

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 15

Bond precision:	C-C = 0.0115 A	Wavelength=0.71073
Cell:	a=24.2350(4)	b=20.8170(4) c=15.3597(2)
	alpha=90	beta=127.925(2) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	6112.5(2)	6112.5(2)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C18 H17 Dy N3 O8), C15 Hg, 2(C14 Hg), 2(H2 O), 2(O)	2(C18 H20 Dy N3 O9), C15 Hg, 2(C14 Hg), H2 O, H3 O
Sum formula	C36 H38 Cl13 Dy2 Hg3 N6 O20	C36 H47 Cl13 Dy2 Hg3 N6 O20
Mr	2262.34	2271.41
Dx, g cm-3	2.458	2.468
Z	4	4
Mu (mm-1)	10.563	10.564
F000	4196.0	4232.0
F000'	4176.83	
h, k, lmax	28, 24, 18	28, 24, 18
Nref	5403	5296
Tmin, Tmax		0.416, 0.655
Tmin'		

Correction method= # Reported T Limits: Tmin=0.416 Tmax=0.655
AbsCorr = MULTI-SCAN

Data completeness= 0.980 Theta(max)= 25.027

R(reflections)= 0.0330(4646) wR2(reflections)= 0.0895(5296)

S = 1.053 Npar= 375

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

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 04W Check

🟢 Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 9.07 Check
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.34 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01147 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C9 - C12 . 1.53 Ang.

🟠 Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C36 H47 Cl13 Dy2 Hg3 N6 O20
Atom count from _chemical_formula_moiety:C36 H45 Cl13 Dy2 Hg3 N6 O20
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:C36 H47 Cl13 Dy2 Hg3 N6 O20
Atom count from the _atom_site data: C36 H38 Cl13 Dy2 Hg3 N6 O20
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 4
From the CIF: _chemical_formula_sum C36 H47 Cl13 Dy2 Hg3 N6 O20
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	144.00	144.00	0.00
H	188.00	152.00	36.00
Cl	52.00	52.00	0.00
Dy	8.00	8.00	0.00
Hg	12.00	12.00	0.00
N	24.00	24.00	0.00
O	80.00	80.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 19 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 66.11 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 14 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Hg1 --Cl2 . 18.0 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Hg1 --Cl3 . 38.0 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Hg1 Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 17% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl2 ..C16 3.03 Ang.

PLAT432_ALERT_2_G Short Inter X...Y Contact	Cl2	1-x,y,5/2-z = ..C15	2_657 Check
			3.13 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	Cl2	1-x,y,5/2-z = ..C4	2_657 Check
			3.16 Ang.
		x,y,1+z =	1_556 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels			4 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF	#		45 Check
HG1 -CL3 -HG1	1.555	1.555 2.657	27.99 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF	#		46 Check
HG1 -CL1 -HG1	2.657	1.555 1.555	28.96 Deg.
PLAT794_ALERT_5_G Tentative Bond Valency for Hg2	(II)	.	2.29 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Dy1	(II)	.	1.96 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints			14 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary		.	Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File		...	92 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged			Please Check

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

13 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
 2 ALERT type 3 Indicator that the structure quality may be low
 9 ALERT type 4 Improvement, methodology, query or suggestion
 4 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.

Datablock 15 - ellipsoid plot

