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 = 0.0148 A              Wavelength=1.54184

Cell:              a=36.1206(14)     b=16.4296(5)          c=14.5113(7)
                   alpha=90          beta=100.380(4)       gamma=90
Temperature:       123 K

                   Calculated                 Reported
Volume             8470.8(6)                  8470.8(6)
Space group        C 2/c                      C 1 2/c 1
Hall group         -C 2yc                     -C 2yc
                   2(C16 Al F36 O4), 4(C19.75 C40 H60 Mo4 P12 Tl,
Moiety formula     H29.25 Mo2 P6 Tl0.50),     0.5(Al2 C32 F72 O8),
                   2(C0.45 H0.90              1.5(C0.3 H0.6 Cl0.6)
                   C112.90 H121.80 Al2 Cl1.80 C56.45 H60.90 Al Cl0.90
Sum formula        F72 Mo8 O8 P24 Tl2         F36 Mo4 O4 P12 Tl
Mr                 5012.03                    2506.00
Dx,g cm-3          1.965                      1.965
Z                  2                          4
Mu (mm-1)          11.921                     11.921
F000               4851.6                     4851.6
F000'              4865.83
h,k,lmax           44,20,18                   44,19,17
Nref               8468                       8068
Tmin,Tmax          0.221,0.875                0.270,0.870
Tmin'              0.113


Correction method= # Reported T Limits: Tmin=0.270 Tmax=0.870
AbsCorr = GAUSSIAN


Data completeness= 0.953           Theta(max)= 73.043


R(reflections)= 0.0836( 6467)      wR2(reflections)= 0.2272( 8068)


S = 1.083                   Npar= 730
```

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 A
PLAT308_ALERT_2_A Single Bonded Metal Atom (Unusual !) ....   *Tl1 Check

Author Response: This compound contains very long and very weak Tl-P dative bonds > 3 \ ang.

🟡 Alert level C
PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms ..   Please Check

Author Response: There is one disordered CH2Cl2 solvent molecule which was refined to 90% occupancy.

PLAT215_ALERT_3_C Disordered F8   has ADP max/min Ratio 3.2

Author Response: The atoms of the weakly coordinating anion show a large degree of thermal motion.

PLAT215_ALERT_3_C Disordered F34   has ADP max/min Ratio 3.4

Author Response: The atoms of the weakly coordinating anion show a large degree of thermal motion.

PLAT215_ALERT_3_C Disordered C42   has ADP max/min Ratio 3.1

Author Response: The atoms of the weakly coordinating anion show a large degree of thermal motion.

PLAT215_ALERT_3_C Disordered C43   has ADP max/min Ratio 3.1

Author Response: The atoms of the weakly coordinating anion show a large degree of thermal motion.

PLAT215_ALERT_3_C Disordered C44   has ADP max/min Ratio 3.1

Author Response: The atoms of the weakly coordinating anion show a large degree of thermal motion.

PLAT220_ALERT_2_C Large Non-Solvent C   Ueq(max)/Ueq(min) Range   4.1 Ratio

Author Response: The atoms of the weakly coordinating anion show a large degree of thermal motion.

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PLAT220_ALERT_2_C Large Non-Solvent  F     Ueq(max)/Ueq(min) Range        3.2 Ratio
```

Author Response: The atoms of the weakly coordinating anion show a large degree of thermal motion.

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PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        3.2 Ratio
```

Author Response: The atoms of the weakly coordinating anion show a large degree of thermal motion.

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PLAT234_ALERT_4_C Large Hirshfeld Difference Al1    --  O4     ..      0.17 Ang.
```

Author Response: The central aluminum atom of the weakly coordinating anion is not affected by the disorder and the thermal motion of the tert-butoxy groups.

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PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............      0.0148 Ang.
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🔘 **Alert level G**
```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       32 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        2 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        1 Report
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
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.     0.11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.   166.37 Why ?
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds        2 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records       12 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        3 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records        8 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records        1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records       11 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo2    -- P8     ..      5.7 su
PLAT300_ALERT_4_G Atom Site Occupancy of *F1    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *F2    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *F3    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *F4    is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *F5    is Constrained at    0.500 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of *F22   is Constrained at    0.500 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of *F23      is Constrained at      0.500 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of >H17B   is Constrained at      0.750 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of <C2S    is Constrained at      0.150 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of <H26B   is Constrained at      0.250 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H26C   is Constrained at      0.250 Check
PLAT301_ALERT_3_G Main Residue  Disorder ........... Percentage =        85 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ........... Percentage =       100 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (  57.50) in Resd. #        2 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   2.25) in Resd. #        3 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....     C16 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....     C17 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....     C18 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....     C19 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C21     -- C26    .     1.81 Ang.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....       ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............     162 Note
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   1 **ALERT level A** = Most likely a serious problem - resolve or explain
   0 **ALERT level B** = A potentially serious problem, consider carefully
  11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 153 **ALERT level G** = General information/check it is not something unexpected

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   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 ALERT type 2 Indicator that the structure model may be wrong or deficient
   8 ALERT type 3 Indicator that the structure quality may be low
 143 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.
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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
```

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