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: pya

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Bond precision:  C-C = 0.0050 A          Wavelength=0.71073

Cell:            a=9.7170(2)    b=17.9672(4)       c=16.2161(3)
                 alpha=90       beta=94.710(2)     gamma=90
Temperature:     110 K
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	Calculated	Reported
Volume	2821.56(10)	2821.56(10)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	?
Moiety formula	2(C31 H17 Cl F4 Ir N3 O2), C H2 Cl2	2(C31 H17 Cl F4 Ir N3 O2), C H2 Cl2
Sum formula	C63 H36 Cl4 F8 Ir2 N6 O4	C63 H36 Cl4 F8 Ir2 N6 O4
Mr	1619.22	1619.18
Dx,g cm-3	1.906	1.906
Z	2	2
Mu (mm-1)	4.984	4.984
F000	1564.0	1564.0
F000’	1560.25	
h,k,lmax	13,24,22	12,24,21
Nref	7669	6574
Tmin,Tmax	0.093,0.248	0.818,1.000
Tmin’	0.048	

```
Correction method= # Reported T Limits: Tmin=0.818 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.857          Theta(max)= 29.220

R(reflections)= 0.0254( 5226)     wR2(reflections)= 0.0519( 6574)

S = 0.953                 Npar= 412
```

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

PLAT336_ALERT_2_C Long Bond Distance for ..... C32 -Cl3 1.892 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact F4 .. O1 .. 2.78 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C31 H17 Cl F4 Ir N3 O2

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT300_ALERT_4_G Atom Site Occupancy of *Cl2 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *Cl3 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C32 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H32A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H32C is Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage = 100 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (2.50) in Resd. # 2 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl2 .. C32 .. 2.10 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl2 .. C31 .. 3.24 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl3 .. C32 .. 0.99 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C32 .. C32 .. 1.30 Ang.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.13 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 120 Check
CL3 -CL2 -C32 3.754 1.555 1.555 38.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 122 Check
C32 -CL2 -C32 1.555 1.555 3.754 38.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 124 Check
C32 -CL3 -C32 3.754 1.555 1.555 40.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 130 Check
C32 -C32 -CL3 3.754 1.555 1.555 29.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 135 Check
CL3 -C32 -CL2 1.555 1.555 3.754 35.80 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C H2 Cl2
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
16 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 11/08/2016; check.def file version of 04/08/2016

Datablock pya - ellipsoid plot