

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: 5

Bond precision:	C-C = 0.0061 A	Wavelength=0.71075
Cell:	a=10.63646(19)	b=19.4945(4) c=15.9469(3)
	alpha=90	beta=102.8964(7) gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	3223.22(11)	3223.22(10)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C27 H47 Ir2 P2, C F3 O3 S	C28 H47 F3 Ir2 O3 P2 S
Sum formula	C28 H47 F3 Ir2 O3 P2 S	C28 H47 F3 Ir2 O3 P2 S
Mr	967.10	967.12
Dx,g cm-3	1.993	1.993
Z	4	4
Mu (mm-1)	8.458	8.481
F000	1864.0	1864.0
F000'	1855.12	
h,k,lmax	13,25,20	13,25,20
Nref	7395	7380
Tmin,Tmax	0.064,0.183	0.060,0.183
Tmin'	0.041	

Correction method= # Reported T Limits: Tmin=0.060 Tmax=0.183
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 27.480

R(reflections)= 0.0314(6781) wR2(reflections)= wR= 0.0453(6798)

S = 1.007 Npar= 399

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

PLAT412_ALERT_2_B Short Intra XH3 .. XHn H9 ..H36 . 1.71 Ang.
x,y,z = 1_555 Check



Alert level C

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S1 Check



Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C28 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C26 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C27 Check
PLAT882_ALERT_1_G No Datum for _diffrn_reflms_av_unetI/netI Please Do !
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT963_ALERT_2_G Both SHELXL WEIGHT Parameters Values Zero Please Check
PLAT983_ALERT_1_G The Ir-f"= 7.9900 Deviates from IT-Value = 7.9887 Check

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

- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
2 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.

