

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1

Bond precision:	C-C = 0.0150 A	Wavelength=0.71073
Cell:	a=14.3769(4)	b=18.7994(5) c=22.2801(6)
	alpha=104.569(1)	beta=106.535(1) gamma=107.314(1)
Temperature:	296 K	
	Calculated	Reported
Volume	5125.8(3)	5125.8(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Mo12 O40 P, 4(C18 H13 N2 O2), C18 H12 N2 O2, 5(O)	Mo12 O40 P, 4(C18 H13 N2 O2), C18 H12 N2 O2, 5(O)
Sum formula	C90 H64 Mo12 N10 O55 P	C90 H74 Mo12 N10 O55 P
Mr	3347.76	3357.84
Dx, g cm-3	2.169	2.176
Z	2	2
Mu (mm-1)	1.540	1.540
F000	3266.0	3286.0
F000'	3226.36	
h,k,lmax	17,23,27	17,23,27
Nref	20226	20180
Tmin,Tmax		
Tmin'		
Correction method=	Not given	
Data completeness=	0.998	Theta(max)= 26.026
R(reflections)=	0.0519(16254)	wR2(reflections)=
		0.1870(20180)
S =	1.011	Npar= 1514

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 B

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	P1	--O17	.	8.5 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	P1	--O26	.	8.5 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	P1	--O30	.	10.5 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	P1	--O44	.	10.5 s.u.
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)				01W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)				02W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)				03W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)				04W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)				05W Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O1W	..03W	.	2.58 Ang.
			x,y,z =		1_555 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O3W	..039	.	2.72 Ang.
			x,y,z =		1_555 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O4W	..011	.	2.83 Ang.
			1-x,1-y,2-z =		2_667 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O31	..031	.	2.79 Ang.
			1-x,1-y,1-z =		2_666 Check

Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ			Please Check
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight	Differ by ..			10.08 Check
PLAT053_ALERT_1_C	Minimum Crystal Dimension	Missing (or Error) ...			Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension	Missing (or Error) ...			Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension	Missing (or Error) ...			Please Check
PLAT068_ALERT_1_C	Reported F000	Differs from Calcd (or Missing)...			Please Check
PLAT234_ALERT_4_C	Large Hirshfeld Difference	N2	--C21	.	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C43	--C69	.	0.22 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C45	--C89	.	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C64	--C69	.	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C69	--C79	.	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C7	--C57	.	0.19 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of				C38 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of				C85 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of				C58 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of				C77 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of				C17 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of				P1 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of				C35 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of				C1 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O1W			0.230 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O2W			0.155 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O3W			0.164 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O4W			0.124 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O5W			0.115 Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds				0.01502 Ang.
PLAT368_ALERT_2_C	Short C(sp2)-C(sp2) Bond	C5	- C43	.	1.23 Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact	O4W	..035	.	2.88 Ang.
			-1+x,y,z =		1_455 Check
PLAT430_ALERT_2_C	Short Inter D...A Contact	O5W	..022	.	2.89 Ang.

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: C90 H74 Mo12 N10 O55 P1
 Atom count from _chemical_formula_moiety: C90 H64 Mo12 N10 O55 P1

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: C90 H74 Mo12 N10 O55 P1
 Atom count from the _atom_site data: C90 H64 Mo12 N10 O55 P1

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 C90 H74 Mo12 N10 O55 P
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	180.00	180.00	0.00
H	148.00	128.00	20.00
Mo	24.00	24.00	0.00
N	20.00	20.00	0.00
O	110.00	110.00	0.00
P	2.00	2.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 8 Note

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 10 Report

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 21.01 Why ?

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree

PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 5 Report

PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 6 Report

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo6 --O44 . 5.5 s.u.

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo10 --O44 . 5.5 s.u.

PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C5 -C43 0.23 Ang.

PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C7 -C57 0.18 Ang.

PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C7 -C83 0.19 Ang.

PLAT432_ALERT_2_G Short Inter X...Y Contact O15 ..C70 . 3.01 Ang.

1-x,1-y,2-z = 2_667 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact O19 ..C28 . 2.99 Ang.

1-x,1-y,1-z = 2_666 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact O34 ..C47 . 2.96 Ang.

1+x,1+y,z = 1_665 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact O43 ..C40 . 3.00 Ang.

x,1+y,z = 1_565 Check

PLAT794_ALERT_5_G Tentative Bond Valency for Mo1 (VI) . 6.05 Info

PLAT794_ALERT_5_G Tentative Bond Valency for Mo2 (VI) . 5.64 Info

PLAT794_ALERT_5_G Tentative Bond Valency for Mo3 (VI) . 5.95 Info

PLAT794_ALERT_5_G Tentative Bond Valency for Mo4 (VI) . 5.69 Info

PLAT794_ALERT_5_G Tentative Bond Valency for Mo5 (VI) . 5.72 Info

PLAT794_ALERT_5_G Tentative Bond Valency for Mo6 (VI) . 6.04 Info

PLAT794_ALERT_5_G Tentative Bond Valency for Mo7 (VI) . 5.99 Info

PLAT794_ALERT_5_G Tentative Bond Valency for Mo8 (VI) . 5.60 Info

PLAT794_ALERT_5_G Tentative Bond Valency for Mo9 (VI) . 5.77 Info

PLAT794_ALERT_5_G Tentative Bond Valency for Mo10 (VI) . 5.84 Info

PLAT794_ALERT_5_G	Tentative Bond Valency for Mo11	(VI)	.	5.72	Info	
PLAT794_ALERT_5_G	Tentative Bond Valency for Mo12	(V)	.	4.82	Info	
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				66	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 13 **ALERT level B** = A potentially serious problem, consider carefully
 29 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 34 **ALERT level G** = General information/check it is not something unexpected

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 43 ALERT type 2 Indicator that the structure model may be wrong or deficient
 2 ALERT type 3 Indicator that the structure quality may be low
 8 ALERT type 4 Improvement, methodology, query or suggestion
 13 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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* or *IUCrData*, 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 18/05/2022; check.def file version of 17/05/2022

