

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: 2

Bond precision: Br-Br = 0.0060 Å Wavelength=0.71073

Cell: a=13.0997(11) b=13.6459(13) c=27.906(3)
 alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	4988.4(8)	4988.4(8)
Space group	P b a m	Pbam
Hall group	-P 2 2ab	?
Moiety formula	Br36 Dy6 Hg9	Br36 Dy6 Hg9
Sum formula	Br36 Dy6 Hg9	Br36 Dy6 Hg9
Mr	5656.71	5656.71
Dx, g cm-3	3.766	3.741
Z	2	2
Mu (mm-1)	32.644	31.850
F000	4752.0	4722.0
F000'	4700.90	
h, k, lmax	15, 16, 33	15, 16, 33
Nref	4514	4402
Tmin, Tmax	0.090, 0.148	0.090, 0.148
Tmin'	0.068	

Correction method= # Reported T Limits: Tmin=0.090 Tmax=0.148
AbsCorr = MULTI-SCAN

Data completeness= 0.975 Theta(max)= 25.030

R(reflections)= 0.1122(2666) wR2(reflections)= 0.3482(4402)

S = 1.032 Npar= 125

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

PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

Author Response: The VOID(S) is actually existed in the structure and no any solvent can be found.

 Alert level B

PLAT241_ALERT_2_B High MainMol Ueq as Compared to Neighbors of Hg1 Check

Author Response: Although we try our best to solve this problem, the problem remains because the quality of the crystal is not high enough. Furthermore, this alert do not affect the main results in this manuscript.

PLAT241_ALERT_2_B High MainMol Ueq as Compared to Neighbors of Hg2 Check

Author Response: Although we try our best to solve this problem, the problem remains because the quality of the crystal is not high enough. Furthermore, this alert do not affect the main results in this manuscript.

PLAT242_ALERT_2_B Low MainMol Ueq as Compared to Neighbors of Br8 Check

Author Response: Although we try our best to solve this problem, the problem remains because the quality of the crystal is not high enough. Furthermore, this alert do not affect the main results in this manuscript

 Alert level C

ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies outside the range 0.99 <> 1.01

Calculated value of mu = 32.644

Value of mu given = 31.850

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -6.423

Test value = -6.000

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.975 Why?

PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 2.49 %

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT082_ALERT_2_C High R1 Value 0.11 Report

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.35 Report

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -6.42 eA-3

PLAT199_ALERT_1_C Reported _cell_measurement_temperature (K) 293 Check

PLAT200_ALERT_1_C Reported _diffrn_ambient_temperature (K) 293 Check

PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of Hg3 Check

Author Response: Although we try our best to solve this problem, the problem remains because the quality of the crystal is not high enough. Furthermore, this alert do not affect the main results in this manuscript.

PLAT242_ALERT_2_C Low MainMol Ueq as Compared to Neighbors of Dy3 Check

Author Response: Although we try our best to solve this problem, the problem remains because the quality of the crystal is not high enough. Furthermore, this alert do not affect the main results in this manuscript

PLAT242_ALERT_2_C Low MainMol Ueq as Compared to Neighbors of Br5 Check

Author Response: Although we try our best to solve this problem, the problem remains because the quality of the crystal is not high enough. Furthermore, this alert do not affect the main results in this manuscript

PLAT260_ALERT_2_C Large Average Ueq of Residue Including Hg1 0.104 Check



Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF	Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.19 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	179.14 Why ?
PLAT794_ALERT_5_G Tentative Bond Valency for Hg1 (II) .	2.19 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Hg3 (II) .	2.07 Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON	85 Info
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL	2018 Note

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

 - 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 13 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
 - 1 ALERT type 4 Improvement, methodology, query or suggestion
 - 5 ALERT type 5 Informative message, check
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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.

