>4</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	(b)	FM	—	HQ	4164
278	Cs <sub>4</sub> (IrO <sub>4</sub> )	<i>C</i> 2/ <i>m</i> (12)	SM	—	FM	—	HQ	72287
279	K <sub>4</sub> (Nb <sub>6</sub> Cl <sub>18</sub> )	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	—	41118
280	K <sub>4</sub> ((NbBr) <sub>6</sub> Br <sub>12</sub> )	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	HQ	49687
281	K <sub>4</sub> (Ta <sub>6</sub> Cl <sub>12</sub> )Cl <sub>6</sub>	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	HQ	59851
282	Tl <sub>4</sub> (Br <sub>12</sub> (NbBr) <sub>6</sub> )	<i>C</i> 2/ <i>m</i> (12)	Triv.	—	NM	—	HQ	402033

283	Rb <sub>4</sub> (Nb <sub>6</sub> Cl <sub>18</sub> )	C2/m (12)	Triv.	—	NM	—	HQ	402272 404165
284	KCr(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	C2/m (12)	SM	—	AFM	—	HQ	172524
285	RbCr(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	C2/m (12)	SM	—	AFM	—	HQ	281565
286	(Ni(NH <sub>3</sub> ) <sub>4</sub> )(NCS) <sub>2</sub>	C2/m (12)	Triv.	—	FM	—	HQ	72515
287	Ni(NH <sub>3</sub> ) <sub>4</sub> (NO <sub>2</sub> ) <sub>2</sub>	C2/m (12)	Triv.	—	FM	—	HQ	201208 201209
288	NiCl <sub>2</sub> (H <sub>2</sub> O) <sub>6</sub>	C2/m (12)	Triv.	—	FM	—	—	22284 64878 64879
289	CoCl <sub>2</sub> (H <sub>2</sub> O) <sub>6</sub>	C2/m (12)	SM	—	AFM	—	—	34429 42744 69393
290	O <sub>8</sub>	C2/m (12)	Triv.	—	NM	—	—	156481 236855 236856 236857 236858
291	(NO <sub>2</sub> )(AsF <sub>6</sub> )	C2/m (12)	TI	—	NM	—	HQ	68906
292	In <sub>2</sub> Ge <sub>2</sub> O <sub>7</sub>	C2/m (12)	Triv.	(b)	NM	—	HQ	20053 74896 239592 409548
293	(V(H <sub>2</sub> O) <sub>6</sub> )(CF <sub>3</sub> SO <sub>3</sub> ) <sub>2</sub>	C2/m (12)	SM	—	FM	—	—	68779
294	(Fe(H <sub>2</sub> O) <sub>6</sub> )((CF <sub>3</sub> )SO <sub>3</sub> ) <sub>2</sub>	C2/m (12)	Triv.	—	FM	—	—	109429 280328
295	Zn <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>8</sub>	C2/m (12)	Triv.	—	NM	—	—	100492
296	TaCl <sub>4</sub>	C2/m (12)	Triv.	(b,s)	NM	—	HQ	402406
297	WOF <sub>4</sub>	C2/m (12)	Triv.	—	NM	—	HQ	10393
298	(Mn(N <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> )Cl <sub>2</sub>	C2/m (12)	SM	—	FM	—	HQ	25784
299	Zr <sub>2</sub> O(PO <sub>4</sub> ) <sub>2</sub>	C2/m (12)	Triv.	(b)	NM	—	—	416014 424511 424513 424514 424515
300	Cs <sub>2</sub> (Sb <sub>2</sub> F <sub>10</sub> O)	P2/c (13)	Triv.	—	NM	—	HQ	21016
301	Sr(Cu(OH) <sub>4</sub> )(H <sub>2</sub> O)	P2/c (13)	SM	—	FM	—	HQ	154808
302	Li(BH <sub>4</sub> )	P2/c (13)	Triv.	—	FM	—	—	168803
303	LiC <sub>2</sub> (CN) <sub>4</sub>	P2/c (13)	SM	—	NM	—	HQ	251418 251419 251420 251421 251422 251423 251424 251425 251426
304	Cs <sub>2</sub> (CO <sub>3</sub> )(H <sub>2</sub> O) <sub>3</sub>	P2/c (13)	Triv.	—	NM	—	HQ	411684 411685
305	CuSr(HCOO) <sub>4</sub>	P2/c (13)	SM	—	FM	—	HQ	150120
306	CaCu(HCOO) <sub>4</sub>	P2/c (13)	SM	—	FM	—	HQ	151315
307	K((CF <sub>3</sub> )BF <sub>3</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	1194
308	Mg <sub>2</sub> (Si <sub>2</sub> O <sub>6</sub> )	P2 <sub>1</sub> /c (14)	Triv.	(b)	NM	—	—	5218
309	(K(H <sub>2</sub> PO <sub>3</sub> ))(HF)	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	9151
310	((POCl <sub>3</sub> )OCl <sub>2</sub> MoCl <sub>2</sub> MoOCl <sub>2</sub> (POCl <sub>3</sub> ))	P2 <sub>1</sub> /c (14)	Triv.	—	FM	—	—	15320
311	K(Au(NO <sub>3</sub> ) <sub>4</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	16141
312	K(PNH <sub>3</sub> O <sub>3</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	23291
313	BF <sub>3</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	24783
314	(PNF <sub>2</sub> ) <sub>4</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	31038 31125
315	S <sub>6</sub> N <sub>4</sub> (SO <sub>3</sub> F) <sub>2</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	31789
316	CsHC <sub>2</sub> O <sub>4</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	39364
317	Cs <sub>2</sub> C <sub>2</sub> O <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	39365
318	K <sub>2</sub> (SbF <sub>5</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	39634
319	Rb(H <sub>2</sub> PO <sub>4</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	47189
320	(Ag(NCCl) <sub>2</sub> )(SbF <sub>6</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	64638
321	Bi <sub>2</sub> Cu(SeO <sub>3</sub> ) <sub>4</sub>	P2 <sub>1</sub> /c (14)	SM	(b,s)	FM	—	—	66826 66827
322	Co(HSeO <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P2 <sub>1</sub> /c (14)	SM	—	FM	—	—	75134
323	Cs(ReF <sub>6</sub> O)	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	78392
324	(Si(NH <sub>3</sub> ) <sub>2</sub> )F <sub>4</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	78902
325	Cs(SO <sub>3</sub> F)	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	82520
326	(Pt(CO) <sub>2</sub> Cl <sub>2</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	82803
327	Na <sub>2</sub> (Pd(NO <sub>3</sub> ) <sub>4</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	92625
328	(NH <sub>4</sub> )(Sn(C <sub>2</sub> O <sub>4</sub> )F)	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	109889
329	((CH <sub>3</sub> ) <sub>2</sub> NH) <sub>2</sub> SnBr <sub>4</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	110028
330	Mo <sub>2</sub> (HCOO) <sub>4</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	151313
331	Rb <sub>2</sub> (Pd(NO <sub>3</sub> ) <sub>4</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	158878
332	K <sub>2</sub> (Pd(NO <sub>3</sub> ) <sub>4</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	166766
333	SnCl <sub>4</sub> (NH(CH <sub>3</sub> ) <sub>2</sub> ) <sub>2</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	170799
334	Cu(IO <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	P2 <sub>1</sub> /c (14)	SM	—	FM	—	HQ	200326
335	BaCu(SeO <sub>3</sub> ) <sub>2</sub>	P2 <sub>1</sub> /c (14)	TI	(b)	FM	—	—	202387
336	LiNH <sub>2</sub> BH <sub>3</sub> (NH <sub>2</sub> NH <sub>2</sub> )	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	238484
337	Na <sub>2</sub> Cu(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub>	P2 <sub>1</sub> /c (14)	SM	—	—	—	—	242098
338	CuCl <sub>2</sub> (C <sub>2</sub> H <sub>4</sub> N <sub>4</sub> ) <sub>2</sub>	P2 <sub>1</sub> /c (14)	SM	—	—	—	—	250269
339	Sr <sub>2</sub> Pt(OH) <sub>8</sub>	P2 <sub>1</sub> /c (14)	Triv.	—	NM	—	—	251043
340	((NH <sub>4</sub> ) <sub>2</sub> (Cu(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> ))	P2 <sub>1</sub> /c (14)	SM	—	—	—	—	253556
341	Rb <sub>2</sub> Cu(VO <sub>2</sub> ) <sub>2</sub> (PO <sub>4</sub> ) <sub>2</sub>	P2 <sub>1</sub> /c (14)	SM	(b)	FM	—	—	260010

342	Cu(H <sub>2</sub> PO <sub>2</sub> ) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	SM	—	FM	—	HQ	280917 280918
343	((CH <sub>3</sub> ) <sub>2</sub> (H <sub>3</sub> B)P <sub>2</sub> (BH <sub>3</sub> )(CH <sub>3</sub> ) <sub>2</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	—	281782
344	Cu(C <sub>2</sub> N <sub>3</sub> ) <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	SM	—	FM	—	—	290326
345	CuMg <sub>2</sub> (V <sub>2</sub> O <sub>8</sub> )	<i>P2</i> <sub>1</sub> /c (14)	SM	(b)	FM	—	HQ	404851
346	(F <sub>3</sub> CSO <sub>3</sub> SiH <sub>2</sub> ) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	—	409803
347	SnAl <sub>2</sub> OCl <sub>6</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	—	411777
348	Na <sub>2</sub> (Cu(NO <sub>3</sub> ) <sub>4</sub> )	<i>P2</i> <sub>1</sub> /c (14)	SM	—	FM	—	—	413267
349	((Co(H <sub>2</sub> O) <sub>2</sub> )Cl <sub>2</sub> )(H <sub>2</sub> SeO <sub>3</sub> ) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	SM	—	FM	—	—	415462
350	K <sub>2</sub> (C <sub>2</sub> )(NH <sub>3</sub> ) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	425116
351	Na <sub>2</sub> AgF <sub>4</sub>	<i>P2</i> <sub>1</sub> /c (14)	SM	(b)	FM	—	HQ	425149
352	Pd(HS <sub>2</sub> O <sub>7</sub> ) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	FM	—	—	426138
353	KNO <sub>3</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	—	—	HQ	428909
354	SrCrO <sub>4</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	—	—	—	670010 40922 159266 160793
355	Na <sub>3</sub> MnF <sub>6</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	(b)	—	—	—	673330 66315
356	(COOH) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	246777 246778
357	Cu(AlCl <sub>4</sub> ) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	SM	(b,s)	FM	—	HQ	14107 80107
358	C <sub>14</sub> H <sub>8</sub> O <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	—	58089 58090
359	Ba <sub>2</sub> (TiO <sub>4</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	2625 <sup>(b)</sup> 15450
360	Sr <sub>2</sub> (GeO <sub>4</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	56382
361	Ni(PO <sub>2</sub> (OH) <sub>2</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	FM	—	—	417429 417430
362	CsHSeO <sub>4</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	290644 290645 411282
363	Na <sub>2</sub> Cu(CO <sub>3</sub> ) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	SM	(b)	FM	—	HQ	10355 60858 426579
364	Sr <sub>2</sub> Cu(BO <sub>3</sub> ) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	SM	(b)	FM	—	HQ	202934
365	Cu(ZrF <sub>6</sub> )(H <sub>2</sub> O) <sub>4</sub>	<i>P2</i> <sub>1</sub> /c (14)	SM	—	FM	—	—	2618
366	(Cu(H <sub>2</sub> O) <sub>4</sub> )(SiF <sub>6</sub> )	<i>P2</i> <sub>1</sub> /c (14)	SM	—	FM	—	—	165385
367	FeY <sub>2</sub> Be <sub>2</sub> Si <sub>2</sub> O <sub>10</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	(b,s)	FM	—	—	109310 109343
368	(NH <sub>2</sub> NH <sub>3</sub> )(NO <sub>3</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	—	162750 170796
369	Rb <sub>2</sub> (CO <sub>3</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	—	14155 414123
370	K <sub>2</sub> (Pd(CN) <sub>4</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	—	413899
371	K(HCO <sub>3</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	2074 2075 2076 43015
372	Ni(IO <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	FM	—	—	10243
373	Co(IO <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub>	<i>P2</i> <sub>1</sub> /c (14)	SM	—	FM	—	—	408060 411878
374	Al <sub>4</sub> Co(BO <sub>4</sub> ) <sub>2</sub> O <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	SM	(b)	FM	—	—	1975
375	Na <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	56906 171458 171459
376	Na <sub>2</sub> (Cu(H <sub>2</sub> O) <sub>2</sub> )(V <sub>2</sub> O <sub>4</sub> F <sub>6</sub> )	<i>P2</i> <sub>1</sub> /c (14)	SM	—	FM	—	—	424346
377	Na <sub>2</sub> (CuF <sub>4</sub> )	<i>P2</i> <sub>1</sub> /c (14)	SM	(b)	FM	—	—	34602
378	K <sub>2</sub> (AgF <sub>4</sub> )	<i>P2</i> <sub>1</sub> /c (14)	SM	(b)	FM	—	HQ	421461
379	Li <sub>2</sub> PtF <sub>6</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	(b,s)	NM	—	—	26168
380	Cs(HCO <sub>3</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	300259
381	Rb <sub>2</sub> (Pt(CN) <sub>4</sub> Br <sub>2</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	852
382	K <sub>2</sub> (Pt(CN) <sub>4</sub> Br <sub>2</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	413705
383	Na <sub>2</sub> Cu(SO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	SM	—	FM	—	—	1915 422593
384	(KrF)(AsF <sub>6</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	—	279624
385	Sr <sub>2</sub> Zn(OH) <sub>6</sub>	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	HQ	66971
386	Sr <sub>2</sub> (Cu(OH) <sub>6</sub> )	<i>P2</i> <sub>1</sub> /c (14)	SM	(b)	FM	—	HQ	260446
387	(XeF)(AsF <sub>6</sub> )	<i>P2</i> <sub>1</sub> /c (14)	Triv.	—	NM	—	—	1691 260951
388	Au(AuF <sub>4</sub> ) <sub>2</sub>	<i>P2</i> <sub>1</sub> /c (14)	SM	(b,s)	FM	—	HQ	89620
389	K <sub>2</sub> (P <sub>2</sub> O <sub>5</sub> F <sub>2</sub> )	<i>C2</i> /c (15)	Triv.	—	NM	—	HQ	1659
390	Na <sub>2</sub> Cu(PO <sub>3</sub> ) <sub>4</sub>	<i>C2</i> /c (15)	SM	(b)	FM	—	—	2822
391	S <sub>10</sub>	<i>C2</i> /c (15)	Triv.	—	NM	—	HQ	38263
392	Ni(NH <sub>2</sub> NHCO <sub>2</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	<i>C2</i> /c (15)	Triv.	—	FM	—	—	48155
393	K <sub>2</sub> (SeO <sub>4</sub> )(Te(OH) <sub>6</sub> )	<i>C2</i> /c (15)	Triv.	(b)	NM	—	—	56856 154512 170043
394	Cs <sub>4</sub> (PbCl <sub>6</sub> )	<i>C2</i> /c (15)	Triv.	(b,s)	NM	—	HQ	62351
395	Be <sub>2</sub> Rb(P <sub>3</sub> O <sub>10</sub> )	<i>C2</i> /c (15)	Triv.	(b,s)	NM	—	—	72985
396	Na <sub>2</sub> O <sub>2</sub> (H <sub>2</sub> O) <sub>8</sub>	<i>C2</i> /c (15)	Triv.	—	NM	—	—	79693
397	Cd((H <sub>3</sub> CO)CS <sub>2</sub> ) <sub>2</sub>	<i>C2</i> /c (15)	Triv.	—	NM	—	—	110011
398	Na <sub>2</sub> (C <sub>4</sub> O <sub>4</sub> )(H <sub>2</sub> O) <sub>3</sub>	<i>C2</i> /c (15)	Triv.	—	NM	—	—	151153
399	CrF(NC(CH <sub>3</sub> )) <sub>2</sub> (BF <sub>4</sub> )	<i>C2</i> /c (15)	Triv.	—	—	—	—	169664
400	Li <sub>2</sub> Pb <sub>2</sub> (CuB <sub>4</sub> O <sub>10</sub> )	<i>C2</i> /c (15)	SM	(b)	FM	—	—	180108
401	Co(C <sub>4</sub> O <sub>4</sub> )(H <sub>2</sub> O) <sub>4</sub>	<i>C2</i> /c (15)	SM	—	FM	—	—	180990

402	Bi <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	C2/c (15)	Triv.	—	NM	—	—	193352
403	((CH <sub>3</sub> )NH <sub>3</sub> ) <sub>2</sub> SiF <sub>6</sub>	C2/c (15)	Triv.	—	NM	—	—	240237
404	Sn(CH <sub>3</sub> ) <sub>2</sub> (Au(CN) <sub>2</sub> ) <sub>2</sub>	C2/c (15)	Triv.	—	—	—	—	249795
405	(C(NH <sub>2</sub> ) <sub>3</sub> )(C(NO <sub>2</sub> ) <sub>3</sub> )(H <sub>2</sub> O)	C2/c (15)	Triv.	—	NM	—	—	417769
406	Cu(C(CN) <sub>3</sub> ) <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub>	C2/c (15)	SM	—	—	—	—	428562
407	Ca(CO <sub>3</sub> )(H <sub>2</sub> O) <sub>6</sub>	C2/c (15)	Triv.	—	NM	—	—	16070 31305 151488 195903 195904 195905 195906 195907
408	Ca(MnF <sub>5</sub> )	C2/c (15)	Triv.	(b)	FM	—	HQ	69632
409	Co(AlCl <sub>4</sub> ) <sub>2</sub>	C2/c (15)	SM	(b,s)	FM	—	—	22143
410	V(AlCl <sub>4</sub> ) <sub>2</sub>	C2/c (15)	SM	(b,s)	FM	—	HQ	415951
411	Ni(GaCl <sub>4</sub> ) <sub>2</sub>	C2/c (15)	TI	(b,s)	FM	—	HQ	417870
412	Ni(AlCl <sub>4</sub> ) <sub>2</sub>	C2/c (15)	TI	(b,s)	FM	—	HQ	417872
413	Mn(NO)(CO) <sub>4</sub>	C2/c (15)	Triv.	—	NM	—	HQ	15221
414	Zn(C <sub>2</sub> O <sub>4</sub> )(H <sub>2</sub> O) <sub>2</sub>	C2/c (15)	Triv.	—	NM	—	HQ	56466
415	K <sub>2</sub> (NH(SO <sub>3</sub> ) <sub>2</sub> )	C2/c (15)	Triv.	—	NM	—	—	15880
416	Co(HSeO <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub>	C2/c (15)	SM	—	—	—	—	79091
417	Ni(HSeO <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub>	C2/c (15)	Triv.	—	FM	—	—	79092
418	Pb <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>	C2/c (15)	Triv.	—	NM	—	HQ	92582 4263 8092 8093 8094 14247 38007 38008 38009 38010 66379 93440 93441 93442 93443 93444 93445
419	(Na <sub>2</sub> (CO <sub>3</sub> ))(Na(HCO <sub>3</sub> ))(H <sub>2</sub> O) <sub>2</sub>	C2/c (15)	Triv.	—	NM	—	—	16641 34627 35191 44802
420	Cs(SbO <sub>2</sub> )	C2/c (15)	Triv.	(b,s)	NM	—	HQ	59329
421	S(NSO) <sub>2</sub>	C2/c (15)	Triv.	—	NM	—	HQ	14197 15795 41538
422	NaCu(SO <sub>4</sub> )F	C2/c (15)	SM	(b)	FM	—	HQ	262273
423	S <sub>10</sub> S <sub>6</sub>	C2/c (15)	Triv.	—	NM	—	—	38264
424	(VO)(H <sub>2</sub> PO <sub>2</sub> ) <sub>2</sub> (H <sub>2</sub> O)	C2/c (15)	SM	—	FM	—	HQ	75435
425	(NH <sub>4</sub> ) <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> )(H <sub>2</sub> O)	P2 <sub>1</sub> 2 <sub>1</sub> (18)	Triv.	—	NM	—	—	64925 64927 64934 64935 64938
426	(Sr <sub>6</sub> N)(CoN <sub>2</sub> )(CN <sub>2</sub> ) <sub>2</sub>	P2 <sub>1</sub> 2 <sub>1</sub> (18)	Triv.	—	FM	—	—	162927
427	(Sr <sub>6</sub> N)(FeN <sub>2</sub> )(CN <sub>2</sub> ) <sub>2</sub>	P2 <sub>1</sub> 2 <sub>1</sub> (18)	SM	—	FM	—	—	409974
428	K(Al(NH <sub>2</sub> ) <sub>4</sub> )	C222 <sub>1</sub> (20)	Triv.	—	NM	—	HQ	2538
429	Cs <sub>3</sub> (VCl <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub> )Cl <sub>4</sub>	I222 (23)	Triv.	—	—	—	HQ	150082
430	(Pd(NH <sub>3</sub> ) <sub>4</sub> )(Ni(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub>	I222 (23)	Triv.	—	FM	—	—	417562
431	(Pt(NH <sub>3</sub> ) <sub>4</sub> )(Ni(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub>	I222 (23)	Triv.	—	FM	—	—	417564
432	(Pt(NH <sub>3</sub> ) <sub>4</sub> )(Co(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub>	I222 (23)	SM	—	FM	—	—	420437
433	(Pt(NH <sub>3</sub> ) <sub>4</sub> )(Zn(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub>	I222 (23)	Triv.	—	NM	—	—	417565
434	NaRb <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub>	Pmc2 <sub>1</sub> (26)	Triv.	—	NM	—	HQ	195082
435	KF(H <sub>2</sub> O) <sub>2</sub>	Pmc2 <sub>1</sub> (26)	Triv.	—	NM	—	HQ	165371 165372 165373
436	Na <sub>2</sub> (CO <sub>3</sub> )(H <sub>2</sub> O)	Pca2 <sub>1</sub> (29)	Triv.	—	NM	—	—	15959 1852 6293 34886
437	(NH <sub>4</sub> )F(NH <sub>3</sub> )	Pca2 <sub>1</sub> (29)	Triv.	—	NM	—	—	419918
438	Cl(CO)SNSO	Pca2 <sub>1</sub> (29)	Triv.	—	NM	—	HQ	91453 410061
439	HF <sub>2</sub> N	Pca2 <sub>1</sub> (29)	Triv.	—	NM	—	HQ	404200
440	Na <sub>2</sub> (HPO <sub>3</sub> )(H <sub>2</sub> O) <sub>5</sub>	Pmn2 <sub>1</sub> (31)	Triv.	—	NM	—	—	1602 16138
441	(VO)(SO <sub>4</sub> )(H <sub>2</sub> O) <sub>5</sub>	Pmn2 <sub>1</sub> (31)	SM	—	FM	—	—	23308 92978
442	MoO <sub>2</sub> Cl <sub>2</sub> (H <sub>2</sub> O)	Pmn2 <sub>1</sub> (31)	Triv.	—	NM	—	HQ	25031
443	Pb <sub>2</sub> (NO <sub>2</sub> )(NO <sub>3</sub> )(SeO <sub>3</sub> )	Pmn2 <sub>1</sub> (31)	Triv.	—	NM	—	HQ	60893
444	K <sub>3</sub> ((SnCl <sub>3</sub> )IrCl <sub>5</sub> )	Pmn2 <sub>1</sub> (31)	Triv.	(b)	NM	—	HQ	69143
445	(N(CH <sub>3</sub> ) <sub>4</sub> )(OCN)	Pmn2 <sub>1</sub> (31)	Triv.	—	NM	—	—	150997
446	(NH <sub>3</sub> )(BH <sub>3</sub> )	Pmn2 <sub>1</sub> (31)	Triv.	—	NM	—	—	180547 182301 159678 182300 187303
447	BaCl(BF <sub>4</sub> )	Pmn2 <sub>1</sub> (31)	Triv.	—	NM	—	HQ	188654
448	Au <sub>2</sub> (SeO <sub>3</sub> ) <sub>2</sub> O	Pba2 (32)	Triv.	(b)	NM	—	HQ	37009
449	CuNa <sub>2</sub> (OH) <sub>4</sub>	Pna2 <sub>1</sub> (33)	SM	—	FM	—	—	65649
450	Be(HPO <sub>4</sub> )(H <sub>2</sub> O)	Pna2 <sub>1</sub> (33)	Triv.	—	NM	—	—	83835
451	Zn(OH)(NO <sub>3</sub> )	Pna2 <sub>1</sub> (33)	Triv.	(b)	NM	—	HQ	415537
452	(H <sub>3</sub> O)(NO <sub>3</sub> )	Pna2 <sub>1</sub> (33)	Triv.	—	NM	—	—	1900 1901
453	KBePO <sub>4</sub>	Pna2 <sub>1</sub> (33)	Triv.	(b)	NM	—	—	4255 202603 <sup>(s)</sup>
454	LiH <sub>2</sub> PO <sub>4</sub>	Pna2 <sub>1</sub> (33)	Triv.	—	NM	—	—	100200 182308 182309
455	(NH <sub>4</sub> )Li(SeO <sub>4</sub> )	Pna2 <sub>1</sub> (33)	Triv.	—	NM	—	—	300031
456	OsOF <sub>5</sub>	Pna2 <sub>1</sub> (33)	SM	—	FM	—	HQ	240332
457	Na <sub>3</sub> (ON(SO <sub>3</sub> ) <sub>2</sub> )(H <sub>2</sub> O) <sub>3</sub>	Cmc2 <sub>1</sub> (36)	Triv.	—	NM	—	—	4288
458	K <sub>2</sub> (OsNCl <sub>5</sub> )	Cmc2 <sub>1</sub> (36)	Triv.	—	—	—	—	43729

459	(NH <sub>4</sub> ) <sub>3</sub> Cr(O <sub>2</sub> ) <sub>4</sub>	Cmc2 <sub>1</sub> (36)	SM	—	FM	—	—	237784 261390
460	(Cl <sub>3</sub> CCN)(NbCl <sub>5</sub> )	Cmc2 <sub>1</sub> (36)	Triv.	—	NM	—	HQ	402856
461	H <sub>2</sub> F <sub>3</sub> P	Cmc2 <sub>1</sub> (36)	Triv.	—	NM	—	HQ	406359 51680
462	ClN <sub>3</sub>	Cmc2 <sub>1</sub> (36)	Triv.	—	NM	—	HQ	424502
463	K <sub>2</sub> S <sub>3</sub>	Cmc2 <sub>1</sub> (36)	Triv.	—	NM	—	HQ	1263
464	K <sub>2</sub> Se <sub>3</sub>	Cmc2 <sub>1</sub> (36)	Triv.	—	NM	—	HQ	1264
465	Rb <sub>2</sub> S <sub>3</sub>	Cmc2 <sub>1</sub> (36)	Triv.	—	NM	—	HQ	14092
466	Rb <sub>2</sub> Se <sub>3</sub>	Cmc2 <sub>1</sub> (36)	Triv.	—	NM	—	HQ	14093 650051
467	Cs <sub>2</sub> S <sub>3</sub>	Cmc2 <sub>1</sub> (36)	Triv.	—	NM	—	HQ	14094
468	K <sub>3</sub> (Pd((SO <sub>3</sub> ) <sub>2</sub> H)Cl <sub>2</sub> )	Cmc2 <sub>1</sub> (36)	Triv.	—	NM	—	HQ	49686
469	Li <sub>2</sub> (PO <sub>2</sub> N)	Cmc2 <sub>1</sub> (36)	Triv.	—	NM	—	—	188493 188494
470	Cs <sub>2</sub> Li(MnO <sub>4</sub> )	Cmc2 <sub>1</sub> (36)	Triv.	(b,s)	AFM	—	HQ	72361
471	((CH <sub>3</sub> ) <sub>4</sub> N)(OsFO <sub>4</sub> )	Aem2 (39)	Triv.	—	NM	—	—	110743
472	Cs(B <sub>3</sub> H <sub>8</sub> )	Ama2 (40)	Triv.	—	NM	—	HQ	65947
473	CrO <sub>3</sub>	Ama2 (40)	Triv.	—	NM	—	HQ	16031 24043 38125 109366
474	NaCa <sub>4</sub> B <sub>3</sub> O <sub>9</sub>	Ama2 (40)	Triv.	—	NM	—	—	239001
475	IF <sub>7</sub>	Aea2 (41)	Triv.	—	NM	—	—	18191 31691
476	(NH <sub>4</sub> ) <sub>3</sub> (AlF <sub>6</sub> )	Aea2 (41)	Triv.	—	NM	—	—	96591
477	(NH <sub>4</sub> ) <sub>4</sub> (H <sub>2</sub> (CO <sub>3</sub> ) <sub>3</sub> )(H <sub>2</sub> O)	Fmm2 (42)	Triv.	—	NM	—	—	281534
478	(CH <sub>3</sub> ) <sub>2</sub> (SO <sub>4</sub> )	Fdd2 (43)	Triv.	—	NM	—	HQ	171689
479	(C <sub>2</sub> F <sub>5</sub> ) <sub>2</sub> GeH <sub>2</sub>	Fdd2 (43)	Triv.	—	NM	—	—	196449
480	NaAg(NO <sub>2</sub> ) <sub>2</sub>	Fdd2 (43)	Triv.	—	NM	—	HQ	200377
481	(C <sub>2</sub> F <sub>5</sub> ) <sub>2</sub> SiH <sub>2</sub>	Fdd2 (43)	Triv.	—	—	—	—	241929
482	K <sub>2</sub> (B(CN) <sub>3</sub> )	Fdd2 (43)	Triv.	—	NM	—	HQ	262588
483	(SeCl <sub>3</sub> ) <sub>2</sub> (ReCl <sub>6</sub> )	Fdd2 (43)	SM	(b)	FM	—	HQ	68655 404534
484	K <sub>2</sub> (Cu(CO <sub>3</sub> ) <sub>2</sub> )	Fdd2 (43)	SM	(b)	FM	—	—	36447 200695 200779
485	K(H <sub>2</sub> PO <sub>4</sub> )	Fdd2 (43)	Triv.	(b)	NM	—	—	31151 68696 183037
486	Rb(H <sub>2</sub> PO <sub>4</sub> )	Fdd2 (43)	Triv.	—	NM	—	HQ	54873 <sup>(b)</sup> 69318 200890 <sup>(b)</sup>
487	(N <sub>2</sub> H <sub>5</sub> )Cl	Fdd2 (43)	Triv.	—	NM	—	—	65334
488	Cs <sub>2</sub> (As <sub>2</sub> Al <sub>2</sub> O <sub>7</sub> )	Imm2 (44)	Triv.	(b,s)	NM	—	HQ	154363
489	K <sub>3</sub> Na <sub>4</sub> (SiF <sub>6</sub> ) <sub>3</sub> (BF <sub>4</sub> )	Imm2 (44)	Triv.	(b)	NM	—	—	160430
490	NaAl(CO <sub>3</sub> )(OH) <sub>2</sub>	Ima2 (46)	Triv.	(b)	NM	—	HQ	67435
491	NaHCN <sub>4</sub> H <sub>2</sub> O	Pmma (51)	Triv.	—	NM	—	HQ	15874
492	RbNb <sub>4</sub> Br <sub>11</sub>	Pmma (51)	Triv.	—	NM	—	—	380397
493	Rb(Nb <sub>4</sub> Cl <sub>11</sub> )	Pmma (51)	Triv.	—	NM	—	—	412126
494	CsNb <sub>4</sub> Cl <sub>11</sub>	Pmma (51)	Triv.	—	NM	—	—	26076
495	Rb <sub>3</sub> IO <sub>5</sub>	Pnna (52)	Triv.	—	NM	—	—	4326
496	CuCl <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	Pmna (53)	SM	—	FM	—	HQ	15087 163013 34239 40290
497	(BrF <sub>2</sub> )(SbF <sub>6</sub> )	Pcca (54)	Triv.	—	NM	—	—	9886
498	CaBi(OF(CO <sub>3</sub> ))	Pcca (54)	Triv.	—	NM	—	—	157756
499	F <sub>2</sub> (OPOPO)F <sub>2</sub>	Pcca (54)	Triv.	—	NM	—	—	248122
500	(ClF <sub>2</sub> )(NbF <sub>6</sub> )	Pcca (54)	Triv.	—	NM	—	—	39501
501	(ClF <sub>2</sub> )(TaF <sub>6</sub> )	Pcca (54)	Triv.	—	NM	—	—	39502
502	NbBr <sub>5</sub>	Pbam (55)	Triv.	—	—	—	—	35410
503	(Mg(XeF <sub>2</sub> ) <sub>2</sub> )(AsF <sub>6</sub> ) <sub>2</sub>	Pbam (55)	Triv.	(b,s)	NM	—	—	281694
504	K <sub>5</sub> I <sub>2</sub> (AuO <sub>2</sub> )	Pbam (55)	Triv.	(b,s)	NM	—	HQ	40376
505	Co(SO <sub>4</sub> )(N <sub>2</sub> H <sub>4</sub> )	Pccn (56)	SM	—	FM	—	—	261204
506	Na <sub>2</sub> N <sub>2</sub> O <sub>3</sub> H <sub>2</sub> O	Pbcm (57)	Triv.	—	NM	—	—	10182
507	K(SCN)	Pbcm (57)	Triv.	—	NM	—	—	36203 28355 36073 65074 65075 67582
508	K <sub>2</sub> (HgS <sub>2</sub> )	Pbcm (57)	Triv.	(b)	NM	—	HQ	74500
509	(NF <sub>4</sub> )(BF <sub>4</sub> )	Pbcm (57)	Triv.	—	NM	—	—	165425
510	((CH <sub>3</sub> ) <sub>2</sub> Se)AlCl <sub>3</sub>	Pbcm (57)	Triv.	—	NM	—	—	250558
511	((CH <sub>3</sub> ) <sub>2</sub> Te)AlCl <sub>3</sub>	Pbcm (57)	Triv.	—	NM	—	—	250561
512	((CH <sub>3</sub> ) <sub>2</sub> Te)AlBr <sub>3</sub>	Pbcm (57)	Triv.	—	NM	—	—	250562
513	K(N(CN) <sub>2</sub> )	Pbcm (57)	Triv.	—	NM	—	HQ	428975
514	K <sub>2</sub> Hg(BrO <sub>3</sub> ) <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub>	Pnnm (58)	Triv.	(b)	NM	—	—	24405
515	(Ag(NCH <sub>2</sub> ) <sub>2</sub> )(SbF <sub>6</sub> )	Pnnm (58)	Triv.	—	NM	—	HQ	63287
516	((CH <sub>3</sub> )NH <sub>3</sub> ) <sub>2</sub> (SiF <sub>6</sub> )	Pnnm (58)	Triv.	—	NM	—	—	110673
517	Ni(N(CN) <sub>2</sub> ) <sub>2</sub>	Pnnm (58)	Triv.	(b)	FM	—	—	85617
518	Co(N(CN) <sub>2</sub> ) <sub>2</sub>	Pnnm (58)	SM	(b)	FM	—	—	85619

519	(N(CH <sub>3</sub> ) <sub>4</sub> )(NO <sub>2</sub> )	<i>Pmmn</i> (59)	Triv.	—	NM	—	—	150985
520	NaB <sub>3</sub> H <sub>8</sub>	<i>Pmmn</i> (59)	Triv.	—	NM	—	HQ	260964
521	Tl((MoOCl <sub>2</sub> ) <sub>2</sub> Cl <sub>3</sub> )	<i>Pmmn</i> (59)	Triv.	(b,s)	FM	—	HQ	408775
522	Rb(I(ICN) <sub>2</sub> )	<i>Pmmn</i> (59)	Triv.	—	NM	—	HQ	35411
523	CsNa <sub>2</sub> (BO <sub>3</sub> )	<i>Pmmn</i> (59)	Triv.	—	NM	—	HQ	67524
524	(NH <sub>4</sub> )(NO <sub>3</sub> )	<i>Pmmn</i> (59)	Triv.	—	NM	—	—	2772 24013
525	CsNO <sub>3</sub>	<i>Pmmn</i> (59)	Triv.	—	NM	—	—	16339 16340
526	Na <sub>2</sub> (TeO <sub>4</sub> )	<i>Pbcn</i> (60)	Triv.	(b,s)	NM	—	—	1108
527	S <sub>4</sub> N <sub>4</sub>	<i>Pbcn</i> (60)	Triv.	—	NM	—	—	51516
528	K <sub>2</sub> (AlF <sub>3</sub> (SO <sub>4</sub> ))	<i>Pbcn</i> (60)	Triv.	(b)	NM	—	—	161272
529	Ba(PdCl <sub>4</sub> )	<i>Pbcn</i> (60)	Triv.	(b)	NM	—	HQ	411837
530	Na <sub>2</sub> WO <sub>2</sub> F <sub>4</sub>	<i>Pbcn</i> (60)	Triv.	(b)	NM	—	—	201173 673329
531	Ca <sub>2</sub> F <sub>2</sub> (CO <sub>3</sub> )	<i>Pbcn</i> (60)	Triv.	—	NM	—	—	100607 158901
532	Cs <sub>2</sub> Re <sub>2</sub> Br <sub>8</sub>	<i>Pbca</i> (61)	Triv.	—	NM	—	—	26060
533	S(CN) <sub>2</sub>	<i>Pbca</i> (61)	Triv.	—	—	—	—	670398 14340 25520
534	Se(CN) <sub>2</sub>	<i>Pbca</i> (61)	Triv.	—	—	—	—	670399 27441
535	B <sub>2</sub> Cl <sub>4</sub>	<i>Pbca</i> (61)	Triv.	—	NM	—	HQ	14213 31693
536	ClO <sub>2</sub>	<i>Pbca</i> (61)	Triv.	—	NM	—	HQ	67663 67664 67665 67666 180778
537	Na <sub>3</sub> (B <sub>3</sub> O <sub>5</sub> (OH) <sub>2</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	—	1939
538	H <sub>3</sub> B <sub>3</sub> O <sub>6</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	—	16545
539	(HgCN) <sub>2</sub> O	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	25708 28398 29037
540	NH <sub>4</sub> HF <sub>2</sub> O <sub>2</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	—	28552
541	K <sub>2</sub> (S <sub>2</sub> CNCN)(H <sub>2</sub> O)	<i>Pnma</i> (62)	Triv.	—	NM	—	—	36006
542	(HBO <sub>2</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	—	39129
543	RbLiO	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	65170
544	Rb(SF <sub>5</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	65221
545	K(NO <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	85491 10289 10290 28077 52376 71397
546	((CH <sub>3</sub> )NH <sub>3</sub> )(NO <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	—	110635
547	Na((CF <sub>3</sub> )SO <sub>3</sub> )(H <sub>2</sub> O)	<i>Pnma</i> (62)	Triv.	—	NM	—	—	151032
548	(CH <sub>3</sub> )S(O) <sub>2</sub> NCl <sub>2</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	—	151036
549	CH <sub>3</sub> FO <sub>2</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	170925
550	Ba <sub>3</sub> Cl <sub>4</sub> (CO <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	—	174065
551	LiGaCl <sub>3</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	—	202641
552	SrF <sub>2</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	—	248433 262349
553	CaCO <sub>3</sub>	<i>Pnma</i> (62)	Triv.	—	—	—	—	252923 252924 15194 15198 32100 34308 52152 56090 157992 157993 157994 157995 157996 157997 161817 166085 166086 166087 169891 169891 169892 169893 169894 169895 169896 169897 169898 169899 169900 169901 169902 169903 169904 169905 169906 169907 169908 169910 169911 169912 170225 190072 252901 252902 252903 252904 252905 252907 252908 252909 252910 252911 252912 252913 252914 252915 252916 252917 252918 252919 252920 252921 252922 27827 157301 157302
554	K <sub>2</sub> (SnCl <sub>3</sub> )Cl(H <sub>2</sub> O)	<i>Pnma</i> (62)	Triv.	—	NM	—	—	290298
555	(TaCl <sub>5</sub> )(SOCl <sub>2</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	—	411518
556	Rb <sub>2</sub> (CO <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	414122
557	Sr(CO <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	15195 27293 56099 166088 202793
558	Ba(CO <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	15196 <sup>(k)</sup> 26718 <sup>(k)</sup> 56100 <sup>(k)</sup> 91888 <sup>(k)</sup> 91889 <sup>(k)</sup> 91890 91891 91892 91893 91894 91895 91896 158378 <sup>(k)</sup> 158379 <sup>(k)</sup> 158380 <sup>(k)</sup> 158381 <sup>(k)</sup> 158382 <sup>(k)</sup> 158383 158384 158385 158386 158387 158388 166090 <sup>(k)</sup> 166091 <sup>(k)</sup> 190075 <sup>(k)</sup>
559	K(BF <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	9875 21081 22260
560	NH <sub>4</sub> SO <sub>3</sub> F	<i>Pnma</i> (62)	Triv.	—	—	—	—	16146

