

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kar201_corr

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: kar201_corr

Bond precision: C-C = 0.0064 Å Wavelength=1.54184

Cell: a=15.7816(3) b=16.8956(4) c=17.5198(4)
 alpha=73.294(2) beta=67.489(2) gamma=84.5748(17)
Temperature: 100 K

	Calculated	Reported
Volume	4132.75(17)	4132.76(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C88 H92 Au2 I2 N8 P4	2(C44 H46 Au I N4 P2)
Sum formula	C88 H92 Au2 I2 N8 P4	C88 H92 Au2 I2 N8 P4
Mr	2033.32	2033.30
Dx, g cm ⁻³	1.634	1.634
Z	2	2
Mu (mm ⁻¹)	13.554	13.554
F000	2000.0	2000.0
F000'	1987.62	
h, k, lmax	19, 21, 22	19, 21, 22
Nref	17417	16836
Tmin, Tmax	0.246, 0.763	0.312, 0.898
Tmin'	0.137	

Correction method= # Reported T Limits: Tmin=0.312 Tmax=0.898
AbsCorr = GAUSSIAN

Data completeness= 0.967 Theta(max)= 76.731

R(reflections)= 0.0394(15034)	wR2(reflections)=
S = 1.084	0.1071(16836)
Npar= 1205	

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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT213_ALERT_2_C	Atom C1V has ADP max/min Ratio	3.4 prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	4.2 Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range	3.1 Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.3 Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N1Q Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C1T Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C1V Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C1W Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C3Q Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C1C Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C1S Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.808 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	16 Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 3.01Ang From C3K	2.11 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.95Ang From I1	1.88 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 2.76Ang From C2V	1.58 eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on Aul	1.30 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H1E .	-0.31 eA-3

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	36 Note
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	10.72 Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	15 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of N2N Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N23 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1N Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2C Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2E Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2F Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2H Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2J Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2K Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2L Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2O Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2P Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2U Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2V Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2W Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2X Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2Y Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2Z Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3D Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3E Constrained at	0.5 Check

[illegible]

[illegible]

PLAT300_ALERT_4_G	Atom Site Occupancy of H21	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H29	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H34	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H45	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H46	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H47A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H47B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48B	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		48%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		40%	Note
PLAT410_ALERT_2_G	Short Intra H...H Contact H1N ..H1TB .		1.81 Ang.	
	x,y,z =	1_555	Check	
PLAT410_ALERT_2_G	Short Intra H...H Contact H1TB ..H2BA .		2.13 Ang.	
	x,y,z =	1_555	Check	
PLAT410_ALERT_2_G	Short Intra H...H Contact H1VA ..H24B .		2.13 Ang.	
	x,y,z =	1_555	Check	
PLAT410_ALERT_2_G	Short Intra H...H Contact H1VA ..H28 .		2.14 Ang.	
	x,y,z =	1_555	Check	
PLAT410_ALERT_2_G	Short Intra H...H Contact H1B ..H3A .		2.06 Ang.	
	x,y,z =	1_555	Check	
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		16	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		9.36 Deg.	
	AU2 -P4 -AU2A 2_656 1_555 2_656	#	40	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		28	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	C88 H92 Au2 I2 N8 P4			
PLAT793_ALERT_4_G	Model has Chirality at C	(Centro SPGR)		S Verify
PLAT793_ALERT_4_G	Model has Chirality at C5	(Centro SPGR)		R Verify
PLAT793_ALERT_4_G	Model has Chirality at C20	(Centro SPGR)		R Verify
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms			! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		57	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		565	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		13	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		3.3	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 24 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
 160 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.

