

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 6300

Bond precision: C-C = 0.0048 A

Wavelength=0.71073

Cell: a=13.0697(2) b=13.5755(3) c=18.2169(3)
 alpha=87.206(1) beta=77.527(1) gamma=64.003(1)
Temperature: 100 K

	Calculated	Reported
Volume	2832.69(9)	2832.69(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C59 H50 Mo N2 O3 Si3, C7	C59 H50 Mo N2 O3 Si3, C7 H8
Sum formula	C66 H50 Mo N2 O3 Si3	C66 H58 MO N2 O3 SI3
Mr	1099.29	1107.35
Dx,g cm-3	1.289	1.298
Z	2	2
Mu (mm-1)	0.343	0.343
F000	1136.0	1152.0
F000'	1133.41	
h,k,lmax	19,20,26	19,19,26
Nref	18999	18892
Tmin,Tmax	0.952,0.966	0.869,0.943
Tmin'	0.927	

Correction method= GAUSSIAN

Data completeness= 0.994

Theta(max)= 31.590

R(reflections)= 0.0586(14883)

wR2(reflections)= 0.1565(18892)

S = 1.048

Npar= 677

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT773_ALERT_2_A	Suspect	C-C Bond in CIF:	C60	--	C63	..	1.85 Ang.
PLAT773_ALERT_2_A	Suspect	C-C Bond in CIF:	C61	--	C62	..	1.76 Ang.
PLAT773_ALERT_2_A	Suspect	C-C Bond in CIF:	C62	--	C64	..	1.70 Ang.
PLAT773_ALERT_2_A	Suspect	C-C Bond in CIF:	C62	--	C61	..	1.76 Ang.
PLAT773_ALERT_2_A	Suspect	C-C Bond in CIF:	C67	--	C68	..	1.74 Ang.

PLAT773_ALERT_2_A Suspect C-C Bond in CIF: C68 -- C75 .. 2.00 Ang.
PLAT773_ALERT_2_A Suspect C-C Bond in CIF: C71 -- C72 .. 1.99 Ang.

Alert level B

DIFMX01_ALERT_2_B The maximum difference density is > 0.1*ZMAX*1.00
 _refine_diff_density_max given = 4.420
 Test value = 4.200

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density. 4.42 eA-3
PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 4.20 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for C21 -- C22 .. 17.90 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for C22 -- C23 .. 9.46 su

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
 The relevant atom site should be identified.

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.71
PLAT213_ALERT_2_C Atom C22 has ADP max/min Ratio 3.10 prola
PLAT222_ALERT_3_C Large Non-Solvent H Ueq(max)/Ueq(min) ... 3.59 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C20 -- C21 .. 6.86 su
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C22
PLAT332_ALERT_2_C Large Phenyl C-C Range C18 -C23 0.17 Ang.
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for C74
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for C66

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and _chemical_formula_moiety. This is
 usually due to the moiety formula being in the wrong format.
 Atom count from _chemical_formula_sum: C66 H58 Mo1 N2 O3 Si3
 Atom count from _chemical_formula_moiety:C66 H58 N2 O4 Si3

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and the formula from the _atom_site* data.
 Atom count from _chemical_formula_sum:C66 H58 Mo1 N2 O3 Si3
 Atom count from the _atom_site data: C66 H50 Mo1 N2 O3 Si3

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
 From the CIF: _cell_formula_units_Z 2
 From the CIF: _chemical_formula_sum C66 H58 Mo N2 O3 Si3
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	132.00	132.00	0.00
H	116.00	100.00	16.00
Mo	2.00	2.00	0.00
N	4.00	4.00	0.00
O	6.00	6.00	0.00
Si	6.00	6.00	0.00

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT unusually Large. 5.16
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal (x 10000) 100 Deg.
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3
PLAT302_ALERT_4_G Note Anion/Solvent Disorder 42.00 Perc.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.18 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF 25.00 Deg.
 C64 -C60 -C61 1.555 1.555 1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF 29.70 Deg.
 C61 -C60 -C63 1.555 1.555 1.555