561	Ba(SO <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	16904 16917 31894 33730 33731 33732 33733 33734 33735 44414 68308 76926 100623 154286 167519 180337 180338 180339 186426 190065 200112
562	Pb(SO <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	16916 31896 44415 75955 75956 92609 109432 154273 190064
563	Pb(BeF <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	24568
564	In(BF <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	50218
565	Tl(BF <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	300222
566	Cs(NH <sub>2</sub> SO <sub>3</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	—	180845
567	Rb <sub>2</sub> PO <sub>3</sub> F	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	172343 172344
568	Cs <sub>2</sub> PO <sub>3</sub> F	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	172345 172346
569	K <sub>2</sub> PO <sub>3</sub> F	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	200441 15691
570	Rb(CN <sub>3</sub> H <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	—	422591 425942
571	Cs(SCN)	<i>Pnma</i> (62)	Triv.	—	NM	—	—	19001 60523 60870 60871 60872 60873 60874 60875 60876 60877 60878 60879
572	Cs(SO <sub>2</sub> F)	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	93070 93072 93074 93076 93078
573	(F <sub>5</sub> S)(CN)	<i>Pnma</i> (62)	Triv.	—	NM	—	—	413755 413756 413757
574	(H <sub>3</sub> O)FSO <sub>3</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	—	33866
575	K <sub>2</sub> OsNCl <sub>5</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	—	27560 28208
576	K <sub>2</sub> (MoOCl <sub>5</sub> )	<i>Pnma</i> (62)	SM	—	FM	—	—	28215
577	K <sub>2</sub> (ReCl <sub>5</sub> O)	<i>Pnma</i> (62)	Triv.	—	NM	—	—	68907
578	K <sub>2</sub> (TcOCl <sub>5</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	—	188005
579	K <sub>2</sub> (Ru(NO)Cl <sub>5</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	—	20436 20713 <sup>(b)</sup> 72617
580	Li(ClO <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	(b)	NM	—	HQ	165579 413238
581	Mg <sub>2</sub> (BO <sub>3</sub> )F	<i>Pnma</i> (62)	Triv.	(b)	NM	—	HQ	28096
582	K <sub>2</sub> TaF <sub>7</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	—	260876 260877
583	CsTeF <sub>5</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	200252
584	Na(TeF <sub>5</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	202879
585	NaY(CO <sub>3</sub> )F <sub>2</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	—	89258
586	LiFe(PO <sub>4</sub> )	<i>Pnma</i> (62)	Triv.	—	AFM	—	—	38209 <sup>(b)</sup> 56291 <sup>(b)</sup> 72545 <sup>(b)</sup> 92198 <sup>(b)</sup> 97764 <sup>(b)</sup> 99860 <sup>(b)</sup> 153699 <sup>(b)</sup> 154117 <sup>(b)</sup> 155580 <sup>(b)</sup> 155635 <sup>(b)</sup> 159107 160776 <sup>(b)</sup> 161479 <sup>(b)</sup> 162282 <sup>(b)</sup> 166815 <sup>(b)</sup> 183874 <sup>(b)</sup> 184652 <sup>(b)</sup> 184862 184863 <sup>(b)</sup> 185308 <sup>(b)</sup> 189057 <sup>(b)</sup> 190771 <sup>(b)</sup> 190772 <sup>(b)</sup> 193797 <sup>(b)</sup> 193799 <sup>(b)</sup> 193800 <sup>(b)</sup> 194331 <sup>(b)</sup> 200155 <sup>(b)</sup> 241942 <sup>(b)</sup> 246855 <sup>(b)</sup> 246857 <sup>(b)</sup> 260569 <sup>(b)</sup> 260570 <sup>(b)</sup> 260571 <sup>(b)</sup> 260572 <sup>(b)</sup> 290334 <sup>(b)</sup> 290335 <sup>(b)</sup> 290336 290339 <sup>(b)</sup> 290718 <sup>(b)</sup> 290719 <sup>(b)</sup>
587	OsOF <sub>5</sub>	<i>Pnma</i> (62)	SM	—	FM	—	HQ	16872
588	K <sub>3</sub> OCl	<i>Pnma</i> (62)	Triv.	(b,s)	NM	—	HQ	78891
589	(NH <sub>4</sub> )(PO <sub>2</sub> F <sub>2</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	—	16152
590	KPO <sub>2</sub> F <sub>2</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	26640
591	Rb(H <sub>2</sub> PO <sub>2</sub> )	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	59834 250131
592	S <sub>3</sub> (CN) <sub>2</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	—	1084 25505
593	Se(SeCN) <sub>2</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	HQ	10072 24054 171333 247099
594	SC(NH <sub>2</sub> ) <sub>2</sub>	<i>Pnma</i> (62)	Triv.	—	NM	—	—	14334 65783 69145 200408
595	K <sub>2</sub> (BiF <sub>5</sub> )	<i>Pnma</i> (62)	Triv.	(b,s)	NM	—	—	418777
596	Ca <sub>3</sub> Cl <sub>2</sub> C <sub>3</sub>	<i>Cmcm</i> (63)	Triv.	—	NM	—	HQ	33818
597	Ba <sub>3</sub> WO <sub>5</sub> Cl <sub>2</sub>	<i>Cmcm</i> (63)	Triv.	—	NM	—	HQ	63518
598	Rb <sub>3</sub> (Re <sub>3</sub> Cl <sub>12</sub> )	<i>Cmcm</i> (63)	Triv.	—	NM	—	—	63585
599	LiBF <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> )	<i>Cmcm</i> (63)	Triv.	—	NM	—	HQ	185384
600	Na(IO <sub>2</sub> F <sub>2</sub> )	<i>Cmcm</i> (63)	Triv.	(b)	NM	—	HQ	260003
601	K <sub>2</sub> (SbF <sub>5</sub> )	<i>Cmcm</i> (63)	Triv.	—	NM	—	—	24742 39630
602	K <sub>2</sub> (TeOF <sub>4</sub> )	<i>Cmcm</i> (63)	Triv.	—	NM	—	HQ	412955
603	Na(B(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> )	<i>Cmcm</i> (63)	Triv.	—	NM	—	HQ	281622
604	Li(NO <sub>3</sub> )(H <sub>2</sub> O) <sub>3</sub>	<i>Cmcm</i> (63)	Triv.	—	NM	—	—	1135 23109 23110 48039 48040
605	RbCd(ZrF <sub>7</sub> )	<i>Cmcm</i> (63)	Triv.	(b,s)	NM	—	HQ	245783
606	(Re(CO) <sub>5</sub> I)	<i>Cmcm</i> (63)	Triv.	—	NM	—	—	71219

607	Mn(CO) <sub>5</sub> I	<i>Cmcm</i> (63)	Triv.	—	NM	—	HQ	71878
608	(Tc(CO) <sub>5</sub> )I	<i>Cmcm</i> (63)	Triv.	—	NM	—	HQ	85335
609	SrV(Si <sub>2</sub> O <sub>7</sub> )	<i>Cmcm</i> (63)	SM	(b)	FM	—	—	64766
610	Sr <sub>2</sub> (V <sub>2</sub> Si <sub>4</sub> O <sub>14</sub> )	<i>Cmcm</i> (63)	SM	(b)	FM	—	HQ	83361
611	Sr <sub>2</sub> CuF <sub>6</sub>	<i>Cmce</i> (64)	SM	(b)	FM	—	—	9926
612	NbP <sub>2</sub> S <sub>8</sub>	<i>Cmce</i> (64)	Triv.	—	NM	—	—	37326
613	Na <sub>2</sub> (W <sub>2</sub> O <sub>7</sub> )	<i>Cmce</i> (64)	Triv.	(b)	NM	—	—	1883 24041 <sup>(s)</sup> 290459
614	(Pt(NH <sub>3</sub> ) <sub>4</sub> )(SnCl <sub>6</sub> )	<i>Cmce</i> (64)	Triv.	—	NM	—	—	74556
615	Ta <sub>6</sub> Br <sub>14</sub>	<i>Cmce</i> (64)	Triv.	—	NM	—	—	402031
616	(Ni(H <sub>2</sub> O) <sub>4</sub> )(C <sub>3</sub> H <sub>2</sub> N <sub>3</sub> O <sub>3</sub> ) <sub>2</sub>	<i>Fmmm</i> (69)	Triv.	—	—	—	—	66806
617	(Co(N <sub>5</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub> )(H <sub>2</sub> O) <sub>4</sub>	<i>Fmmm</i> (69)	SM	—	—	—	—	432489
618	TaI <sub>2</sub> Cl <sub>2</sub>	<i>Immm</i> (71)	Triv.	—	NM	—	HQ	69688
619	Cs(BrF <sub>4</sub> )	<i>Immm</i> (71)	Triv.	—	NM	—	HQ	426292
620	Na <sub>3</sub> (AlF <sub>6</sub> )	<i>Immm</i> (71)	Triv.	—	NM	—	HQ	74210 74211
621	NaAl(OH) <sub>2</sub> (CO <sub>3</sub> )	<i>Imma</i> (74)	Triv.	(b)	NM	—	HQ	100140
622	CrOF <sub>3</sub>	<i>P4</i> <sub>1</sub> (76)	SM	(b,s)	FM	—	—	59123
623	C(HCO <sub>2</sub> ) <sub>2</sub>	<i>P4</i> <sub>1</sub> (76)	Triv.	—	—	—	—	109620
624	(Ni(SC(NH <sub>2</sub> ) <sub>2</sub> ) <sub>4</sub> Cl <sub>2</sub> )	<i>I</i> 4 (79)	Triv.	—	FM	—	—	61122 61123
625	Na <sub>4</sub> (CO(PO <sub>3</sub> ) <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub>	<i>P</i> 4̄ (81)	Triv.	—	NM	—	—	19
626	K <sub>5</sub> (Nb(CN) <sub>8</sub> )	<i>I</i> 4̄ (82)	Triv.	—	NM	—	HQ	16458
627	CsCo(CO) <sub>4</sub>	<i>I</i> 4̄ (82)	Triv.	—	NM	—	HQ	31359 31360
628	LiNH <sub>2</sub>	<i>I</i> 4̄ (82)	Triv.	—	NM	—	HQ	173179 10354 51679 161017 165467 168792 168793 182470 182471 237203
629	Cu(XeF <sub>2</sub> ) <sub>4</sub> (SbF <sub>6</sub> ) <sub>2</sub>	<i>I</i> 4̄ (82)	SM	—	FM	—	HQ	249656
630	Li <sub>3</sub> Na(NH <sub>2</sub> ) <sub>4</sub>	<i>I</i> 4̄ (82)	Triv.	—	NM	—	HQ	201147 201148
631	Re <sub>4</sub> Te <sub>4</sub> (TeBr <sub>2</sub> ) <sub>4</sub> Br <sub>8</sub>	<i>I</i> 4̄ (82)	Triv.	—	NM	—	HQ	78924
632	((S <sub>4</sub> Re <sub>4</sub> )Cl <sub>8</sub> (TeCl <sub>2</sub> ) <sub>4</sub> )	<i>I</i> 4̄ (82)	Triv.	—	NM	—	HQ	165333
633	((Te <sub>4</sub> Re <sub>4</sub> )Cl <sub>8</sub> (TeCl <sub>2</sub> ) <sub>4</sub> )	<i>I</i> 4̄ (82)	Triv.	—	NM	—	HQ	165335
634	(PCl <sub>4</sub> )(SbF <sub>6</sub> )	<i>P4</i> /n (85)	Triv.	—	NM	—	HQ	71876
635	(Li(NH <sub>3</sub> ) <sub>4</sub> )(C <sub>2</sub> )H	<i>P4</i> /n (85)	Triv.	—	NM	—	—	425119
636	PCl <sub>5</sub>	<i>P4</i> /n (85)	Triv.	—	NM	—	—	26048 26661
637	Cs(Al(NH <sub>2</sub> ) <sub>4</sub> )	<i>P4</i> /n (85)	Triv.	—	NM	—	HQ	2537 40169
638	(VO)(SO <sub>4</sub> )	<i>P4</i> /n (85)	SM	(b)	AFM	—	HQ	18307
639	MoO(PO <sub>4</sub> )	<i>P4</i> /n (85)	SM	(b)	FM	—	HQ	24894 36095
640	(PNCl <sub>2</sub> ) <sub>4</sub>	<i>P4</i> <sub>2</sub> /n (86)	Triv.	—	NM	—	—	23897 33711
641	KSb <sub>4</sub> F <sub>13</sub>	<i>I</i> 4/m (87)	Triv.	—	NM	—	—	24740
642	Ba(VSi <sub>2</sub> O <sub>7</sub> )	<i>I</i> 4/m (87)	Triv.	(b)	AFM	—	HQ	78029
643	(N(CH <sub>3</sub> ) <sub>4</sub> ) <sub>2</sub> (PtF <sub>6</sub> )	<i>I</i> 4/m (87)	Triv.	—	NM	—	—	151176
644	Ba <sub>2</sub> Zr <sub>6</sub> Cl <sub>17</sub> B	<i>I</i> 4/m (87)	Triv.	(b)	NM	—	HQ	203141
645	Cs <sub>8</sub> (Ta <sub>6</sub> O <sub>19</sub> )	<i>I</i> 4/m (87)	Triv.	(b,s)	NM	—	—	411856
646	((CH <sub>3</sub> ) <sub>4</sub> N) <sub>2</sub> K(Mn(CN) <sub>6</sub> )	<i>I</i> 4/m (87)	Triv.	—	FM	—	—	107665
647	((CH <sub>3</sub> ) <sub>4</sub> N) <sub>2</sub> Rb(Co(CN) <sub>6</sub> )	<i>I</i> 4/m (87)	Triv.	—	NM	—	—	107666
648	((CH <sub>3</sub> ) <sub>4</sub> N) <sub>2</sub> (KFe(CN) <sub>6</sub> )	<i>I</i> 4/m (87)	SM	—	FM	—	—	239245
649	Na <sub>4</sub> (IrO <sub>4</sub> )	<i>I</i> 4/m (87)	SM	(b)	FM	—	HQ	67826
650	Na <sub>2</sub> TiOSi <sub>4</sub> O <sub>10</sub>	<i>I</i> 4/m (87)	Triv.	(b,s)	NM	—	—	16899
651	XeF <sub>2</sub> IF <sub>5</sub>	<i>I</i> 4/m (87)	Triv.	—	NM	—	HQ	26059
652	(XeOF <sub>4</sub> )(XeF <sub>2</sub> )	<i>I</i> 4/m (87)	Triv.	—	—	—	HQ	422962
653	B <sub>10</sub> F <sub>12</sub>	<i>I</i> 4 <sub>1</sub> /a (88)	Triv.	—	NM	—	—	412618
654	TlB(CN) <sub>4</sub>	<i>I</i> 4 <sub>1</sub> /a (88)	Triv.	—	NM	—	HQ	414564
655	SO <sub>2</sub> F <sub>2</sub>	<i>P</i> 4 <sub>1</sub> 2 <sub>1</sub> 2 (92)	Triv.	—	NM	—	HQ	62968
656	Pb <sub>2</sub> Cu(OH) <sub>4</sub> Cl <sub>2</sub>	<i>P</i> 4mm (99)	SM	—	FM	—	HQ	81589
657	Cs <sub>2</sub> V <sub>3</sub> O <sub>8</sub>	<i>P</i> 4bm (100)	SM	(b,s)	FM	—	HQ	251010 430710 430711 430708 430709
658	(H <sub>3</sub> O) <sub>2</sub> V <sub>3</sub> O <sub>8</sub>	<i>P</i> 4bm (100)	SM	—	FM	—	—	421914
659	K <sub>2</sub> (VO)(V <sub>2</sub> O <sub>7</sub> )	<i>P</i> 4bm (100)	SM	(b,s)	FM	—	HQ	1925 245500
660	Rb <sub>2</sub> (VO)(V <sub>2</sub> O <sub>7</sub> )	<i>P</i> 4bm (100)	SM	(b,s)	FM	—	HQ	72285 79378 150326
661	(NH <sub>4</sub> ) <sub>2</sub> V <sub>3</sub> O <sub>8</sub>	<i>P</i> 4bm (100)	SM	—	FM	—	—	201900
662	Cs <sub>2</sub> V <sub>5</sub> O <sub>13</sub>	<i>I</i> 4mm (107)	SM	(b)	FM	—	HQ	849
663	KNa <sub>2</sub> (CuO <sub>2</sub> )	<i>I</i> 4mm (107)	Triv.	(b)	NM	—	HQ	47105
664	Ta <sub>4</sub> S <sub>9</sub> Br <sub>8</sub>	<i>I</i> 4mm (107)	Triv.	(b)	NM	—	HQ	171236
665	Cu(Fe(CN) <sub>5</sub> NO)	<i>I</i> 4mm (107)	SM	—	FM	—	HQ	414021

666	(Os(NO)(NH <sub>3</sub> ) <sub>4</sub> Cl)Cl <sub>2</sub>	<i>I</i> 4 <i>mm</i> (107)	Triv.	—	NM	—	—	39306
667	K <sub>3</sub> (NO <sub>3</sub> )	<i>I</i> 4 <i>cm</i> (108)	Triv.	(b,s)	NM	—	—	37204
668	(NO)(ClF <sub>4</sub> )	<i>I</i> 4 <i>cm</i> (108)	Triv.	—	NM	—	HQ	50216
669	Li <sub>2</sub> VO(SO <sub>4</sub> ) <sub>2</sub>	<i>I</i> 4 <i>cm</i> (108)	SM	(b)	—	—	—	241829
670	(NH <sub>4</sub> )(ClO <sub>2</sub> )	<i>P</i> 4 <i>2</i> <sub>1</sub> <i>m</i> (113)	Triv.	—	NM	—	—	26511 59921
671	(PCl <sub>4</sub> )(ICl <sub>2</sub> )	<i>P</i> 4 <i>2</i> <sub>1</sub> <i>m</i> (113)	Triv.	—	NM	—	—	26594
672	(S <sub>3</sub> N <sub>3</sub> O <sub>4</sub> ) <sub>2</sub> S	<i>P</i> 4 <i>2</i> <sub>1</sub> <i>m</i> (113)	Triv.	(b)	NM	—	—	49015
673	(NF <sub>4</sub> )(BF <sub>4</sub> )	<i>P</i> 4 <i>2</i> <sub>1</sub> <i>m</i> (113)	Triv.	—	NM	—	—	63311 68017
674	Li(ReO <sub>2</sub> F <sub>4</sub> )	<i>P</i> 4 <i>2</i> <sub>1</sub> <i>m</i> (113)	Triv.	(b)	NM	—	HQ	280011
675	CO(NH <sub>2</sub> ) <sub>2</sub>	<i>P</i> 4 <i>2</i> <sub>1</sub> <i>m</i> (113)	Triv.	—	NM	—	HQ	15432 15433 16692 29364 29365 29366 40049 43490 56901 100303 100304 100305 170090 280179
676	C <sub>10</sub> H <sub>16</sub>	<i>P</i> 4 <i>2</i> <sub>1</sub> <i>c</i> (114)	Triv.	—	NM	—	—	5284
677	(NSF) <sub>4</sub>	<i>P</i> 4 <i>2</i> <sub>1</sub> <i>c</i> (114)	Triv.	—	NM	—	—	15422 18202 71039
678	H <sub>10</sub> O <sub>8</sub> Se	<i>P</i> 4 <i>2</i> <sub>1</sub> <i>c</i> (114)	Triv.	—	—	—	—	404660
679	CsLi <sub>2</sub> I <sub>3</sub>	<i>P</i> 4 <i>m</i> 2 (115)	Triv.	(b)	NM	—	—	245988
680	RbCuO	<i>I</i> 4 <i>m</i> 2 (119)	Triv.	—	NM	—	HQ	49758 188523
681	CsSbClF <sub>3</sub>	<i>I</i> 4 <i>2m</i> (121)	Triv.	—	NM	—	HQ	28222 200296
682	(TcBr <sub>2</sub> )(P(CH <sub>3</sub> ) <sub>3</sub> ) <sub>4</sub>	<i>I</i> 4 <i>2m</i> (121)	SM	—	FM	—	—	166912
683	WCl <sub>2</sub> (P(CH <sub>3</sub> ) <sub>3</sub> ) <sub>4</sub>	<i>I</i> 4 <i>2m</i> (121)	Triv.	—	FM	—	—	185488
684	MoCl <sub>2</sub> (P(CH <sub>3</sub> ) <sub>3</sub> ) <sub>4</sub>	<i>I</i> 4 <i>2m</i> (121)	Triv.	—	FM	—	—	185489
685	Cs(NH <sub>4</sub> ) <sub>2</sub> Cr(O <sub>2</sub> ) <sub>4</sub>	<i>I</i> 4 <i>2m</i> (121)	SM	—	FM	—	HQ	237787 261393
686	Ba <sub>4</sub> Na(CuO <sub>4</sub> )(CO <sub>3</sub> ) <sub>2</sub>	<i>I</i> 4 <i>2m</i> (121)	Triv.	—	NM	—	HQ	66776 80606
687	K <sub>3</sub> (Cr(O <sub>2</sub> ) <sub>4</sub> )	<i>I</i> 4 <i>2m</i> (121)	SM	—	FM	—	HQ	9356 9676 23536 30404 280253
688	K <sub>3</sub> (VO <sub>4</sub> )	<i>I</i> 4 <i>2m</i> (121)	Triv.	—	NM	—	—	4138
689	K <sub>3</sub> (MnO <sub>4</sub> )	<i>I</i> 4 <i>2m</i> (121)	Triv.	—	AFM	—	—	108935
690	K <sub>4</sub> (CO <sub>4</sub> )	<i>I</i> 4 <i>2m</i> (121)	Triv.	—	NM	—	—	245419 245420
691	Be(OH <sub>2</sub> ) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub>	<i>I</i> 4 <i>2d</i> (122)	Triv.	—	NM	—	—	15858
692	K(HC(NO) <sub>2</sub> )	<i>I</i> 4 <i>2d</i> (122)	Triv.	—	NM	—	HQ	170586
693	(NH <sub>4</sub> )(H <sub>2</sub> PO <sub>4</sub> )	<i>I</i> 4 <i>2d</i> (122)	Triv.	(b)	NM	—	HQ	28154 54776 63494 63634 84114 174048 174049 174050 246299 <sup>(s)</sup>
694	(NH <sub>4</sub> )(H <sub>2</sub> AsO <sub>4</sub> )	<i>I</i> 4 <i>2d</i> (122)	Triv.	(b)	NM	—	HQ	28155 66203 66204 <sup>(s)</sup> 66205 <sup>(s)</sup> 66206 <sup>(s)</sup> 174061 <sup>(s)</sup> 200219
695	Co(B(CN) <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	<i>I</i> 4 <i>2d</i> (122)	SM	—	—	—	—	260263
696	Rb(H <sub>2</sub> PO <sub>4</sub> )	<i>I</i> 4 <i>2d</i> (122)	Triv.	(b)	NM	—	HQ	69317
697	Na <sub>5</sub> (NiO <sub>2</sub> )S	<i>P</i> 4/ <i>mmm</i> (123)	SM	(b,s)	FM	—	HQ	412972
698	Na <sub>5</sub> (CuO <sub>2</sub> )S	<i>P</i> 4/ <i>mmm</i> (123)	Triv.	(b,s)	NM	—	HQ	412977
699	(P(NH <sub>2</sub> ) <sub>4</sub> )I	<i>P</i> 4/ <i>nbm</i> (125)	Triv.	—	NM	—	HQ	74814
700	((NH <sub>2</sub> ) <sub>4</sub> P)I	<i>P</i> 4/ <i>nbm</i> (125)	TI	—	—	—	HQ	400461
701	(P(NH <sub>2</sub> ) <sub>4</sub> )Br	<i>P</i> 4/ <i>nbm</i> (125)	Triv.	—	FM	—	HQ	410797
702	Cs <sub>3</sub> (SiF <sub>6</sub> )F	<i>P</i> 4/ <i>mbm</i> (127)	Triv.	—	NM	—	—	9588
703	Rb <sub>2</sub> CsSiF <sub>7</sub>	<i>P</i> 4/ <i>mbm</i> (127)	Triv.	—	NM	—	—	9592
704	Cs <sub>3</sub> TiF <sub>7</sub>	<i>P</i> 4/ <i>mbm</i> (127)	Triv.	—	NM	—	—	9594
705	Cs <sub>3</sub> CrF <sub>7</sub>	<i>P</i> 4/ <i>mbm</i> (127)	Triv.	—	FM	—	—	9596
706	Rb <sub>3</sub> CrF <sub>7</sub>	<i>P</i> 4/ <i>mbm</i> (127)	Triv.	—	FM	—	—	9597
707	Cs <sub>3</sub> (MnF <sub>6</sub> )F	<i>P</i> 4/ <i>mbm</i> (127)	SM	—	FM	—	—	9598
708	Rb <sub>3</sub> (MnF <sub>6</sub> )F	<i>P</i> 4/ <i>mbm</i> (127)	SM	—	FM	—	—	9599
709	K <sub>3</sub> Cl(ReF <sub>6</sub> )	<i>P</i> 4/ <i>mbm</i> (127)	SM	—	FM	—	—	80170
710	Pb <sub>2</sub> Cl <sub>2</sub> (CO <sub>3</sub> )	<i>P</i> 4/ <i>mbm</i> (127)	Triv.	—	NM	—	—	4240 29113 36241
711	Pb <sub>2</sub> Br <sub>2</sub> (CO <sub>3</sub> )	<i>P</i> 4/ <i>mbm</i> (127)	Triv.	—	NM	—	—	29114 250396
712	Cs <sub>2</sub> Li(Cr(CN) <sub>6</sub> )	<i>P</i> 4/ <i>mnc</i> (128)	SM	—	FM	—	—	804
713	Na <sub>2</sub> Cl(B(OH) <sub>4</sub> )	<i>P</i> 4/ <i>nmm</i> (129)	Triv.	—	NM	—	—	32518
714	(N(CH <sub>3</sub> ) <sub>4</sub> )I	<i>P</i> 4/ <i>nmm</i> (129)	Triv.	—	NM	—	—	55080
715	Cs(ReF <sub>8</sub> )	<i>P</i> 4/ <i>nmm</i> (129)	Triv.	—	NM	—	—	410829
716	KNaWO <sub>2</sub> F <sub>4</sub>	<i>P</i> 4/ <i>nmm</i> (129)	Triv.	(b)	NM	—	—	422709
717	KNaMoO <sub>2</sub> F <sub>4</sub>	<i>P</i> 4/ <i>nmm</i> (129)	Triv.	(b)	NM	—	—	422707
718	BaFCl	<i>P</i> 4/ <i>nmm</i> (129)	Triv.	—	NM	—	—	2350 35487 35488 35489 35490 35491 35492 35493 85319 155004 183925 201514 201515 201516 201517 201518 201519
719	(VO)(P <sub>2</sub> SiO <sub>8</sub> )	<i>P</i> 4/ <i>ncc</i> (130)	SM	(b,s)	FM	—	—	628

720	Mo(AlP <sub>2</sub> O <sub>9</sub> )	<i>P4/ncc</i> (130)	SM	(b,s)	—	—	—	67221
721	PtZn(CN) <sub>4</sub>	<i>P4<sub>2</sub>/mcm</i> (132)	Triv.	—	NM	—	HQ	169758
722	PdZn(CN) <sub>4</sub>	<i>P4<sub>2</sub>/mcm</i> (132)	Triv.	—	—	—	HQ	169759
723	NiZn(CN) <sub>4</sub>	<i>P4<sub>2</sub>/mcm</i> (132)	Triv.	—	—	—	HQ	169760
724	Cs <sub>4</sub> K <sub>2</sub> Cu(SiO <sub>4</sub> ) <sub>2</sub>	<i>P4<sub>2</sub>/mnmm</i> (136)	SM	(b,s)	FM	—	—	92493
725	Li <sub>2</sub> PtF <sub>6</sub>	<i>P4<sub>2</sub>/mnmm</i> (136)	Triv.	(b)	NM	—	HQ	248725 165216
726	K <sub>3</sub> NiO <sub>2</sub>	<i>P4<sub>2</sub>/mnmm</i> (136)	SM	(b)	FM	—	HQ	262579
727	Cs <sub>3</sub> NiO <sub>2</sub>	<i>P4<sub>2</sub>/mnmm</i> (136)	SM	(b)	—	—	HQ	424578
728	Rb <sub>3</sub> NiO <sub>2</sub>	<i>P4<sub>2</sub>/mnmm</i> (136)	SM	(b)	FM	—	HQ	424579
729	K <sub>2</sub> (CuCl <sub>4</sub> )(H <sub>2</sub> O) <sub>2</sub>	<i>P4<sub>2</sub>/mnmm</i> (136)	SM	—	FM	—	—	15943 16052
730	(NH <sub>4</sub> ) <sub>2</sub> (CuCl <sub>4</sub> )(H <sub>2</sub> O) <sub>2</sub>	<i>P4<sub>2</sub>/mnmm</i> (136)	SM	—	FM	—	—	23750 163014 420586
731	Rb <sub>2</sub> CuCl <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub>	<i>P4<sub>2</sub>/mnmm</i> (136)	SM	—	FM	—	HQ	71867
732	(NH <sub>4</sub> ) <sub>2</sub> (Cu(H <sub>2</sub> O) <sub>2</sub> Br <sub>2</sub> )Br <sub>2</sub>	<i>P4<sub>2</sub>/mnmm</i> (136)	SM	—	FM	—	—	88887 88888 88889
733	Li <sub>2</sub> (MoF <sub>6</sub> )	<i>P4<sub>2</sub>/mnmm</i> (136)	Triv.	(b)	FM	—	HQ	74565
734	Li <sub>2</sub> (RhF <sub>6</sub> )	<i>P4<sub>2</sub>/mnmm</i> (136)	SM	(b)	FM	—	HQ	95778 165211
735	Li <sub>2</sub> (PdF <sub>6</sub> )	<i>P4<sub>2</sub>/mnmm</i> (136)	Triv.	(b)	NM	—	HQ	165212
736	Li <sub>2</sub> (CrF <sub>6</sub> )	<i>P4<sub>2</sub>/mnmm</i> (136)	Triv.	(b)	FM	—	HQ	418676
737	Mg(ClO <sub>2</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>6</sub>	<i>P4<sub>2</sub>/nmcm</i> (137)	Triv.	—	NM	—	—	69587
738	(CsF <sub>2</sub> )(Br <sub>2</sub> )	<i>I4/mmm</i> (139)	Triv.	—	NM	—	HQ	84021 84022
739	Rb <sub>2</sub> Na(MnF <sub>6</sub> )	<i>I4/mmm</i> (139)	Triv.	(b)	FM	—	—	9708
740	Cs <sub>2</sub> K(MnF <sub>6</sub> )	<i>I4/mmm</i> (139)	Triv.	—	FM	—	—	22110 91036 91197(b)
741	K <sub>2</sub> NaMnF <sub>6</sub>	<i>I4/mmm</i> (139)	Triv.	(b,s)	FM	—	—	61117
742	Cs <sub>3</sub> (O(ReCl <sub>5</sub> ) <sub>2</sub> )	<i>I4/mmm</i> (139)	SM	—	FM	—	HQ	31
743	CsNi(CN) <sub>2</sub> Br	<i>I4/mmm</i> (139)	TI	—	—	—	HQ	380468
744	CsNi(CN) <sub>2</sub> Cl	<i>I4/mmm</i> (139)	TI	—	—	—	HQ	380469
745	RbNi(CN) <sub>2</sub> Br	<i>I4/mmm</i> (139)	TI	—	FM	—	HQ	380470
746	RbNi(CN) <sub>2</sub> Cl	<i>I4/mmm</i> (139)	TI	—	FM	—	HQ	380471
747	K <sub>2</sub> (OsO <sub>2</sub> Cl <sub>4</sub> )	<i>I4/mmm</i> (139)	Triv.	—	NM	—	HQ	15454 36231
748	Cs <sub>2</sub> NiO <sub>2</sub>	<i>I4/mmm</i> (139)	Triv.	(b)	AFM	—	HQ	423923
749	KrF <sub>2</sub>	<i>I4/mmm</i> (139)	Triv.	—	NM	—	HQ	279623
750	Rb(BrF <sub>4</sub> )	<i>I4/mcm</i> (140)	Triv.	—	NM	—	HQ	65713 670019
751	Ba(C <sub>4</sub> O <sub>4</sub> )	<i>I4/mcm</i> (140)	Triv.	—	NM	—	HQ	412830
752	Cs <sub>3</sub> (MnCl <sub>5</sub> )	<i>I4/mcm</i> (140)	SM	(b)	FM	—	HQ	24
753	Cs <sub>3</sub> FeBr <sub>5</sub>	<i>I4/mcm</i> (140)	SM	(b)	FM	—	—	4065
754	Cs <sub>3</sub> (CoCl <sub>4</sub> )Cl	<i>I4/mcm</i> (140)	SM	—	FM	—	HQ	14087 <sup>(b)</sup> 15245 <sup>(b)</sup> 16397 <sup>(b)</sup> 16556 28533 <sup>(b)</sup> 31032 280443 <sup>(b)</sup>
755	Cs <sub>3</sub> NiCl <sub>5</sub>	<i>I4/mcm</i> (140)	Triv.	—	FM	—	HQ	59372
756	Cs <sub>3</sub> CoBr <sub>5</sub>	<i>I4/mcm</i> (140)	SM	(b)	FM	—	HQ	201135
757	SrCuF <sub>4</sub>	<i>I4/mcm</i> (140)	SM	(b)	FM	—	—	9927
758	CaCuF <sub>4</sub>	<i>I4/mcm</i> (140)	SM	(b)	FM	—	—	9928
759	SrPdF <sub>4</sub>	<i>I4/mcm</i> (140)	Triv.	—	NM	—	—	108990
760	NaBrF <sub>4</sub>	<i>I4/mcm</i> (140)	Triv.	(b)	—	—	—	431176
761	(Pd(NH <sub>3</sub> ) <sub>4</sub> )(CrO <sub>4</sub> )	<i>I4<sub>1</sub>/amd</i> (141)	Triv.	—	NM	—	—	72997
762	Cr(H <sub>2</sub> O) <sub>6</sub> F <sub>3</sub> (H <sub>2</sub> O) <sub>3</sub>	<i>R3</i> (146)	SM	—	FM	—	—	2379
763	Cl <sub>3</sub> (Co(CO) <sub>4</sub> )Sn	<i>R3</i> (146)	Triv.	—	NM	—	HQ	69685
764	KNi(PO <sub>3</sub> ) <sub>3</sub>	<i>R3</i> (146)	SM	(b)	AFM	—	HQ	91527
765	(Cs <sub>2</sub> (SO <sub>4</sub> ))(Te(OH) <sub>6</sub> )	<i>R3</i> (146)	Triv.	—	—	—	HQ	93016
766	Li <sub>3</sub> VO <sub>4</sub> (H <sub>2</sub> O) <sub>6</sub>	<i>R3</i> (146)	Triv.	—	NM	—	HQ	174238
767	(Mg(H <sub>2</sub> O) <sub>6</sub> )(HPO <sub>3</sub> )	<i>R3</i> (146)	Triv.	—	NM	—	HQ	74520 74521
768	Cs <sub>2</sub> Na(Bi(SCN) <sub>6</sub> )	<i>P3</i> (147)	Triv.	—	—	—	—	79593
769	Li <sub>2</sub> Pt(OH) <sub>6</sub>	<i>P3</i> (147)	Triv.	—	NM	—	HQ	251041
770	Na <sub>2</sub> Pt(OH) <sub>6</sub>	<i>P3</i> (147)	Triv.	—	NM	—	HQ	251042
771	Cs <sub>2</sub> Sn(OOH) <sub>6</sub>	<i>P3</i> (147)	Triv.	—	NM	—	HQ	260828
772	Ca <sub>10</sub> (PO <sub>4</sub> ) <sub>6</sub> Se	<i>P3</i> (147)	Triv.	—	NM	—	—	410781
773	Ba <sub>10</sub> (PO <sub>4</sub> ) <sub>6</sub> S	<i>P3</i> (147)	Triv.	—	NM	—	—	410785
774	Cd <sub>2</sub> (Os(CN) <sub>6</sub> )	<i>P3</i> (147)	Triv.	(b)	—	—	HQ	417821
775	Cd <sub>2</sub> (Ru(CN) <sub>6</sub> )	<i>P3</i> (147)	Triv.	(b)	—	—	HQ	417822
776	Te(OTeF <sub>5</sub> ) <sub>6</sub>	<i>R3</i> (148)	Triv.	—	NM	—	—	2174
777	C <sub>2</sub> H <sub>30</sub> MgO <sub>18</sub> S <sub>2</sub>	<i>R3</i> (148)	Triv.	—	NM	—	—	5391 169171
778	(Re(CO) <sub>3</sub> I <sub>3</sub> ) <sub>2</sub> Re	<i>R3</i> (148)	SM	—	FM	—	HQ	15497

