

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ga_80425a_a_sq

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: ga_80425a_a_sq

Bond precision: C-C = 0.0076 Å

Wavelength=1.34138

Cell: a=18.3185(6) b=18.3357(5) c=19.5491(6)
 alpha=106.191(1) beta=92.557(1) gamma=97.633(1)
Temperature: 170 K

	Calculated	Reported
Volume	6226.9(3)	6226.9(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C48 H48 N32 O16), 4(C21 H17 N2), 2(Cd2 Cl7), 2(Cd ? Cl4), Cl, 2	
Sum formula	C180 H164 Cd6 Cl23 N72 O54	C90 H107.50 Cd3 Cl111.50
Mr	5689.64	2870.49
Dx,g cm-3	1.517	1.531
Z	1	2
Mu (mm-1)	4.731	4.732
F000	2859.0	2910.0
F000'	2873.17	
h,k,lmax	22,22,24	22,22,24
Nref	25482	25389
Tmin,Tmax	0.706,0.753	0.617,0.772
Tmin'	0.566	

Correction method= # Reported T Limits: Tmin=0.617 Tmax=0.772
AbsCorr = MULTI-SCAN

Data completeness= 0.996

Theta(max)= 56.976

R(reflections)= 0.0546(19734)

wR2(reflections)= 0.1586(25389)

S = 1.042

Npar= 1689

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 A

PLAT430_ALERT_2_A Short Inter D...A Contact	O20	..026		2.50 Ang.
		x,y,z =	1_555	Check
PLAT430_ALERT_2_A Short Inter D...A Contact	O21	..023		2.49 Ang.
		x,y,z =	1_555	Check
PLAT430_ALERT_2_A Short Inter D...A Contact	O22	..025		2.07 Ang.
		x,y,z =	1_555	Check
PLAT430_ALERT_2_A Short Inter D...A Contact	O23	..025		2.39 Ang.
		1-x,1-y,1-z =	2_666	Check

Alert level B

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)			019	Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)			020	Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)			021	Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)			022	Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)			023	Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)			024	Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)			025	Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)			026	Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)			027	Check
PLAT430_ALERT_2_B Short Inter D...A Contact	O1	..023		2.73 Ang.	
		x,y,1+z =	1_556	Check	
PLAT430_ALERT_2_B Short Inter D...A Contact	O2	..020		2.73 Ang.	
		-1+x,y,1+z =	1_456	Check	
PLAT430_ALERT_2_B Short Inter D...A Contact	O4	..024		2.76 Ang.	
		-1+x,y,1+z =	1_456	Check	
PLAT430_ALERT_2_B Short Inter D...A Contact	O5	..019		2.82 Ang.	
		x,y,z =	1_555	Check	
PLAT430_ALERT_2_B Short Inter D...A Contact	O7	..N33		2.65 Ang.	
		x,y,1+z =	1_556	Check	
PLAT430_ALERT_2_B Short Inter D...A Contact	O11	..027		2.76 Ang.	
		x,y,z =	1_555	Check	
PLAT430_ALERT_2_B Short Inter D...A Contact	O15	..017		2.74 Ang.	
		x,-1+y,z =	1_545	Check	
PLAT430_ALERT_2_B Short Inter D...A Contact	O17	..N35		2.66 Ang.	
		x,y,z =	1_555	Check	
PLAT430_ALERT_2_B Short Inter D...A Contact	O20	..024		2.72 Ang.	
		x,y,z =	1_555	Check	
PLAT430_ALERT_2_B Short Inter D...A Contact	N35	..017'		2.79 Ang.	
		x,y,z =	1_555	Check	
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers				2	Check

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for	O6	--C15		5.7 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of			C53	Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of			Cd3	Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance			2.048	Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=	0.600		24	Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens.	1.00A	From O24	0.61	eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.	1.04A	From O20	0.61	eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.	0.52A	From O23	-0.94	eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.	1.04A	From O23	-0.66	eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.	1.01A	From O22	-0.63	eA-3

PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.47A	From O26	-0.59 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.41A	From O25	-0.51 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.50A	From O22	-0.47 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.60A	From O21	-0.46 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.52A	From O21	-0.44 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.64A	From O22	-0.43 eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.			0 Info

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and the formula from the _atom_site* data.
 Atom count from _chemical_formula_sum: C90 H107.5 Cd3 Cl11.5 N36 O27
 Atom count from the _atom_site data: C90. H82 Cd3 Cl11.5 N36 O27

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
 not performed for this radiation type.

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
 From the CIF: _cell_formula_units_Z 2
 From the CIF: _chemical_formula_sum C90 H107.50 Cd3 Cl11.50 N36 O27
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	180.00	180.00	0.00
H	215.00	164.00	51.00
Cd	6.00	6.00	0.00
Cl	23.00	23.00	0.00
N	72.00	72.00	0.00
O	54.00	54.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 19 Note

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 49 Report

PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check

PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 12.85 Why ?

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report

PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report

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 5 Report

PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Cd2 --Cl4 10.8 s.u.

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 48% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 48% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 7) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 8) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 9) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 20) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 21) 100% Note

PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 7 0.35 Check

PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 8 0.15 Check

PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 9 0.80 Check

PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 10 0.51 Check

PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 20 0.20 Check

PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 21 0.49 Check

PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) 017 Check

PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) 018' Check

PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) 017' Check

PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) 018 Check

PLAT431_ALERT_2_G Short Inter HL..A Contact Cl10 ..O21 3.12 Ang.
 x,y,z = 1_555 Check

PLAT431_ALERT_2_G Short Inter HL..A Contact	Cl11	..O22	3.12 Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	Cl10	..C19	3.11 Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	O3	..C90'	2.96 Ang.
		x,y,l+z =	1_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	O7	..C49	2.99 Ang.
		x,y,l+z =	1_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	O10	..C70	3.01 Ang.
		1-x,1-y,1-z =	2_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	O12	..C76	3.01 Ang.
		1-x,1-y,1-z =	2_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	O14	..C69'	2.95 Ang.
		1-x,1-y,1-z =	2_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	O22	..C77	2.98 Ang.
		1-x,1-y,1-z =	2_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	O22	..C71	3.01 Ang.
		1-x,1-y,1-z =	2_666 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure			! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1	(II)	.	2.07 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd2	(II)	.	1.99 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd3	(II)	.	1.94 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints			402 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed			! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).			2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600			67 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...			1 Note

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 56 ALERT type 2 Indicator that the structure model may be wrong or deficient
 5 ALERT type 3 Indicator that the structure quality may be low
 23 ALERT type 4 Improvement, methodology, query or suggestion
 3 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.

