checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a23061303a0229

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: a23061303a0229

Bond precision: C-C = 0.0064 A Wavelength=1.54184

Cell: a=10.6791(3) b=12.5175(4) c=13.8170(4)
alpha=81.202(2) beta=84.247(2) gamma=82.229(2)
Temperature: 150 K

	Calculated	Reported
Volume	1802.52(9)	1802.52(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C34 H32 Ir N4 O2, F6 P [+ solvent]	0.267(C34 H28 Ir N4 O2), 0.267(F6 P), 0.267[CHCL3]
Sum formula	C34 H32 F6 Ir N4 O2 P [+ solvent]	C34 H32 F6 Ir N4 O2 P
Mr	865.83	865.80
Dx,g cm-3	1.595	1.595
Z	2	2
Mu (mm-1)	8.171	8.171
F000	852.0	852.0
F000'	845.53	
h,k,lmax	13,15,17	13,15,17
Nref	7215	6987
Tmin,Tmax		0.090,0.189
Tmin'		

Correction method= # Reported T Limits: Tmin=0.090 Tmax=0.189
AbsCorr = SPHERE

Data completeness= 0.968 Theta(max)= 73.055

R(reflections)= 0.0329(6429)

wR2(reflections)= 0.0807(6987)

S = 1.039 Npar= 435

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

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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.11 Report
PLAT414_ALERT_2_C Short Intra D-H..H-X       H2       ..H4A      .       1.90 Ang.
                                                      x,y,z  =      1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H3A      ..H17      .       1.91 Ang.
                                                      x,y,z  =      1_555 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N3       --H3A      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N4       --H4B      .     Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          8 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.99Ang From Ir1             1.51 eA-3
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Alert level G

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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:   C34 H32 F6 Ir1 N4 O2 P1
           Atom count from _chemical_formula_moiety:C9.345 H7.743 C10.801 F1.602
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          4 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.002 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          3 Report
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of         P1 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        264 A**3
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          3 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        220 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          4 Info
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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
  13 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 06/07/2023; check.def file version of 30/06/2023

Datablock a23061303a0229 - ellipsoid plot