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: = 0.0000 A Wavelength=1.54184

Cell: a=8.0528(4) b=15.3282(6) c=11.4000(6)
alpha=90 beta=104.970(5) gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	1359.40(12)	1359.41(12)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	1.9(C20 H30 Mo2 P10), 0.1(Mo2 P6)	0.05(Mo2 P6), 0.95(C20 H30 Mo2 P10)
Sum formula	C38 H57 Mo4 P19.60	C19 H28.50 Mo2 P9.80
Mr	1504.61	752.30
Dx,g cm-3	1.838	1.838
Z	1	2
Mu (mm-1)	13.087	13.087
F000	747.0	747.0
F000’	753.32	
h,k,lmax	10,19,14	9,19,14
Nref	2842	2718
Tmin,Tmax	0.320,0.672	0.301,0.707
Tmin’	0.062	

Correction method= # Reported T Limits: Tmin=0.301 Tmax=0.707
AbsCorr = GAUSSIAN

Data completeness= 0.956 Theta(max)= 76.165

R(reflections)= 0.0474(2346) wR2(reflections)= 0.1324(2718)

S = 1.069 Npar= 166

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

Author Response: The measured crystal was a co-crystallization of (Cp*Mo)2P10 and \ (Cp*Mo)2P6 with occupancies of 95% and 5%. The positions of the Cp* ligands with 5% \ occupancy could not be determined.

Alert level G

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ..... 0.50 Ratio
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo1 -- P1 .. 5.3 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo1 -- P2 .. 5.9 su
PLAT300_ALERT_4_G Atom Site Occupancy of >Mo1 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >P1 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >P2 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >P3 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >P4 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >P5 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C1 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C2 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C3 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C4 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C5 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C6 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C7 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C8 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C9 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C10 is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H6A is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H6B is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H6C is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H7A is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H7B is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H7C is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H8A is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H8B is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H8C is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H9A is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H9B is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H9C is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10A is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10B is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10C is Constrained at 0.950 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Mo2 is Constrained at 0.050 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <P6 is Constrained at 0.050 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <P7 is Constrained at 0.050 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <P8 is Constrained at 0.050 Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 100 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage = 100 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (58.90) in Resd. # 1 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.40) in Resd. # 2 Check

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PLAT328_ALERT_4_G Possible Missing H on sp3? Phosphorus .........        >P1 Check
PLAT328_ALERT_4_G Possible Missing H on sp3? Phosphorus .........        >P2 Check
PLAT328_ALERT_4_G Possible Missing H on sp3? Phosphorus .........        >P4 Check
PLAT328_ALERT_4_G Possible Missing H on sp3? Phosphorus .........        >P5 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.22 Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        15 Note
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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   0 **ALERT level B** = A potentially serious problem, consider carefully
   1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  50 **ALERT level G** = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 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
  45 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check

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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.
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   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

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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 21/06/2015; check.def file version of 21/06/2015

Datablock I - ellipsoid plot