

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: I

Bond precision: C-C = 0.0081 Å

Wavelength=0.71073

Cell: a=11.9193(4) b=9.5228(3) c=32.7149(7)
 alpha=90 beta=94.100(2) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	3703.81(19)	3703.81(19)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety	C18 H12 Cl6	
formula	Hg3 N3 O8 Tb, [TB(IA)3(H2O)2(HG2CL4)]N.N(HGCL2).NH2O	
Sum	C18 H12 Cl6	
formula	Hg3 N3 O9 Tb	C18 H18 Cl6 Hg3 N3 O9 Tb
Mr	1387.71	1393.74
Dx, g cm-3	2.489	2.499
Z	4	4
Mu (mm-1)	14.756	14.756
F000	2480.0	2504.0
F000'	2457.64	
h, k, lmax	14, 11, 38	14, 11, 38
Nref	6549	6285
Tmin, Tmax	0.301, 0.554	0.301, 0.554
Tmin'	0.024	

Correction method= # Reported T Limits: Tmin=0.301 Tmax=0.554
AbsCorr = MULTI-SCAN

Data completeness= 0.960

Theta(max)= 25.030

R(reflections)= 0.0880(5261)

wR2(reflections)= 0.2133(6285)

S = 1.135

Npar= 360

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 [VOLT](#) LARGE Solvent Accessible VOID(S) in Structure [! Info](#)

 Alert level C

PLAT029_ALERT_3_C [_diffn_measured_fraction_theta_full](#) value Low . 0.960 [Why?](#)
PLAT041_ALERT_1_C [Calc. and Reported SumFormula](#) Strings Differ [Please Check](#)
PLAT043_ALERT_1_C [Calculated and Reported Mol. Weight](#) Differ by .. 6.03 [Check](#)
PLAT068_ALERT_1_C [Reported F000](#) Differs from Calcd (or Missing)... [Please Check](#)
PLAT125_ALERT_4_C [No '_symmetry_space_group_name_Hall'](#) Given [Please Do !](#)
PLAT202_ALERT_3_C [Isotropic non-H Atoms in Anion/Solvent](#) 1 [Check](#)
PLAT242_ALERT_2_C [Low 'MainMol' Ueq as Compared to Neighbors of](#) Tb1 [Check](#)
PLAT342_ALERT_3_C [Low Bond Precision on C-C Bonds](#) 0.00813 [Ang.](#)
PLAT369_ALERT_2_C [Long C\(sp2\)-C\(sp2\) Bond](#) C3 - C6 . 1.53 [Ang.](#)
PLAT369_ALERT_2_C [Long C\(sp2\)-C\(sp2\) Bond](#) C9 - C12 . 1.54 [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](#): C18 H18 Cl6 Hg3 N3 O9 Tb1
 Atom count from [_chemical_formula_moiety](#):
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](#): C18 H18 Cl6 Hg3 N3 O9 Tb1
 Atom count from the [_atom_site](#) data: C18 H12 Cl6 Hg3 N3 O9 Tb1
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](#) C18 H18 Cl6 Hg3 N3 O9 Tb
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	72.00	72.00	0.00
H	72.00	48.00	24.00
Cl	24.00	24.00	0.00
Hg	12.00	12.00	0.00
N	12.00	12.00	0.00
O	36.00	36.00	0.00
Tb	4.00	4.00	0.00

PLAT003_ALERT_2_G [Number of Uiso or Uij Restrained non-H Atoms](#) ... 17 [Report](#)
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 !](#)
PLAT042_ALERT_1_G [Calc. and Reported MoietyFormula Strings](#) Differ [Please Check](#)
PLAT066_ALERT_1_G [Predicted and Reported Tmin&Tmax Range](#) Identical [? Check](#)
PLAT083_ALERT_2_G [SHELXL Second Parameter in WGHT](#) Unusually Large 213.61 [Why ?](#)
PLAT093_ALERT_1_G [No s.u.'s on H-positions, Refinement Reported as](#) mixed [Check](#)
PLAT199_ALERT_1_G [Reported _cell_measurement_temperature](#) (K) 293 [Check](#)
PLAT200_ALERT_1_G [Reported _diffn_ambient_temperature](#) (K) 293 [Check](#)
PLAT300_ALERT_4_G [Atom Site Occupancy of O3WB](#) Constrained at 0.7 [Check](#)
PLAT300_ALERT_4_G [Atom Site Occupancy of O3WA](#) Constrained at 0.3 [Check](#)
PLAT302_ALERT_4_G [Anion/Solvent/Minor-Residue Disorder \(Resd 2 \)](#) 100% [Note](#)
PLAT302_ALERT_4_G [Anion/Solvent/Minor-Residue Disorder \(Resd 3 \)](#) 100% [Note](#)
PLAT311_ALERT_2_G [Isolated Disordered Oxygen Atom \(No H's ?\)](#) O3WB [Check](#)

PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	03WA	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	2	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Hg3 (II) .	2.13	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Tb1 (III) .	3.23	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	102	Note
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
0 **ALERT level B** = A potentially serious problem, consider carefully
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected

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

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
_publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
```

```

RESPONSE: ...
;
_vrf_PLAT602_I
;
PROBLEM: VERY LARGE Solvent Accessible VOID(S) in Structure      ! Info
RESPONSE: ...
;
# end Validation Reply Form

```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 19/10/2018; check.def file version of 15/10/2018

Datablock I - ellipsoid plot