779	(Co(NH <sub>3</sub> ) <sub>6</sub> )(Os(SCN) <sub>6</sub> )	R <sub>3</sub> (148)	SM	—	—	—	—	92479
780	(N(CH <sub>3</sub> ) <sub>4</sub> ) <sub>2</sub> (OsF <sub>6</sub> )	R <sub>3</sub> (148)	Triv.	—	FM	—	—	151185
781	(Cu(XeF <sub>2</sub> ) <sub>6</sub> )(SbF <sub>6</sub> ) <sub>2</sub>	R <sub>3</sub> (148)	SM	—	—	—	—	416303
782	Ba <sub>2</sub> Co(B <sub>3</sub> O <sub>6</sub> ) <sub>2</sub>	R <sub>3</sub> (148)	SM	(b)	AFM	—	HQ	391014
783	Co(ClO <sub>4</sub> ) <sub>2</sub>	R <sub>3</sub> (148)	SM	(b)	FM	—	—	33288
784	Ni(ClO <sub>4</sub> ) <sub>2</sub>	R <sub>3</sub> (148)	Triv.	(b)	FM	—	—	33289
785	(Co(H <sub>2</sub> O) <sub>6</sub> )(SiF <sub>6</sub> )	R <sub>3</sub> (148)	SM	—	FM	—	HQ	2900
786	Zn(TiF <sub>6</sub> )(H <sub>2</sub> O) <sub>6</sub>	R <sub>3</sub> (148)	Triv.	—	NM	—	HQ	62375 202787
787	Co(SnF <sub>6</sub> )(H <sub>2</sub> O) <sub>6</sub>	R <sub>3</sub> (148)	SM	—	FM	—	HQ	75984
788	Mn(TiF <sub>6</sub> )(H <sub>2</sub> O) <sub>6</sub>	R <sub>3</sub> (148)	SM	—	AFM	—	HQ	202786
789	(Co(NH <sub>3</sub> ) <sub>6</sub> )(Cr(CN) <sub>6</sub> )	R <sub>3</sub> (148)	SM	—	FM	—	—	805 806
790	(Co(NH <sub>3</sub> ) <sub>6</sub> )(Mn(CN) <sub>6</sub> )	R <sub>3</sub> (148)	Triv.	—	—	—	—	260055
791	(Co(NH <sub>3</sub> ) <sub>6</sub> )(Fe(CN) <sub>6</sub> )	R <sub>3</sub> (148)	SM	—	FM	—	—	411630 421507
792	K <sub>2</sub> SrNb <sub>6</sub> Cl <sub>18</sub>	R <sub>3</sub> (148)	Triv.	—	—	—	HQ	280933
793	Cs <sub>2</sub> Pb(NbCl <sub>3</sub> ) <sub>6</sub>	R <sub>3</sub> (148)	Triv.	—	NM	—	HQ	409544
794	(HSiO <sub>1.5</sub> ) <sub>8</sub>	R <sub>3</sub> (148)	Triv.	(b,s)	NM	—	HQ	27154 75244
795	K(Os(NH <sub>3</sub> ) <sub>6</sub> )(ClO <sub>4</sub> ) <sub>2</sub> Cl <sub>2</sub>	R <sub>3</sub> (148)	SM	—	FM	—	—	87619
796	K(Cr(NH <sub>3</sub> ) <sub>6</sub> )(ClO <sub>4</sub> ) <sub>2</sub> Cl <sub>2</sub>	R <sub>3</sub> (148)	SM	—	FM	—	—	87621
797	Rb(Ru(NH <sub>3</sub> ) <sub>6</sub> )(ClO <sub>4</sub> ) <sub>2</sub> Cl <sub>2</sub>	R <sub>3</sub> (148)	SM	—	FM	—	—	280492 280493
798	Cs(Ru(NH <sub>3</sub> ) <sub>6</sub> )(ClO <sub>4</sub> ) <sub>2</sub> Cl <sub>2</sub>	R <sub>3</sub> (148)	SM	—	FM	—	—	280495
799	Cs(Cr(NH <sub>3</sub> ) <sub>6</sub> )(ClO <sub>4</sub> ) <sub>2</sub> Cl <sub>2</sub>	R <sub>3</sub> (148)	SM	—	FM	—	—	280497
800	Cs(Cr(NH <sub>3</sub> ) <sub>6</sub> )(ClO <sub>4</sub> ) <sub>2</sub> Br <sub>2</sub>	R <sub>3</sub> (148)	SM	—	FM	—	—	280499
801	CsReF <sub>6</sub>	R <sub>3</sub> (148)	SM	—	FM	—	HQ	201511
802	Ba(IrF <sub>6</sub> )	R <sub>3</sub> (148)	SM	—	—	—	HQ	240981
803	Li <sub>8</sub> (IrO <sub>6</sub> )	R <sub>3</sub> (148)	SM	—	FM	—	HQ	61217
804	CdCrF <sub>6</sub>	R <sub>3</sub> (148)	Triv.	(b)	FM	—	—	10346
805	NiSnF <sub>6</sub>	R <sub>3</sub> (148)	SM	(b,s)	FM	—	—	25015
806	CuSnF <sub>6</sub>	R <sub>3</sub> (148)	SM	(b,s)	FM	—	—	25016
807	CaPtF <sub>6</sub>	R <sub>3</sub> (148)	Triv.	(b,s)	NM	—	—	37443
808	ZnPtF <sub>6</sub>	R <sub>3</sub> (148)	Triv.	(b,s)	NM	—	—	37444
809	Cd(PtF <sub>6</sub> )	R <sub>3</sub> (148)	Triv.	(b,s)	NM	—	—	37445 78906
810	NiPtF <sub>6</sub>	R <sub>3</sub> (148)	SM	(b,s)	FM	—	—	37448 78905
811	PdPtF <sub>6</sub>	R <sub>3</sub> (148)	SM	(b,s)	FM	—	—	64661
812	Li(IrF <sub>6</sub> )	R <sub>3</sub> (148)	Triv.	(b,s)	FM	—	HQ	95777 165207
813	Li(OsF <sub>6</sub> )	R <sub>3</sub> (148)	SM	(b,s)	FM	—	HQ	165206 165213 165214
814	Li(PtF <sub>6</sub> )	R <sub>3</sub> (148)	SM	(b,s)	FM	—	HQ	165208
815	Ca(SiF <sub>6</sub> )	R <sub>3</sub> (148)	Triv.	—	—	—	HQ	183914
816	Na(AsF <sub>6</sub> )	R <sub>3</sub> (148)	Triv.	—	NM	—	HQ	184562 184563
817	Na <sub>2</sub> Mg(CO <sub>3</sub> ) <sub>2</sub>	R <sub>3</sub> (148)	Triv.	(b)	NM	—	HQ	9518 100482
818	AgGe <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub>	R <sub>3</sub> (148)	Triv.	(b)	—	—	—	425869
819	Na <sub>2</sub> Pt(IO <sub>3</sub> ) <sub>6</sub>	R <sub>3</sub> (148)	Triv.	(b)	—	—	—	291621
820	K <sub>2</sub> Pt(IO <sub>3</sub> ) <sub>6</sub>	R <sub>3</sub> (148)	Triv.	(b)	—	—	—	291622
821	Rb <sub>2</sub> Pt(IO <sub>3</sub> ) <sub>6</sub>	R <sub>3</sub> (148)	Triv.	—	—	—	—	291623
822	Cs <sub>2</sub> Pt(IO <sub>3</sub> ) <sub>6</sub>	R <sub>3</sub> (148)	Triv.	—	—	—	—	291624
823	KCo(Au(CN) <sub>2</sub> ) <sub>3</sub>	P312 (149)	SM	(k*,b)	FM	—	HQ	201056
824	K(Ni(Au(CN) <sub>2</sub> ) <sub>3</sub> )	P312 (149)	SM	(k*,b)	FM	—	—	249724
825	KMn(Ag(CN) <sub>2</sub> ) <sub>3</sub>	P312 (149)	SM	(k*,b)	FM	—	HQ	281280 262503 262504 262505 262506 262507
826	BaCa(CO <sub>3</sub> ) <sub>2</sub>	P321 (150)	Triv.	—	NM	—	HQ	100477
827	CaCl <sub>2</sub> (H <sub>2</sub> O) <sub>6</sub>	P321 (150)	Triv.	—	NM	—	—	1140 59142
828	CaBr <sub>2</sub> (H <sub>2</sub> O) <sub>6</sub>	P321 (150)	Triv.	—	—	—	—	1141
829	SrCl <sub>2</sub> (H <sub>2</sub> O) <sub>6</sub>	P321 (150)	Triv.	—	—	—	HQ	48110 59143
830	K <sub>2</sub> (S <sub>2</sub> O <sub>6</sub> )	P321 (150)	Triv.	—	NM	—	HQ	16661 36154 <sup>(b)</sup> 82843
831	CaMg <sub>3</sub> (CO <sub>3</sub> ) <sub>4</sub>	R32 (155)	Triv.	(b)	NM	—	HQ	201729
832	Sr(Al <sub>2</sub> B <sub>2</sub> O <sub>7</sub> )	R32 (155)	Triv.	(b)	—	—	HQ	89423
833	NaK(TeO <sub>3</sub> )(H <sub>2</sub> O) <sub>3</sub>	P31c (159)	Triv.	—	NM	—	HQ	24781
834	KLi(SO <sub>4</sub> )	P31c (159)	Triv.	(b)	NM	—	—	62981 71365
835	Ca <sub>3</sub> (SiO <sub>4</sub> )O	R3m (160)	Triv.	(k*,b)	NM	—	HQ	22501 24625
836	(V(H <sub>2</sub> O) <sub>3</sub> F <sub>3</sub> )	R3m (160)	SM	—	AFM	—	HQ	69571
837	(N(CH <sub>3</sub> ) <sub>3</sub> )(BH <sub>3</sub> )	R3m (160)	Triv.	—	—	—	HQ	249799
838	(Cl <sub>2</sub> B) <sub>3</sub> B(CO)	R3m (160)	Triv.	—	NM	—	HQ	280617

839	Ba(CO <sub>3</sub> )	<i>R</i> 3 <i>m</i> (160)	Triv.	—	NM	—	HQ	158389 158390
840	Rb <sub>4</sub> (CO <sub>4</sub> )	<i>R</i> 3 <i>m</i> (160)	Triv.	—	NM	—	—	245430
841	(NH <sub>3</sub> OH) <sub>3</sub> FeF <sub>6</sub>	<i>R</i> 3 <i>c</i> (161)	SM	—	FM	—	—	424249
842	(CH <sub>2</sub> ) <sub>3</sub> O <sub>3</sub>	<i>R</i> 3 <i>c</i> (161)	Triv.	—	NM	—	HQ	151224 151343
843	Ca <sub>3</sub> (C <sub>6</sub> N <sub>6</sub> O <sub>6</sub> )	<i>R</i> 3 <i>c</i> (161)	Triv.	—	NM	—	—	428357
844	LiCaNiF <sub>6</sub>	<i>P</i> 3 <i>1c</i> (163)	SM	(b,s)	FM	—	—	32732
845	LiSrNiF <sub>6</sub>	<i>P</i> 3 <i>1c</i> (163)	SM	(b,s)	FM	—	—	32733
846	LiCaCrF <sub>6</sub>	<i>P</i> 3 <i>1c</i> (163)	SM	(b)	FM	—	—	73985
847	Na <sub>3</sub> (CrCl <sub>6</sub> )	<i>P</i> 3 <i>1c</i> (163)	SM	(b)	FM	—	HQ	62035
848	Hg(B(CN) <sub>4</sub> ) <sub>2</sub>	<i>P</i> 3 <i>m1</i> (164)	Triv.	(b)	—	—	HQ	412297
849	Cs <sub>2</sub> Na(TiF <sub>6</sub> )	<i>P</i> 3 <i>m1</i> (164)	SM	(b,s)	FM	—	HQ	67160
850	(Hg(H <sub>2</sub> O) <sub>6</sub> )(ClO <sub>4</sub> ) <sub>2</sub>	<i>P</i> 3 <i>m1</i> (164)	Triv.	—	NM	—	HQ	1640
851	(Co(H <sub>2</sub> O) <sub>6</sub> )(BrO <sub>4</sub> ) <sub>2</sub>	<i>P</i> 3 <i>m1</i> (164)	SM	—	AFM	—	HQ	73397
852	K <sub>2</sub> (ReF <sub>6</sub> )	<i>P</i> 3 <i>m1</i> (164)	SM	(k*)	FM	—	HQ	1528
853	K <sub>2</sub> PtF <sub>6</sub>	<i>P</i> 3 <i>m1</i> (164)	Triv.	—	NM	—	—	16892 87360 <sup>(k)</sup>
854	Cs <sub>2</sub> PtF <sub>6</sub>	<i>P</i> 3 <i>m1</i> (164)	Triv.	—	NM	—	HQ	35107
855	Rb <sub>2</sub> PtF <sub>6</sub>	<i>P</i> 3 <i>m1</i> (164)	Triv.	(k*)	NM	—	HQ	35108
856	K <sub>2</sub> (IrF <sub>6</sub> )	<i>P</i> 3 <i>m1</i> (164)	SM	(k*)	FM	—	HQ	95779
857	Cs <sub>2</sub> (TcF <sub>6</sub> )	<i>P</i> 3 <i>m1</i> (164)	SM	—	FM	—	HQ	425912
858	K <sub>2</sub> (TcF <sub>6</sub> )	<i>P</i> 3 <i>m1</i> (164)	SM	(k*)	FM	—	HQ	425914
859	Na <sub>2</sub> (TcF <sub>6</sub> )	<i>P</i> 3 <i>m1</i> (164)	SM	—	FM	—	HQ	425915
860	Rb <sub>2</sub> (TcF <sub>6</sub> )	<i>P</i> 3 <i>m1</i> (164)	SM	(k*)	—	—	HQ	425918
861	K <sub>2</sub> (SO <sub>3</sub> )	<i>P</i> 3 <i>m1</i> (164)	Triv.	—	NM	—	HQ	60762
862	NaK <sub>3</sub> (PO <sub>3</sub> F) <sub>2</sub>	<i>P</i> 3 <i>m1</i> (164)	Triv.	—	—	—	HQ	1904
863	BaNa <sub>2</sub> Co(VO <sub>4</sub> ) <sub>2</sub>	<i>P</i> 3 <i>m1</i> (164)	SM	(k*,b)	—	—	—	429826
864	Rb <sub>2</sub> (IrF <sub>6</sub> )	<i>P</i> 3 <i>m1</i> (164)	SM	(k*)	FM	—	HQ	240955
865	Cs <sub>2</sub> (IrF <sub>6</sub> )	<i>P</i> 3 <i>m1</i> (164)	SM	—	FM	—	HQ	240956
866	Os(S <sub>2</sub> Cl <sub>12</sub> )	<i>R</i> 3 <i>m</i> (166)	Triv.	—	FM	—	HQ	74680
867	K <sub>4</sub> Xe <sub>3</sub> O <sub>12</sub>	<i>R</i> 3 <i>m</i> (166)	Triv.	(k*,b)	—	—	—	253443
868	Cs <sub>2</sub> Na(FeF <sub>6</sub> )	<i>R</i> 3 <i>m</i> (166)	TI	—	FM	—	—	9003 <sup>(b,s)</sup> 16255
869	Cs <sub>2</sub> NaMnF <sub>6</sub>	<i>R</i> 3 <i>m</i> (166)	Triv.	(b,s)	FM	—	HQ	37006
870	Cs <sub>2</sub> Na(NiF <sub>6</sub> )	<i>R</i> 3 <i>m</i> (166)	TI	(b,s)	—	—	—	42152
871	Cs <sub>2</sub> Na(TiF <sub>6</sub> )	<i>R</i> 3 <i>m</i> (166)	Triv.	(b,s)	FM	—	—	42153
872	Cs <sub>4</sub> K(Li(FeF <sub>6</sub> ) <sub>2</sub> )	<i>R</i> 3 <i>m</i> (166)	TI	(b,s)	FM	—	HQ	78928
873	PbPtF <sub>6</sub>	<i>R</i> 3 <i>m</i> (166)	Triv.	—	NM	—	—	4057
874	Ba(RhF <sub>6</sub> )	<i>R</i> 3 <i>m</i> (166)	SM	—	FM	—	—	6038
875	BaCrF <sub>6</sub>	<i>R</i> 3 <i>m</i> (166)	SM	—	FM	—	—	10341
876	SrCrF <sub>6</sub>	<i>R</i> 3 <i>m</i> (166)	SM	—	FM	—	—	10342
877	Sr(RhF <sub>6</sub> )	<i>R</i> 3 <i>m</i> (166)	SM	—	FM	—	—	42158
878	K(AuF <sub>6</sub> )	<i>R</i> 3 <i>m</i> (166)	Triv.	—	—	—	HQ	415874
879	K <sub>2</sub> Mg(CO <sub>3</sub> ) <sub>2</sub>	<i>R</i> 3 <i>m</i> (166)	Triv.	(b)	NM	—	HQ	31295
880	K(Cr(NH <sub>3</sub> ) <sub>6</sub> )(ClO <sub>4</sub> ) <sub>2</sub> Cl <sub>2</sub>	<i>R</i> 3 <i>m</i> (166)	SM	—	FM	—	—	87620
881	K(Ru(NH <sub>3</sub> ) <sub>6</sub> )(ClO <sub>4</sub> ) <sub>2</sub> Cl <sub>2</sub>	<i>R</i> 3 <i>m</i> (166)	SM	—	FM	—	—	280489 280490
882	O <sub>2</sub>	<i>R</i> 3 <i>m</i> (166)	Triv.	—	FM	SC*	HQ	15535 43430 173934 190368 190369
883	Re <sub>3</sub> Cl <sub>9</sub>	<i>R</i> 3 <i>m</i> (166)	Triv.	(k*)	NM	—	HQ	14209
884	ReCl <sub>3</sub>	<i>R</i> 3 <i>m</i> (166)	Triv.	—	NM	—	HQ	62222
885	Rb(C(CN) <sub>3</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	—	—	—	HQ	428450
886	Cs(C(CN) <sub>3</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	—	—	—	HQ	428451
887	((H <sub>2</sub> O) <sub>6</sub> Cr)Cl <sub>3</sub>	<i>R</i> 3 <i>c</i> (167)	SM	—	FM	—	—	66000
888	(Bi <sub>5</sub> )(GaCl <sub>4</sub> ) <sub>3</sub>	<i>R</i> 3 <i>c</i> (167)	Triv.	(b,s)	NM	—	—	81468
889	Bi <sub>5</sub> (AlCl <sub>4</sub> ) <sub>3</sub>	<i>R</i> 3 <i>c</i> (167)	Triv.	(b,s)	NM	—	—	201993 420082
890	Sr <sub>3</sub> (BO <sub>3</sub> ) <sub>2</sub>	<i>R</i> 3 <i>c</i> (167)	Triv.	—	NM	—	HQ	93395
891	K <sub>3</sub> (Cr(OH) <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	SM	—	AFM	—	—	62653
892	Rb <sub>3</sub> (Cr(OH) <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	SM	—	FM	—	—	72315
893	InSr <sub>3</sub> (NiO <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	SM	(b,s)	AFM	—	HQ	81660
894	K <sub>3</sub> NaMnCl <sub>6</sub>	<i>R</i> 3 <i>c</i> (167)	SM	(b,s)	FM	—	HQ	290109
895	Rb <sub>6</sub> Cl <sub>4</sub> O	<i>R</i> 3 <i>c</i> (167)	Triv.	(b)	NM	—	HQ	405193
896	Cs <sub>6</sub> Cl <sub>4</sub> O	<i>R</i> 3 <i>c</i> (167)	Triv.	(b,s)	NM	—	HQ	411634
897	Rb <sub>6</sub> Br <sub>4</sub> O	<i>R</i> 3 <i>c</i> (167)	Triv.	—	NM	—	HQ	411955
898	Rb <sub>3</sub> B <sub>3</sub> O <sub>6</sub>	<i>R</i> 3 <i>c</i> (167)	Triv.	—	NM	—	HQ	59826

899	Cs(BO <sub>2</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	—	NM	—	HQ	74888
900	Rb <sub>3</sub> (B <sub>3</sub> S <sub>6</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	—	NM	—	HQ	79615
901	K <sub>3</sub> F(CO <sub>3</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	(b,s)	NM	—	HQ	66028
902	Rb <sub>3</sub> F(CO <sub>3</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	(b,s)	NM	—	HQ	66029
903	K <sub>3</sub> (AuSe <sub>2</sub> )	<i>R</i> 3 <i>c</i> (167)	Triv.	—	NM	—	HQ	402000
904	K <sub>3</sub> SbS <sub>3</sub> (Sb <sub>2</sub> O <sub>3</sub> ) <sub>3</sub>	<i>P</i> 6 <sub>3</sub> (173)	Triv.	(b,s)	NM	—	—	4215
905	NaPO <sub>3</sub> NH <sub>3</sub>	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	NM	—	—	16608
906	PS(N(CH <sub>3</sub> )NH <sub>2</sub> ) <sub>3</sub>	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	NM	—	—	189680
907	(Sn(H <sub>2</sub> O) <sub>3</sub> )(ClO <sub>4</sub> ) <sub>2</sub>	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	NM	—	—	237716 253553
908	Sn(SnCl)(W <sub>3</sub> Cl <sub>13</sub> )	<i>P</i> 6 <sub>3</sub> (173)	Triv.	—	NM	—	—	421915
909	Al(IO <sub>3</sub> ) <sub>3</sub>	<i>P</i> 6 <sub>3</sub> (173)	Triv.	(b,s)	NM	—	HQ	152758
910	Li(IO <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> (173)	Triv.	(b)	NM	—	—	9508 <sup>(s)</sup> 14344 14377 <sup>(s)</sup> 35472 35473 35474 35475 <sup>(s)</sup> 35476 40358 40359 40360 40361 40362 <sup>(s)</sup> 40363 40364 40365 46025 46026 46027 <sup>(s)</sup> 80025 <sup>(s)</sup> 80026 <sup>(s)</sup> 20851 33251 36038 36471 48136 56106 71364 88827 88828 280391
911	KLi(SO <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> (173)	Triv.	(b)	NM	—	HQ	20851 33251 36038 36471 48136 56106 71364 88827 88828 280391
912	LiNa(CO <sub>3</sub> )	<i>P</i> 6̄ (174)	Triv.	(b)	NM	—	—	80459 89650 89651
913	TcOF <sub>4</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	—	FM	—	—	16143
914	B(OTeF <sub>5</sub> ) <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	Triv.	—	NM	—	—	27200
915	TlCu(OH)(CO <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	SM	(k,b)	FM	—	—	74875
916	Na(W <sub>6</sub> NCl <sub>18</sub> )	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	Triv.	(b)	—	—	—	414409
917	Sr <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> Cl	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	Triv.	—	NM	—	—	2089 80084 80085 253053
918	Sr <sub>10</sub> (PO <sub>4</sub> ) <sub>6</sub> F <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	Triv.	(b)	NM	—	—	163792
919	Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> Cl	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	Triv.	—	NM	—	—	184824 184825 670545
920	B(OCH <sub>3</sub> ) <sub>3</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	Triv.	—	NM	—	—	245045
921	BaZn(CO <sub>3</sub> )F <sub>2</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	Triv.	(b)	NM	—	HQ	95739
922	Fe <sub>2</sub> (CO) <sub>9</sub>	<i>P</i> 6 <sub>3</sub> / <i>m</i> (176)	Triv.	(b)	NM	—	—	6010 31030
923	SiO <sub>2</sub>	<i>P</i> 622 (177)	Triv.	(b,s)	NM	—	—	170519 170520 170522
924	CsLi(NH <sub>2</sub> ) <sub>2</sub>	<i>P</i> 6222 (180)	Triv.	—	NM	—	HQ	62654
925	Ba <sub>5</sub> (ReO <sub>5</sub> ) <sub>3</sub> Cl	<i>P</i> 6 <sub>3</sub> cm (185)	Triv.	—	NM	—	—	73928
926	Li <sub>8</sub> CoO <sub>6</sub>	<i>P</i> 6 <sub>3</sub> cm (185)	SM	(b,s)	FM	—	—	21026
927	BiCo <sub>3</sub> (CO) <sub>9</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	—	—	—	62542 66163
928	(NH <sub>4</sub> )(In(HPO <sub>3</sub> ) <sub>2</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	(k*,b)	—	—	—	188660
929	((CH <sub>3</sub> ) <sub>4</sub> P)(FeCl <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	SM	(k*)	FM	—	—	194586
930	Cl <sub>4</sub> H <sub>12</sub> N <sub>3</sub> O <sub>3</sub> Re	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	(k*)	—	—	—	419767
931	(NH <sub>4</sub> ) <sub>2</sub> (SiF <sub>6</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	NM	—	—	280755
932	(NH <sub>4</sub> ) <sub>2</sub> (MnF <sub>6</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	SM	—	FM	—	—	406381
933	Rb <sub>2</sub> (MnF <sub>6</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	SM	—	—	—	—	25578
934	K <sub>2</sub> (MnF <sub>6</sub> )	<i>P</i> 6 <sub>3</sub> mc (186)	SM	—	FM	—	HQ	60417 61275 76273
935	Li(ClO <sub>4</sub> )(H <sub>2</sub> O) <sub>3</sub>	<i>P</i> 6 <sub>3</sub> mc (186)	Triv.	—	NM	—	HQ	1321 1913 1914 27730 32534
936	SrKF(CO <sub>3</sub> )	<i>P</i> 6̄m2 (187)	Triv.	—	NM	—	HQ	262231
937	SrRbF(CO <sub>3</sub> )	<i>P</i> 6̄m2 (187)	Triv.	—	NM	—	HQ	262233
938	KCo(PO <sub>3</sub> ) <sub>3</sub>	<i>P</i> 6̄c2 (188)	SM	(b)	AFM	—	HQ	193216
939	KZn(BeF <sub>3</sub> ) <sub>3</sub>	<i>P</i> 6̄c2 (188)	Triv.	(b)	NM	—	HQ	18022
940	RbMgCO <sub>3</sub> F	<i>P</i> 6̄2m (189)	Triv.	(b)	NM	—	HQ	238611 670338 <sup>(s)</sup>
941	CaRbF(CO <sub>3</sub> )	<i>P</i> 6̄2m (189)	Triv.	—	NM	—	HQ	262232
942	CaCsF(CO <sub>3</sub> )	<i>P</i> 6̄2m (189)	Triv.	—	—	—	HQ	262234
943	K <sub>2</sub> (HfF <sub>6</sub> )	<i>P</i> 6̄2m (189)	Triv.	—	NM	—	—	47246
944	N <sub>2</sub> O <sub>5</sub>	<i>P</i> 6 <sub>3</sub> /mmc (194)	Triv.	—	NM	—	—	30638
945	N <sub>2</sub> O <sub>5</sub>	<i>P</i> 6 <sub>3</sub> /mmc (194)	SM	—	NM	—	—	30639
946	K <sub>6</sub> (BiCl <sub>6</sub> )Cl <sub>2</sub> (H <sub>3</sub> F <sub>4</sub> )	<i>P</i> 6 <sub>3</sub> /mmc (194)	Triv.	(k)	NM	—	—	68226
947	K <sub>4</sub> (O <sub>3</sub> (IO <sub>3</sub> ) <sub>2</sub> )	<i>P</i> 6 <sub>3</sub> /mmc (194)	Triv.	(b,s)	NM	—	—	25694
948	(K <sub>2</sub> (SiF <sub>6</sub> ))(K(NO <sub>3</sub> ))	<i>P</i> 6 <sub>3</sub> /mmc (194)	Triv.	—	NM	—	HQ	159390 417735
949	Cs(NiF <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> /mmc (194)	SM	(b,s)	FM	—	—	15092 61278
950	Cs <sub>2</sub> Ni <sub>2</sub> F <sub>6</sub>	<i>P</i> 6 <sub>3</sub> /mmc (194)	SM	(b,s)	FM	—	—	410394
951	Rb <sub>3</sub> ((OsBr <sub>3</sub> ) <sub>2</sub> Br <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> /mmc (194)	Triv.	(k*)	NM	—	—	56896
952	He	<i>P</i> 6 <sub>3</sub> /mmc (194)	Triv.	—	NM	—	—	43426 44394 44396 426943
953	K <sub>2</sub> (CO <sub>3</sub> )	<i>P</i> 6 <sub>3</sub> /mmc (194)	Triv.	—	NM	—	—	52535

954	$\text{Na}_2(\text{CO}_3)$	$P\bar{6}3/mmc$ (194)	Triv.	—	NM	—	—	$81004\ 81005\ 81006$ $81007\ 81008\ 81009$ $81010\ 81011\ 81012$ $81013$
955	$\text{Cs}_3(\text{Mo}_2\text{O}_7)\text{Br}$	$P\bar{6}3/mmc$ (194)	Triv.	—	—	—	HQ	$260595$
956	$\text{PF}_5$	$P\bar{6}3/mmc$ (194)	Triv.	(k*)	NM	—	—	$62554$
957	$\text{AsF}_5$	$P\bar{6}3/mmc$ (194)	Triv.	(k*)	NM	—	—	$65477$
958	$\text{K}_2\text{Pb}(\text{Cu}(\text{NO}_2)_6)$	$F2\bar{3}$ (196)	SM	—	FM	—	—	$36135$
959	$\text{Bi}_{12}\text{MnO}_{20}$	$I2\bar{3}$ (197)	SM	(b)	FM	—	—	$75079$
960	$\text{Bi}_{24}\text{Mn}_2\text{O}_{40}$	$I2\bar{3}$ (197)	SM	(b)	FM	—	—	$75390$
961	$\text{Ba}(\text{NO}_3)_2$	$P2_{13}$ (198)	Triv.	—	—	—	—	$34902$
962	$\text{CsXeF}_7$	$P2_{13}$ (198)	Triv.	—	NM	—	—	$404986$
963	$\text{NH}_3$	$P2_{13}$ (198)	Triv.	—	NM	—	—	$638341\ 29321\ 84461$ $300149$
964	$\text{Na}(\text{ClO}_3)$	$P2_{13}$ (198)	Triv.	—	NM	—	—	$1117\ 1301\ 16714$ $22395\ 26684\ 28830$ $31121\ 31167\ 31168$ $80337\ 80338\ 80339$ $80340\ 80341$
965	$\text{Na}(\text{BrO}_3)$	$P2_{13}$ (198)	Triv.	—	NM	—	HQ	$1302^{(b)}\ 22396\ 28831$ $30208^{(b)}\ 31166\ 47174^{(b)}$
966	$\text{Tl}(\text{Co}(\text{CO})_4)$	$P2_{13}$ (198)	Triv.	—	NM	—	—	$6011\ 31361\ 31362$
967	$\text{Tl}(\text{Fe}(\text{CO})_3(\text{NO}))$	$P2_{13}$ (198)	Triv.	—	NM	—	—	$66317$
968	$\text{K}_2\text{Pb}(\text{Ni}(\text{NO}_2)_6)$	$Fm\bar{3}$ (202)	SM	—	FM	—	HQ	$1937$
969	$\text{Cs}_2\text{PbCu}(\text{NO}_2)_6$	$Fm\bar{3}$ (202)	SM	—	FM	—	HQ	$2381\ 56254$
970	$\text{K}_2\text{Pb}(\text{Cu}(\text{NO}_2)_6)$	$Fm\bar{3}$ (202)	SM	—	FM	—	HQ	$16127\ 26228\ 26749$
971	$\text{K}_2\text{Ca}(\text{Ni}(\text{NO}_2)_6)$	$Fm\bar{3}$ (202)	SM	—	FM	—	—	$26748$
972	$\text{N}_2\text{O}_4$	$I\bar{m}3$ (204)	Triv.	—	NM	—	—	$52347\ 29047\ 201140$ $201141\ 201142$
973	$\text{CaCu}_3\text{Ge}_4\text{O}_{12}$	$I\bar{m}3$ (204)	SM	(k,b)	FM	—	—	$1303\ 184279$
974	$\text{CaCu}_3(\text{Sn}_4\text{O}_{12})$	$I\bar{m}3$ (204)	SM	(k,b)	FM	—	HQ	$162100\ 184281$
975	$\text{SrCu}_3(\text{Sn}_4\text{O}_{12})$	$I\bar{m}3$ (204)	SM	(k,b)	FM	—	HQ	$162101$
976	$\text{PbCu}_3(\text{Sn}_4\text{O}_{12})$	$I\bar{m}3$ (204)	SM	(k,b)	FM	—	HQ	$162102$
977	$\text{Cs}(\text{NO}_3)$	$P\bar{a}3$ (205)	Triv.	—	NM	—	—	$35555$
978	$(\text{IF}_6)(\text{AsF}_6)$	$P\bar{a}3$ (205)	Triv.	—	NM	—	—	$249129$
979	$\text{N}$	$P\bar{a}3$ (205)	Triv.	—	NM	—	—	$426956$
980	$\text{N}_2$	$P\bar{a}3$ (205)	Triv.	—	NM	—	—	$15472\ 26482\ 28179$
981	$\text{NaO}_2$	$P\bar{a}3$ (205)	SM	—	FM	—	—	$26582\ 87178$
982	$\text{Ba}(\text{NO}_3)_2$	$P\bar{a}3$ (205)	Triv.	—	NM	—	—	$35495\ 52353\ 95594$ $95595\ 109281$
983	$(\text{O}_2)(\text{SbF}_6)$	$I\bar{a}3$ (206)	SM	—	FM	—	—	$78849$
984	$\text{K}(\text{SbF}_6)$	$I\bar{a}3$ (206)	Triv.	—	NM	—	—	$76422\ 76653$
985	$\text{Li}_2\text{NiGe}_3\text{O}_8$	$P4_{3}32$ (212)	SM	(k*,b)	FM	—	—	$68339$
986	$\text{Cs}_3(\text{Mo}_4\text{O}_4)(\text{PO}_4)_3$	$P\bar{4}3m$ (215)	Triv.	(k,b)	FM	—	HQ	$62225$
987	$\text{K}_4(\text{CO}_4)$	$P\bar{4}3m$ (215)	Triv.	—	NM	—	—	$245417$
988	$\text{Rb}_4(\text{CO}_4)$	$P\bar{4}3m$ (215)	Triv.	—	NM	—	—	$245429$
989	$\text{LiCo}(\text{CO})_4$	$P\bar{4}3m$ (215)	Triv.	—	NM	—	HQ	$30854$
990	$\text{Ag}(\text{B}(\text{CN})_4)$	$P\bar{4}3m$ (215)	Triv.	—	NM	—	HQ	$411179$
991	$\text{Ba}(\text{SO}_4)$	$P\bar{4}3m$ (216)	Triv.	(k*,p*)	NM	—	—	$23743\ 62368$
992	$\text{SrSO}_4$	$P\bar{4}3m$ (216)	Triv.	(k*,p*)	NM	—	—	$23744$
993	$\text{K}(\text{ClO}_4)$	$P\bar{4}3m$ (216)	Triv.	(k*,p*)	NM	—	—	$33562$
994	$\text{Tl}(\text{ClO}_4)$	$P\bar{4}3m$ (216)	Triv.	(k*,p*)	NM	—	—	$33564$
995	$\text{Cs}(\text{ClO}_4)$	$P\bar{4}3m$ (216)	Triv.	(k*,p*)	NM	—	—	$33566$
996	$\text{Na}(\text{ClO}_4)$	$P\bar{4}3m$ (216)	Triv.	(k*,p*)	NM	—	—	$33567$
997	$\text{Ag}(\text{ClO}_4)$	$P\bar{4}3m$ (216)	Triv.	(k*,p*)	NM	—	—	$33568$
998	$\text{CsFe}(\text{H}_2\text{O})_6\text{PO}_4$	$P\bar{4}3m$ (216)	Triv.	—	FM	—	HQ	$172377$
999	$\text{Cs}(\text{Mg}(\text{H}_2\text{O})_6)(\text{AsO}_4)$	$P\bar{4}3m$ (216)	Triv.	—	NM	—	HQ	$260150$
1000	$\text{Cs}(\text{Mg}(\text{H}_2\text{O})_6)(\text{PO}_4)$	$P\bar{4}3m$ (216)	Triv.	—	NM	—	HQ	$281563$
1001	$\text{CsNi}(\text{Cr}(\text{CN})_6)$	$P\bar{4}3m$ (216)	SM	—	—	—	—	$56603$
1002	$\text{KI}$	$P\bar{4}3m$ (216)	Triv.	—	—	—	—	$674991$
1003	$\text{NaF}$	$P\bar{4}3m$ (216)	Triv.	—	—	—	—	$674994$
1004	$\text{RbI}$	$P\bar{4}3m$ (216)	Triv.	—	—	—	—	$674999$
1005	$(\text{Zn}(\text{NH}_3)_4)(\text{ClO}_4)_2$	$P\bar{4}3m$ (216)	Triv.	—	NM	—	HQ	$74790$
1006	$(\text{Zn}(\text{NH}_3)_4)(\text{MnO}_4)_2$	$P\bar{4}3m$ (216)	Triv.	—	NM	—	—	$162384$
1007	$(\text{Ru}(\text{CO})_3)_4\text{Se}_4$	$I\bar{4}3m$ (217)	Triv.	—	NM	—	—	$92913$
1008	$(\text{Li}(\text{NH}_3)_4)_3(\text{AsSe}_4)$	$I\bar{4}3m$ (217)	Triv.	(k)	NM	—	—	$409539$
1009	$\text{K}_3(\text{BiO}_3)$	$I\bar{4}3m$ (217)	Triv.	(b)	NM	—	HQ	$407293$
1010	$\text{Cs}_8(\text{Al}_{12}\text{O}_{24})\text{S}_2$	$I\bar{4}3m$ (217)	Triv.	(b,s)	NM	—	HQ	$67589$

1011	Sr <sub>8</sub> (Al <sub>12</sub> O <sub>24</sub> )S <sub>2</sub>	<i>I</i> 43 <i>m</i> (217)	Triv.	(b,s)	NM	—	HQ	67590
1012	Sr <sub>8</sub> (AlO <sub>2</sub> ) <sub>12</sub> Te <sub>2</sub>	<i>I</i> 43 <i>m</i> (217)	Triv.	(b,s)	NM	—	HQ	82609
1013	Na <sub>8</sub> (Al <sub>6</sub> Ge <sub>6</sub> O <sub>24</sub> )I <sub>2</sub>	<i>P</i> 43 <i>n</i> (218)	Triv.	(b,s)	NM	—	—	65666 85349
1014	Na <sub>8</sub> (Al <sub>6</sub> Si <sub>6</sub> O <sub>24</sub> )I <sub>2</sub>	<i>P</i> 43 <i>n</i> (218)	Triv.	(b,s)	NM	—	—	68960 71434
1015	Li <sub>8</sub> Br <sub>2</sub> (Be <sub>6</sub> P <sub>6</sub> O <sub>24</sub> )	<i>P</i> 43 <i>n</i> (218)	Triv.	(b,s)	NM	—	—	80472
1016	Li <sub>8</sub> (GaSiO <sub>4</sub> ) <sub>6</sub> Br <sub>2</sub>	<i>P</i> 43 <i>n</i> (218)	Triv.	(b,s)	NM	—	—	87988
1017	Li <sub>8</sub> (GaSiO <sub>4</sub> ) <sub>6</sub> I <sub>2</sub>	<i>P</i> 43 <i>n</i> (218)	Triv.	(b,s)	NM	—	—	87989
1018	Li <sub>8</sub> (AlGeO <sub>4</sub> ) <sub>6</sub> Br <sub>2</sub>	<i>P</i> 43 <i>n</i> (218)	Triv.	(b)	NM	—	—	87991
1019	Li <sub>8</sub> (AlGeO <sub>4</sub> ) <sub>6</sub> I <sub>2</sub>	<i>P</i> 43 <i>n</i> (218)	Triv.	(b)	NM	—	—	87992
1020	Mg <sub>3</sub> (B <sub>7</sub> O <sub>13</sub> Cl)	<i>F</i> 43 <i>c</i> (219)	Triv.	(k,b)	NM	—	—	30351 <sup>(s)</sup> 30615
1021	(Si <sub>5</sub> Cl <sub>12</sub> )(SiCl <sub>4</sub> )	<i>F</i> 43 <i>c</i> (219)	Triv.	—	NM	—	—	2767
1022	YF <sub>3</sub>	<i>P</i> m $\bar{3}$ <i>m</i> (221)	Triv.	(k)	NM	—	—	15961
1023	LaF <sub>3</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	—	NM	—	—	164054 167556
1024	Cs <sub>2</sub> Li(Fe(CN) <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	HQ	1000 1001 10179 60540 60541 60542
1025	Cs <sub>2</sub> Li(Cr(CN) <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	—	6085 68068
1026	Cs <sub>2</sub> MgFe(CN) <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	—	NM	—	—	6086
1027	Cs <sub>2</sub> LiIr(CN) <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	—	NM	—	—	9032
1028	Cs <sub>2</sub> LiMn(CN) <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	—	FM	—	HQ	10180 68067
1029	Cs <sub>2</sub> Li(Co(CN) <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	—	NM	—	HQ	10181 23204 60538 60539
1030	MnCs <sub>2</sub> (Fe(CN) <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	HQ	151695
1031	CdCs <sub>2</sub> (Fe(CN) <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	—	NM	—	HQ	151696
1032	NiCs <sub>2</sub> (Fe(CN) <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	HQ	151706
1033	Cs <sub>2</sub> Co(Fe(CN) <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	—	—	HQ	416443
1034	Rb <sub>2</sub> NaFeF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(b)	FM	—	—	4030 <sup>(k,s)</sup> 40966 <sup>(k,s)</sup> 42146
1035	Cs <sub>2</sub> KMoF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(b)	FM	—	—	4053
1036	Cs <sub>2</sub> K(RhF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	—	NM	—	—	4056
1037	K <sub>3</sub> MoF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(b)	FM	—	HQ	4403
1038	Cs <sub>2</sub> K(TiF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	—	6035 67146
1039	Cs <sub>2</sub> Tl(FeF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	—	6036
1040	Cs <sub>2</sub> K(CoF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	—	NM	—	—	6037
1041	Cs <sub>2</sub> K(NiF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	—	6039
1042	Rb <sub>2</sub> K(FeF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	—	9001 40967 42145
1043	Cs <sub>2</sub> NaBiF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	(k*,b,s)	NM	—	—	9382
1044	Rb <sub>2</sub> NaBiF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	(k*,b,s)	NM	—	—	9386
1045	Cs <sub>2</sub> KCrF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	—	9705
1046	Rb <sub>2</sub> NaCrF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(k*,b,s)	FM	—	—	9706
1047	Rb <sub>2</sub> K(CrF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(b)	FM	—	—	9707
1048	Cs <sub>2</sub> TlMoF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(b)	FM	—	—	15772
1049	KRb <sub>2</sub> MoF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(b)	FM	—	—	15773
1050	K <sub>2</sub> NaMoF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(k*,b,s)	FM	—	—	15777
1051	Cs <sub>2</sub> K(AgF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(k*,b,s)	FM	—	—	16783
1052	K <sub>2</sub> NaCrF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(k*,b,s)	FM	—	—	22199 40965
1053	K <sub>2</sub> Na(FeF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(k*,b,s)	FM	—	—	22200 61277
1054	Rb <sub>2</sub> KRhF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	(b)	NM	—	—	27339
1055	Rb <sub>2</sub> NaRhF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	(k*,b,s)	NM	—	—	27341
1056	K <sub>2</sub> NaRhF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	(k*,b,s)	NM	—	—	27342
1057	Cs <sub>2</sub> TlVF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	—	27343
1058	Cs <sub>2</sub> KVF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	—	27344
1059	Rb <sub>2</sub> KVF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(b)	FM	—	—	27345
1060	Cs <sub>2</sub> NaMnF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	(b)	FM	—	—	37005
1061	Rb <sub>2</sub> K(TiF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(b)	FM	—	—	42142 67147
1062	Rb <sub>2</sub> Na(TiF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(k*,b,s)	FM	—	—	42143
1063	Cs <sub>2</sub> K(FeF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	—	42144
1064	Rb <sub>2</sub> K(NiF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(b)	FM	—	—	42149
1065	Tl <sub>3</sub> (TiF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(k*,b,s)	FM	—	—	42154
1066	Cs <sub>2</sub> K(CuF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	—	FM	—	HQ	59102
1067	Cs <sub>2</sub> NaFeF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(b)	FM	—	HQ	65503
1068	Cs <sub>2</sub> KMnF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	Triv.	—	FM	—	HQ	91037
1069	K <sub>2</sub> NaVF <sub>6</sub>	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(k*,b,s)	FM	—	—	186883
1070	(NH <sub>4</sub> ) <sub>2</sub> Na(CrF <sub>6</sub> )	<i>F</i> m $\bar{3}$ <i>m</i> (225)	SM	(k*)	FM	—	—	418735

