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: C5Me5IrMsenDMNHCOPh

```
Bond precision:  C-C = 0.0136 A          Wavelength=0.71075

Cell:             a=8.5166(8)      b=15.794(2)      c=17.528(2)
                  alpha=90         beta=90          gamma=90
Temperature:      193 K
```

	Calculated	Reported
Volume	2357.7(5)	2357.7(5)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C22 H34 Ir N3 O3 S	C22 H34 Ir N3 O3 S
Sum formula	C22 H34 Ir N3 O3 S	C22 H34 Ir N3 O3 S
Mr	612.80	612.81
Dx,g cm-3	1.726	1.726
Z	4	4
Mu (mm-1)	5.779	5.795
F000	1216.0	1216.0
F000’	1211.31	
h,k,lmax	11,20,22	11,20,22
Nref	5407[3061]	5296
Tmin,Tmax	0.566,0.560	0.360,0.560
Tmin’	0.555	

```
Correction method= # Reported T Limits: Tmin=0.360 Tmax=0.560
AbsCorr = MULTI-SCAN

Data completeness= 1.73/0.98      Theta(max)= 27.482

R(reflections)= 0.0297( 5203)     wR2(reflections)= 0.0730( 5296)

S = 1.010                 Npar= 271
```

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

```
PLAT213_ALERT_2_B Atom C7              has ADP max/min Ratio .....        4.5 prolat
```

Alert level C

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PLAT213_ALERT_2_C Atom O1              has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C6              has ADP max/min Ratio .....        3.7 prolat
PLAT213_ALERT_2_C Atom C8              has ADP max/min Ratio .....        3.7 prolat
PLAT213_ALERT_2_C Atom C9              has ADP max/min Ratio .....        3.8 prolat
PLAT213_ALERT_2_C Atom C10             has ADP max/min Ratio .....        3.5 prolat
PLAT213_ALERT_2_C Atom C22             has ADP max/min Ratio .....        3.1 prolat
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        5.8 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range        6.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C19      --C20      .       0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C19 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Ir1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         S1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C5 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2 Note
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01356 Ang.
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Alert level G

```
CHEMS02_ALERT_1_G  Please check that you have entered the correct
           _publ_requested_category classification of your compound;
           FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
           FO or CO or EO for organic.
           From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or A
           From the CIF: _chemical_formula_sum :C22 H34 Ir1 N3 O3 S1
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0      0.994 Report
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C6 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C7 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C8 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C9 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C10 Check
PLAT963_ALERT_2_G Both SHELXL WEIGHT Parameters Values Zero ......     Please Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  18 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 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
   6 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 C5Me5IrMsenDMNHCOPh - ellipsoid plot