

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 = 0.0117 Å

Wavelength=0.71073

Cell: a=12.4435(3) b=13.3321(3) c=14.0134(4)
 alpha=81.649(2) beta=71.018(2) gamma=63.354(2)
Temperature: 123 K

	Calculated	Reported
Volume	1964.89(10)	1964.90(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H12 Hg3, C14 H10 Mo2 O4 Sb2, C H2 Cl2	C14 H10 Mo2 O4 Sb2, C18 F12 Hg3, C H2 Cl2
Sum formula	C33 H12 Cl2 F12 Hg3 Mo2 O4 Sb2	C33 H12 Cl2 F12 Hg3 Mo2 O4 Sb2
Mr	1808.50	1808.48
Dx, g cm ⁻³	3.057	3.057
Z	2	2
Mu (mm ⁻¹)	13.877	13.877
F000	1620.0	1620.0
F000'	1598.71	
h,k,lmax	15,17,17	15,17,17
Nref	8657	8644
Tmin,Tmax	0.255,0.579	0.331,0.621
Tmin'	0.178	

Correction method= # Reported T Limits: Tmin=0.331 Tmax=0.621
AbsCorr = GAUSSIAN

Data completeness= 0.998

Theta(max)= 27.103

R(reflections)= 0.0297(5727)

wR2(reflections)= 0.0482(8644)

S = 0.813

Npar= 550

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

PLAT213_ALERT_2_C	Atom F10	has ADP max/min Ratio	3.9	prolat
PLAT213_ALERT_2_C	Atom C30	has ADP max/min Ratio	3.7	prolat
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.0117	Ang.
PLAT431_ALERT_2_C	Short Inter HL..A Contact F10 .. O4 ..		2.80	Ang.
PLAT431_ALERT_2_C	Short Inter HL..A Contact F12 .. O3 ..		2.88	Ang.



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		6	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		1	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ			Please Check
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal		0.00200	Degree
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Hg1 -- C15 ..		5.7	su
PLAT300_ALERT_4_G	Atom Site Occupancy of >C11 is Constrained at		0.620	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C12 is Constrained at		0.620	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C33 is Constrained at		0.620	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C13 is Constrained at		0.380	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C14 is Constrained at		0.380	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C34 is Constrained at		0.380	Check
PLAT302_ALERT_4_G	Anion/Solvent Disorder	Percentage =	100	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (3.10) in Resd. #		3	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (1.90) in Resd. #		4	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F3 .. C11 ..		2.87	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F2 .. F2 ..		2.75	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F4 .. F5 ..		2.82	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F10 .. F11 ..		2.82	Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		12	Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 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
10 ALERT type 4 Improvement, methodology, query or suggestion
0 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 29/01/2015; check.def file version of 29/01/2015

Datablock I - ellipsoid plot

