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 = 0.0126 A          Wavelength=0.71075

Cell:              a=13.240(3)      b=11.975(2)      c=32.330(6)
                   alpha=90         beta=90          gamma=90
Temperature:       143 K
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	Calculated	Reported
Volume	5125.9(17)	5125.9(18)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	2(C23 H29 Cl Ir N2 O2), C H4 O, 2(Cl)	2(C1 H29 C23 Ir N2 O2), 2 (Cl), C H4 O
Sum formula	C47 H62 Cl4 Ir2 N4 O5	C47 H62 Cl4 Ir2 N4 O5
Mr	1289.25	1289.20
Dx,g cm-3	1.671	1.671
Z	4	4
Mu (mm-1)	5.442	5.442
F000	2536.0	2536.0
F000’	2528.00	
h,k,lmax	17,15,42	17,15,41
Nref	6174	6136
Tmin,Tmax	0.350,0.897	0.706,1.000
Tmin’	0.324	

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Correction method= # Reported T Limits: Tmin=0.706 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994          Theta(max)= 27.500

R(reflections)= 0.0584( 5744)     wR2(reflections)= 0.1387( 6136)

S = 1.170                 Npar= 312
```

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

```
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.4 Ratio
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01262 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         95 Ang**3
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Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C47 H62 Cl4 Ir2 N4 O5
           Atom count from _chemical_formula_moiety:C49 H62 Cl2 Ir2 N4 O5
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          3 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      54.43 Why ?
PLAT300_ALERT_4_G Atom Site Occupancy of H00V       Constrained at     0.8124 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H          Constrained at     0.0938 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H00W       Constrained at     0.4062 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H00X       Constrained at     0.4062 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H00Y       Constrained at     0.1876 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ha         Constrained at     0.0938 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9C        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H011       Constrained at        0.5 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  4           0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  5           0.50 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C00S     - C00V     .       1.53 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C00R     - C00W     .       1.53 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         70 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          3 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  20 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 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
  14 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.

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

Datablock shelx - ellipsoid plot