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: 4

Bond precision: C-C = 0.0111 A Wavelength=0.71075

Cell: a=17.2066(5) b=13.4578(3) c=17.4402(4)
alpha=90 beta=118.3955(8) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	3552.62(16)	3552.61(16)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C29 H45 Ir2 O P2, C F3 O3 S	C30 H51 F3 Ir2 O4 P2 S
Sum formula	C30 H45 F3 Ir2 O4 P2 S	C30 H51 F3 Ir2 O4 P2 S
Mr	1005.10	1011.17
Dx,g cm-3	1.879	1.890
Z	4	4
Mu (mm-1)	7.680	7.701
F000	1936.0	1960.0
F000’	1927.14	
h,k,lmax	22,17,22	22,17,22
Nref	8137	8112
Tmin,Tmax	0.260,0.315	0.131,0.315
Tmin’	0.065	

Correction method= # Reported T Limits: Tmin=0.131 Tmax=0.315
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 27.470

R(reflections)= 0.0411(6327) wR2(reflections)= wR= 0.0629(6354)

S = 1.003 Npar= 449

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

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of O1 Check

---

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 6.07 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.01 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C27 --C28 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C27 --C30 . 0.18 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C27 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Ir2 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S1 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..... O1 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0111 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H5 ..H10 . 2.09 Ang.
-x,1/2+y,1/2-z = 2_555 Check
PLAT430_ALERT_2_C Short Inter D...A Contact O1 ..O3 . 2.88 Ang.
1-x,-1/2+y,1/2-z = 2_645 Check

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C30 H51 F3 Ir2 O4 P2 S1
Atom count from the _atom_site data: C30 H45 F3 Ir2 O4 P2 S1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C30 H51 F3 Ir2 O4 P2 S
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	120.00	120.00	0.00
H	204.00	180.00	24.00
F	12.00	12.00	0.00
Ir	8.00	8.00	0.00
O	16.00	16.00	0.00
P	8.00	8.00	0.00
S	4.00	4.00	0.00

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
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C32 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C28 Constrained at 0.61 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C29 Constrained at 0.61 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C30 Constrained at 0.39 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31 Constrained at 0.39 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 6% Note
PLAT303_ALERT_2_G Full Occupancy Atom H45 with # Connections 2.00 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 75 Check
C(29)-O(1) -C(31) 1.555 1.555 1.555 36.00 Deg.
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_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
 14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 17 ALERT level G = General information/check it is not something unexpected

  9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 11 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
  9 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.

PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock 4 - ellipsoid plot