1071	$(\text{NH}_4)_2\text{Na}(\text{FeF}_6)$	$Fm\bar{3}m$ (225)	SM	$(k^*)$	FM	—	HQ	418736
1072	$\text{Rb}_2\text{CoF}_6$	$Fm\bar{3}m$ (225)	SM	—	FM	—	—	9701
1073	$\text{Cs}_2\text{CoF}_6$	$Fm\bar{3}m$ (225)	SM	—	FM	—	—	9702
1074	$\text{Rb}_2(\text{MnF}_6)$	$Fm\bar{3}m$ (225)	SM	—	FM	—	—	25579 47207 202536
1075	$\text{Cs}_2\text{SiF}_6$	$Fm\bar{3}m$ (225)	Triv.	—	NM	—	—	26871 38548
1076	$\text{Rb}_2(\text{PdF}_6)$	$Fm\bar{3}m$ (225)	Triv.	—	NM	—	—	28675
1077	$\text{Rb}_2(\text{CrF}_6)$	$Fm\bar{3}m$ (225)	SM	—	FM	—	—	29006
1078	$\text{Cs}_2(\text{CrF}_6)$	$Fm\bar{3}m$ (225)	SM	—	FM	—	—	29007
1079	$\text{K}_2\text{SiF}_6$	$Fm\bar{3}m$ (225)	Triv.	—	NM	—	HQ	29407 38546 64763 73722
1080	$\text{Cs}_2(\text{GeF}_6)$	$Fm\bar{3}m$ (225)	Triv.	—	NM	—	—	35547
1081	$\text{Rb}_2(\text{SiF}_6)$	$Fm\bar{3}m$ (225)	Triv.	—	NM	—	—	38547
1082	$\text{Cs}_2(\text{MnF}_6)$	$Fm\bar{3}m$ (225)	SM	—	FM	—	—	47201 76272
1083	$\text{K}_2(\text{MnF}_6)$	$Fm\bar{3}m$ (225)	SM	$(k^*)$	FM	—	—	47213
1084	$\text{Rb}_2(\text{GeF}_6)$	$Fm\bar{3}m$ (225)	Triv.	—	NM	—	HQ	68982
1085	$\text{Cs}_2(\text{IrCl}_6)$	$Fm\bar{3}m$ (225)	SM	$(k^*)$	FM	—	HQ	69142
1086	$\text{Cs}_2(\text{PtF}_6)$	$Fm\bar{3}m$ (225)	Triv.	—	NM	—	HQ	78955
1087	$\text{Sr}_2\text{OsH}_6$	$Fm\bar{3}m$ (225)	Triv.	$(k^*)$	NM	—	—	638409
1088	$\text{Na}_6\text{MnCl}_8$	$Fm\bar{3}m$ (225)	SM	(k,b)	FM	—	HQ	1845
1089	$\text{Li}_6\text{FeCl}_8$	$Fm\bar{3}m$ (225)	Triv.	(k,b)	FM	—	HQ	73217
1090	$\text{Li}_6\text{VCl}_8$	$Fm\bar{3}m$ (225)	SM	(k,b)	FM	—	—	100834
1091	$\text{Na}_6\text{O}(\text{SO}_4)_2$	$Fm\bar{3}m$ (225)	Triv.	$(k^*)$	NM	—	HQ	411442 52241 53824 64686 671925 673325 673985 674974
1092	KF	$Fm\bar{3}m$ (225)	Triv.	—	NM	—	—	52274 61515 674969
1093	$\text{CsCl}$	$Fm\bar{3}m$ (225)	Triv.	—	NM	—	—	53828 673989 674982
1094	RbF	$Fm\bar{3}m$ (225)	Triv.	—	NM	—	—	27484 31033
1095	$\text{Na}(\text{MoF}_6)$	$Fm\bar{3}m$ (225)	SM	—	FM	—	—	90615
1096	$\text{Na}(\text{PF}_6)$	$Fm\bar{3}m$ (225)	Triv.	—	NM	—	HQ	184564 184565 170476 35536 <sup>(k,p)</sup> 77458 <sup>(k,p)</sup> 77459 <sup>(k,p)</sup> 77460 <sup>(k,p)</sup> 162620 <sup>(k,p)</sup>
1097	$\text{Na}(\text{AsF}_6)$	$Fm\bar{3}m$ (225)	Triv.	—	NM	—	HQ	23994 168524
1098	$\text{SiO}_2$	$Fd\bar{3}m$ (227)	Triv.	(b,s)	NM	—	—	27791
1099	$\text{K}_2\text{Cd}(\text{CN})_4$	$Fd\bar{3}m$ (227)	Triv.	(k,p,b)	NM	—	—	25769 415950
1100	$\text{Mg}_2\text{Na}_6(\text{CO}_3)_4\text{Br}_2$	$Fd\bar{3}m$ (227)	Triv.	(k,p)	NM	—	—	63362 252619 252620
1101	$\text{Nb}_6\text{F}_{15}$	$Im\bar{3}m$ (229)	SM	(b,s)	NM	—	—	108651, SG 221 ( $Pm\bar{3}m$ )
1102	$\text{SF}_6$	$Im\bar{3}m$ (229)	Triv.	—	NM	—	HQ	193

### 3. Best flat bands near or at the Fermi level

Among the 2,379 curated flat-band materials given in Table XII of non-atomic flat-band materials, we present in this subsection the 345 best candidates (corresponding to 949 ICSD entries). They have been selected with their experimental relevance in mind: we have targeted materials where flat bands are located at or close to the Fermi level, without any gating/doping. For that purpose, we have applied the following two criteria:

1. The highest occupied band or the lowest unoccupied band near the Fermi level is classified as a flat band according to the definition given in Appendix C 2a.
2. The highest occupied or lowest unoccupied flat band is perfectly flat, *i.e.*, almost dispersionless, along at least one high-symmetry line of the BZ. Note that we did not apply here any bandwidth threshold.

The band structure and projected density of states of each of these 345 best candidates are given in Figs. 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70 and 71. In Fig. 27, we detail the information provided for each material. Note that the materials KAg[CN]<sub>2</sub> [ICSD 30275, SG 163 ( $P\bar{3}1c$ )], Pb<sub>2</sub>Sb<sub>2</sub>O<sub>7</sub> [ICSD 27120, SG 227 ( $Fd\bar{3}m$ )], Rb<sub>2</sub>CaH<sub>4</sub> [ICSD 65196, SG 139 ( $I4/mmm$ )], Ca<sub>2</sub>NCl [ICSD 62555, SG 166 ( $R\bar{3}m$ )] and WO<sub>3</sub> [ICSD 108651, SG 221 ( $Pm\bar{3}m$ )] have been used as prototypical cases with line-graph or bipartite sublattice in the main text. The five materials and CaNi<sub>5</sub> [ICSD 54474, SG 191 ( $P6/mmm$ )] appearing in this list of best candidates are discussed in details in Appendix F, focusing on the origin of their flat bands. As pointed out in Appendix H 1, some candidates presented here have been reported theoretically or experimentally to host flat bands near the Fermi level: Co<sub>3</sub>Sn<sub>2</sub>S<sub>2</sub> [ICSD 624867, SG 166 ( $R\bar{3}m$ )]<sup>86,96,97</sup>, Sr<sub>2</sub>FeMoO<sub>6</sub> [ICSD 181752, SG 225 ( $Fm\bar{3}m$ )]<sup>94</sup> and Pd<sub>3</sub>Pb [ICSD 42600, SG 221 ( $Pm\bar{3}m$ )]<sup>93</sup>.

Compounds with the same crystal structure and varying chemical composition can have remarkably similar band structures. In the following subsections, we briefly describe structural and composition requirements for the 8 most prominent groups of these 122 unique materials (including 323 ICSDs) among the list of best compounds.

### a. Heusler-AlCu<sub>2</sub>Mn

Heusler compounds are a class of intermetallic crystals with generic chemical formula X<sub>2</sub>YZ, which crystallize in the cubic space group SG 225 ( $Fm\bar{3}m$ ). X and Y are transition metals and Z is a main-group element. In some cases, Y can be an alkaline earth element. Atoms of X, Y, and Z elements occupy 8c, 4a, and 4b Wyckoff positions, respectively. They are known for easily-tunable band gaps, diverse magnetic properties, such as magneto-optical, magnetocaloric, and magneto-structural characteristics, half-metallic ferromagnetism, and flat bands<sup>98,99</sup>. Moreover, Heusler compounds with electron counts near 27 electrons are superconductive<sup>98,100–103</sup>. We refer the reader to the review Ref.<sup>98</sup> for a detailed discussion about Heusler compounds.

The list of best compounds contains 35 unique materials (corresponding to 100 ICSD entries) that are Heusler compounds. These materials are given in Table XIV.

Table XIV: List of best compounds belonging to the family of Heusler-AlCu<sub>2</sub>Mn compounds. The first column is the chemical formula, the second column is the representative ICSD used for the band structure and projected DOS plots. The third column is the space group, the fourth column is the link to figure showing the corresponding band structure and projected DOS. The last two columns provide the magnetic and superconducting properties, following the same notations than Table XII.

chem. formula	ICSD	space group	figure	magn.	super-conduct.
LiCo <sub>2</sub> Ge	<a href="#">25324</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 64	NM	—
CoFe <sub>2</sub> Ge	<a href="#">52954</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 64	FM	—
Co <sub>2</sub> ZnGe	<a href="#">52994</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 64	FM	—
Co <sub>2</sub> TiSi	<a href="#">53080</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 64	FM	—
Co <sub>2</sub> VSi	<a href="#">53086</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 64	FM	—
FeRu <sub>2</sub> Si	<a href="#">53525</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 67	FM	—
Fe <sub>2</sub> VSi	<a href="#">53555</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 64	FM	—
ZrNi <sub>2</sub> In	<a href="#">54546</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 64	NM	—
HfNi <sub>2</sub> In	<a href="#">54595</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 65	NM	—
AlCrFe <sub>2</sub>	<a href="#">57654</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 65	FM	—
AlFe <sub>3</sub>	<a href="#">57793</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 65	FM	—
AlFe <sub>2</sub> Mo	<a href="#">57807</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 65	FM	—
Mn <sub>3</sub> Si	<a href="#">76227</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 65	FM	SC
CoFe <sub>2</sub> Ga	<a href="#">102385</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 63	FM	—
Co <sub>2</sub> HfGa	<a href="#">102433</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 65	FM	—
Co <sub>2</sub> HfSn	<a href="#">102483</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 63	FM	—
Co <sub>2</sub> SnTi	<a href="#">102682</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 63	FM	—
Co <sub>2</sub> SnZr	<a href="#">102687</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 63	FM	—
CrFe <sub>2</sub> Ga	<a href="#">102755</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 65	FM	—
Cu <sub>2</sub> MnIn	<a href="#">102996</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 63	FM	—
Fe <sub>2</sub> GaV	<a href="#">103473</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 67	NM	—
Fe <sub>2</sub> SnTi	<a href="#">103641</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 65	NM	—
Fe <sub>2</sub> SnV	<a href="#">103644</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 66	FM	—
MnNi <sub>2</sub> Sn	<a href="#">104926</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 66	FM	—
NiRh <sub>2</sub> Sn	<a href="#">105327</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 64	FM	—
Ni <sub>2</sub> ScSn	<a href="#">105339</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 66	NM	—
Fe <sub>3</sub> Ga	<a href="#">108436</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 66	FM	—
Co <sub>2</sub> TiGe	<a href="#">169468</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 66	FM	—
Co <sub>2</sub> TiAl	<a href="#">185966</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 66	FM	—
Fe <sub>2</sub> CrSn	<a href="#">185999</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 66	FM	—
Fe <sub>2</sub> TiGe	<a href="#">186057</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 67	NM	—
Fe <sub>2</sub> TiAs	<a href="#">186059</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 66	FM	—
Fe <sub>2</sub> TiSb	<a href="#">186060</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 67	FM	—
Ru <sub>2</sub> VGe	<a href="#">671340</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 67	n.a.	—
Fe <sub>2</sub> ZrP	<a href="#">675102</a>	SG 225 ( $Fm\bar{3}m$ )	Fig. 67	n.a.	—

b. *Heusler-AlLiSi*

Heusler-AlLiSi compounds, a sub-class of half-Heusler compounds, have the XYZ general formula and non-centrosymmetric SG 216 ( $F\bar{4}3m$ ). There is a wide range of choices for X, Y, and Z elements. The compounds can contain main-group elements, transition metals, and elements whose atoms form cations, which can be an alkaline, alkaline earth, or transition-metal, or rare-earth elements. The lattice can be viewed as zinc blende-type sub-lattice ( $4a$  and  $4c$  Wyckoff positions) with occupied  $4b$  positions.<sup>98</sup>. Members of half-Heusler family are known for superconductivity<sup>104–106</sup> and thermoelectric properties<sup>107,108</sup>.

The list of best compounds contains 6 unique materials (corresponding to 21 ICSD entries) that are Heusler-AlLiSi compounds. These materials are given in Table XV.

Table XV: List of best compounds belonging to the family of Heusler-AlLiSi compounds. The first column is the chemical formula, the second column is the representative ICSD used for the band structure and projected DOS plots. The third column is the space group, the fourth column is the link to figure showing the corresponding band structure and projected DOS. The last two columns provide the magnetic and superconducting properties, following the same notations than Table. XII.

chem. formula	ICSD	space group	figure	magn.	super-conduct.
CoMnSb	<a href="#">53001</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 52	FM	—
NiMnSb	<a href="#">54255</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 52	FM	—
RhMnSb	<a href="#">54343</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 53	FM	—
CoNbSn	<a href="#">102552</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 53	FM	—
MnPtSn	<a href="#">104955</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 53	FM	—
LiCaC	<a href="#">672030</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 53	n.a.	—

c. *Heusler-CuHg<sub>2</sub>Ti*

Intermetallic compounds in the CuHg<sub>2</sub>Ti structure type, known as inverse Heusler structure, have a X<sub>2</sub>YZ generalized chemical formula. Similarly to the Heusler compounds discussed in Appendix H 3a, they are composed of transition metals X and Y, and a main-group element Z. They crystallize in the cubic space group SG 216 ( $F\bar{4}3m$ ), like half-Heusler compounds (Appendix H 3b). However, the coordination around all sites is tetrahedral, unlike in the Heusler compounds. Two X atoms occupy non-equivalent  $4a$  and  $4d$  Wyckoff positions, while Y and Z atoms occupy  $4b$  and  $4c$  positions, respectively. This lattice type arises in cases when Y element is more electronegative than X element. Sometimes atoms at  $4a$  and  $4d$  positions belong to different element leading to XX'YZ structure<sup>98</sup>.

The list of best compounds contains 10 unique materials (corresponding to 11 ICSD entries) that have CuHg<sub>2</sub>Ti structure type. These materials are given in Table XVI.

Table XVI: List of best compounds belonging to the family of CuHg<sub>2</sub>Ti compounds. The first column is the chemical formula, the second column is the representative ICSD used for the band structure and projected DOS plots. The third column is the space group, the fourth column is the link to figure showing the corresponding band structure and projected DOS. The last two columns provide the magnetic and superconducting properties, following the same notations than Table. XII.

chem. formula	ICSD	space group	figure	magn.	super-conduct.
Mn <sub>2</sub> CoAs	<a href="#">191648</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 51	FM	—
CoFeTiAl	<a href="#">191657</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 52	NM	—
CoFeTiGa	<a href="#">191658</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 51	NM	—
CoFeTiSi	<a href="#">191659</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 51	FM	—
CoFeTiGe	<a href="#">191660</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 52	FM	—
CoFeTiAs	<a href="#">191661</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 52	FM	—
CoFeTiSb	<a href="#">191662</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 52	FM	—
CoFeVGa	<a href="#">191664</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 52	FM	—
Fe <sub>2</sub> MnGe	<a href="#">671982</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 52	n.a.	—
Fe <sub>2</sub> MnAl	<a href="#">672261</a>	SG 216 ( $F\bar{4}3m$ )	Fig. 51	n.a.	—

d. *Perovskite-CaTiO<sub>3</sub>*

Cubic perovskites which crystallize in SG 221 ( $Pm\bar{3}m$ ) have a generalized chemical formula XYZ<sub>3</sub>, where X and Y are cations, while Z is an anion. In traditional structures, smaller Y atoms are octahedrally coordinated by 6

Z atoms, while larger X atoms have XII-fold Z shell. X atoms are at  $1a$ , Y atoms are at  $1b$ , and Z atoms are at  $3c$  Wyckoff positions<sup>109</sup>. The covalent framework of these compounds is formed by Y-Z bonds, while X-Z bonds are ionic in character, and X cations provide the charge balance. Perovskites are known for magnetism<sup>110–115</sup>, and superconductivity<sup>116–118</sup>.

The list of best compounds contains 27 unique materials (corresponding to 69 ICSD entries) that are Perovskite-CaTiO<sub>3</sub> compounds. These materials are given in Table XVII.

Table XVII: List of best compounds belonging to the family of Perovskite-CaTiO<sub>3</sub> compounds. The first column is the chemical formula, the second column is the representative ICSD used for the band structure and projected DOS plots. The third column is the space group, the fourth column is the link to figure showing the corresponding band structure and projected DOS. The last two columns provide the magnetic and superconducting properties, following the same notations than Table. XII.

chem. formula	ICSD	space group	figure	magn.	super-conduct.
KMnF <sub>3</sub>	<a href="#">15423</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 56	FM	—
KFeF <sub>3</sub>	<a href="#">15424</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 59	FM	—
Cs(HgBr <sub>3</sub> )	<a href="#">24479</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 56	NM	—
KVF <sub>3</sub>	<a href="#">28145</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 56	FM	—
RbVF <sub>3</sub>	<a href="#">28146</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 56	FM	—
La(CrO <sub>3</sub> )	<a href="#">28930</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 56	FM	—
La(MnO <sub>3</sub> )	<a href="#">29119</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 59	FM	—
Rb(MnF <sub>3</sub> )	<a href="#">43722</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 57	FM	—
Rh <sub>3</sub> YB	<a href="#">44568</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 57	NM	—
NaVF <sub>3</sub>	<a href="#">60611</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 57	FM	—
Sr(RuO <sub>3</sub> )	<a href="#">69360</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 57	FM	—
Fe <sub>3</sub> ZnC	<a href="#">76763</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 57	FM	—
Co <sub>3</sub> MgC	<a href="#">76790</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 57	FM	—
Co <sub>3</sub> ZnC	<a href="#">76797</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 57	FM	—
YRh <sub>3</sub> C	<a href="#">77389</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 57	NM	—
Sr(VO <sub>3</sub> )	<a href="#">88982</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 58	FM	—
Sr(TcO <sub>3</sub> )	<a href="#">109076</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 58	NM	—
Ca(MnO <sub>3</sub> )	<a href="#">168902</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 58	FM	—
Pb(VO <sub>3</sub> )	<a href="#">187637</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 58	FM	—
Sr(MnO <sub>3</sub> )	<a href="#">188415</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 58	AFM	—
Ba(VO <sub>3</sub> )	<a href="#">191203</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 58	FM	—
InNCo <sub>3</sub>	<a href="#">247066</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 58	FM	—
CdCo <sub>3</sub> N	<a href="#">422858</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 58	FM	—
CaTcO <sub>3</sub>	<a href="#">671082</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 59	n.a.	—
BaTcO <sub>3</sub>	<a href="#">671086</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 59	n.a.	—
ZnSnO <sub>3</sub>	<a href="#">673496</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 59	n.a.	—
KSbO <sub>3</sub>	<a href="#">674060</a>	SG 221 ( $Pm\bar{3}m$ )	Fig. 59	n.a.	—

#### e. Double perovskite crystal structure: K<sub>2</sub>PtCl<sub>6</sub>, Elpasolite-K<sub>2</sub>NaAlF<sub>6</sub>, and Sr<sub>2</sub>NiWO<sub>6</sub>

Unit cell of double perovskites is created by the doubling of perovskite unit cell, XYZ<sub>3</sub> along all three crystallographic axes and introducing a change every other Y site. In K<sub>2</sub>PtCl<sub>6</sub> lattice type, with a generalized formula X<sub>2</sub>YZ<sub>6</sub>, a vacancy is introduced. In elpasolites, with a X<sub>2</sub>Y'YZ<sub>6</sub> general formula, Y atom is substitute by Y' atom. The symmetry reduces from SG 221 ( $Pm\bar{3}m$ ) to SG 225 ( $Fm\bar{3}m$ ). Finally, in compounds of Sr<sub>2</sub>NiWO<sub>6</sub> lattice type elpasolite lattice is tetragonally distorted as the size of X cations decreases with respect to sizes of Y and Y' cations. Space group reduces farther to SG 87 ( $I4/m$ )<sup>119,120</sup>.

Usually, X is an alkaline, alkaline earth, or rare-earth elements, Y is a transition metal or a main-group element, and Z is a halide. In elpasolites, Y' can be an alkaline or alkaline earth metal, a transition metal, or a main-group element. Moreover, Y and Y' can be the same element, but in different oxidation states<sup>121</sup>. Additionally, Z element in elpasolites can be an oxide anion instead of a halide. Transition from elpasolite to the Sr<sub>2</sub>NiWO<sub>6</sub> lattice is the most common when Y and Y' are transition metals<sup>119,120,122,123</sup>.

The list of best compounds contains 8 unique materials (20 ICSD entries), 20 unique materials (44 ICSD entries) and 11 unique materials (41 ICSD entries) that are K<sub>2</sub>PtCl<sub>6</sub>, elpasolites, and Sr<sub>2</sub>NiWO<sub>6</sub> compounds, respectively. These materials are given in Tables XIX, XVIII and XX.

Table XVIII: List of best compounds belonging to the family of Elpasolite- $K_2NaAlF_6$  compounds. The first column is the chemical formula, the second column is the representative ICSD used for the band structure and projected DOS plots. The third column is the space group, the fourth column is the link to figure showing the corresponding band structure and projected DOS. The last two columns provide the magnetic and superconducting properties, following the same notations than Table. XII.

chem. formula	ICSD	space group	figure	magn.	super-conduct.
$Ba_2Mn(ReO_6)$	4169	SG 225 ( $Fm\bar{3}m$ )	Fig. 61	FM	—
$K_2Na(AlF_6)$	6027	SG 225 ( $Fm\bar{3}m$ )	Fig. 61	NM	—
$KTl_2MoF_6$	15775	SG 225 ( $Fm\bar{3}m$ )	Fig. 60	FM	—
$NaTl_2MoF_6$	15776	SG 225 ( $Fm\bar{3}m$ )	Fig. 60	FM	—
$K_2NaTlF_6$	22114	SG 225 ( $Fm\bar{3}m$ )	Fig. 61	NM	—
$Cs_2NaTlF_6$	22118	SG 225 ( $Fm\bar{3}m$ )	Fig. 62	NM	—
$Ba_2CoWO_6$	27425	SG 225 ( $Fm\bar{3}m$ )	Fig. 60	FM	—
$Sr_2Co(WO_6)$	28598	SG 225 ( $Fm\bar{3}m$ )	Fig. 60	FM	—
$Sr_2Co(MoO_6)$	28601	SG 225 ( $Fm\bar{3}m$ )	Fig. 61	AFM	—
$Ba_2FeMoO_6$	96688	SG 225 ( $Fm\bar{3}m$ )	Fig. 62	FM	—
$Ba_2(CoMoO_6)$	97028	SG 225 ( $Fm\bar{3}m$ )	Fig. 61	AFM	—
$Ba_2(FeWO_6)$	99061	SG 225 ( $Fm\bar{3}m$ )	Fig. 62	AFM	—
$Ba_2Fe(ReO_6)$	109252	SG 225 ( $Fm\bar{3}m$ )	Fig. 61	FM	—
$Sr_2(GaSbO_6)$	157016	SG 225 ( $Fm\bar{3}m$ )	Fig. 62	NM	—
$Sr_2(FeMoO_6)$	157603	SG 225 ( $Fm\bar{3}m$ )	Fig. 62	AFM	—
$Sr_2Y(SbO_6)$	157886	SG 225 ( $Fm\bar{3}m$ )	Fig. 62	NM	—
$Ba_2CaTeO_6$	246112	SG 225 ( $Fm\bar{3}m$ )	Fig. 62	NM	—
$Sr_2FeOsO_6$	251068	SG 225 ( $Fm\bar{3}m$ )	Fig. 61	AFM	—
$Cs_2InAgCl_6$	257115	SG 225 ( $Fm\bar{3}m$ )	Fig. 62	n.a.	—
$Pb_2NaIO_6$	427115	SG 225 ( $Fm\bar{3}m$ )	Fig. 61	NM	—

Table XIX: List of best compounds belonging to the family of  $K_2PtCl_6$  compounds. The first column is the chemical formula, the second column is the representative ICSD used for the band structure and projected DOS plots. The third column is the space group, the fourth column is the link to figure showing the corresponding band structure and projected DOS. The last two columns provide the magnetic and superconducting properties, following the same notations than Table. XII.

chem. formula	ICSD	space group	figure	magn.	super-conduct.
$K_2(SnCl_6)$	604	SG 225 ( $Fm\bar{3}m$ )	Fig. 68	NM	—
$(NH_4)_2(SnCl_6)$	605	SG 225 ( $Fm\bar{3}m$ )	Fig. 68	NM	—
$Rb_2SnCl_6$	9022	SG 225 ( $Fm\bar{3}m$ )	Fig. 68	NM	—
$Cs_2SnCl_6$	9023	SG 225 ( $Fm\bar{3}m$ )	Fig. 68	NM	—
$Rb_2MnCl_6$	9347	SG 225 ( $Fm\bar{3}m$ )	Fig. 67	FM	—
$K_2TaCl_6$	59894	SG 225 ( $Fm\bar{3}m$ )	Fig. 68	FM	—
$Rb_2(NbCl_6)$	245747	SG 225 ( $Fm\bar{3}m$ )	Fig. 68	FM	—
$Y_2Ni_6C$	673582	SG 225 ( $Fm\bar{3}m$ )	Fig. 67	n.a.	—

Table XX: List of best compounds belonging to the family of  $Sr_2NiWO_6$  compounds. The first column is the chemical formula, the second column is the representative ICSD used for the band structure and projected DOS plots. The third column is the space group, the fourth column is the link to figure showing the corresponding band structure and projected DOS. The last two columns provide the magnetic and superconducting properties, following the same notations than Table. XII.

chem. formula	ICSD	space group	figure	magn.	super-conduct.
$Sr_2Ni(WO_6)$	91791	SG 87 ( $I4/m$ )	Fig. 34	AFM	—
$Ba_2(FeWO_6)$	95518	SG 87 ( $I4/m$ )	Fig. 34	AFM	—
$Sr_2(FeMoO_6)$	150701	SG 87 ( $I4/m$ )	Fig. 34	FM	—
$Sr_2(FeReO_6)$	150702	SG 87 ( $I4/m$ )	Fig. 33	FM	—
$Sr_2Mg(WO_6)$	151703	SG 87 ( $I4/m$ )	Fig. 34	NM	—
$Sr_2(CoMoO_6)$	153544	SG 87 ( $I4/m$ )	Fig. 33	FM	—
$Sr_2CoReO_6$	173488	SG 87 ( $I4/m$ )	Fig. 33	AFM	—
$Sr_2MgMoO_6$	187662	SG 87 ( $I4/m$ )	Fig. 34	NM	—
$Sr_2MnMoO_6$	187669	SG 87 ( $I4/m$ )	Fig. 33	FM	—
$Sr_2CoWO_6$	190593	SG 87 ( $I4/m$ )	Fig. 33	AFM	—
$Sr_2CoNbO_6$	192327	SG 87 ( $I4/m$ )	Fig. 34	n.a.	—

f. Shandite- $\text{Ni}_3\text{Pb}_2\text{S}_2$ 

$\text{Ni}_3\text{Pb}_2\text{S}_2$  lattice type in SG 166 ( $R\bar{3}m$ ), known as shandite, is a lattice with a  $X_3Y_2Z_2$  general formula. But this lattice type also includes compounds with a  $X_3YY'Z_2$  formula. X atoms belong to a transition metal element, while Y (Y') and Z atoms are main-group elements. X atoms occupy  $3a$  Wyckoff positions, Y atoms are at  $3b$  positions, and Z atoms are at  $6c$  positions. The bonding in these compounds can be approximated by a Kagome Hamiltonian for  $d$  orbitals, though small contributions from Y's and Z's orbitals to the bands near the Fermi level are possible<sup>124,125</sup>.

The list of best compounds contains 5 unique materials (corresponding to 17 ICSD entries) that are Shandite- $\text{Ni}_3\text{Pb}_2\text{S}_2$  compounds, and are listed in Table XXI. Note that all of them host a rigorous Kagome sublattice, as expected.

Table XXI: List of best compounds belonging to the family of  $\text{Ni}_3\text{Pb}_2\text{S}_2$  compounds. The first column is the chemical formula, the second column is the representative ICSD used for the band structure and projected DOS plots. The third column is the space group, the fourth column is the link to figure showing the corresponding band structure and projected DOS. The last two columns provide the magnetic and superconducting properties, following the same notations than Table XII.

chem. formula	ICSD	space group	figure	magn.	super-conduct.
$\text{Co}_3\text{Sn}_2\text{S}_2$	5435	SG 166 ( $R\bar{3}m$ )	Fig. 44	FM	—
$\text{Co}_3\text{InSn}_2\text{S}_2$	5437	SG 166 ( $R\bar{3}m$ )	Fig. 44	NM	—
$\text{Rh}_3\text{InPb}_2\text{S}_2$	5440	SG 166 ( $R\bar{3}m$ )	Fig. 44	NM	—
$\text{Rh}_3\text{Sn}_2\text{S}_2$	420728	SG 166 ( $R\bar{3}m$ )	Fig. 44	NM	—
$\text{InSnCo}_3\text{S}_2$	425137	SG 166 ( $R\bar{3}m$ )	Fig. 44	n.a.	—

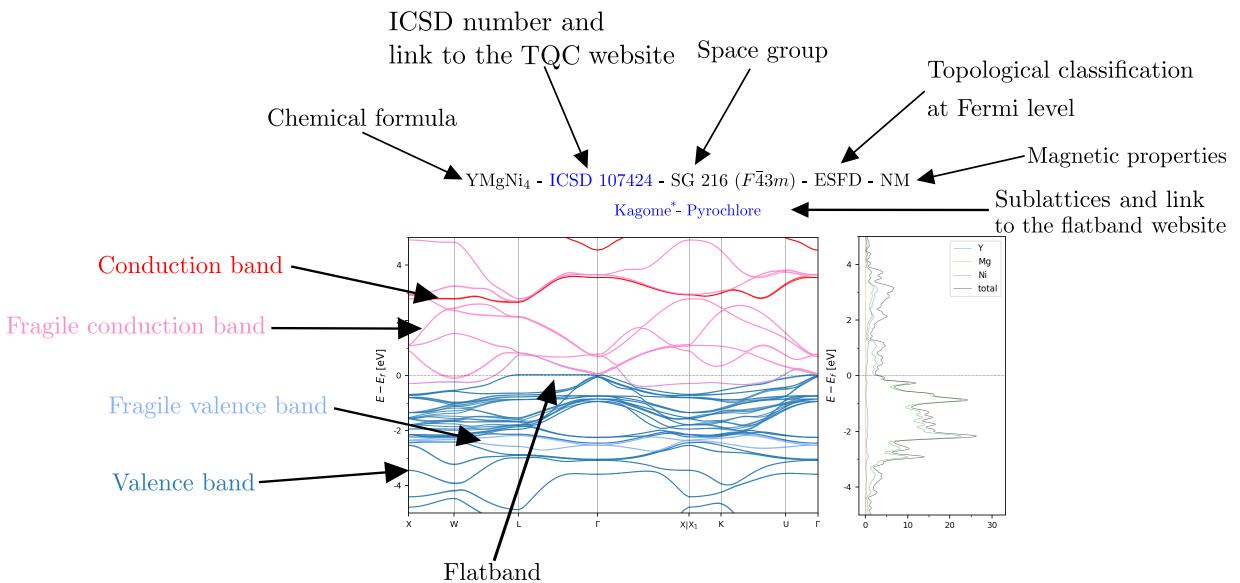


Figure 27. Example band structure and projected density of states plots. In this figure, we show the band structure and the projected density of states of  $\text{YMgNi}_4$  [ICSD 107424, SG 216  $F\bar{4}3m$ ] as an example of the labeling scheme and information contained within each of the band structure plots shown in this section. First, at the top of each band structure plot, we provide the chemical formula, ICSD number with a hyperlink to <https://www.topologicalquantumchemistry.org/>, space group symbol and number, the topological classification at the Fermi level (LCEBR, NLC, SEBR, ES, or ESFD) and the magnetic properties as available from Materials Project (NM for non-magnetic, FM for ferromagnetic, AFM for anti-ferromagnetic, FiM for ferrimagnetic and n.a. when the information is not available). Then we further list the hosted sublattices: Kagome, pyrochlore, bipartite, split or Lieb. A superscript \* for Kagome (Lieb) means that only approximate sublattices exist for Kagome (Lieb), as defined in Appendix D. In the band structure plot, trivial and stable topological conduction (valence) bands are labeled in red (blue), and fragile conduction (valence) bands are labeled in pink (light blue).

