

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1_a

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: 1_a

Bond precision: C-C = 0.0126 Å Wavelength=1.34139

Cell: a=20.757(7) b=20.007(6) c=10.946(4)
 alpha=90 beta=90 gamma=90
Temperature: 193 K

	Calculated	Reported
Volume	4546(3)	4546(3)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C41 H75 Ir3 N8 P2 U	C41 H75 Ir3 N8 P2 U
Sum formula	C41 H75 Ir3 N8 P2 U	C41 H75 Ir3 N8 P2 U
Mr	1556.72	1556.66
Dx, g cm-3	2.274	2.275
Z	4	4
Mu (mm-1)	19.107	19.108
F000	2920.0	2920.0
F000'	2841.93	
h, k, lmax	24, 24, 13	24, 24, 13
Nref	4287	4265
Tmin, Tmax	0.222, 0.148	0.354, 0.751
Tmin'	0.099	

Correction method= # Reported T Limits: Tmin=0.354 Tmax=0.751
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 53.878

R(reflections)= 0.0336(3825) wR2(reflections)= 0.0865(4265)

S = 1.041 Npar= 263

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

PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01256 Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C36 - C36_a .	1.43 Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C40 - C40_a .	1.42 Ang.
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of .	33 Ang**3
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	11 Report
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.67A From N4	-0.63 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.79A From N6	-0.61 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H23	-0.35 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H25A	-0.36 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H40A	-0.47 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H40B	-0.37 eA-3

● Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.	
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	14.85 Why ?
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	42.60 Deg.
	N1 -P1 -U1 1_555 1_555 1_555 #	99 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	48 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	11 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

8 **ALERT level G** = General information/check it is not something unexpected

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

12 ALERT type 2 Indicator that the structure model may be wrong or deficient

3 ALERT type 3 Indicator that the structure quality may be low

3 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.

