checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mjl18097_0m

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: mjl18097_0m

```
Bond precision:   C-C = 0.0046 A              Wavelength=1.34139

Cell:          a=31.9259(6)     b=7.9828(2)          c=20.1715(4)
               alpha=90          beta=100.614(1)     gamma=90
Temperature:   170 K

               Calculated                Reported
Volume         5052.91(19)               5052.91(19)
Space group    C 2/c                     C 1 2/c 1
Hall group     -C 2yc                    -C 2yc
Moiety formula C23 H43 Cl Ir N O P2      C23 H43 Cl Ir N O P2
Sum formula    C23 H43 Cl Ir N O P2      C23 H43 Cl Ir N O P2
Mr             639.19                    639.17
Dx,g cm-3      1.681                     1.680
Z              8                         8
Mu (mm-1)      8.293                     8.585
F000           2560.0                    2560.0
F000'          2524.08
h,k,lmax       38,9,24                   38,9,24
Nref           4812                      4804
Tmin,Tmax      0.627,0.773               0.391,0.751
Tmin'          0.479

Correction method= # Reported T Limits: Tmin=0.391 Tmax=0.751
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 54.911

R(reflections)= 0.0219( 4405)      wR2(reflections)= 0.0460( 4804)

S = 1.107                 Npar= 279
```

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 B
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PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on       Ir1        1.57 eA-3
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Author Response: Inadequate absorption correction of iridium which strongly absorbs X-r

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🟡 Alert level C
```
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .      3.40 %
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=     0.600         4 Report
PLAT927_ALERT_1_C Reported and Calculated  wR2 Differ by ........   -0.0013 Check
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⚪ Alert level G
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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                 not performed for this radiation type.
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      12.09 Why ?
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600          2 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         3 Info
PLAT984_ALERT_1_G The   C-f'=    0.0150 Deviates from the B&C-Value   0.0137 Check
PLAT984_ALERT_1_G The  Ir-f'=   -5.4390 Deviates from the B&C-Value  -5.7005 Check
PLAT984_ALERT_1_G The   O-f'=    0.0410 Deviates from the B&C-Value   0.0389 Check
PLAT984_ALERT_1_G The   P-f'=    0.2600 Deviates from the B&C-Value   0.2543 Check
PLAT985_ALERT_1_G The Cl-f"=    0.5400 Deviates from the B&C-Value   0.5435 Check
PLAT985_ALERT_1_G The Ir-f"=    5.4710 Deviates from the B&C-Value   5.2682 Check
PLAT985_ALERT_1_G The  P-f"=    0.3350 Deviates from the B&C-Value   0.3332 Check
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 0 ALERT level A = Most likely a serious problem - resolve or explain
 1 ALERT level B = A potentially serious problem, consider carefully
 3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
14 ALERT level G = General information/check it is not something unexpected

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

It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/12/2019; check.def file version of 13/12/2019