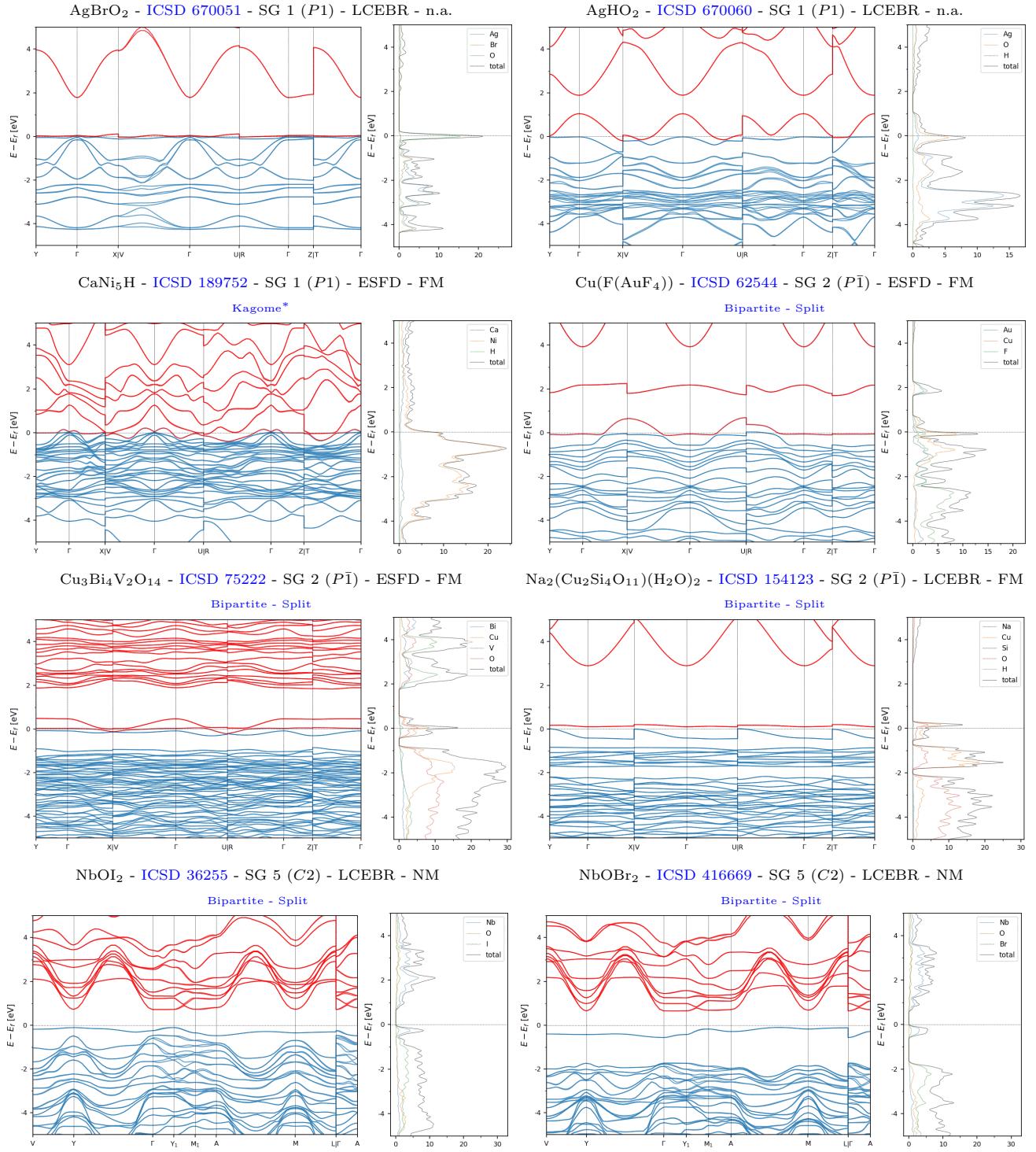


Figure 28. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 1/44)

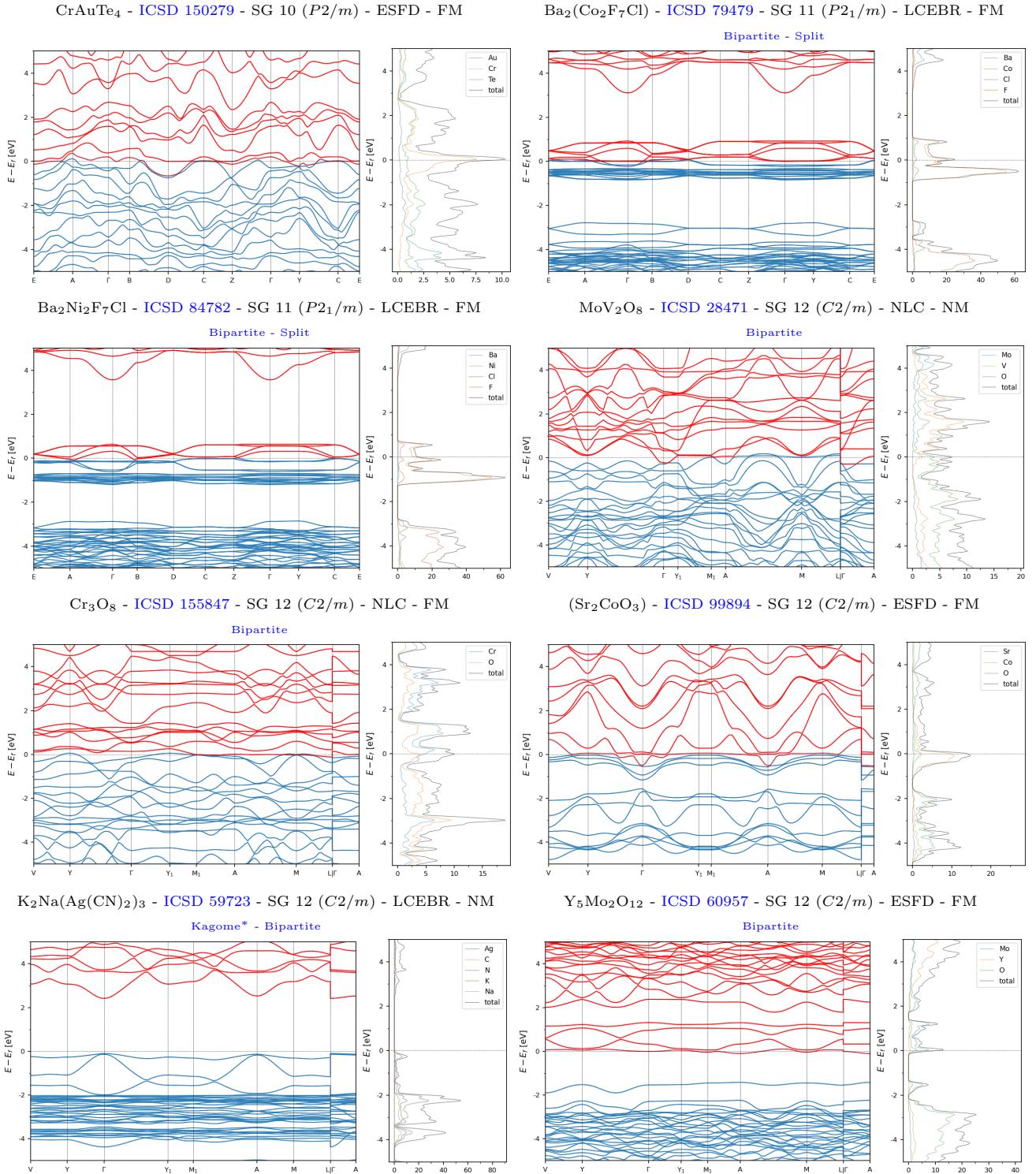


Figure 29. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 2/44)

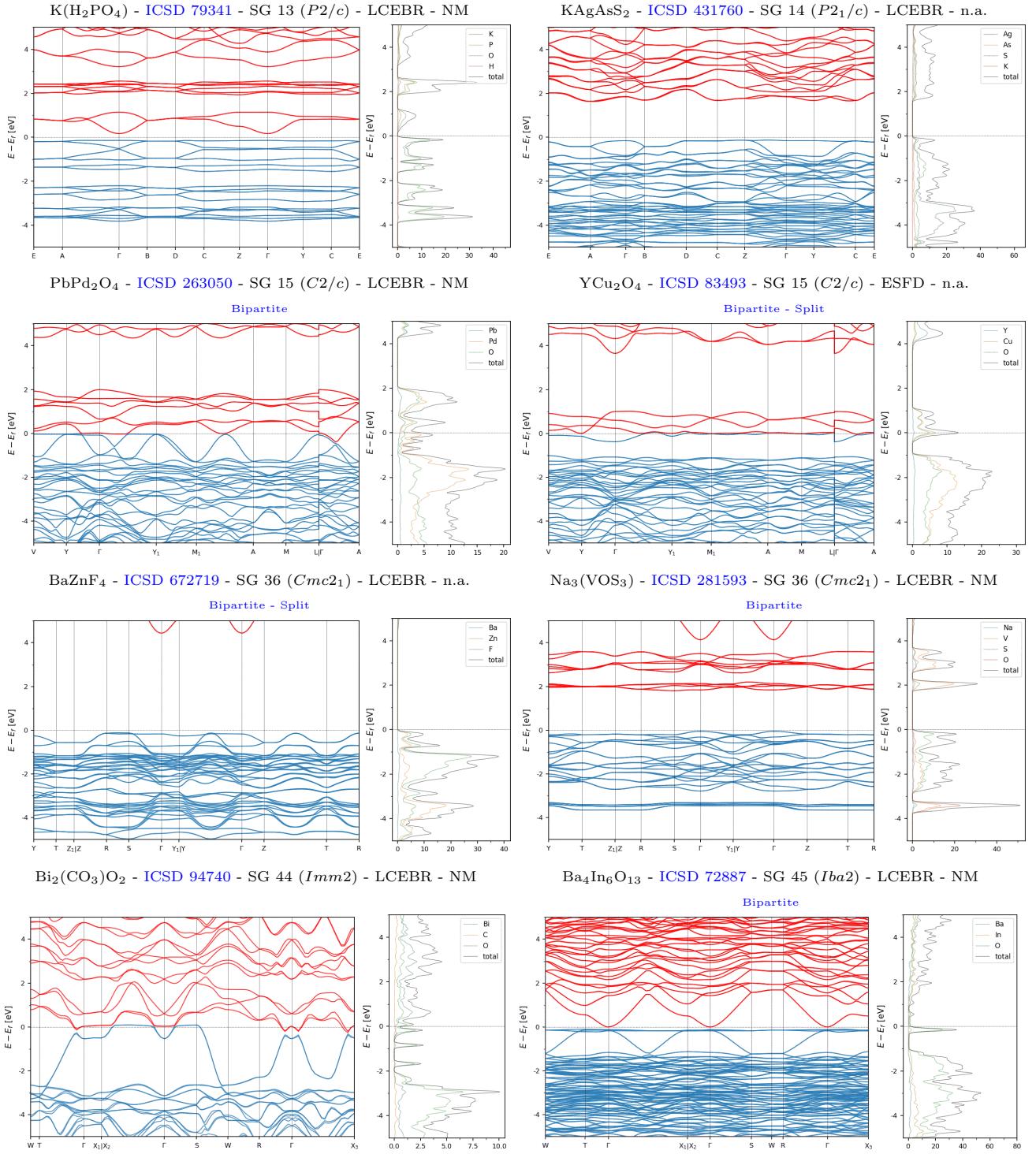


Figure 30. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 3/44)

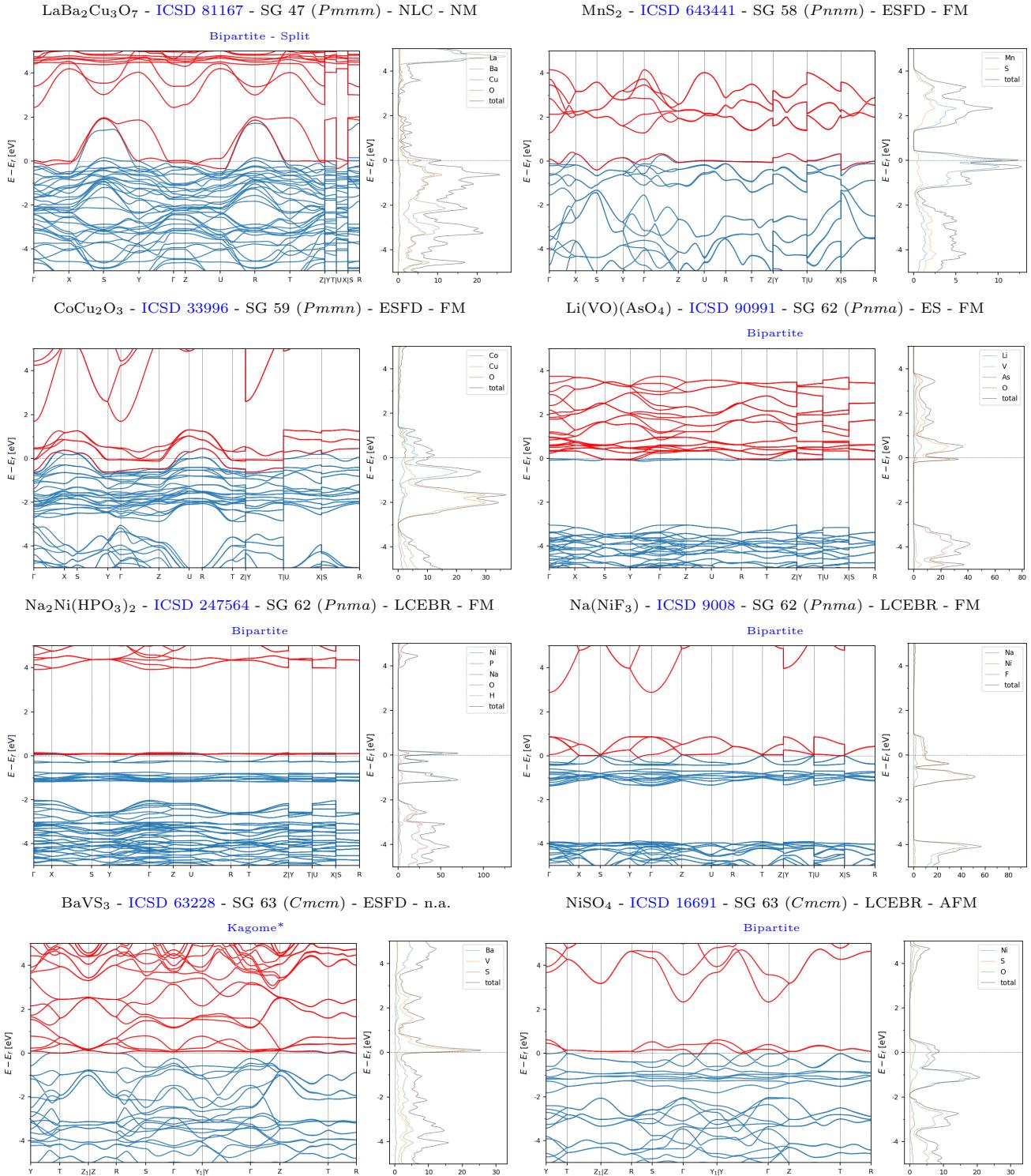


Figure 31. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 4/44)

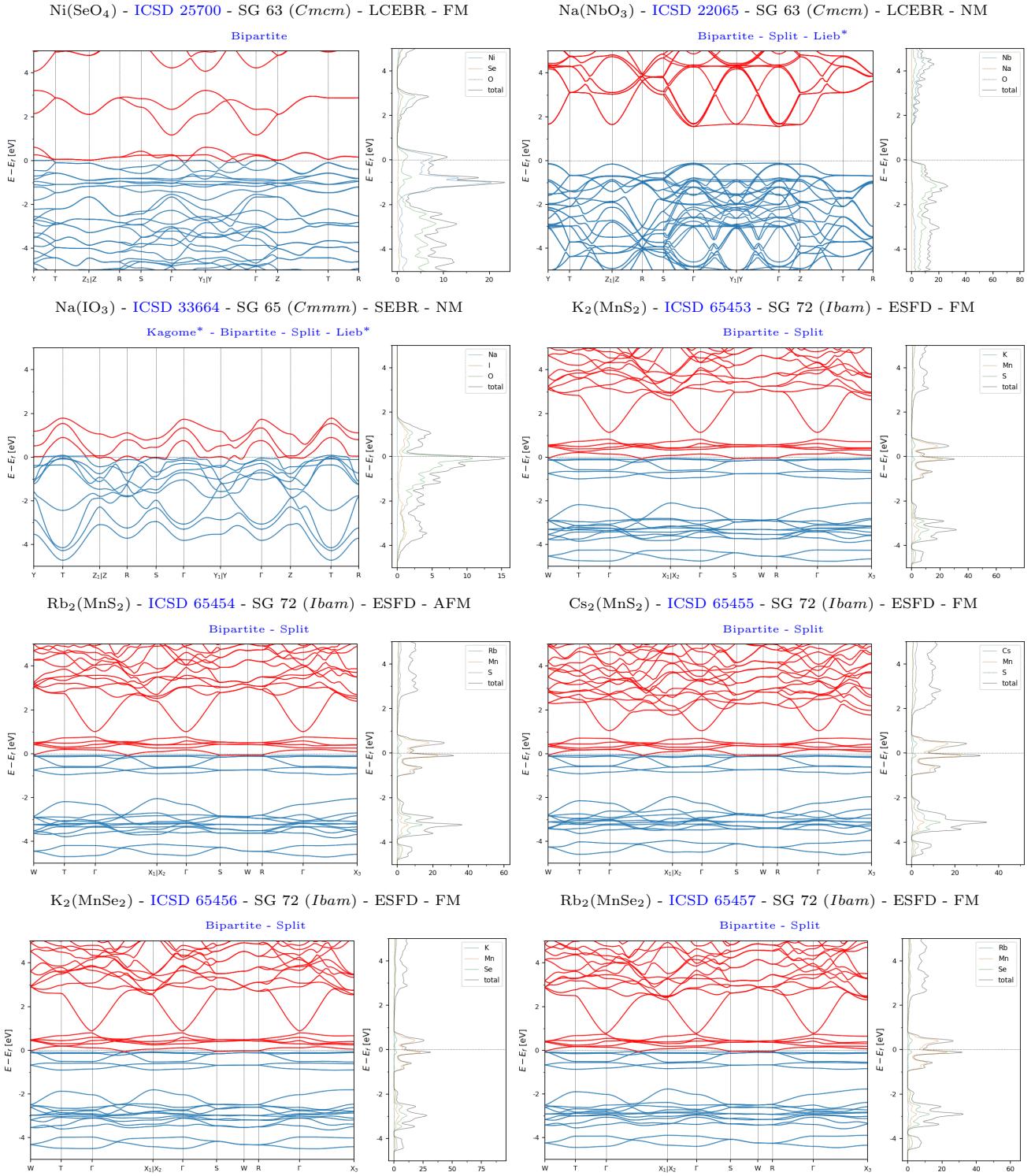


Figure 32. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 5/44)

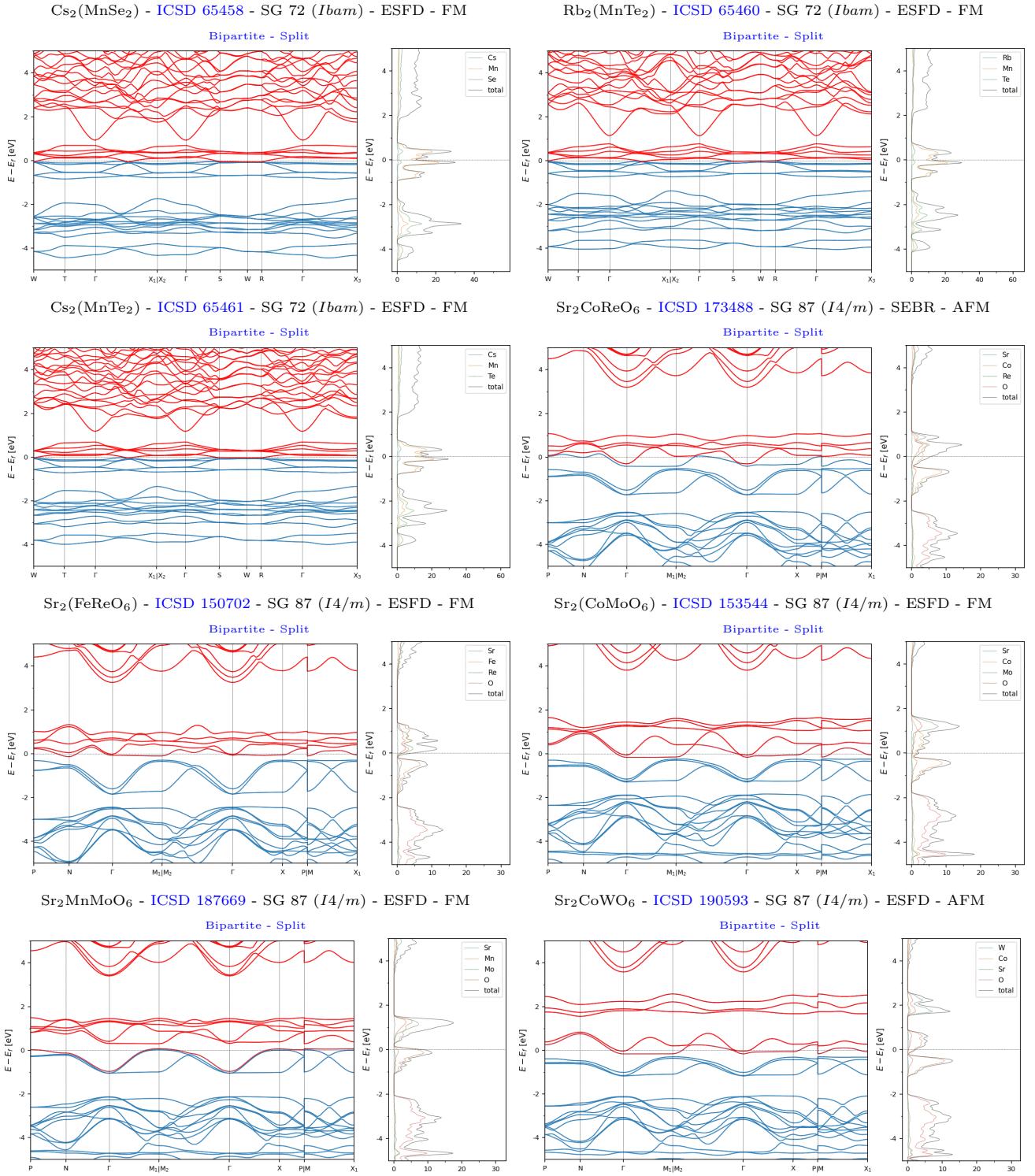


Figure 33. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 6/44)

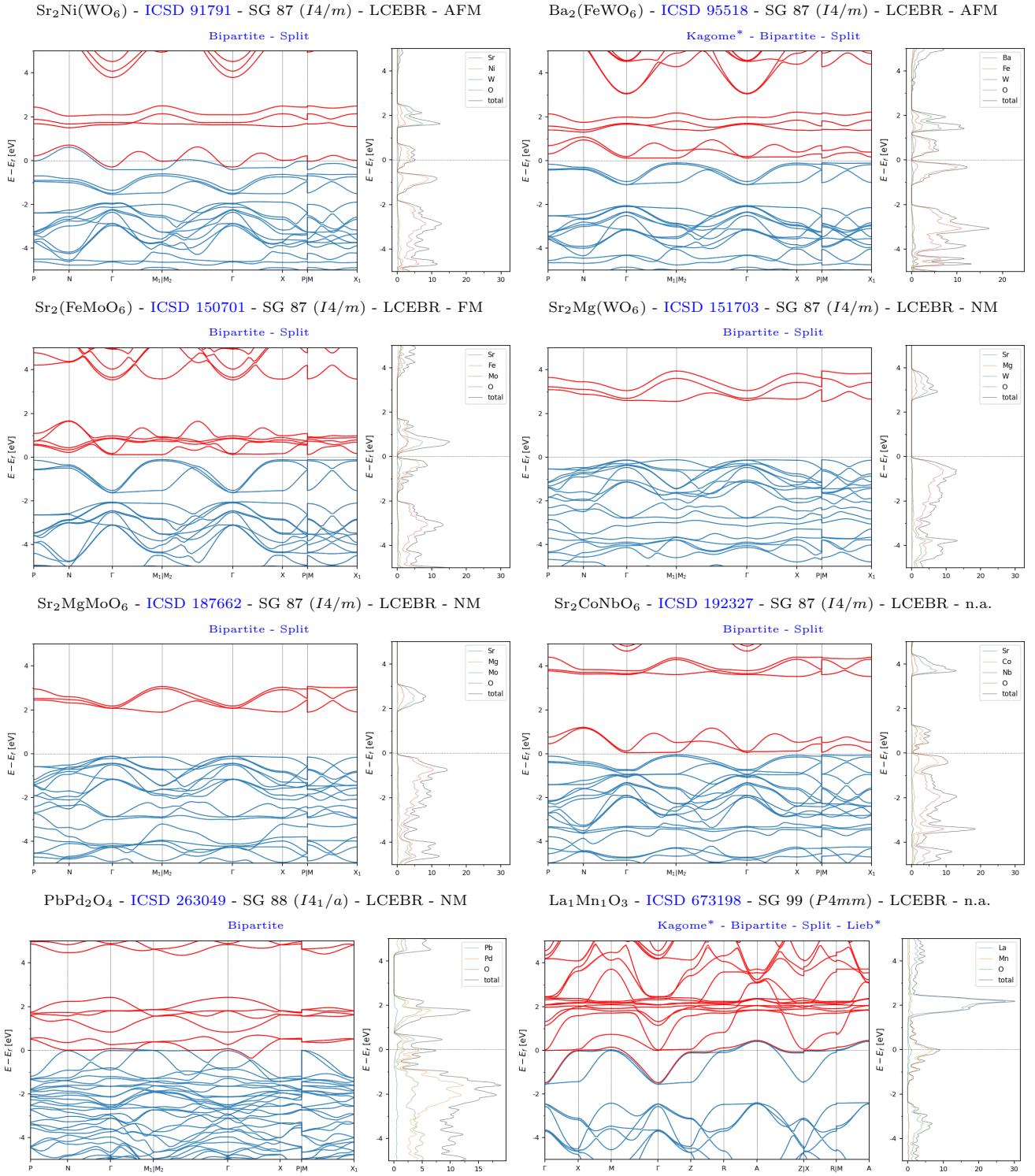


Figure 34. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 7/44)

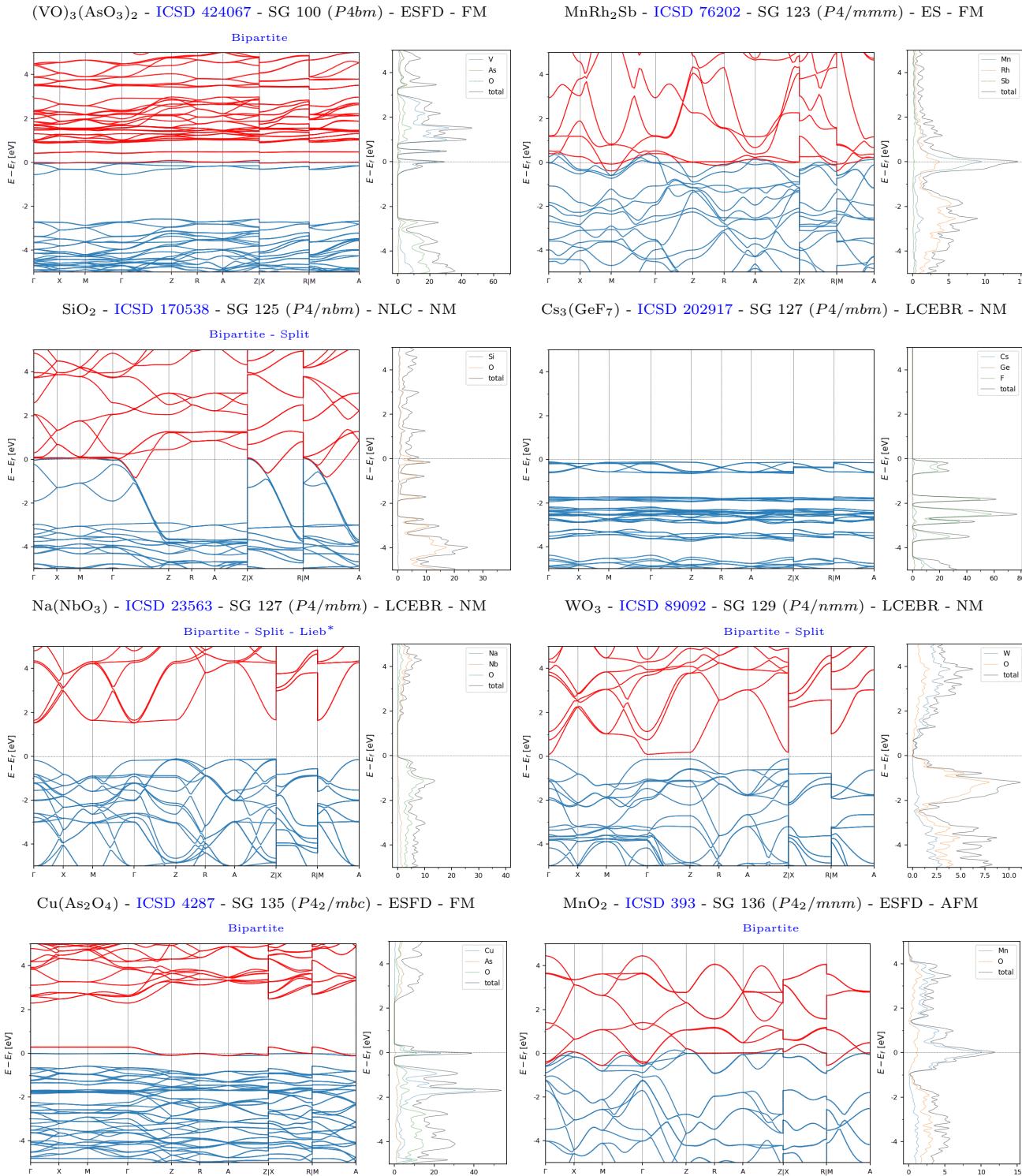


Figure 35. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 8/44)

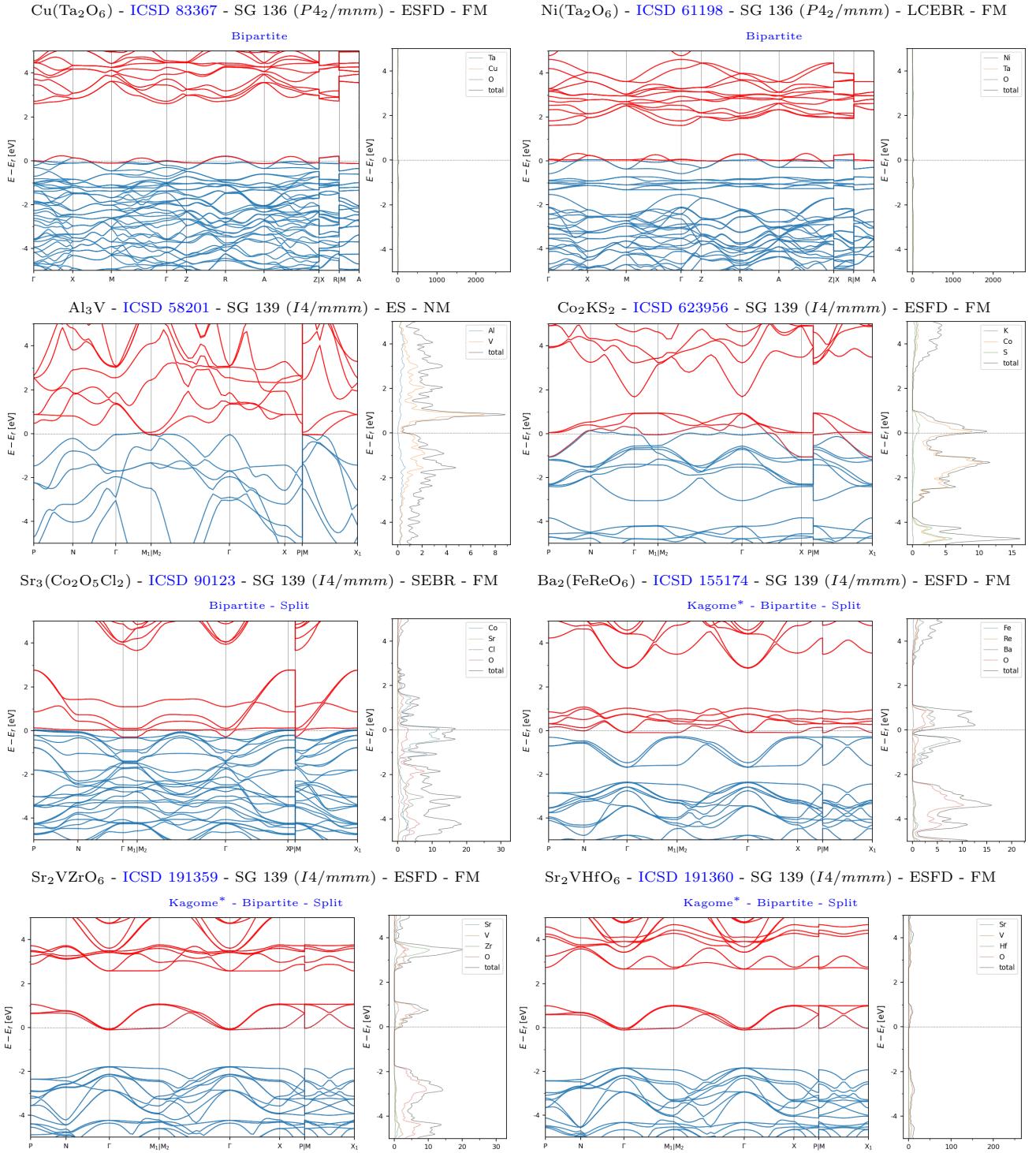


Figure 36. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 9/44)

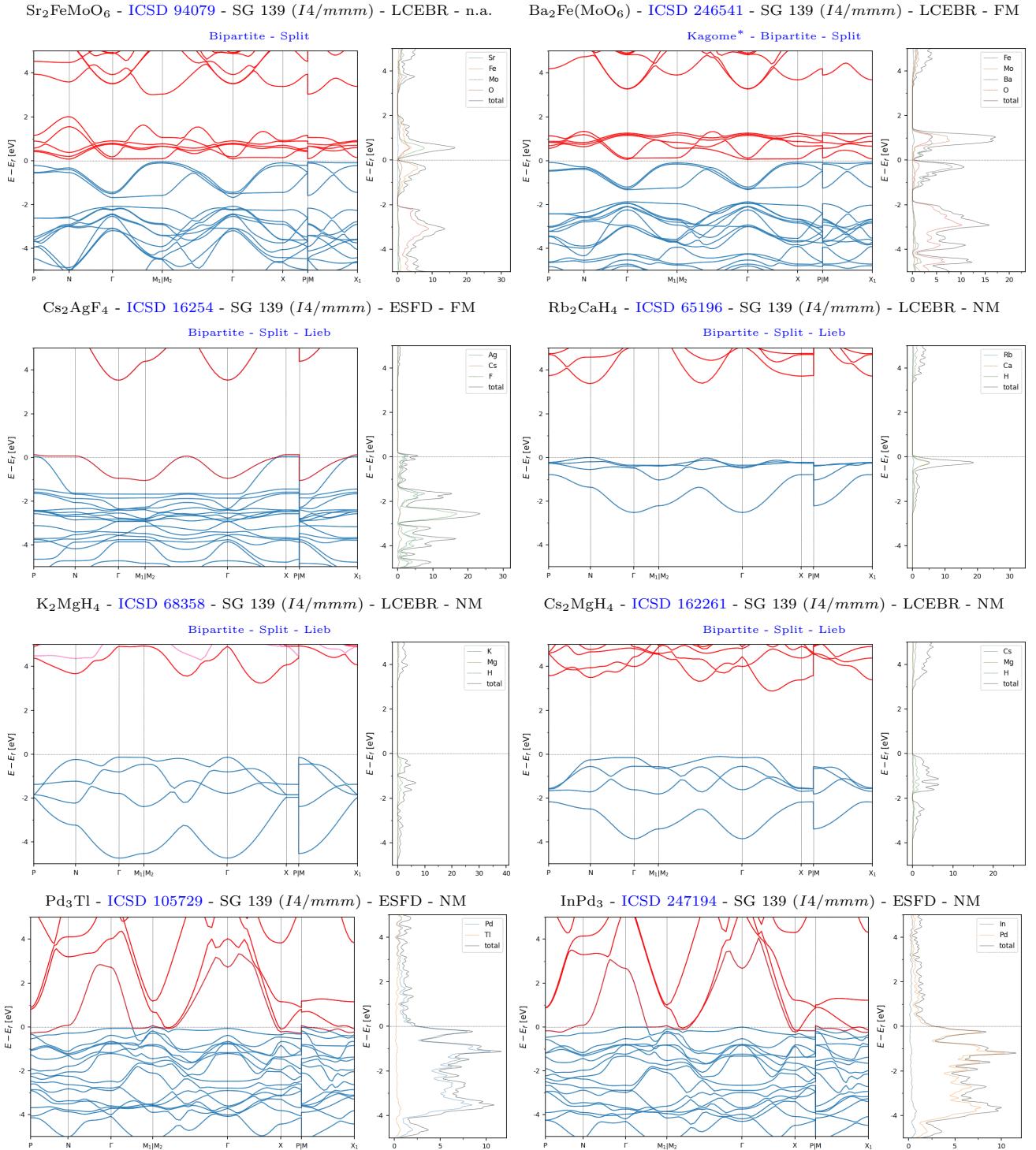


Figure 37. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 10/44)

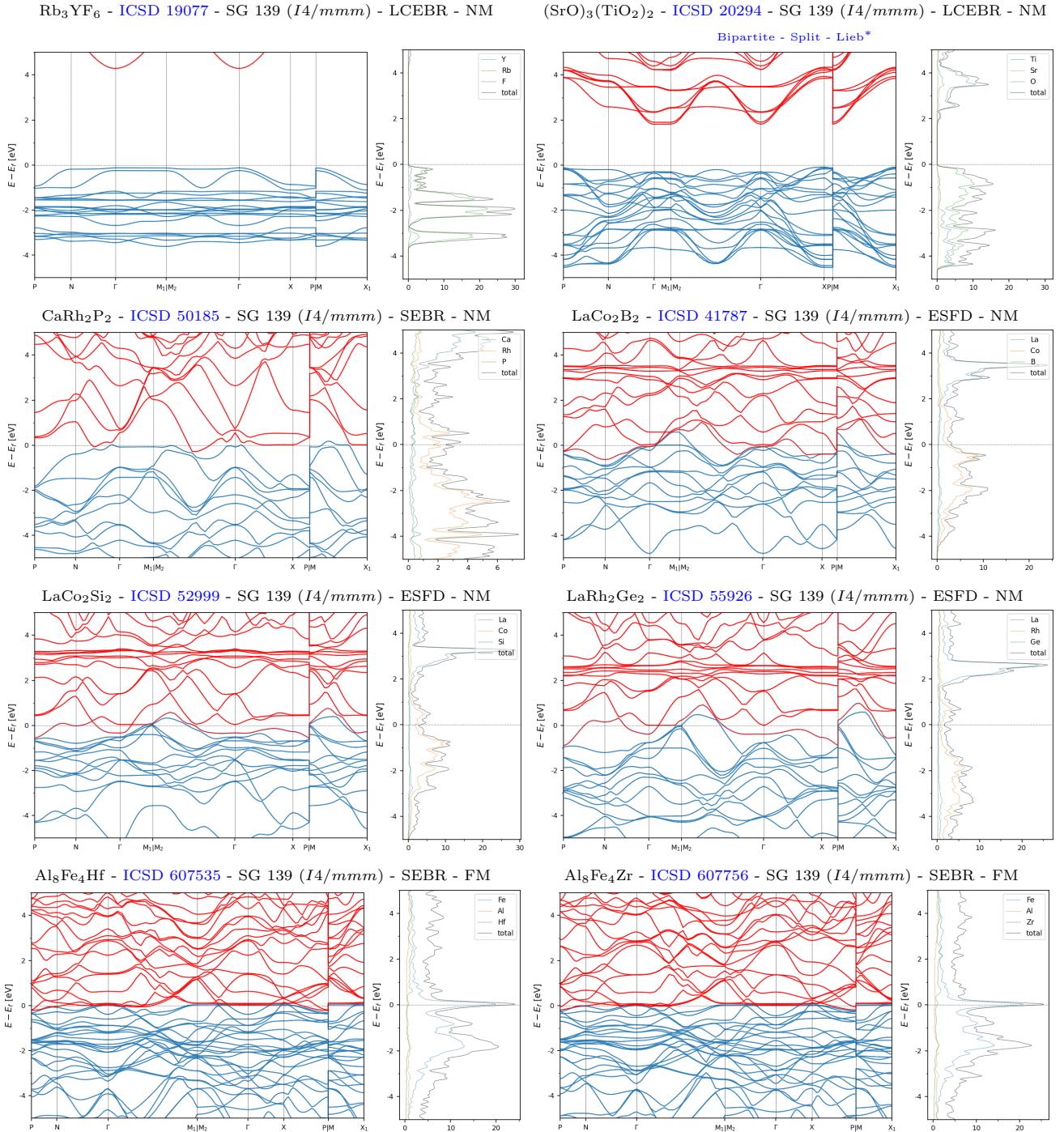


Figure 38. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 11/44)

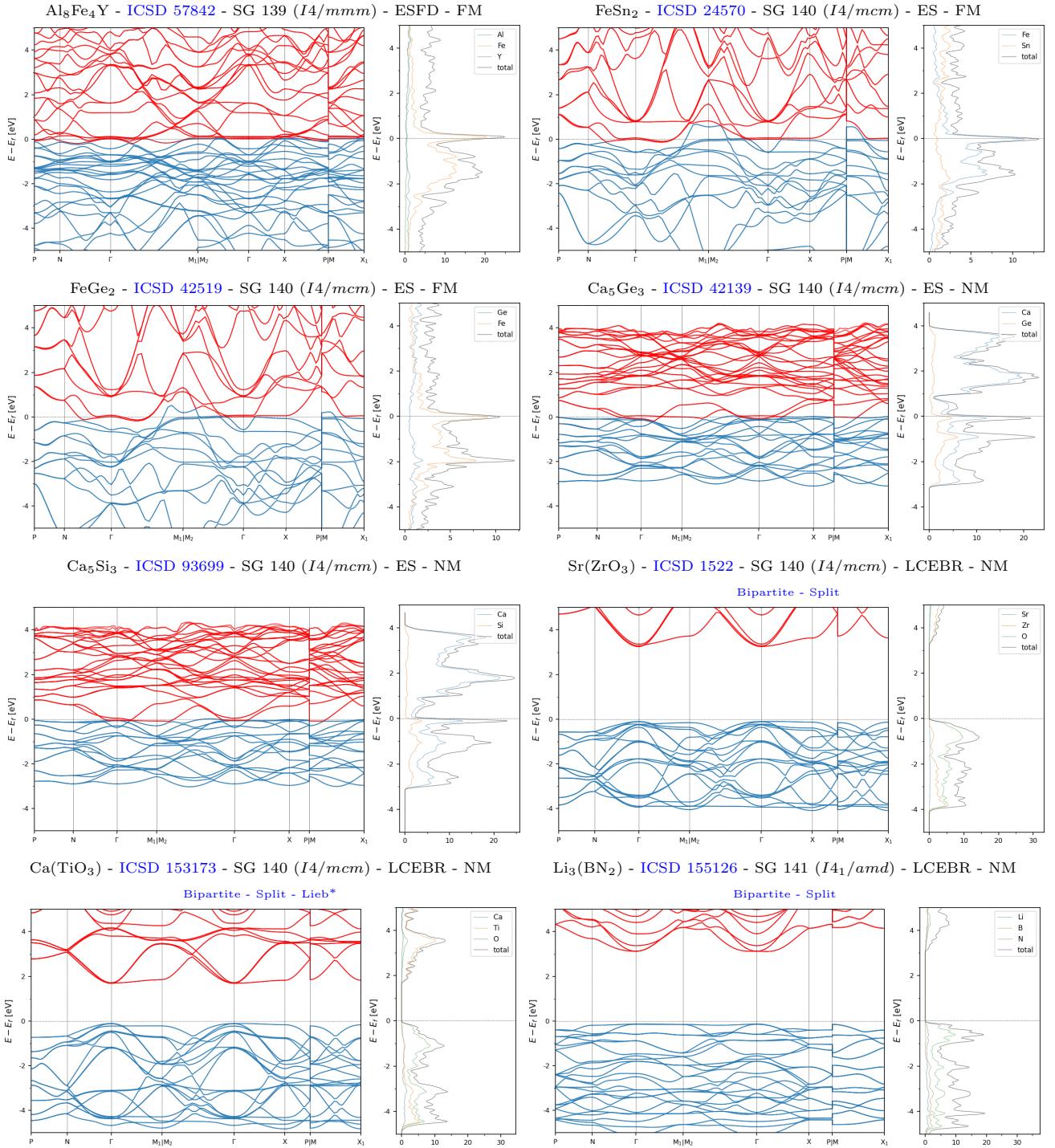


Figure 39. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 12/44)