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	27.00 Deg.
C63 -C61 -C66	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	29.60 Deg.
C64 -C61 -C60	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	28.40 Deg.
C62 -C61 -C65	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	24.50 Deg.
C66 -C61 -C62	1.555	1.555	2.566	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	20.00 Deg.
C66 -C62 -C63	2.566	1.555	2.566	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	26.70 Deg.
C61 -C62 -C64	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	31.50 Deg.
C63 -C62 -C61	2.566	1.555	2.566	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	21.30 Deg.
C66 -C63 -C62	1.555	1.555	2.566	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	24.40 Deg.
C61 -C63 -C64	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	28.60 Deg.
C64 -C63 -C60	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	30.00 Deg.
C61 -C64 -C63	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	24.80 Deg.
C65 -C64 -C62	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	21.60 Deg.
C62 -C65 -C66	1.555	1.555	2.566	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	30.30 Deg.
C64 -C65 -C61	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	20.90 Deg.
C62 -C66 -C65	2.566	1.555	2.566	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	36.20 Deg.
C63 -C66 -C61	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	41.00 Deg.
C72 -C67 -C71	1.555	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	31.20 Deg.
C73 -C67 -C71	2.666	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	10.80 Deg.
C69 -C67 -C68	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	14.90 Deg.
C69 -C68 -C74	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	12.60 Deg.
C71 -C68 -C73	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	28.30 Deg.
C69 -C68 -C67	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	30.80 Deg.
C72 -C68 -C67	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	33.00 Deg.
C74 -C68 -C67	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	34.90 Deg.
C71 -C68 -C75	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	32.10 Deg.
C73 -C68 -C75	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	39.80 Deg.
C67 -C69 -C72	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	9.20 Deg.
C68 -C69 -C71	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	37.50 Deg.
C71 -C69 -C72	1.555	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	41.80 Deg.
C67 -C70 -C74	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	33.00 Deg.
C67 -C70 -C72	1.555	1.555	1.555	

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	27.00 Deg.
C73 -C70 -C71	2.666	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	37.00 Deg.
C72 -C70 -C71	1.555	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	5.10 Deg.
C68 -C71 -C69	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	35.60 Deg.
C72 -C71 -C67	2.666	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	42.00 Deg.
C73 -C71 -C70	1.555	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	32.30 Deg.
C67 -C71 -C70	2.666	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	40.60 Deg.
C72 -C71 -C72	2.666	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	41.20 Deg.
C69 -C71 -C72	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	44.70 Deg.
C71 -C72 -C68	2.666	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	32.90 Deg.
C71 -C72 -C73	2.666	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	32.70 Deg.
C67 -C72 -C70	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	19.70 Deg.
C69 -C72 -C68	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	34.20 Deg.
C67 -C72 -C74	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	41.40 Deg.
C69 -C72 -C74	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	16.40 Deg.
C68 -C72 -C69	2.666	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	28.00 Deg.
C72 -C72 -C71	2.666	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	26.70 Deg.
C68 -C72 -C71	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	43.20 Deg.
C71 -C73 -C72	1.555	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	36.60 Deg.
C70 -C73 -C67	2.666	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	35.70 Deg.
C72 -C73 -C67	2.666	1.555	2.666	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	14.80 Deg.
C71 -C73 -C68	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	38.30 Deg.
C67 -C74 -C70	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	7.40 Deg.
C69 -C74 -C68	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	31.80 Deg.
C67 -C74 -C72	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	36.50 Deg.
C73 -C75 -C71	1.555	1.555	1.555	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle in CIF	23.60 Deg.
C71 -C75 -C68	1.555	1.555	1.555	

7 **ALERT level A** = In general: serious problem

5 **ALERT level B** = Potentially serious problem

11 **ALERT level C** = Check and explain

68 **ALERT level G** = General alerts; check

7 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data

19 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
64 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Publication of your CIF in IUCr Journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr Journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C or E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 09/04/2009; check.def file version of 08/04/2009

Datablock 6300 - ellipsoid plot

