

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: C5Me5IrMsenDMCN

Bond precision:	C-C = 0.0160 A	Wavelength=0.71075
Cell:	a=15.158(5)	b=8.800(3) c=14.210(5)
	alpha=90	beta=101.968(4) gamma=90
Temperature:	93 K	
	Calculated	Reported
Volume	1854.3(11)	1854.3(11)
Space group	C 2	C 1 2 1
Hall group	C 2y	C 2y
Moiety formula	C16 H28 Ir N3 O2 S	C16 H28 Ir N3 O2 S
Sum formula	C16 H28 Ir N3 O2 S	C16 H28 Ir N3 O2 S
Mr	518.69	518.70
Dx,g cm-3	1.858	1.858
Z	4	4
Mu (mm-1)	7.325	7.345
F000	1016.0	1016.0
F000'	1011.30	
h,k,lmax	19,11,18	19,11,18
Nref	4276[2276]	4151
Tmin,Tmax	0.485,0.480	0.392,0.480
Tmin'	0.475	

Correction method= # Reported T Limits: Tmin=0.392 Tmax=0.480
AbsCorr = MULTI-SCAN

Data completeness= 1.82/0.97 Theta(max)= 27.480
R(reflections)= 0.0333(3720) wR2(reflections)= 0.0762(4151)

S = 0.973 Npar= 208

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

PLAT213_ALERT_2_C Atom Cl has ADP max/min Ratio 3.1 prolat
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.016 Ang.

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 :C16 H28 Ir1 N3 O2 S1
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0 0.996 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
PLAT432_ALERT_2_G Short Inter X...Y Contact O2 ..C14 3.00 Ang.
1/2-x,-1/2+y,2-z = 4_547 Check
PLAT963_ALERT_2_G Both SHELXL WEIGHT Parameters Values Zero Please Check

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
9 **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
1 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