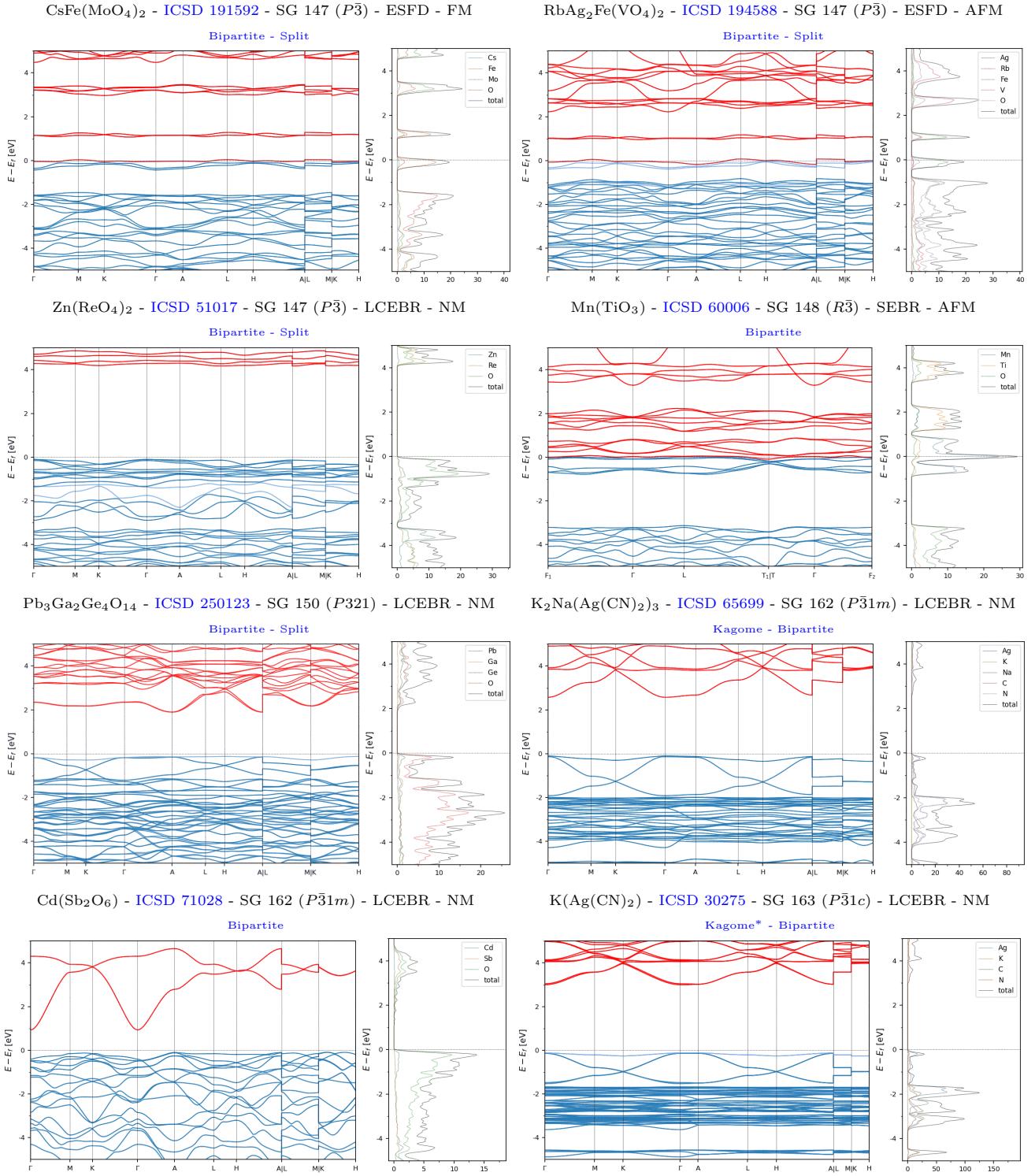


Figure 40. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 13/44)

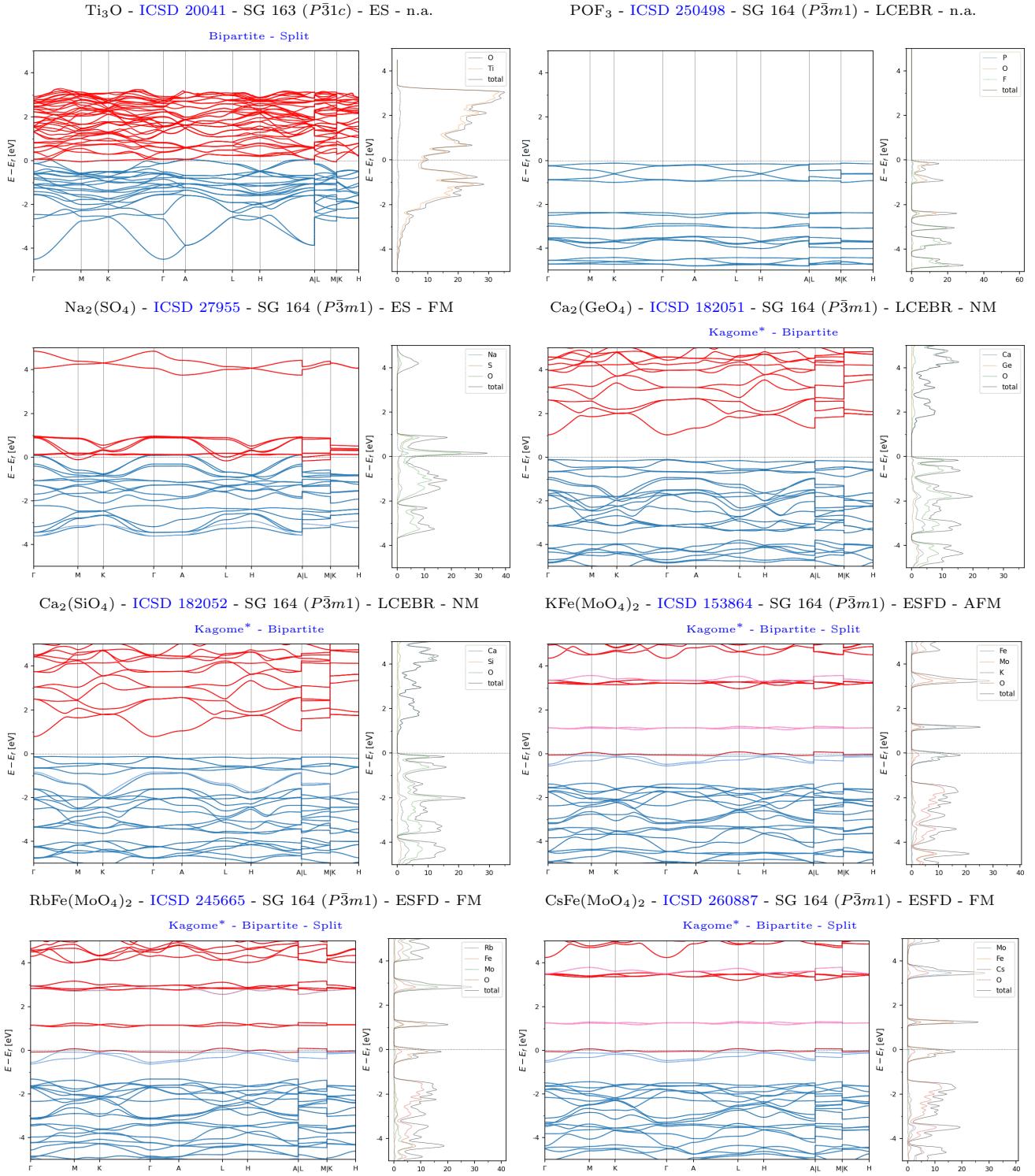


Figure 41. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 14/44)

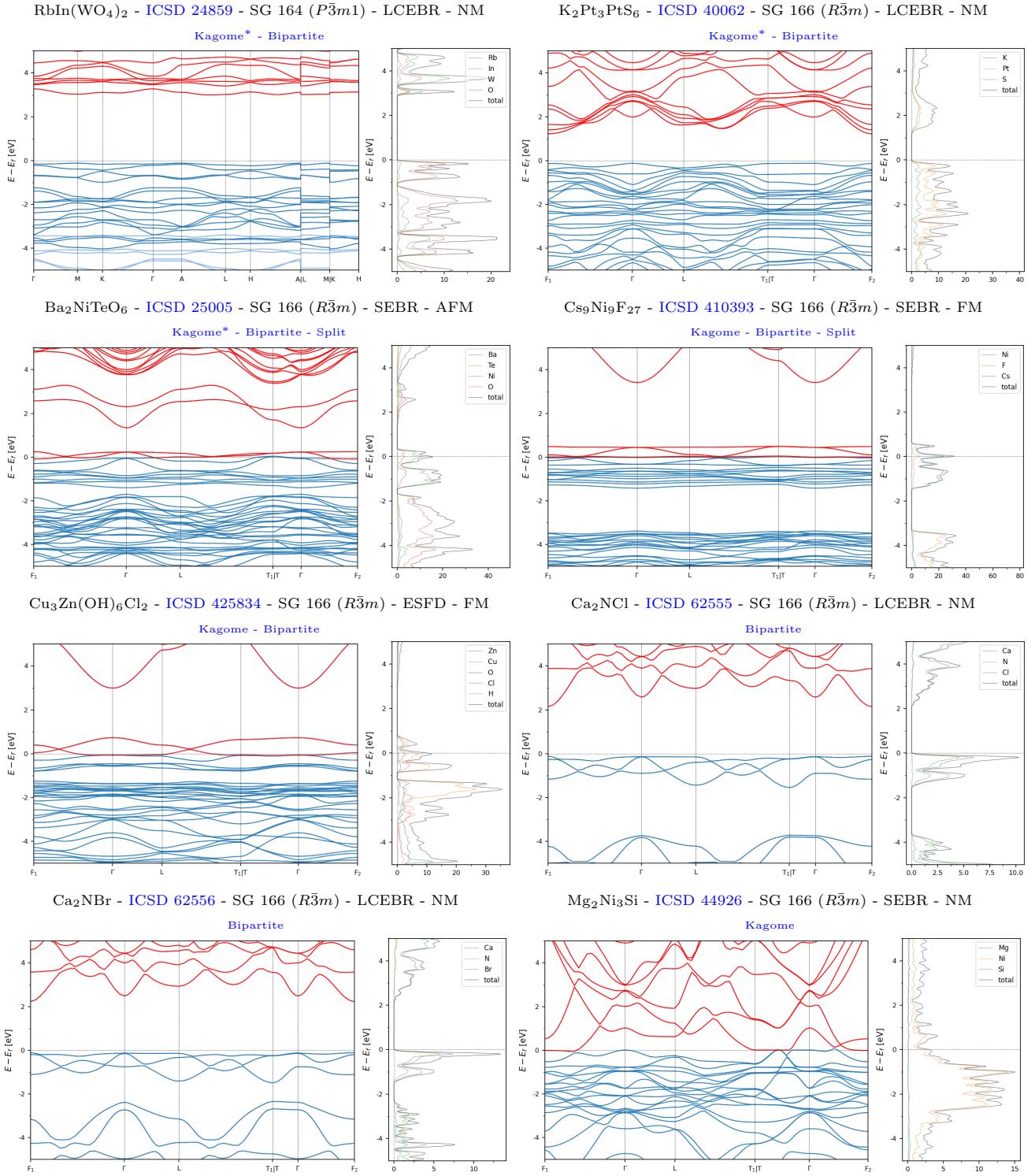


Figure 42. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 15/44)

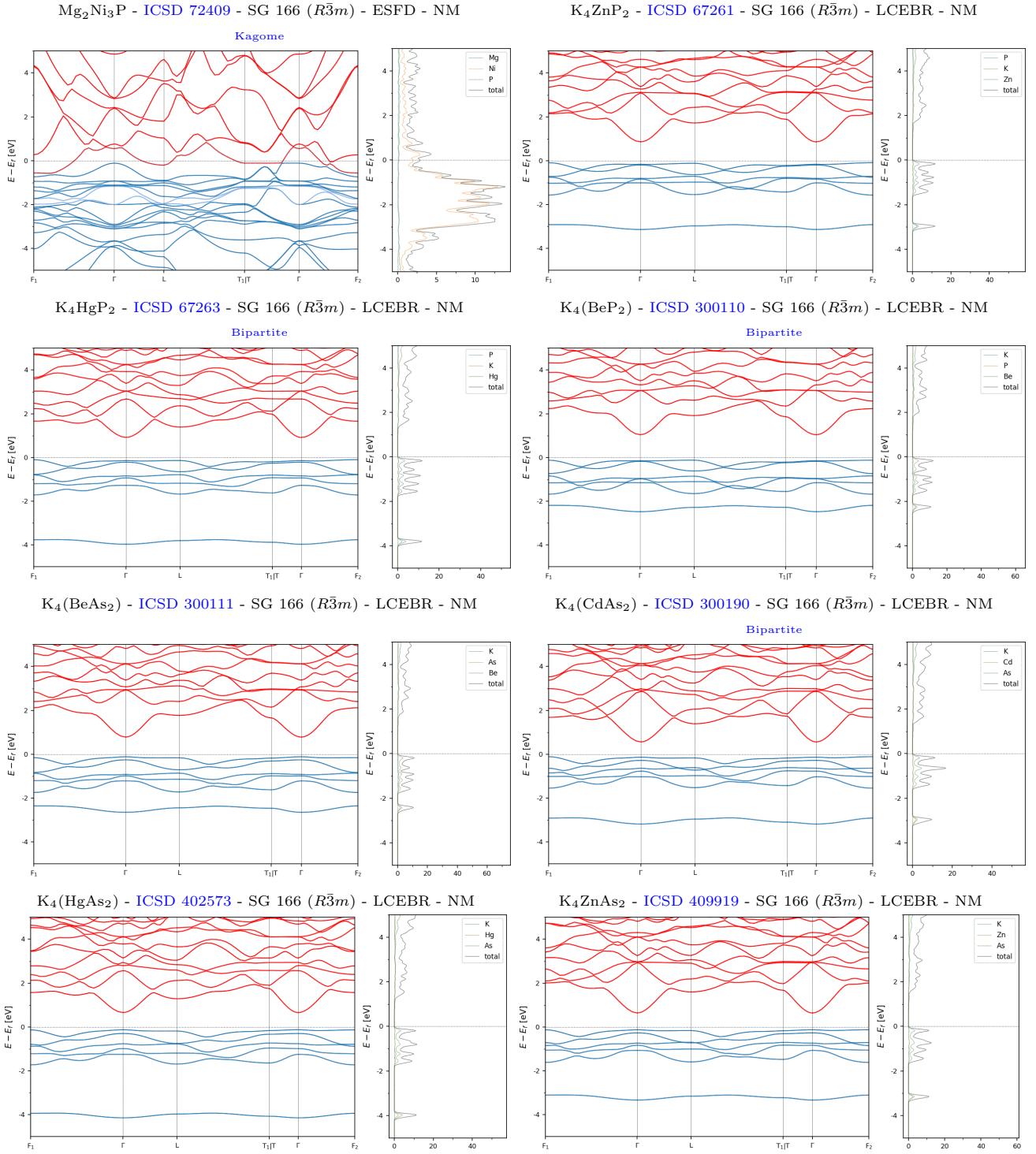


Figure 43. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 16/44)

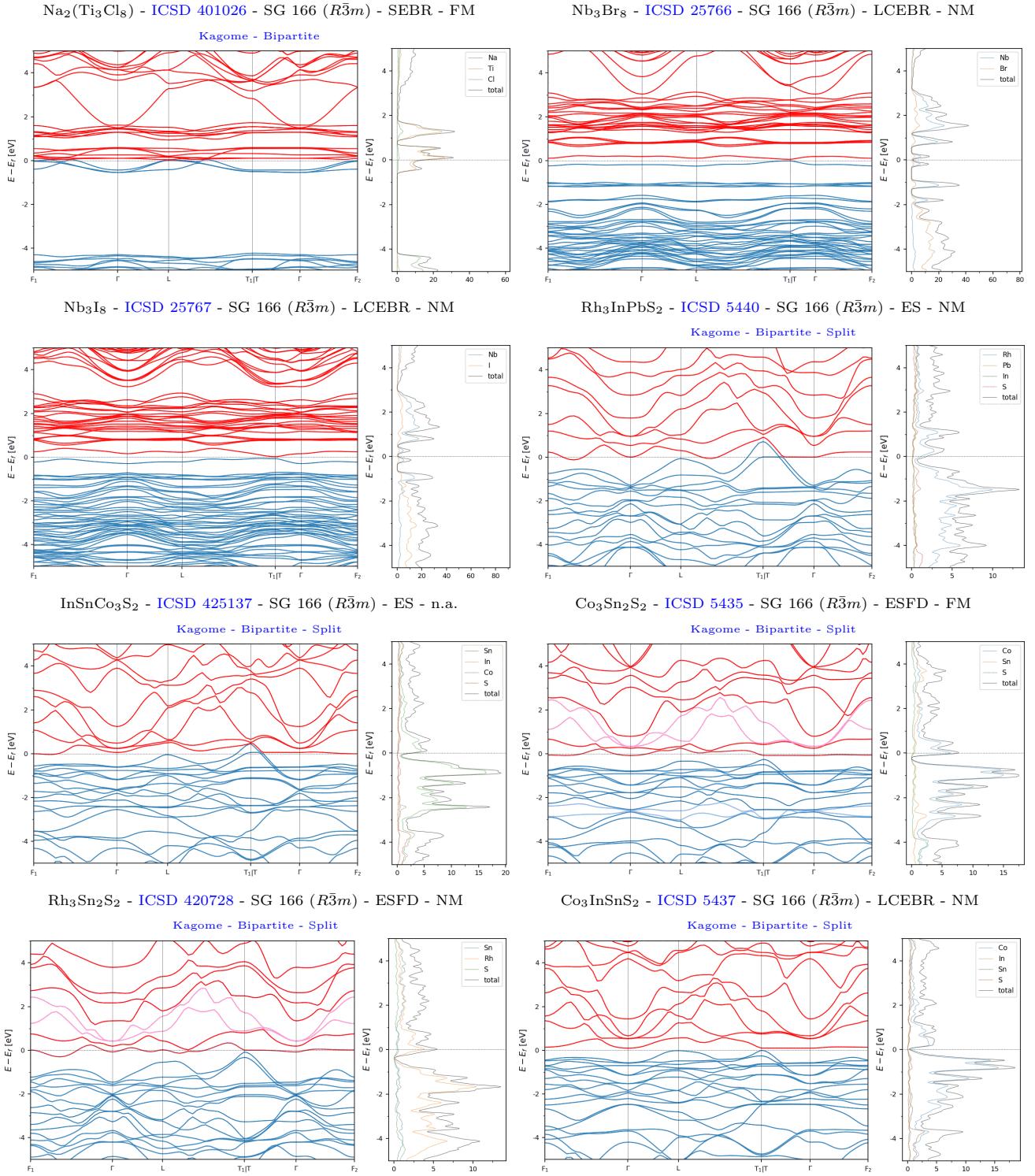


Figure 44. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 17/44)

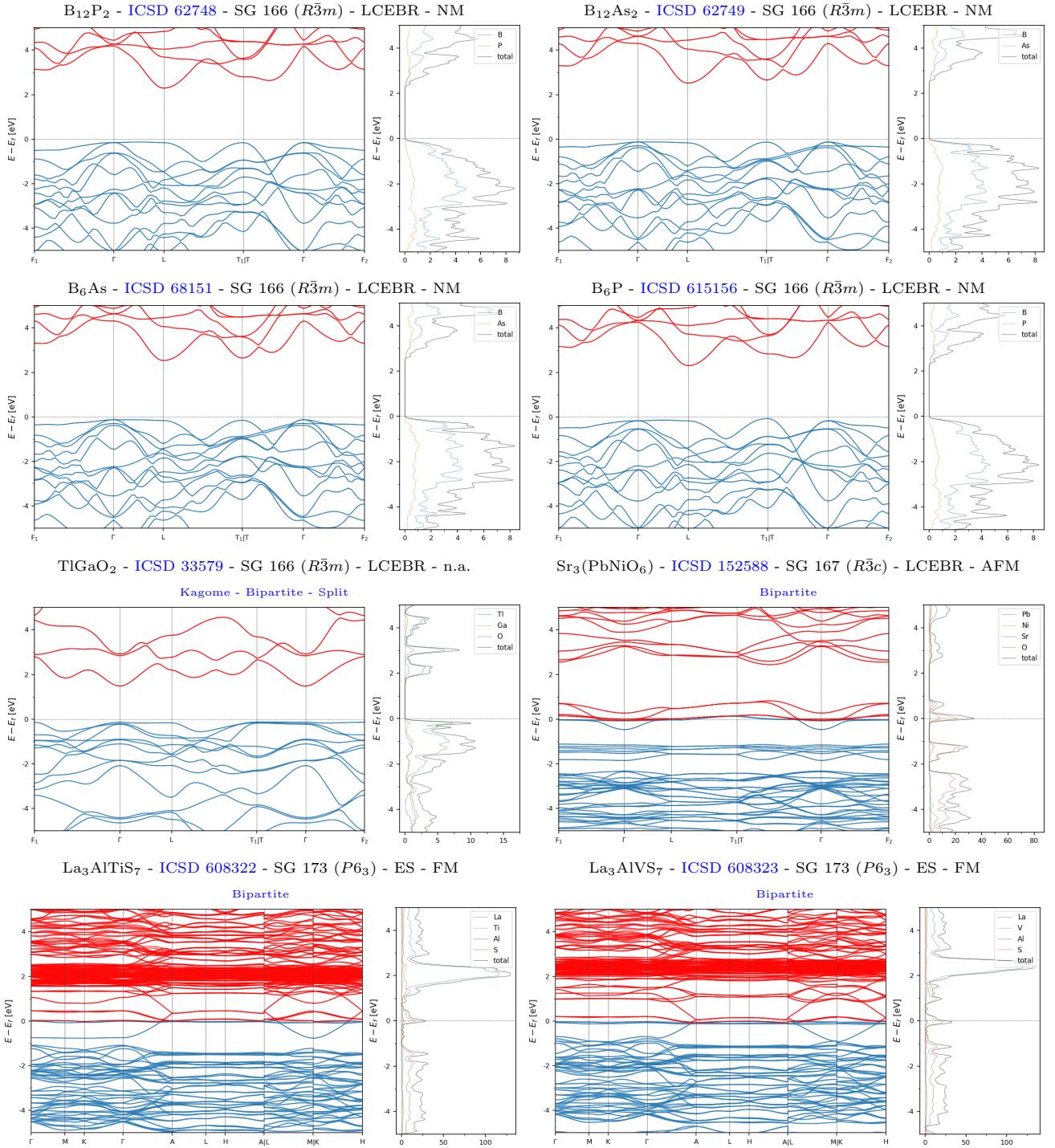


Figure 45. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 18/44)

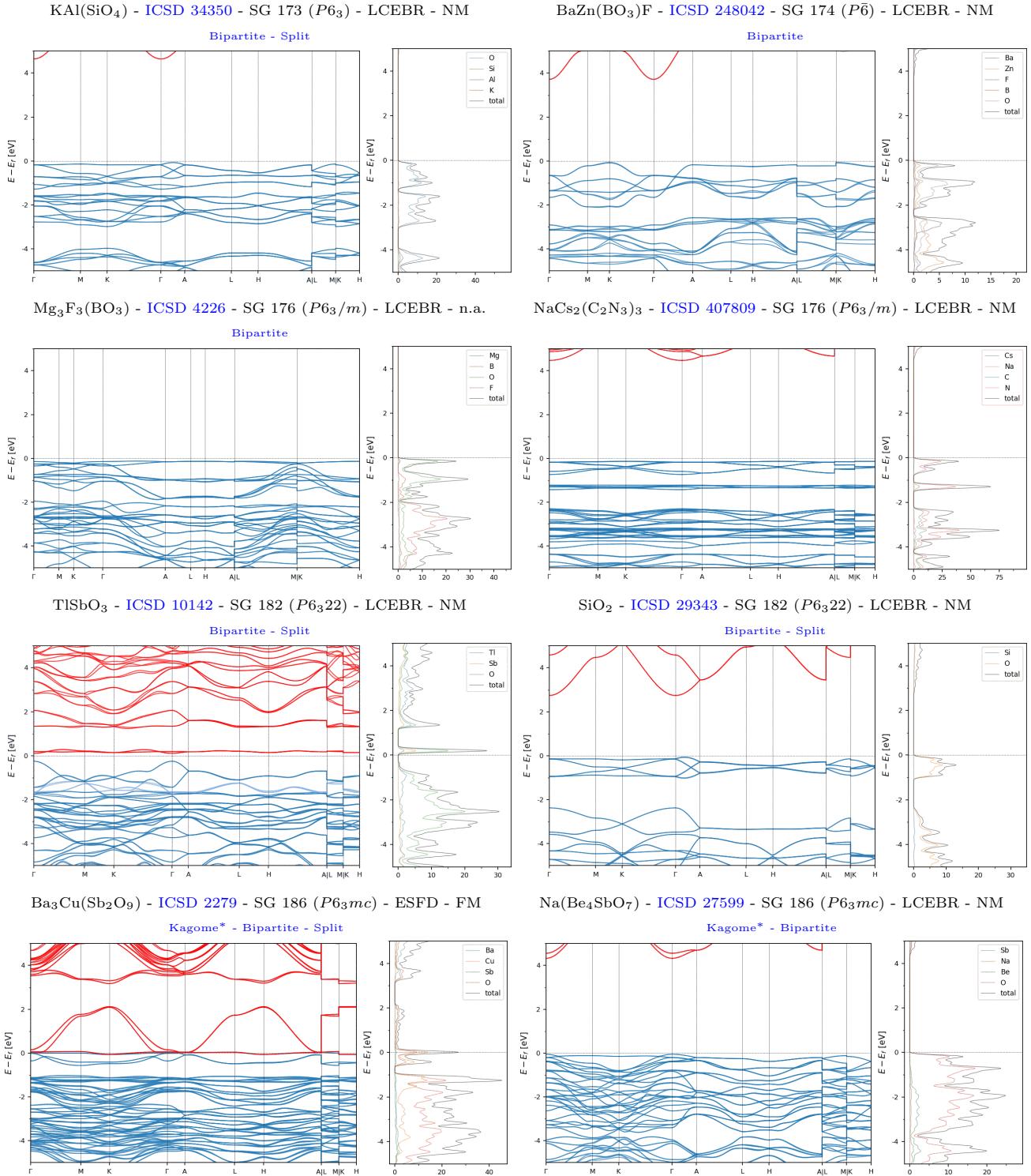


Figure 46. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 19/44)

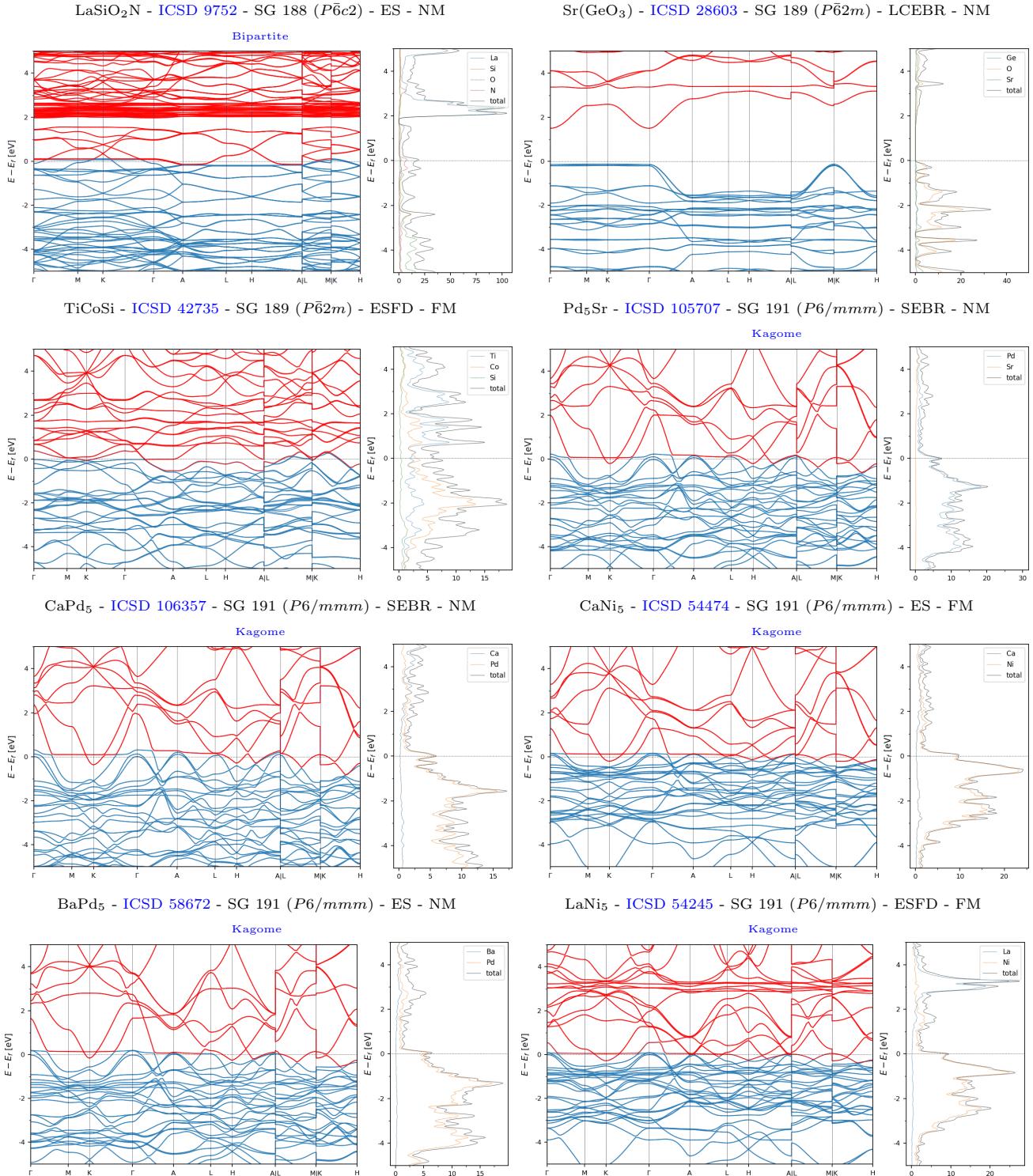


Figure 47. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 20/44)

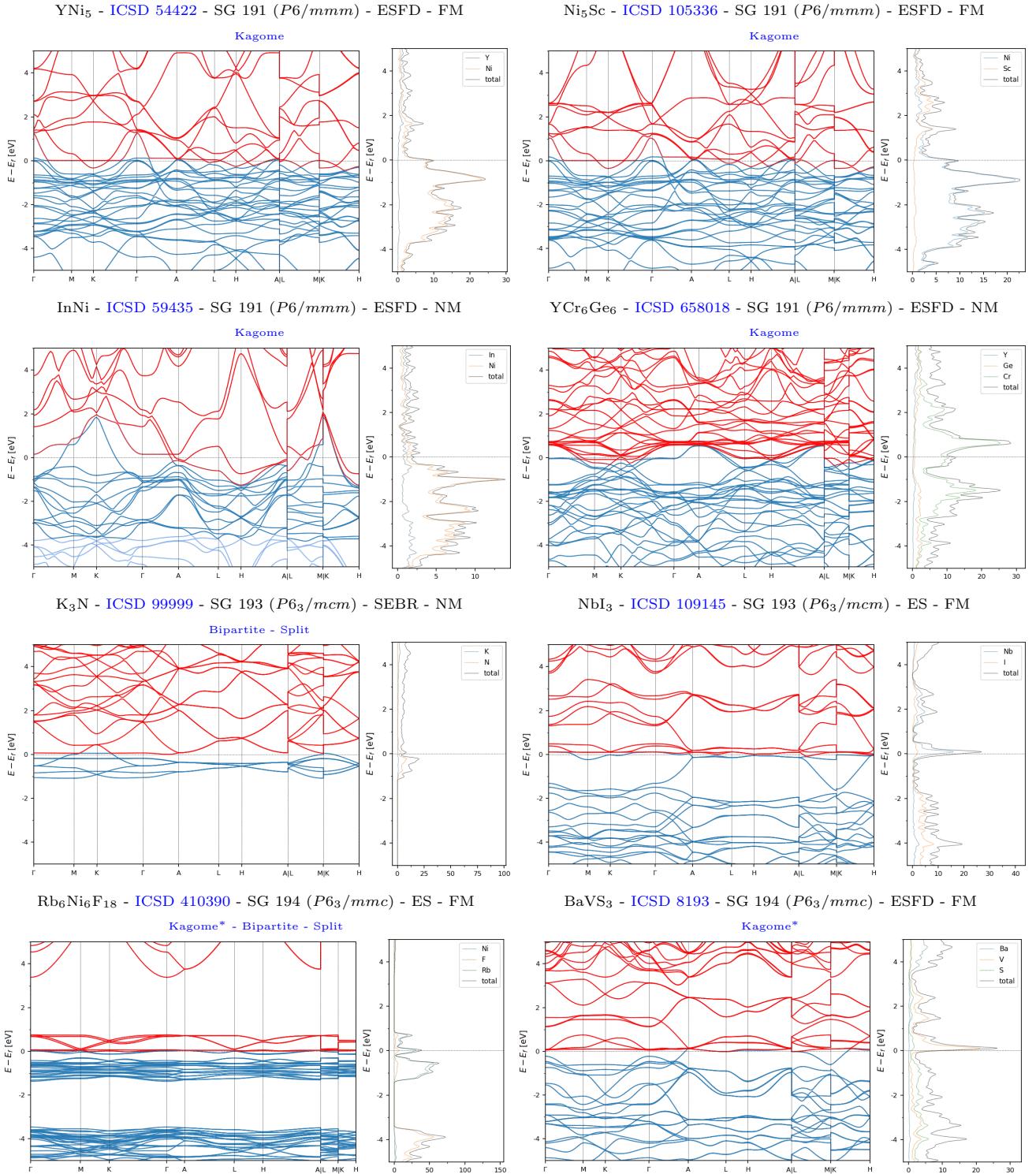


Figure 48. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 21/44)

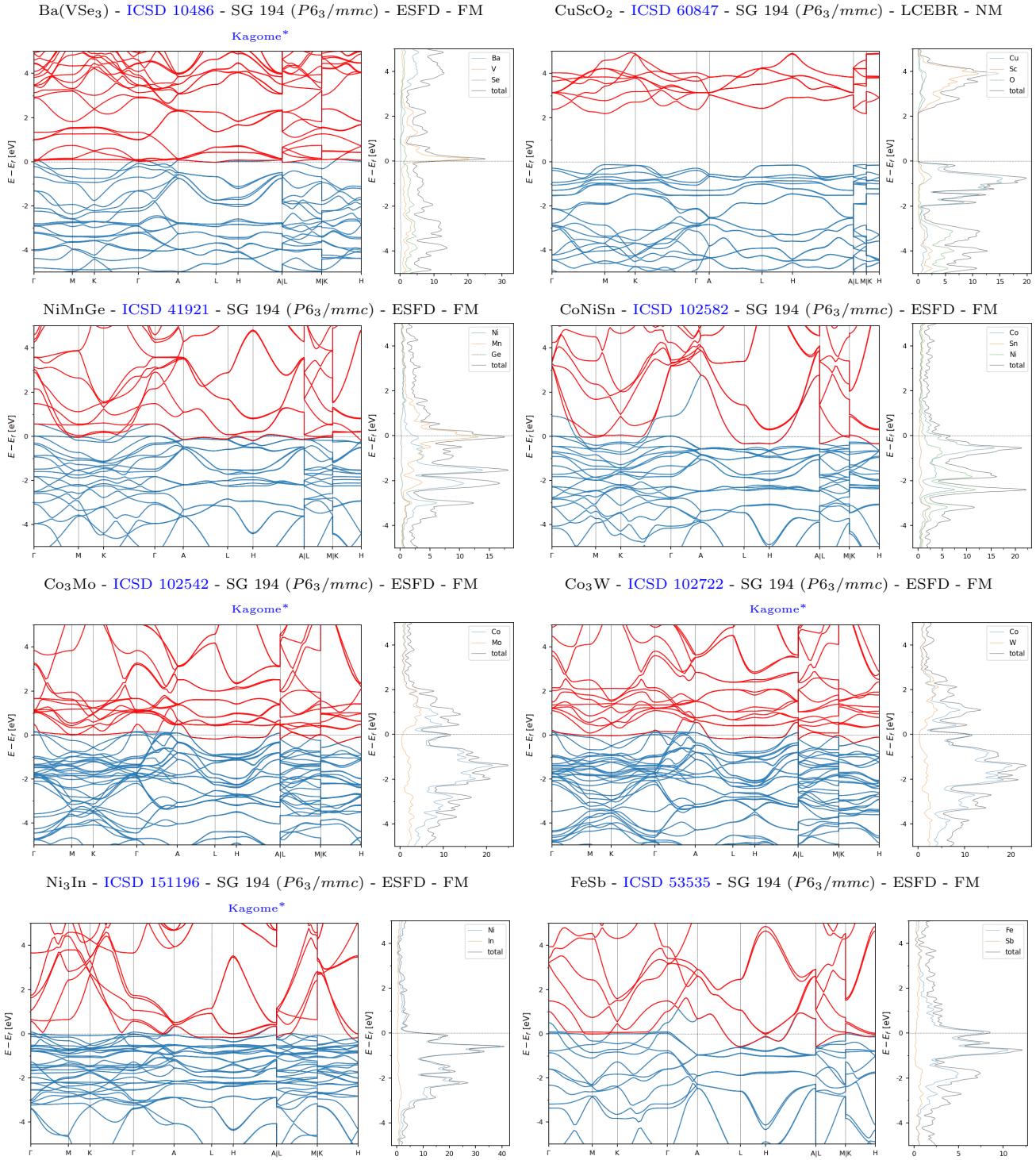


Figure 49. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 22/44)

