

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) deh097_raj_sad

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: deh097_raj_sad

Bond precision: C-C = 0.0058 A

Wavelength=0.71073

Cell: a=21.0960(18) b=10.6127(8) c=24.0691(19)
 alpha=90 beta=108.277(4) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	5116.9(7)	5116.9(7)
Space group	P 2/n	P 2/n
Hall group	-P 2yac	-P 2yac
Moiety formula	C52 H40 Cu2 I2 N2 P2, 2(C H2 Cl2)	C52 H40 Cu2 I2 N2 P2, 2(C H2 Cl2)
Sum formula	C54 H44 Cl4 Cu2 I2 N2 P2	C54 H44 Cl4 Cu2 I2 N2 P2
Mr	1305.55	1305.53
Dx,g cm-3	1.695	1.695
Z	4	4
Mu (mm-1)	2.348	2.348
F000	2576.0	2576.0
F000'	2578.55	
h,k,lmax	27,13,31	27,13,31
Nref	11853	11817
Tmin,Tmax	0.798,0.889	0.633,0.746
Tmin'	0.671	

Correction method= # Reported T Limits: Tmin=0.633 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 0.997

Theta(max)= 27.582

R(reflections)= 0.0378(8446)

wR2(reflections)= 0.0749(11817)

S = 1.017

Npar= 649

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 B

PLAT213_ALERT_2_B Atom C49B has ADP max/min Ratio 4.2 prolat



Alert level C

PLAT213_ALERT_2_C Atom C40 has ADP max/min Ratio 3.2 prolat
 PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.2 Ratio
 PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 5.0 Ratio
 PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of Cl2 Check
 PLAT336_ALERT_2_C Long Bond Distance for C53B -Cl2 1.867 Ang.
 PLAT411_ALERT_2_C Short Inter H...H Contact H26 .. H48A .. 2.10 Ang.
 PLAT413_ALERT_2_C Short Inter XH3 .. XHn H40A .. H50B .. 2.14 Ang.
 PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min) 5 Note
 PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density 0 Note



Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.96 Why ?
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 -- Cu1 .. 8.0 s.u.
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 -- Cu2 .. 10.0 s.u.
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I2 -- Cu1 .. 22.0 s.u.
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I2 -- Cu2 .. 10.0 s.u.
 PLAT300_ALERT_4_G Atom Site Occupancy of *Cl5 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of *C55 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of *H55A is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of *H55B is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of *H54A is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of *H54B is Constrained at 0.5 Check
 PLAT301_ALERT_3_G Main Residue Disorder Percentage = 10 Note
 PLAT302_ALERT_4_G Anion/Solvent Disorder Percentage = 33 Note
 PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 4 Check
 PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 31 Note

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

- 0 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
 11 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.

