

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_3482

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: exp_3482

Bond precision:	C-C = 0.0082 A	Wavelength=1.54184	
Cell:	a=10.5816(1)	b=18.5399(2)	c=17.3118(2)
	alpha=90	beta=90.374(1)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	3396.19(6)	3396.19(6)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C34 H28 Ir N4 O2, F6 P [+ solvent]	0.267(C34 H28 Ir N4 O2), 0.267(F6 P), 0.267[CHCL3]	
Sum formula	C34 H28 F6 Ir N4 O2 P [+ solvent]	C34 H28 F6 Ir N4 O2 P	
Mr	861.79	861.77	
Dx, g cm-3	1.686	1.685	
Z	4	4	
Mu (mm-1)	8.674	8.674	
F000	1688.0	1688.0	
F000'	1675.07		
h, k, lmax	13, 23, 21	13, 23, 21	
Nref	6793	6708	
Tmin, Tmax	0.562, 0.707	0.562, 1.000	
Tmin'	0.400		

Correction method= # Reported T Limits: Tmin=0.562 Tmax=1.000

AbsCorr = MULTII-SCAN

Data completeness= 0.987

Theta(max)= 73.048

R(reflections)= 0.0392(5530)

wR2(reflections)=
0.1010(6708)

S = 1.062

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

PLAT244_ALERT_4_C Low	'Solvent' Ueq as Compared to Neighbors of	P1 Check
PLAT342_ALERT_3_C Low Bond Precision on	C-C Bonds	0.00815 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: C34 H28 F6 Ir1 N4 O2 P1 Atom count from _chemical_formula_moiety:C9.345 H7.743 Cl0.801 F1.602	
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	8.44 Why ?
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	242 A**3
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # F6 P	2 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	85 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.2 Low
PLAT954_ALERT_1_G	Reported (CIF) and Actual (FCF) Kmax Differ by .	1 Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info

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

2 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
2 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

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.

