

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: shelx

Bond precision:	C-C = 0.0071 A	Wavelength=0.71075
Cell:	a=16.891(2)	b=14.4978(18) c=17.310(2)
	alpha=90	beta=90 gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	4238.9(9)	4238.8(9)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C19 H21 Cl Ir N2 O2, C H4 O, Cl	C19 H21 Cl Ir N2 O2, Cl, C H4 O
Sum formula	C20 H25 Cl2 Ir N2 O3	C20 H25 Cl2 Ir N2 O3
Mr	604.54	604.52
Dx,g cm-3	1.895	1.895
Z	8	8
Mu (mm-1)	6.575	6.575
F000	2352.0	2352.0
F000'	2344.04	
h,k,lmax	21,18,22	21,18,22
Nref	4863	4852
Tmin,Tmax	0.225,0.518	0.551,1.000
Tmin'	0.128	

Correction method= # Reported T Limits: Tmin=0.551 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 27.485

R(reflections)= 0.0416(4208) wR2(reflections)= 0.1095(4852)

S = 1.033 Npar= 261

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.146



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	3	Report
PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12	0.146	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	51	Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
1 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.

Datablock shelx - ellipsoid plot

