

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: I

Bond precision:	C-C = 0.0138 A	Wavelength=1.54184	
Cell:	a=19.44134(16)	b=17.47231(13)	c=34.8842(2)
	alpha=90	beta=101.9624(7)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	11592.32(15)	11592.33(15)	
Space group	I 2/a	I 1 2/a 1	
Hall group	-I 2ya	-I 2ya	
Moiety formula	2(C21 H15 Ag Mo3 O6 P3), 2(C15.35 Al F34.05 O4), C5.60 H6.40, 2	2(Al C16 F36 O4), 0.5(C84 H60 Ag4 Mo12 O24 P12), C5.6 H6.4, 0.4	
Sum formula	C80 H37.20 Ag2 Al2 Cl0.80 F72 Mo6 O20 P6	C80 H37.20 Ag2 Al2 Cl0.80 F72 Mo6 O20 P6	
Mr	3745.82	3745.82	
Dx,g cm-3	2.146	2.146	
Z	4	4	
Mu (mm-1)	10.554	10.554	
F000	7203.2	7203.0	
F000'	7243.34		
h,k,lmax	23,20,41	22,20,41	
Nref	10327	10155	
Tmin,Tmax	0.179,0.232	0.229,0.406	
Tmin'	0.083		

Correction method= # Reported T Limits: Tmin=0.229 Tmax=0.406
AbsCorr = GAUSSIAN

Data completeness= 0.983 Theta(max)= 66.994

R(reflections)= 0.0577(8861) wR2(reflections)= 0.1711(10155)

S = 1.055 Npar= 1180

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 C**

PLAT077_ALERT_4_C	Unitcell contains non-integer number of atoms ..	Please Check
PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	8.75 Note
PLAT213_ALERT_2_C	Atom F2 has ADP max/min Ratio	3.5 prolat
PLAT215_ALERT_3_C	Disordered F50 has ADP max/min Ratio	3.1
PLAT234_ALERT_4_C	Large Hirshfeld Difference C1AA -- C11 ..	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F5 -- C43 ..	0.23 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F20 -- C50 ..	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F21 -- C50 ..	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F26 -- C52 ..	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F36 -- C56 ..	0.20 Ang.
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	C1AA Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	O11 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	Mo1 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	Mo2 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	All Check
PLAT330_ALERT_2_C	Large Average Phenyl C-C Dist. C600 -C601_d	1.42 Ang.
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0138 Ang.

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	140 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	12 Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1 Info
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
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.	67.36 Why ?
PLAT142_ALERT_4_G	su on b - Axis Small or Missing	0.00013 Ang.
PLAT143_ALERT_4_G	su on c - Axis Small or Missing	0.00020 Ang.
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	5 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	37 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	34 Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	1 Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	2 Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for F3 -- C42 ..	7.0 su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for F9 -- C44 ..	5.3 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mo4 -- P3 ..	5.2 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mo4 -- C16 ..	6.0 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mo4 -- C17 ..	5.8 su
PLAT300_ALERT_4_G	Atom Site Occupancy of >Mo4 is Constrained at	0.530 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <Mo3 is Constrained at	0.235 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <Mo5 is Constrained at	0.235 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >O5 is Constrained at	0.530 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >O106 is Constrained at	0.530 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <O6 is Constrained at	0.235 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <O105 is Constrained at	0.235 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <O205 is Constrained at	0.235 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <O206 is Constrained at	0.235 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C15 is Constrained at	0.530 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C16 is Constrained at	0.530 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C17 is Constrained at	0.530 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C18 is Constrained at	0.530 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C19 is Constrained at	0.530 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C20 is Constrained at	0.530 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of <C59	is Constrained at	0.400	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C60	is Constrained at	0.400	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C65	is Constrained at	0.350	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C66	is Constrained at	0.350	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C67	is Constrained at	0.350	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C68	is Constrained at	0.350	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C69	is Constrained at	0.470	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C70	is Constrained at	0.470	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C71	is Constrained at	0.470	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C72	is Constrained at	0.470	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C600	is Constrained at	0.800	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C601	is Constrained at	0.800	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C602	is Constrained at	0.800	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C603	is Constrained at	0.800	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C604	is Constrained at	0.800	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >H601	is Constrained at	0.800	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >H602	is Constrained at	0.800	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >H603	is Constrained at	0.800	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >H60A	is Constrained at	0.400	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H60B	is Constrained at	0.400	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H60C	is Constrained at	0.400	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F22	is Constrained at	0.450	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F23	is Constrained at	0.450	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F24	is Constrained at	0.450	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C51	is Constrained at	0.450	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F122	is Constrained at	0.200	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F123	is Constrained at	0.200	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F124	is Constrained at	0.200	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C151	is Constrained at	0.200	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <Cl1	is Constrained at	0.100	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <Cl2	is Constrained at	0.100	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C702	is Constrained at	0.100	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H70A	is Constrained at	0.100	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H70B	is Constrained at	0.100	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <Cl3	is Constrained at	0.100	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <Cl4	is Constrained at	0.100	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C701	is Constrained at	0.100	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H70C	is Constrained at	0.100	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H70D	is Constrained at	0.100	Check
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage =	48	Note
PLAT302_ALERT_4_G	Anion/Solvent Disorder	Percentage =	100	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		12	Note
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		10	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms			! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		312	Note

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

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

checkCIF publication errors

Alert level A

PUBL002_ALERT_1_A The contact author's address is missing,
_publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

7 **ALERT level A** = Data missing that is essential or data in wrong format
0 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL002_GLOBAL
;
PROBLEM: The contact author's address is missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
```

```
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 21/04/2015; check.def file version of 09/03/2015