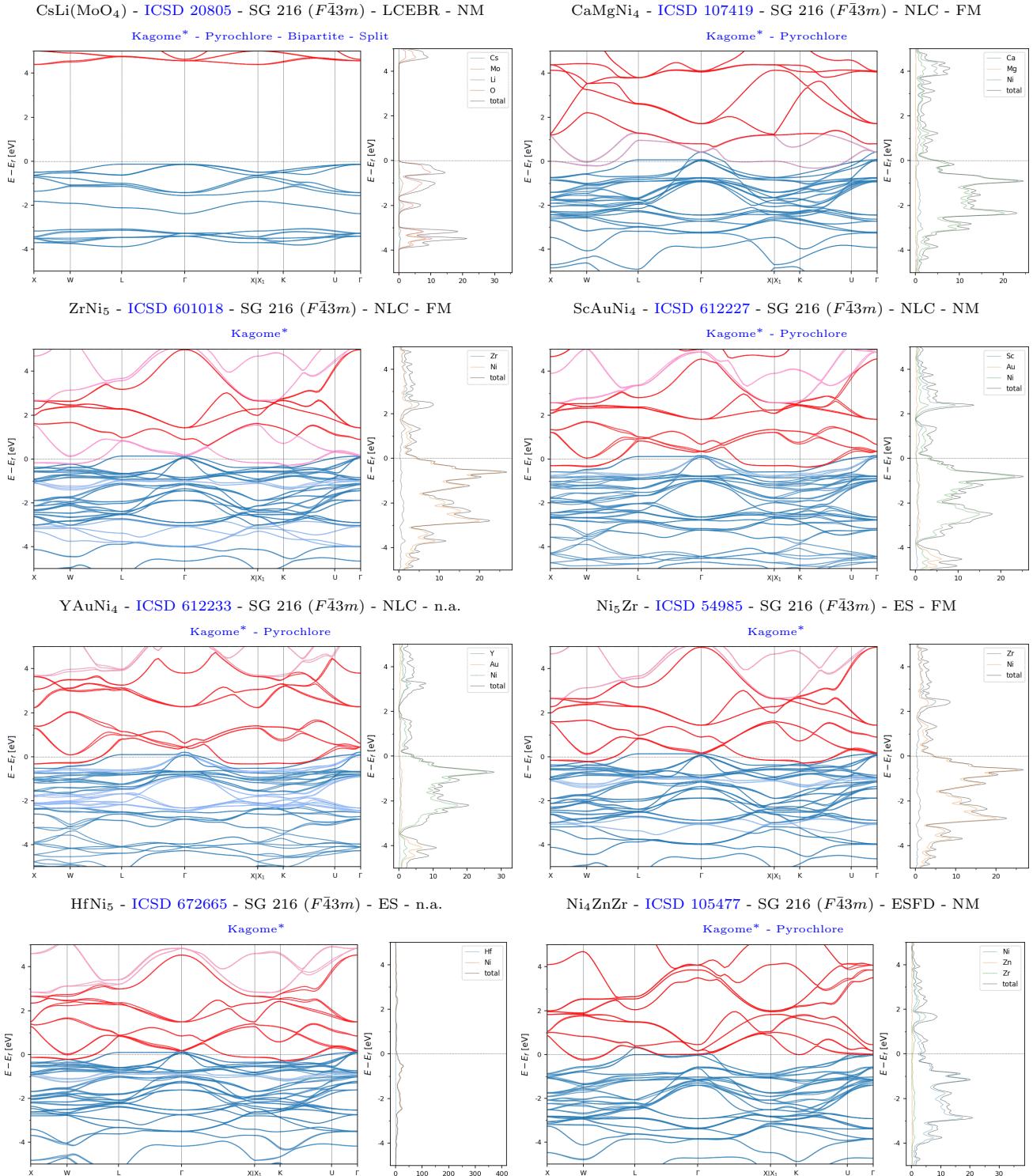


Figure 50. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 23/44)

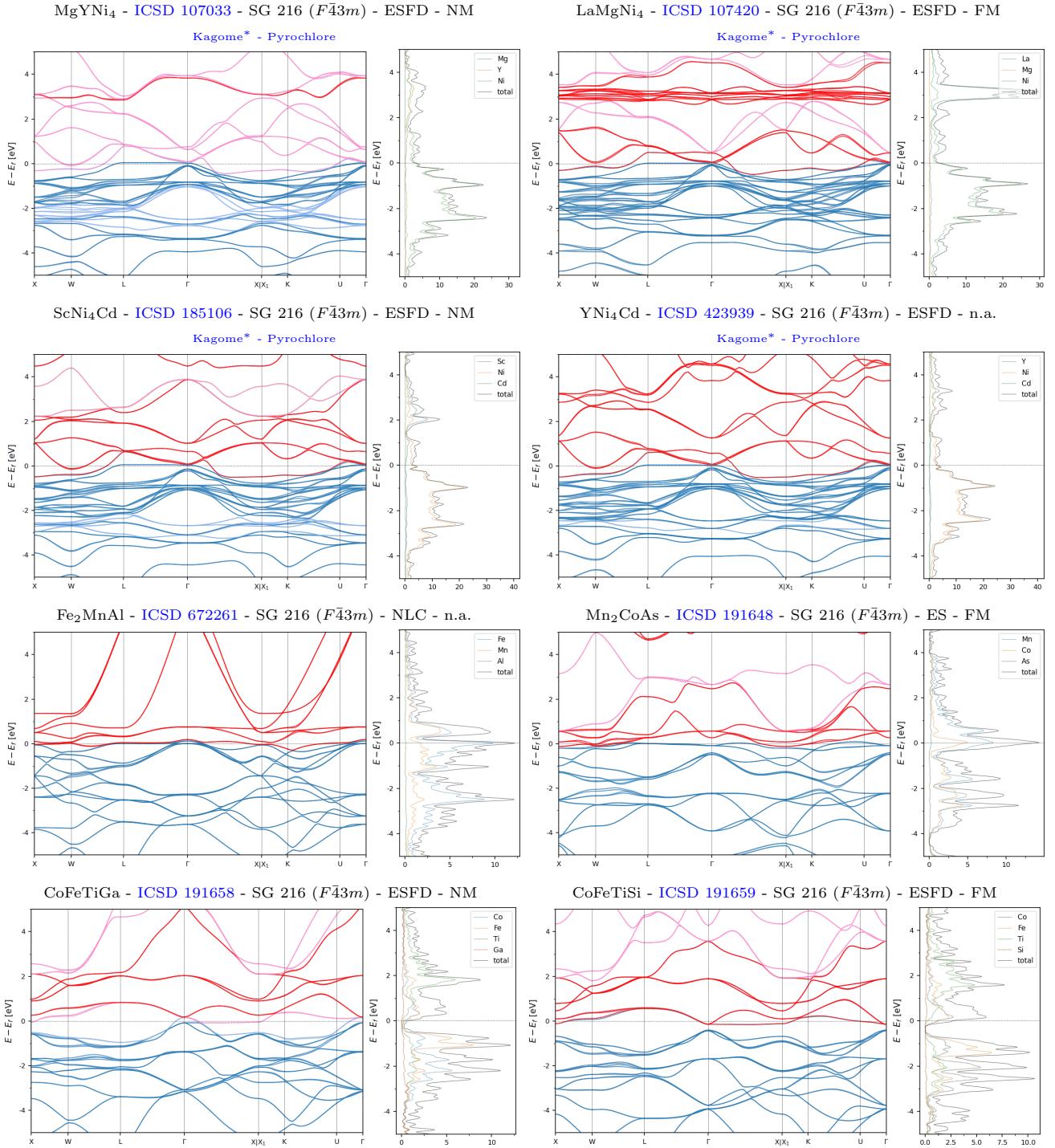


Figure 51. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 24/44)

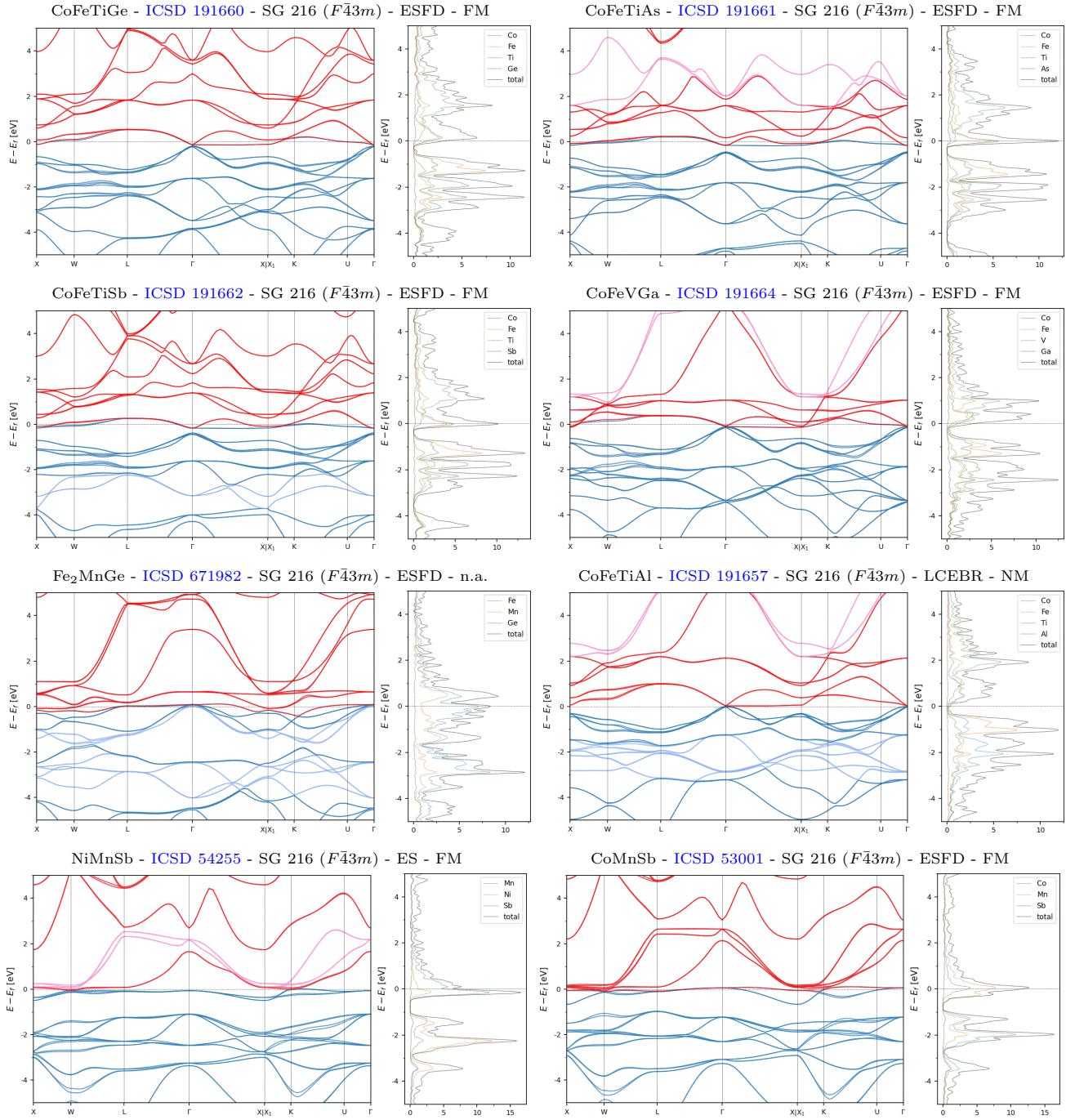


Figure 52. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 25/44)

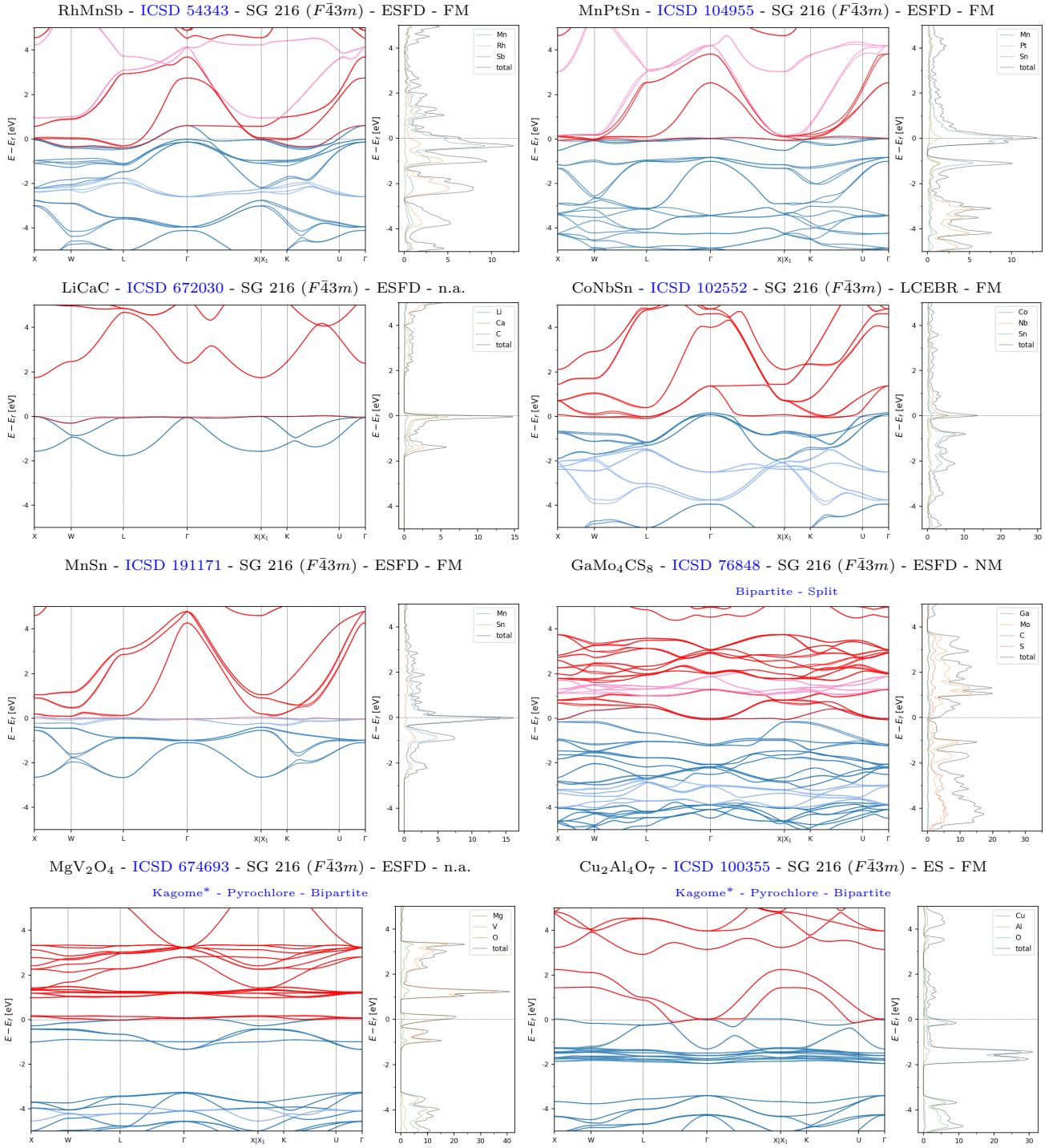


Figure 53. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 26/44)

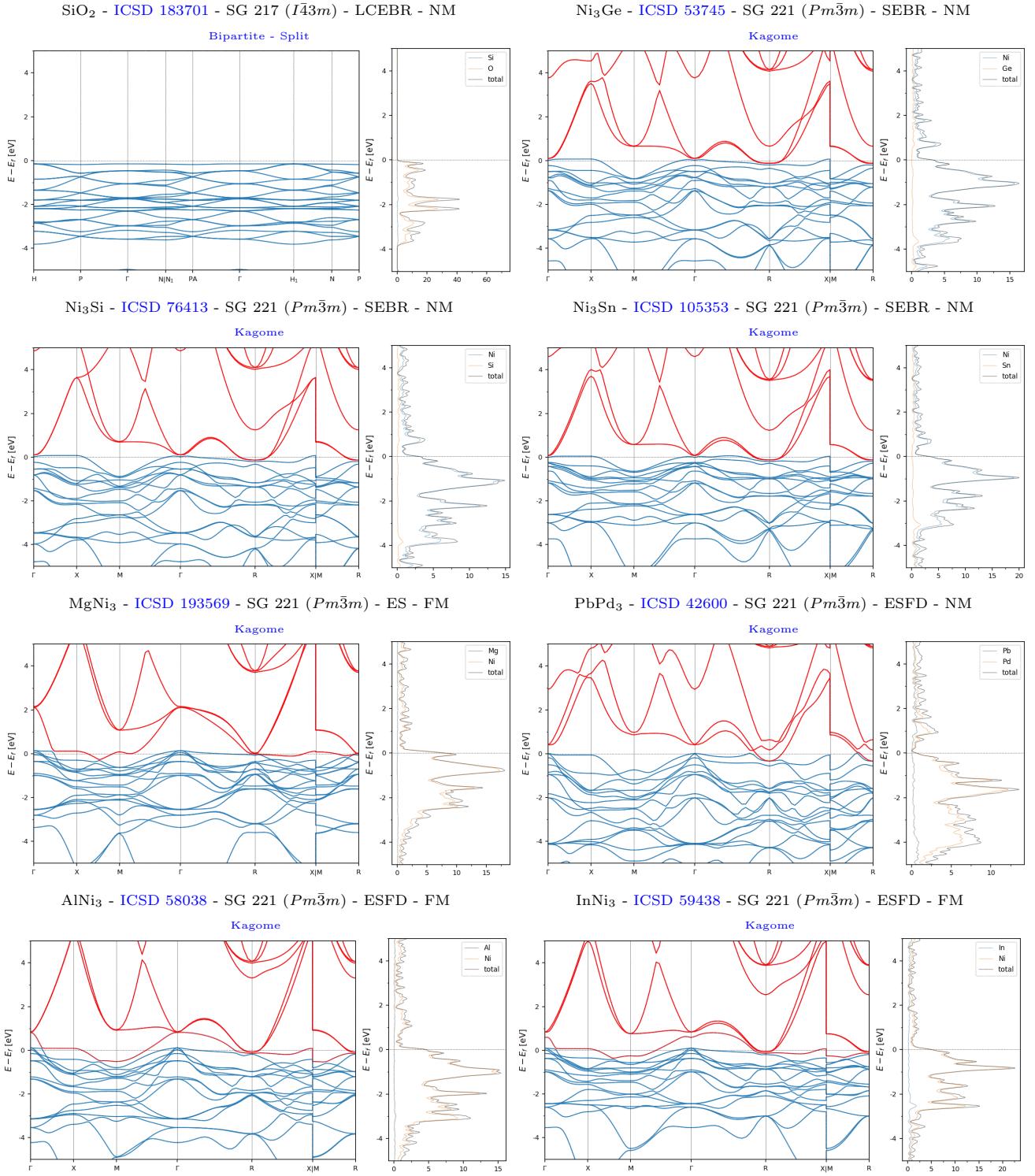


Figure 54. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 27/44)

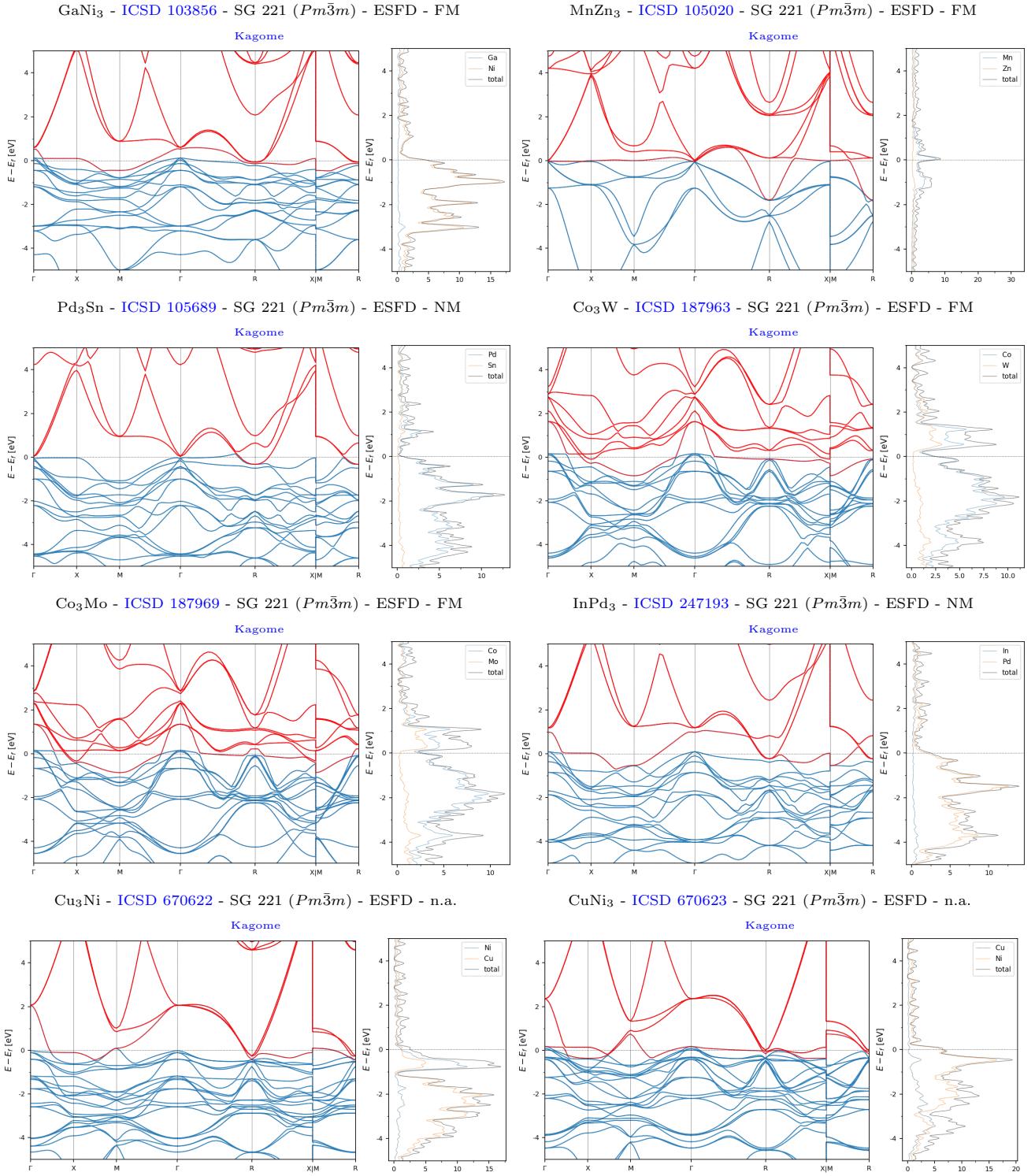


Figure 55. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 28/44)

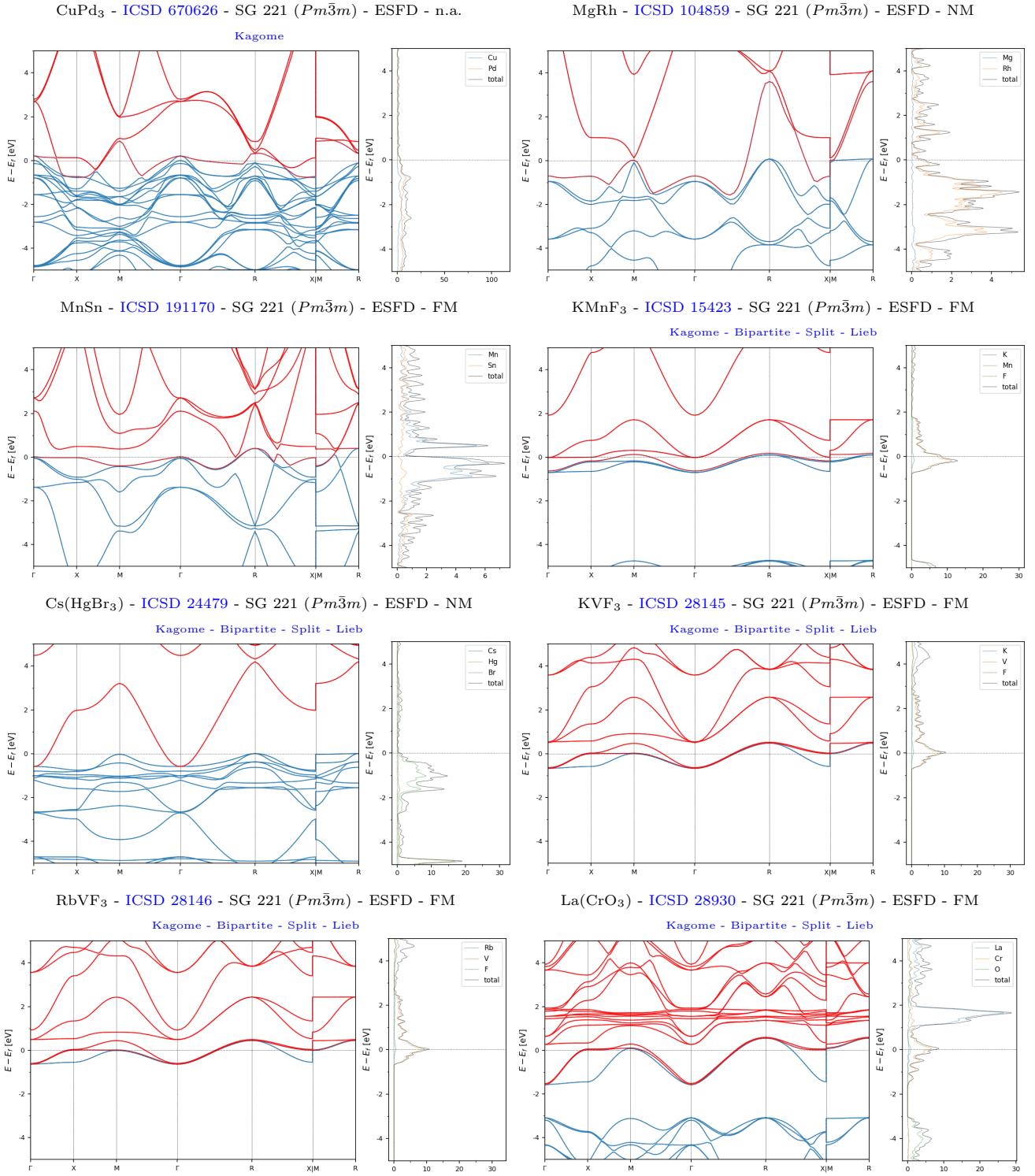


Figure 56. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 29/44)

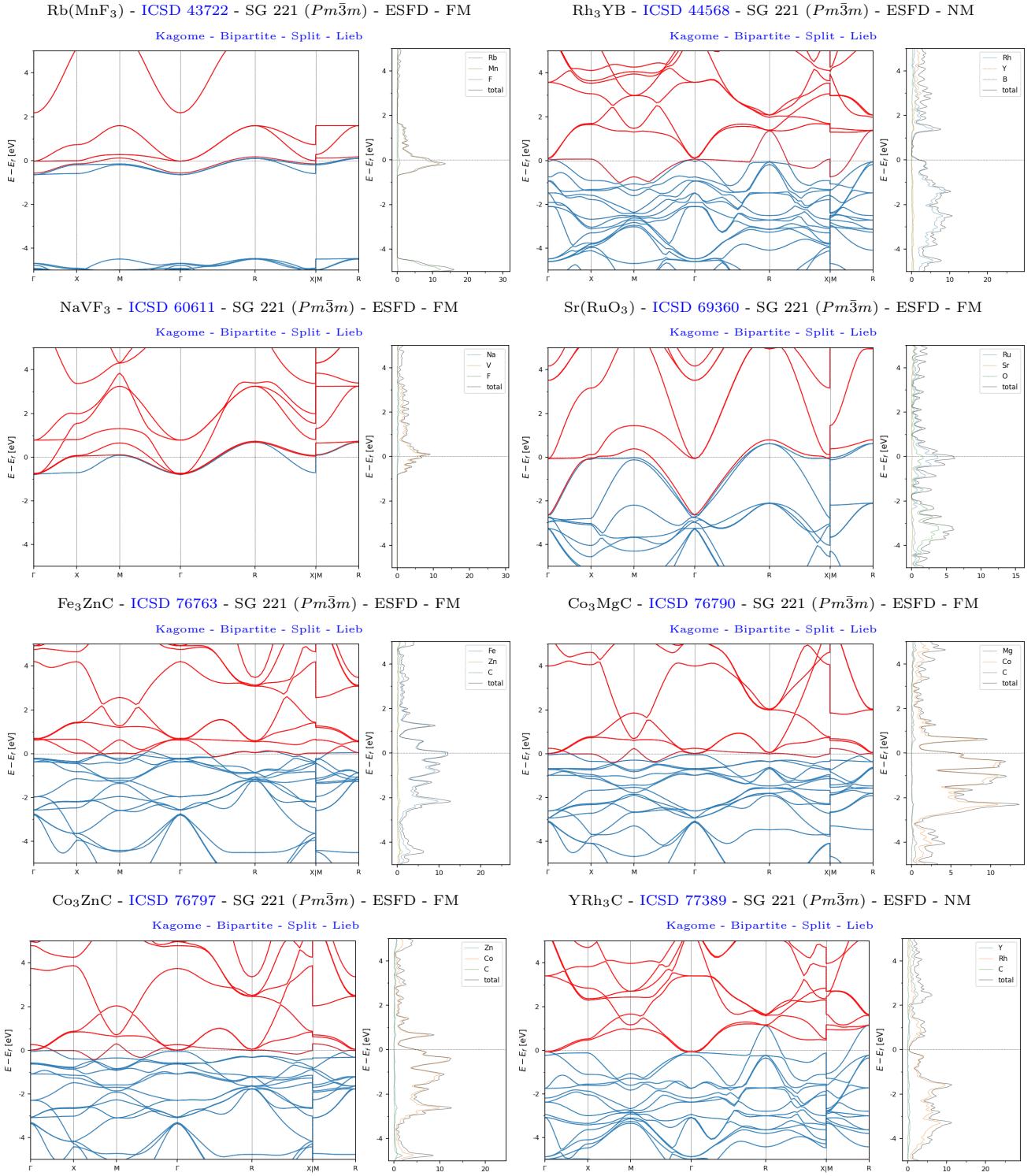


Figure 57. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 30/44)

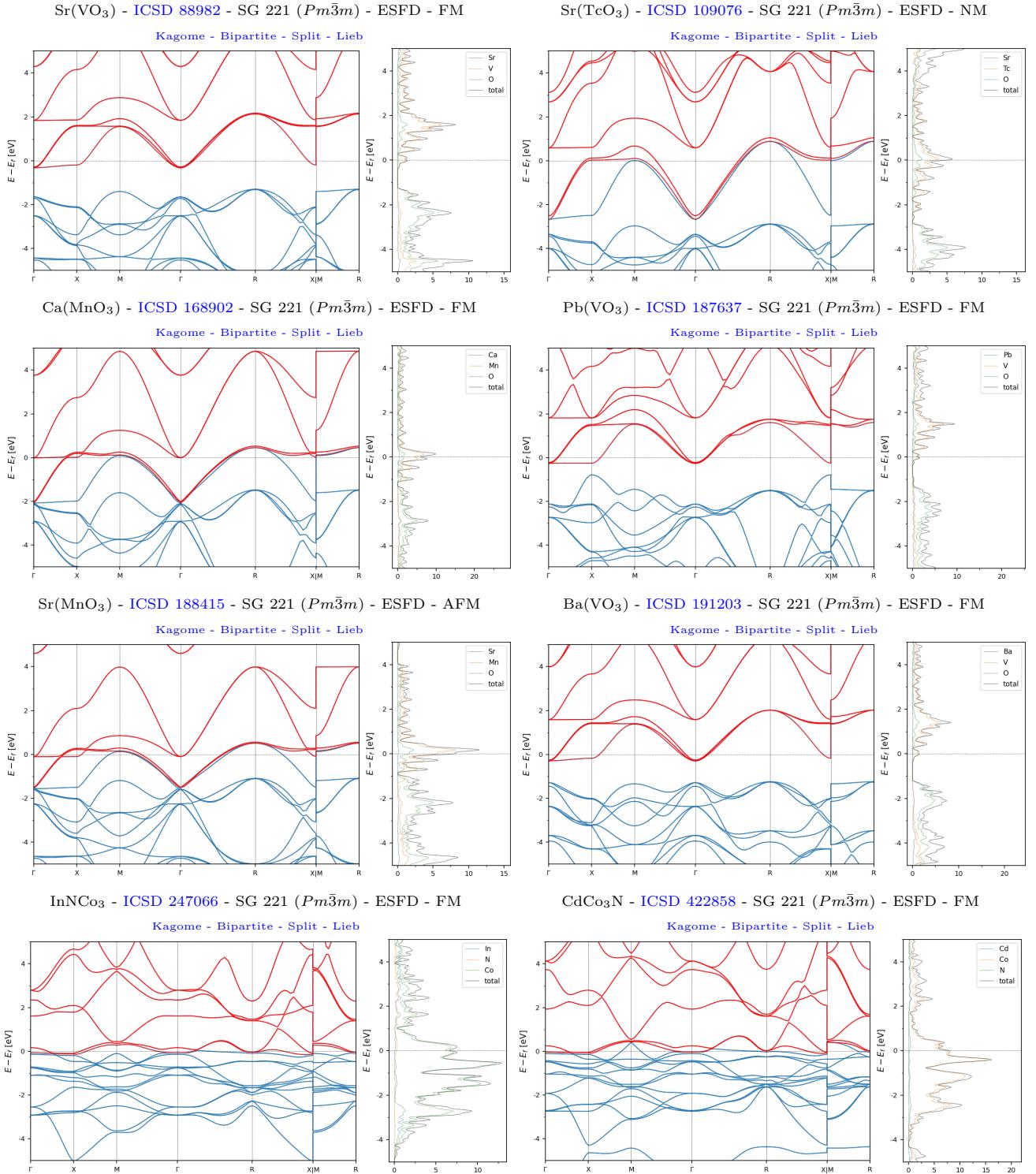


Figure 58. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 31/44)

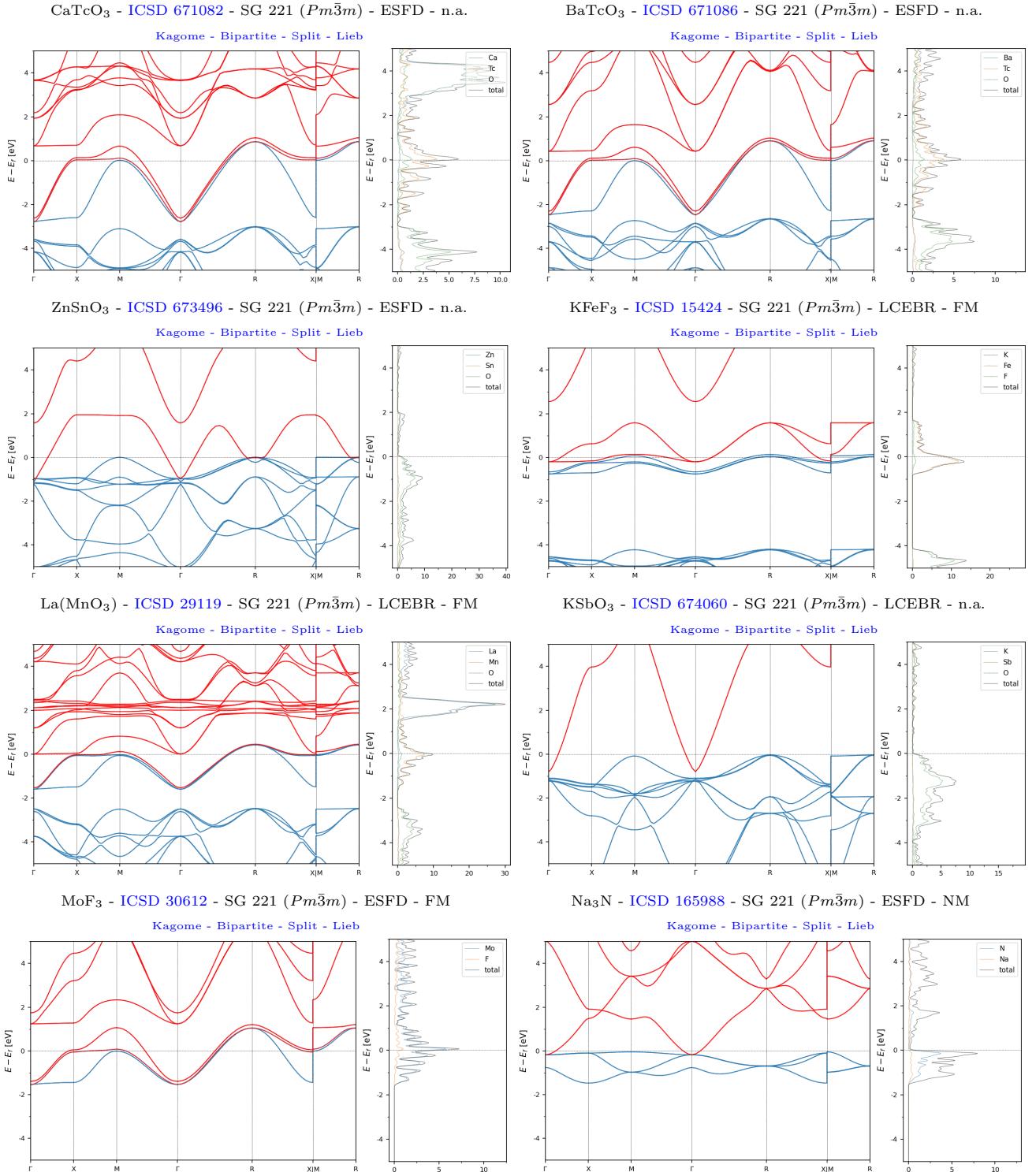


Figure 59. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 32/44)

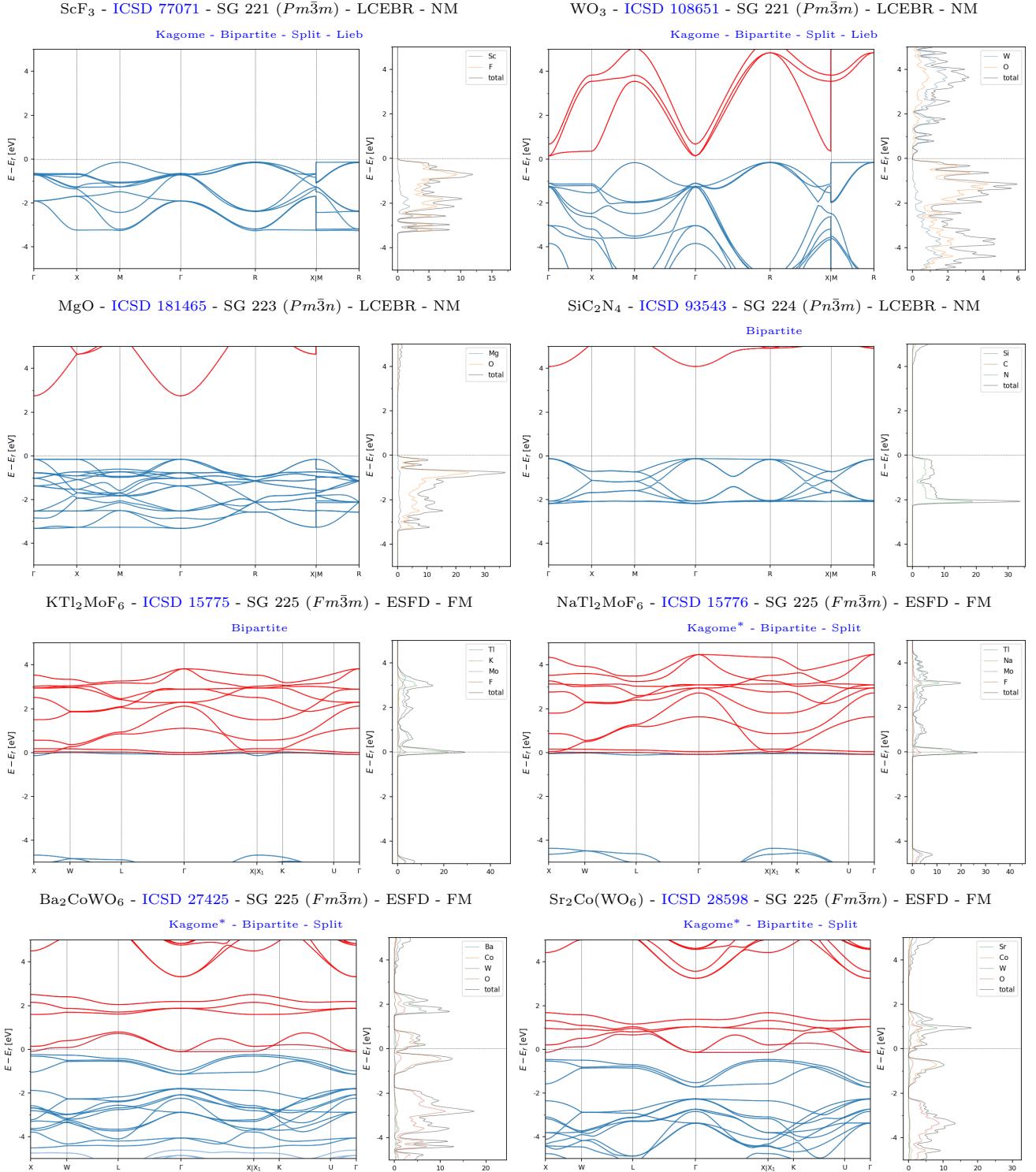


Figure 60. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 33/44)

