checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mjl18140_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: mjl18140_0m

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Bond precision:  C-C = 0.0198 A          Wavelength=1.34139

Cell:           a=36.270(2)    b=7.8548(4)         c=36.2929(17)
                alpha=90       beta=113.602(3)     gamma=90
Temperature:    170 K

                Calculated                Reported
Volume          9474.7(9)                 9474.6(9)
Space group     C 2/c                     C 1 2/c 1
Hall group      -C 2yc                    -C 2yc
Moiety formula  C21 H36 Ir N O2 P2        C21 H36 Ir N O2 P2
Sum formula     C21 H36 Ir N O2 P2        C21 H36 Ir N O2 P2
Mr              588.67                    588.65
Dx,g cm-3       1.651                     1.651
Z               16                        16
Mu (mm-1)       8.155                     8.479
F000            4672.0                    4672.0
F000'           4595.02
h,k,lmax        44,9,44                   44,9,44
Nref            9100                      8847
Tmin,Tmax       0.774,0.844               0.457,0.751
Tmin'           0.408

Correction method= # Reported T Limits: Tmin=0.457 Tmax=0.751
AbsCorr = MULTI-SCAN

Data completeness= 0.972          Theta(max)= 55.119

R(reflections)= 0.0708( 6205)     wR2(reflections)= 0.1670( 8847)

S = 1.032                 Npar= 505
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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

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Ir1 2.18 eA-3

Author Response: Inadequate absorption correction of iridium which strongly absorbs X-r

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Alert level B

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Ir2 1.82 eA-3

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 . 3.82 %
PLAT234_ALERT_4_C Large Hirshfeld Difference Ir1 --C2 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C40 --C41 . 0.17 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01977 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 5.601 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 166 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.96A From Ir1 2.04 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.02A From Ir1 1.89 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.13A From Ir1 1.72 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.15A From Ir2 1.57 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.99A From Ir2 1.55 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.02A From C22 1.52 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H33B -0.44 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

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Alert level G

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 409.09 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). 3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 84 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 152 Note
PLAT984_ALERT_1_G The C-f'= 0.0148 Deviates from the B&C-Value 0.0137 Check
PLAT984_ALERT_1_G The Ir-f'= -5.4392 Deviates from the B&C-Value -5.7005 Check
PLAT984_ALERT_1_G The O-f'= 0.0412 Deviates from the B&C-Value 0.0389 Check
PLAT984_ALERT_1_G The P-f'= 0.2596 Deviates from the B&C-Value 0.2543 Check
PLAT985_ALERT_1_G The Ir-f"= 5.4712 Deviates from the B&C-Value 5.2682 Check
PLAT985_ALERT_1_G The P-f"= 0.3354 Deviates from the B&C-Value 0.3332 Check

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

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  8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 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
  4 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
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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

Datablock mjl18140_0m - ellipsoid plot