

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 = 0.0087 Å

Wavelength=0.71073

Cell: a=10.4461(3) b=15.7690(5) c=18.4599(7)
 alpha=84.440(1) beta=73.937(1) gamma=78.725(1)
Temperature: 193 K

	Calculated	Reported
Volume	2862.73(16)	2862.73(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C41 H75 Ir3 N13 P2 U), 3(C7 H8)	C41 H75 Ir3 N13 P2 U, 1.5(C7 H8)
Sum formula	C103 H174 Ir6 N26 P4 U2	C51.50 H87 Ir3 N13 P2 U
Mr	3529.95	1764.91
Dx, g cm ⁻³	2.048	2.047
Z	1	2
Mu (mm ⁻¹)	9.873	9.873
F000	1680.0	1680.0
F000'	1653.70	
h, k, lmax	13, 20, 23	13, 20, 23
Nref	13170	13033
Tmin, Tmax	0.387, 0.373	0.366, 0.746
Tmin'	0.358	

Correction method= # Reported T Limits: Tmin=0.366 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 0.990

Theta(max)= 27.520

R(reflections)= 0.0270(11570)

wR2(reflections)= 0.0625(13033)

S = 1.051

Npar= 666

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	NonSolvent	Resd 1 N	Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor			3.0	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor			2.4	Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C49		0.101	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds			0.00873	Ang.
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).			7	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		87	Report
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.61A	From Ir3	-1.77	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.67A	From Ir3	-1.60	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H6			-0.32	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H41B			-0.33	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H47			-0.43	eA-3

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...			14	Report
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ			Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...			0.50	Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)			0.001	Degree
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records			2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records			2	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C49	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C50	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C51	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C52	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C53	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C54	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C55	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H49A	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H49B	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H49C	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H51	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H53	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H54	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H55	Constrained at		0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)			100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)			7.50	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...			39.34	Deg.
	N1 -P1 -U1 1_555 1_555 1_555	#	110	Check	
PLAT789_ALERT_4_G	Atoms with Negative_atom_site_disorder_group #			15	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #			2	Note
	C7 H8				
PLAT794_ALERT_5_G	Tentative Bond Valency for U1 (IV)			4.76	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints			168	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		43	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF			2	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...			2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity			2.1	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			2	Info

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

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

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

33 **ALERT level 6** = General information/check it is not something unexpected

3 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
6 ALERT type 3 Indicator that the structure quality may be low
23 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 16/05/2021; check.def file version of 13/05/2021