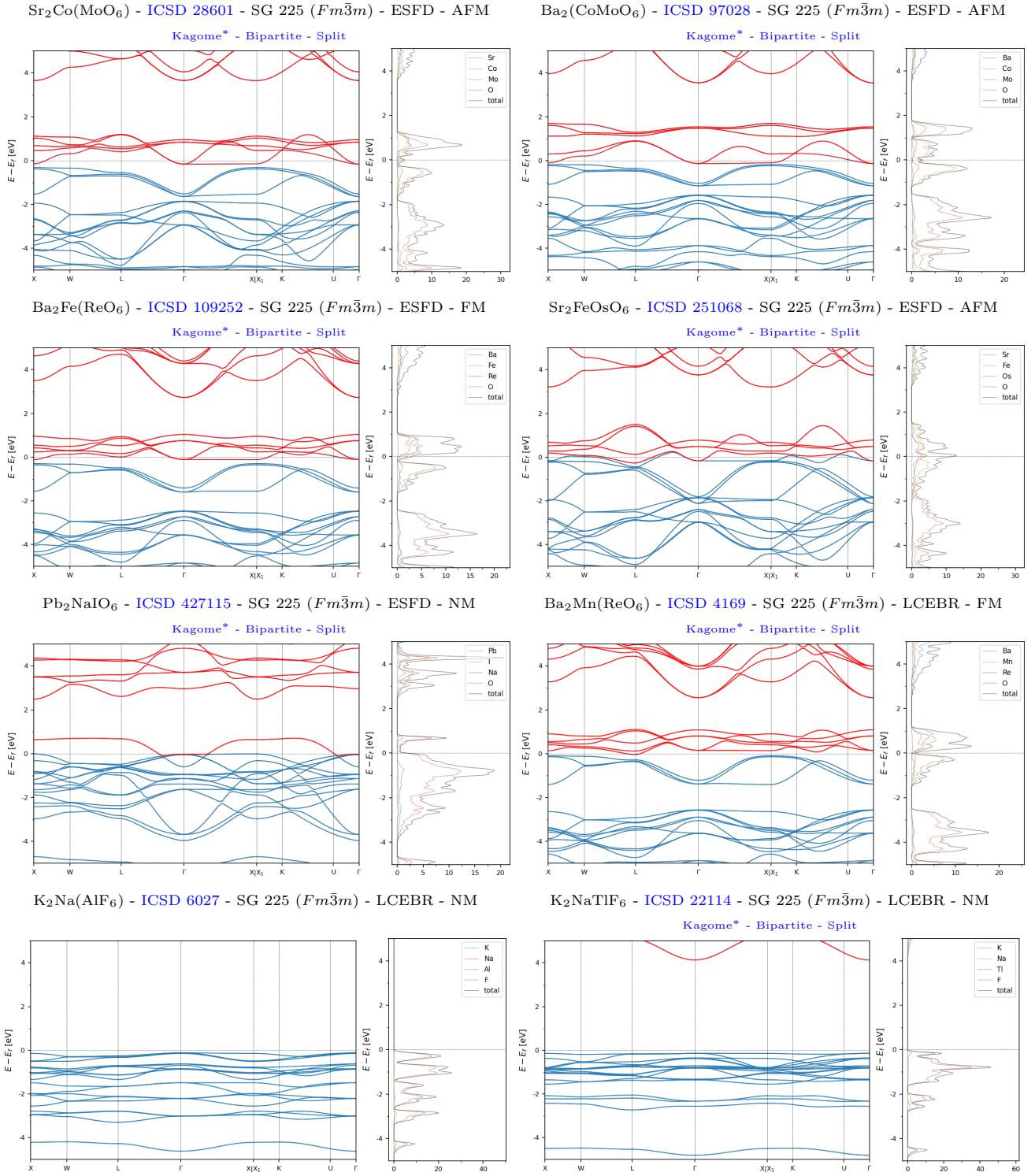


Figure 61. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 34/44)

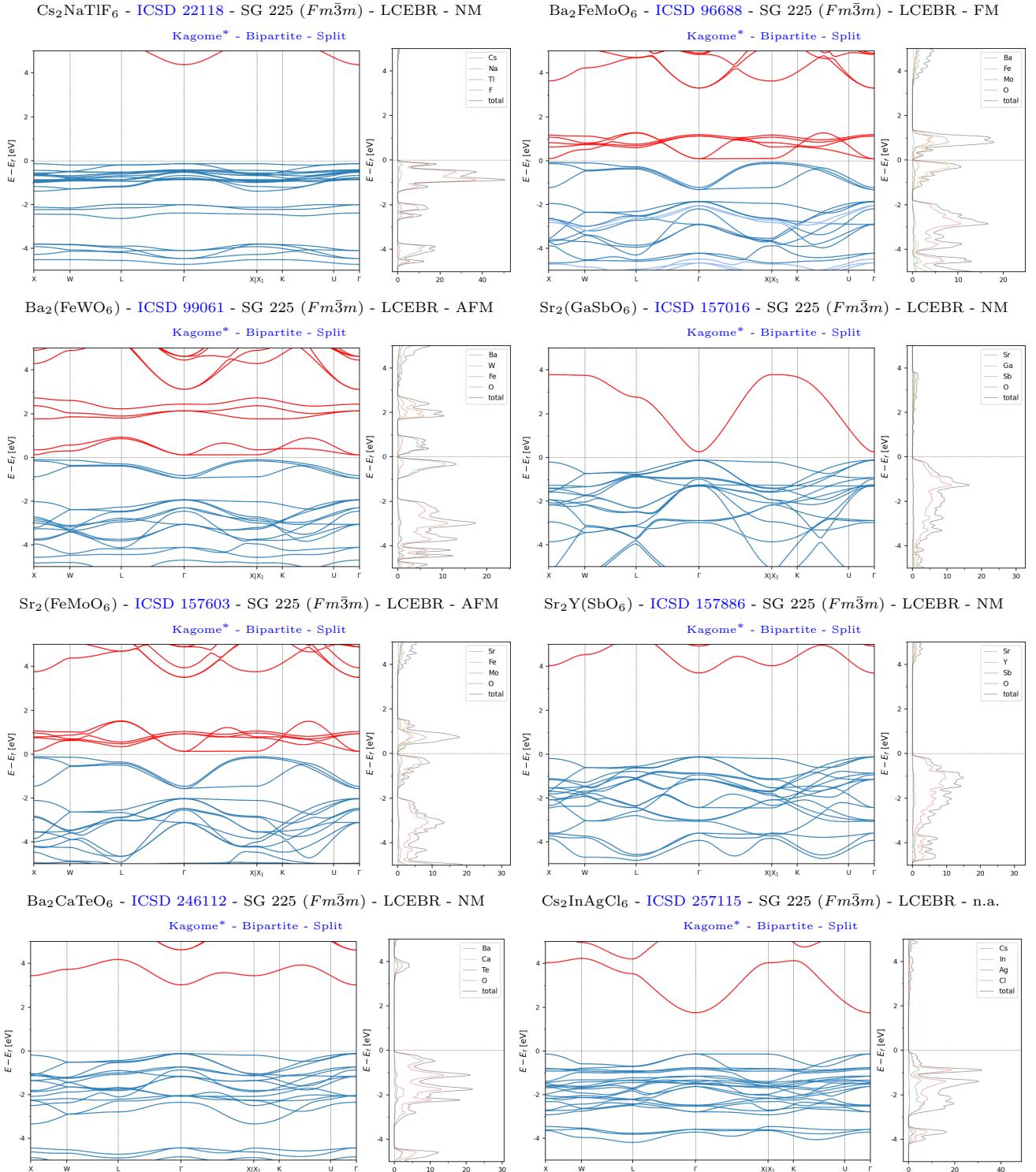


Figure 62. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 35/44)

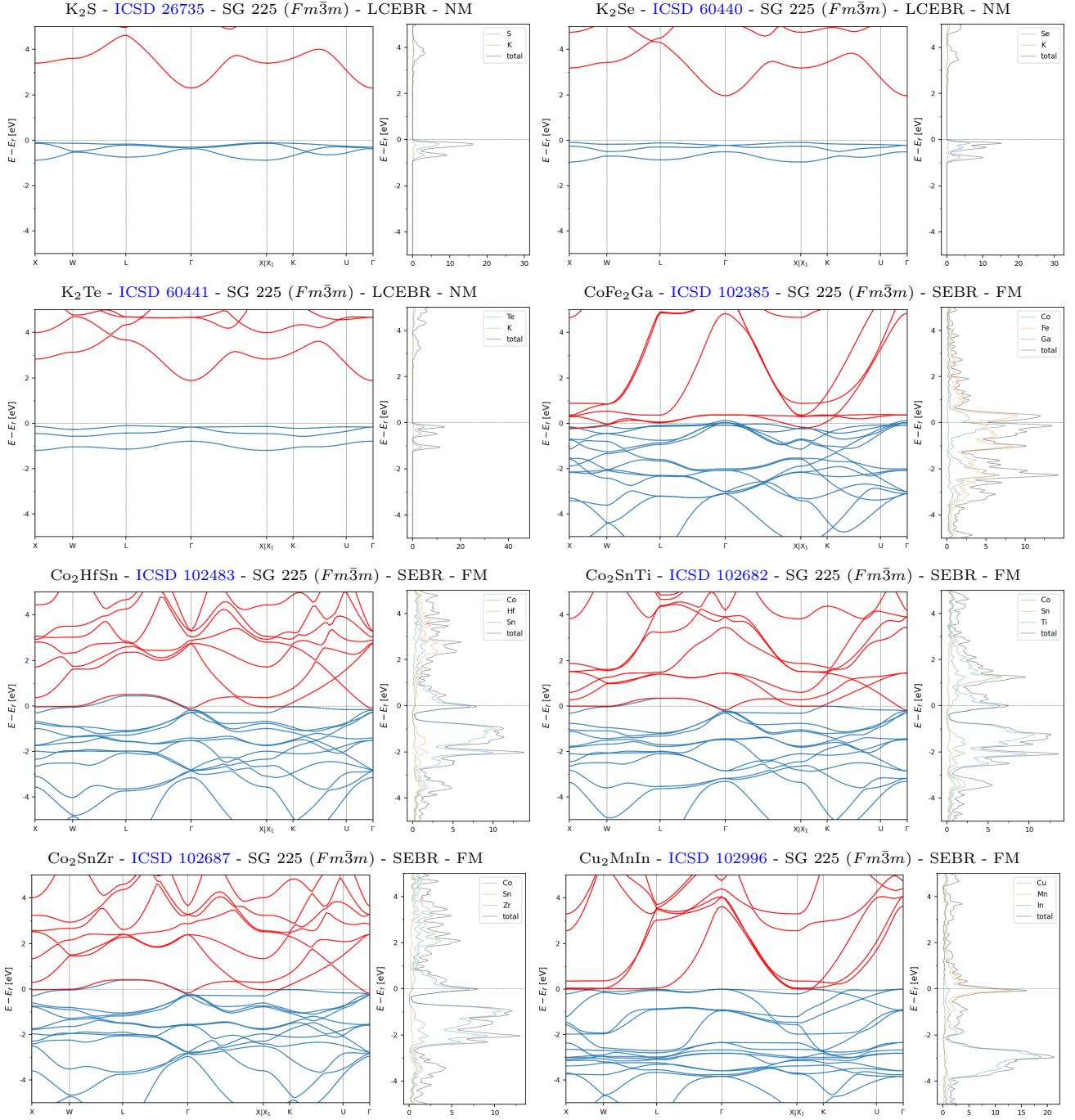


Figure 63. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 36/44)

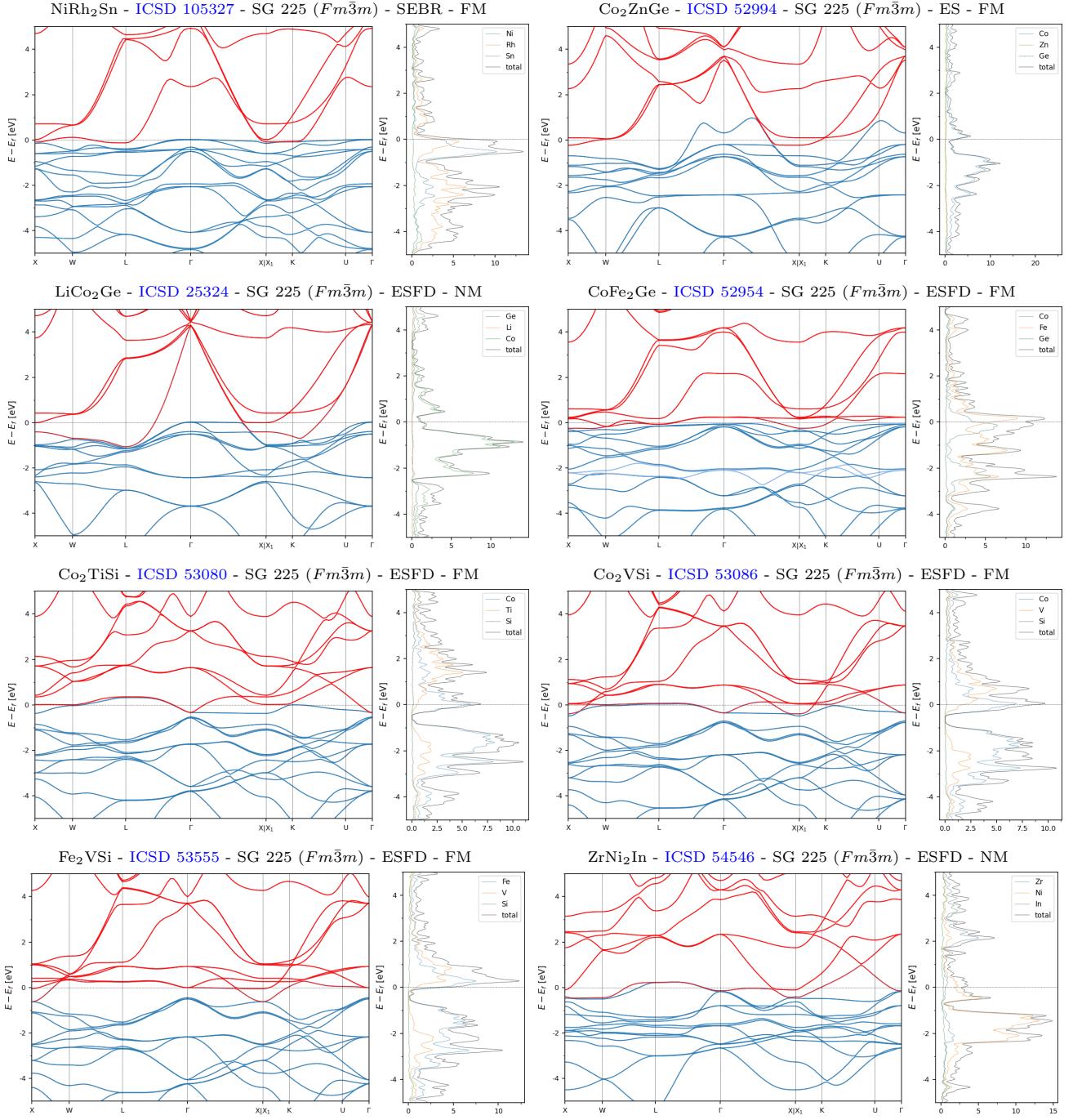


Figure 64. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 37/44)

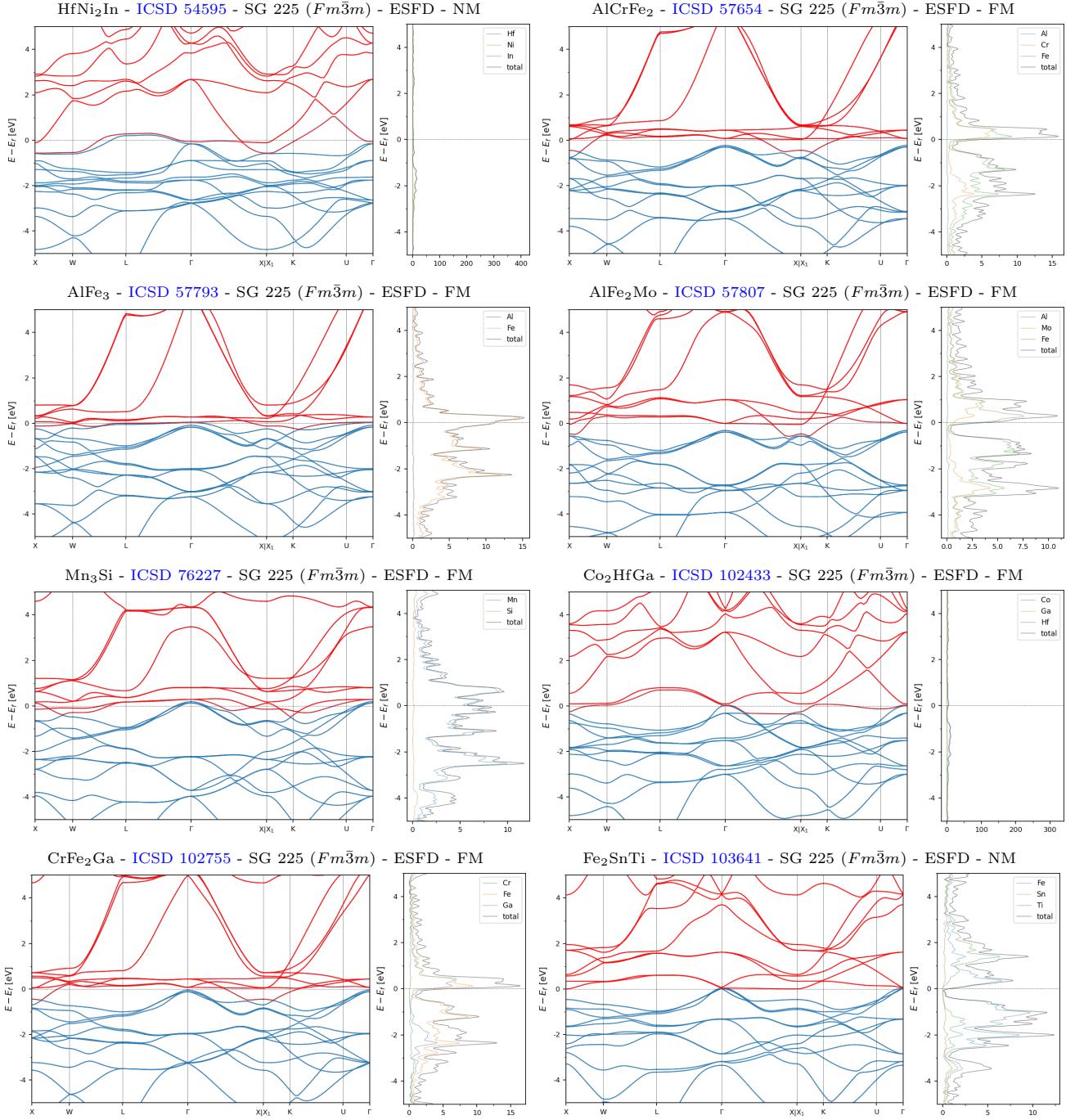


Figure 65. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 38/44)

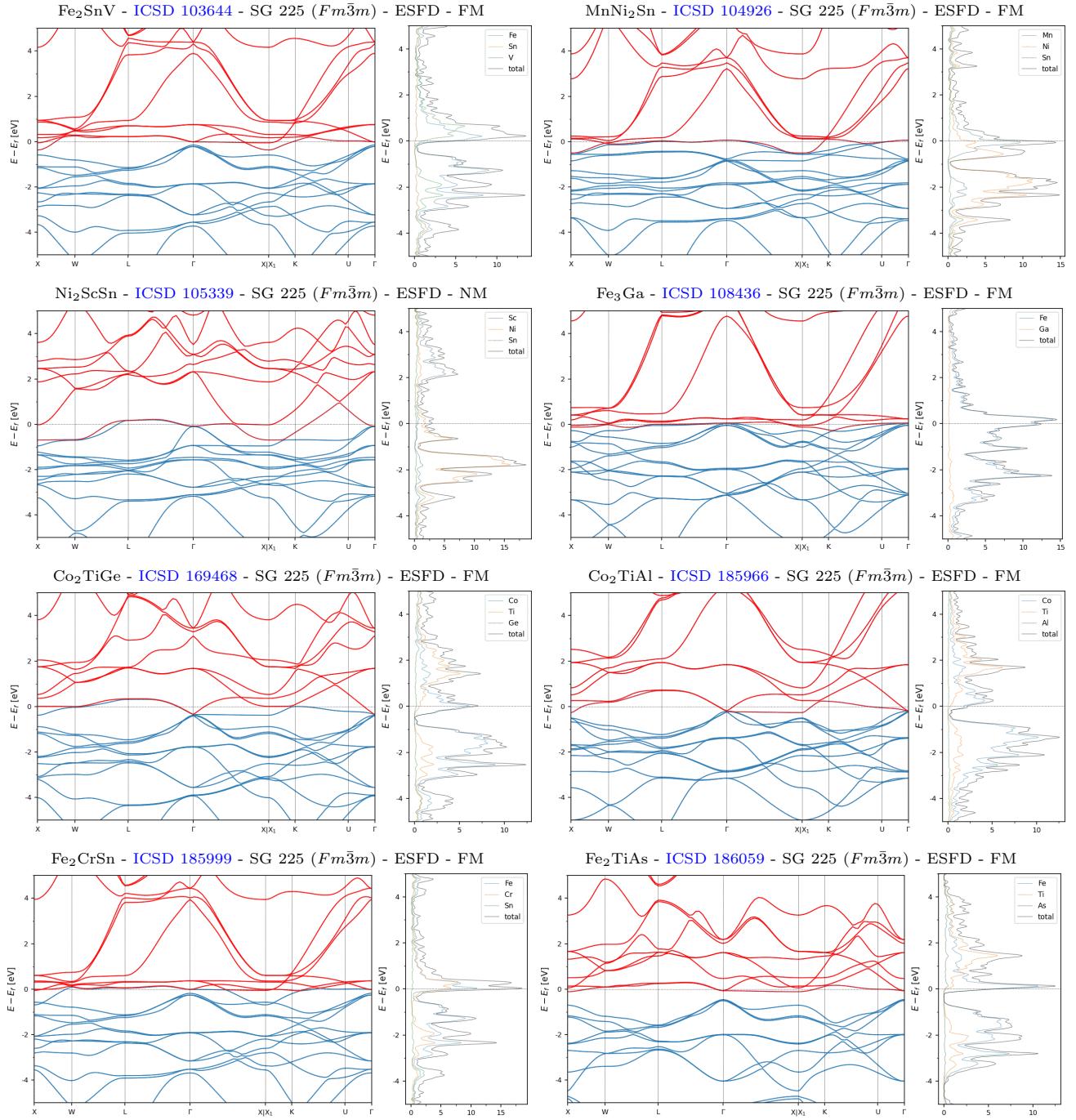


Figure 66. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 39/44)

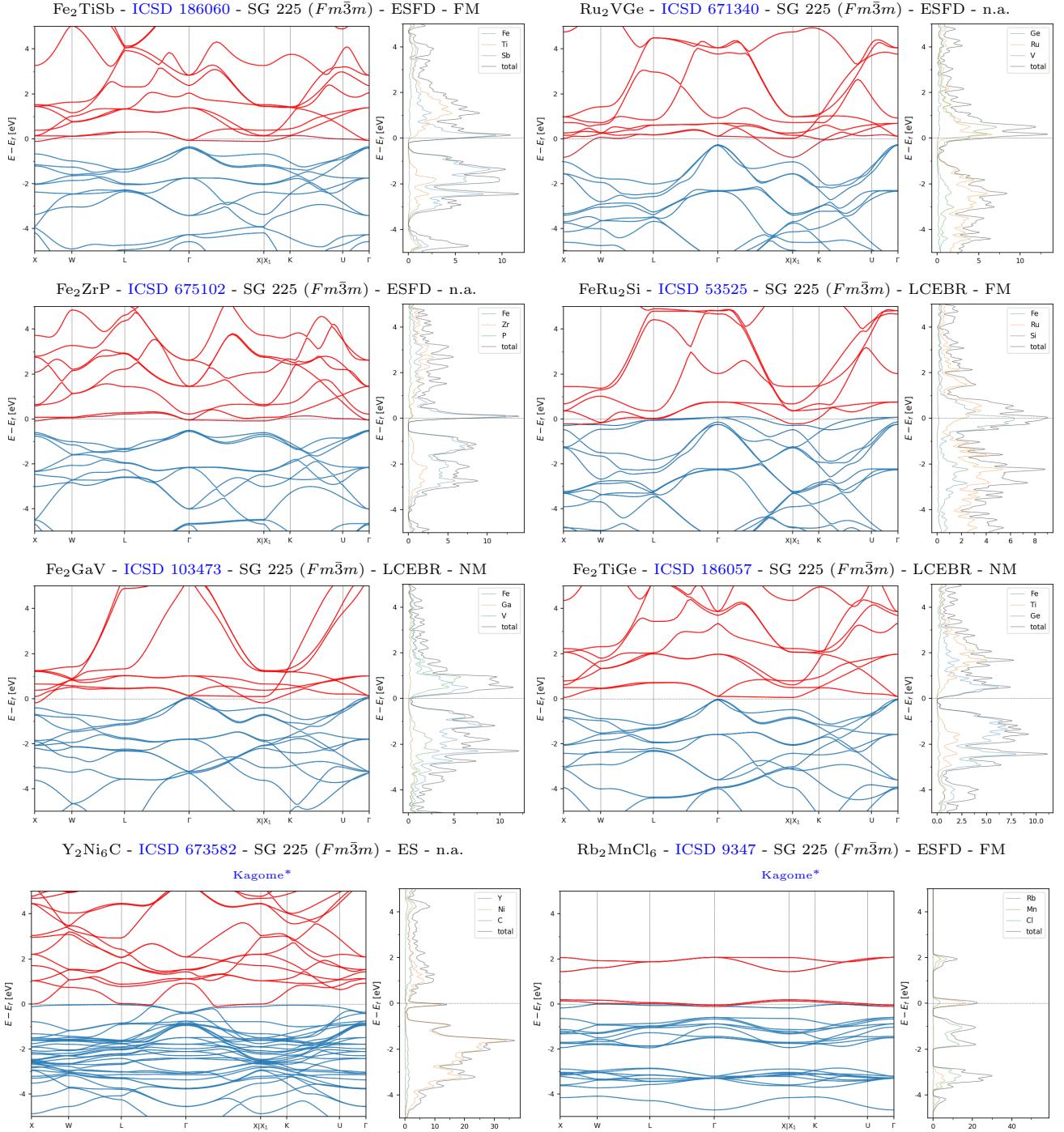


Figure 67. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 40/44)

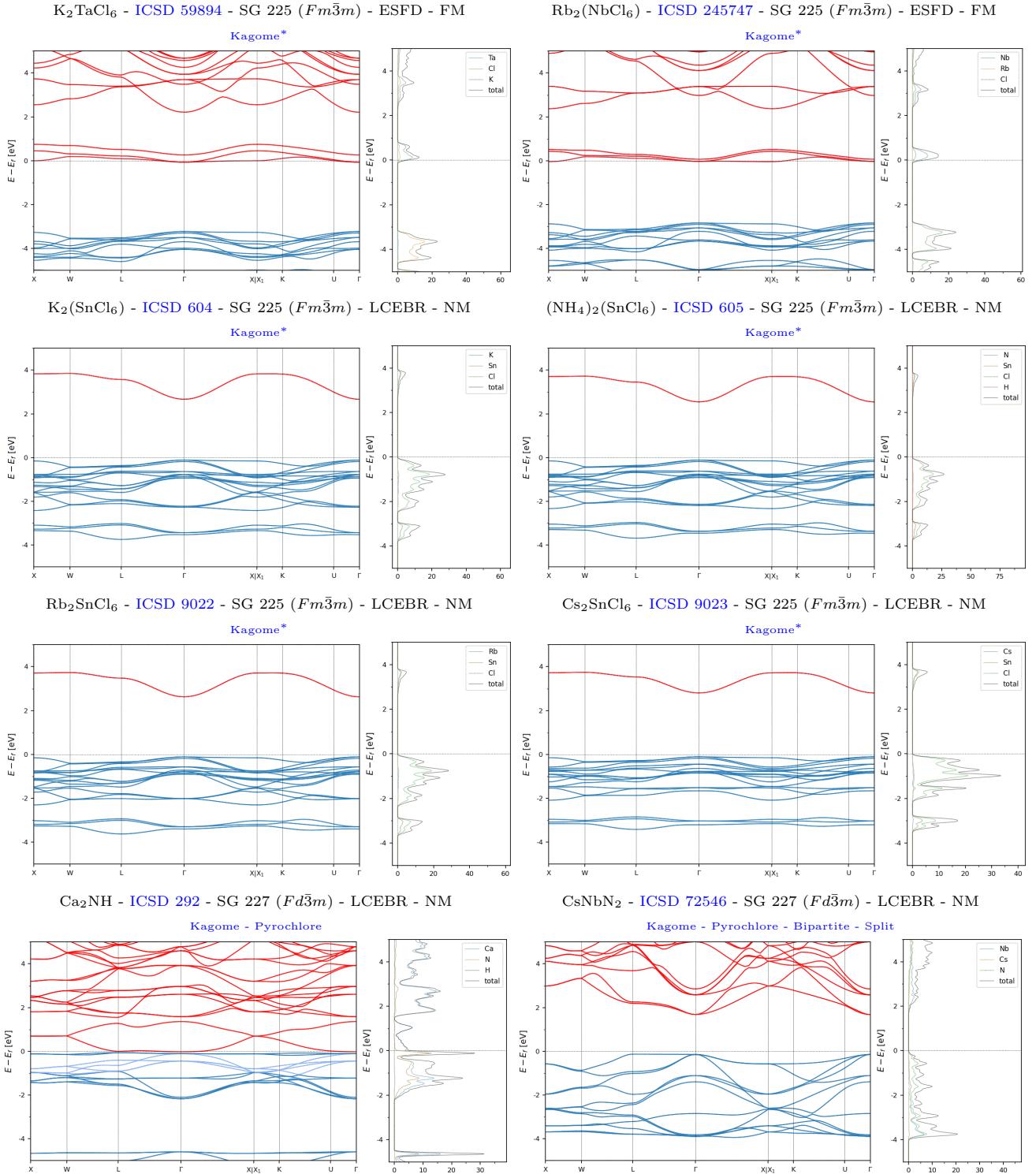


Figure 68. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 41/44)

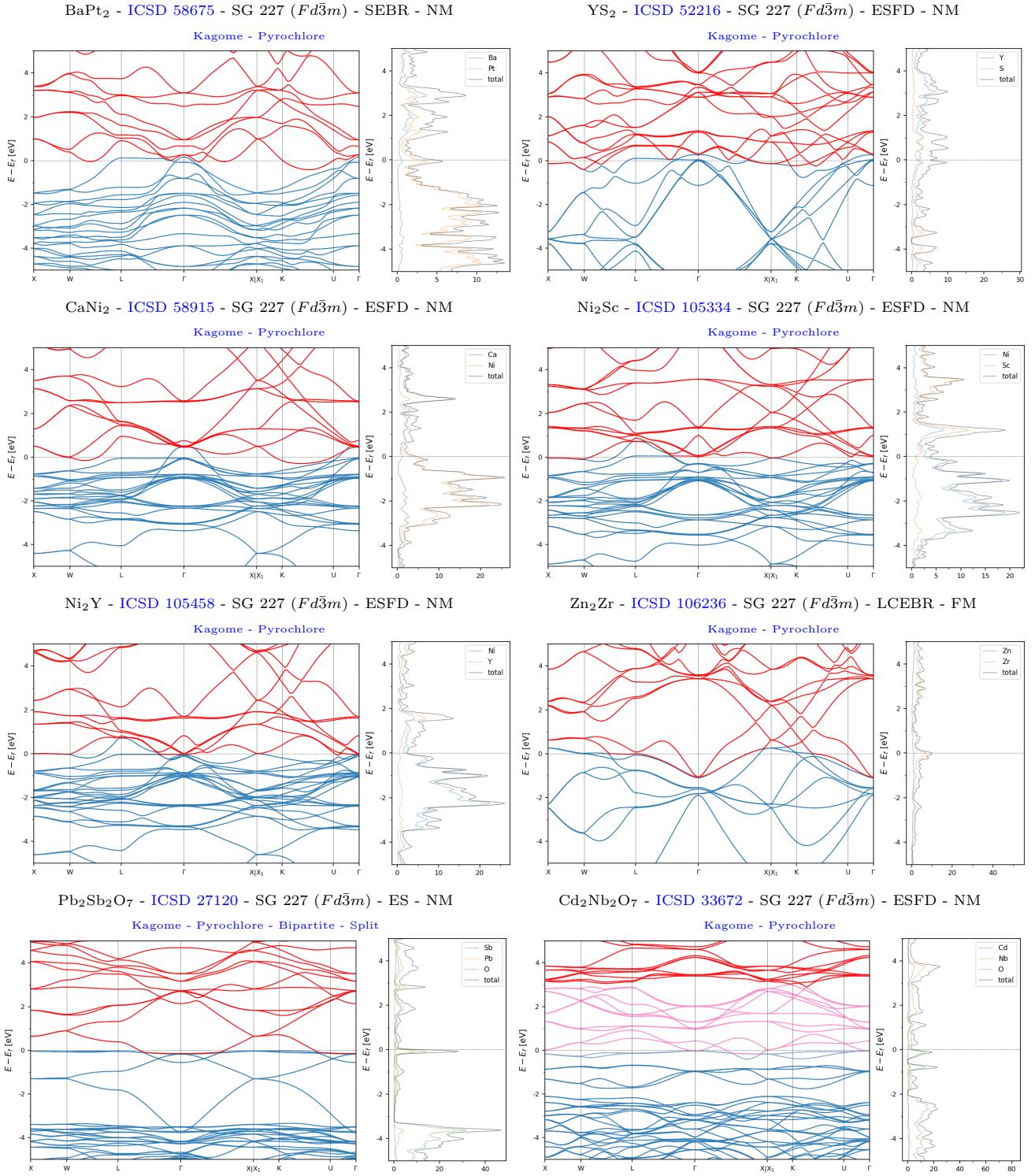


Figure 69. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 42/44)

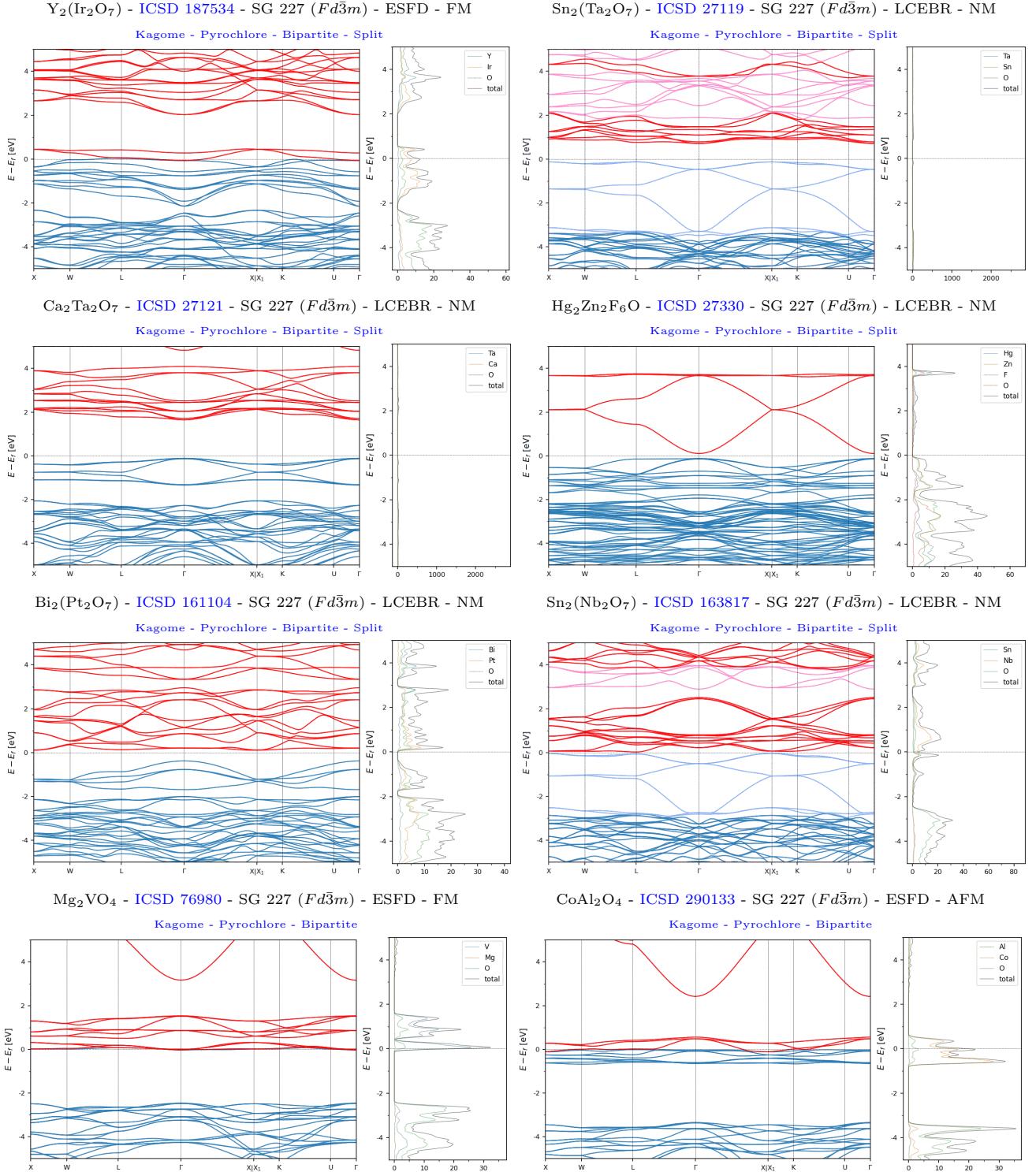


Figure 70. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 43/44)

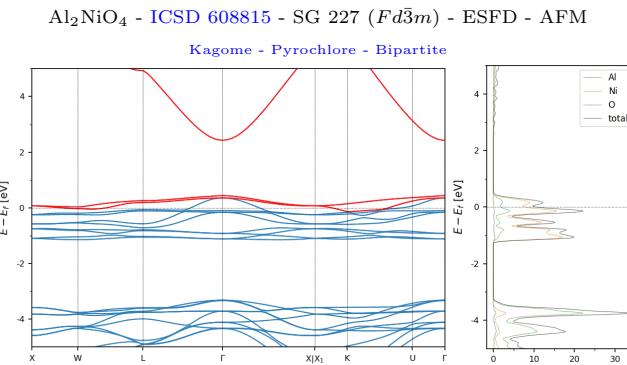


Figure 71. Band structure and density of states for materials with the most remarkable flat-band features near the Fermi energy. (part 44/44)