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 = 0.0082 A   Wavelength=1.54184

Cell: a=29.9487(4)   b=21.10640(19)   c=33.3294(4)
                 alpha=90   beta=113.6367(15)   gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	19300.4(4)	19300.4(4)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C56 H40 Ag2 Mo8 O16 P8, 2(C36 Al F46 O3), 2(C3), 2(C7 H8), 0.6(	\ 2(Al C36 F46 O3), C42 H30 Ag2 Mo6 O12 P8, 2(C7 H5 Mo O2), 2(C
Sum formula	C159.22 H56.36 Ag2 Al2 Cl0.36 F92 Mo8 O22 P8	C159.22 H56.36 Ag2 Al2 Cl0.36 F92 Mo8 O22 P8
Mr	5366.79	5366.78
Dx,g cm-3	1.847	1.847
Z	4	4
Mu (mm-1)	7.830	7.829
F000	10391.2	10391.0
F000'	10444.01	
h,k,lmax	36,26,41	36,25,41
Nref	19069	18317
Tmin,Tmax	0.433,0.691	0.500,0.748
Tmin'	0.327	

Correction method= # Reported T Limits: Tmin=0.500 Tmax=0.748
AbsCorr = GAUSSIAN

Data completeness= 0.961   Theta(max)= 72.264

R(reflections)= 0.0484(14955)   wR2(reflections)= 0.1396(18317)

S = 1.042   Npar= 1357

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 unit cell contains disordered CH2Cl2 and toluene molecules.

PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent   2

Author Response: These atoms are part of disordered toluene molecules.

PLAT242_ALERT_2_C Low   Ueq as Compared to Neighbors for .....   Mo4 Check
PLAT331_ALERT_2_C Small Average Phenyl   C-C Dist. C101   -C106   1.37 Ang.

Author Response: These atoms are part of disordered toluene molecules.

PLAT332_ALERT_2_C Large Phenyl C-C Range   C101   -C106   0.19 Ang.

Author Response: These atoms are part of disordered toluene molecules.

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.0082 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact F27   .. O7   ..   2.88 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: C159.2199 H56.36 Ag2 Al2 Cl
           Atom count from _chemical_formula_moiety:C78 H56 Ag2 Mo8 O16 P8
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   9 Note
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
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.   42.90 Why ?
PLAT142_ALERT_4_G su on b - Axis Small or Missing .... 0.00019 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records   2 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ag1   -- P2   ..   7.3 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ag1   -- P3   ..   6.7 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo1   -- C1   ..   5.3 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo2   -- C8   ..   7.0 su
PLAT300_ALERT_4_G Atom Site Occupancy of *C17   is Constrained at   0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C18   is Constrained at   0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C19   is Constrained at   0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C20   is Constrained at   0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C21   is Constrained at   0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C22   is Constrained at   0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C23   is Constrained at   0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C24   is Constrained at   0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C25   is Constrained at   0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C26   is Constrained at   0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H17   is Constrained at   0.500 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of *H18    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H19    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H20    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H21    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H22    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H24    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H25    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H26    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C115   is Constrained at    0.400 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C116   is Constrained at    0.400 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of <C118   is Constrained at    0.400 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C119   is Constrained at    0.400 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C400   is Constrained at    0.200 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C401   is Constrained at    0.200 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of <C405   is Constrained at    0.200 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C101   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C102   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C103   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C104   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C105   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C106   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C107   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10A   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10B   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H10C   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H102   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H103   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H104   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H105   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H106   is Constrained at    0.670 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C108   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C109   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C110   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C111   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C112   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C113   is Constrained at    0.330 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of <H11A   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H11B   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H11C   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H109   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H110   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H111   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H112   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H113   is Constrained at    0.330 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C140   is Constrained at    0.300 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C141   is Constrained at    0.300 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C142   is Constrained at    0.300 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C143   is Constrained at    0.300 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C144   is Constrained at    0.300 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C145   is Constrained at    0.300 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C500   is Constrained at    0.370 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C502   is Constrained at    0.370 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C503   is Constrained at    0.370 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C504   is Constrained at    0.370 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C505   is Constrained at    0.370 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Cl1    is Constrained at    0.090 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Cl4    is Constrained at    0.090 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of <C977   is Constrained at      0.090 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H97A   is Constrained at      0.090 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H97B   is Constrained at      0.090 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C120   is Constrained at      0.600 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C404   is Constrained at      0.600 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C501   is Constrained at      0.670 Check
PLAT301_ALERT_3_G Main Residue  Disorder ............ Percentage =         6 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ........... Percentage =       100 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (  10.05) in Resd. #       4 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   4.95) in Resd. #       5 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.80) in Resd. #       6 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.85) in Resd. #       7 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.45) in Resd. #       8 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.60) in Resd. #       9 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.60) in Resd. #      10 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.67) in Resd. #      11 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl1    .. C120    ..    2.23 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F40    .. C56     ..    2.92 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C120   .. C405    ..    1.89 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C120   .. C404    ..    2.52 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C120   .. C400    ..    3.04 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C404   .. C403    ..    1.39 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C404   .. C405    ..    1.39 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C404   .. C400    ..    2.41 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C404   .. C402    ..    2.41 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C404   .. C401    ..    2.78 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C501   .. C140    ..    1.53 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C501   .. C142    ..    2.40 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C501   .. C145    ..    2.76 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F10    .. F14     ..    2.77 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F15    .. F15     ..    2.81 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F29    .. F40     ..    2.71 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F29    .. F32     ..    2.83 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C120   -- C405    .     1.90 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C142   -- C145    .     2.04 Ang.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #      11 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       4 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
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 122 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  29 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  93 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.
```

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

Datablock I - ellipsoid plot