checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

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Bond precision:   C-C = 0.0183 A          Wavelength=0.71073

Cell:             a=15.954(4)     b=28.0512(19)       c=26.982(3)
                  alpha=90        beta=90.462(9)      gamma=90
Temperature:      100 K
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	Calculated	Reported
Volume	12075(3)	12074(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	4(C54 H78 Bi3 Ce3 Tl), 8(C18 H36 K N2 O6), C9 H14, 0.5(C6 H14),	C54 H78 Bi4 Ce3 Tl, 2(C18 H36 K N2 O6), 0.25(C9 H14), 0.25(C3 H
Sum formula	C372 H621 Bi16 Ce12 K8 N16 O48 Tl4 [+ solvent]	C93 H155.25 Bi4 Ce3 K2 N4 O12 Tl
Mr	12241.31	3060.30
Dx,g cm-3	1.683	1.683
Z	1	4
Mu (mm-1)	8.359	8.359
F000	5849.0	5849.0
F000'	5775.64	
h,k,lmax	18,33,32	18,33,32
Nref	21258	21239
Tmin,Tmax	0.009,0.081	0.561,0.746
Tmin'	0.005	

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Correction method= # Reported T Limits: Tmin=0.561 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.999           Theta(max)= 25.000
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R(reflections)= 0.0567(15425)

wR2(reflections)= 0.1235(21239)

S = 1.062 Npar= 1139

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

PLAT307_ALERT_2_A Isolated Metal Atom found in Structure (Unusual) Bi4A Check

Author Response: This is an error of the software, which does not consider the (normal) Bi-Atom bond lengths as bonds. All Bi atoms are properly connected to other atoms.

PLAT307_ALERT_2_A Isolated Metal Atom found in Structure (Unusual) Bi4B Check

Author Response: This is an error of the software, which does not consider the (normal) Bi-Atom bond lengths as bonds. All Bi atoms are properly connected to other atoms.

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 11 Note

Author Response: This is due to the geometry of our measurement device, but does not affect the validation of the data and the correctness of the refinement result.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.146
PLAT213_ALERT_2_C Atom C48 has ADP max/min Ratio ..... 3.1 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C24 --C25 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C37 --C44 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O1 --C56 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O1 --C57 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C73 --C74 . 0.20 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C57 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of K2 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01828 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.834 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 6 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.01Ang From Bi4B 1.73 eA-3

PLAT977_ALERT_2_C Check Negative Difference Density on H1 . -0.53 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H9C . -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H12B . -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H19 . -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H21C . -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H23A . -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H50A . -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H56A . -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H58B . -0.40 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H62B . -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H65A . -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H81A . -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H84A . -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H89B . -0.34 eA-3

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 3 Report
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.146 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.250 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 109.07 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Tl1A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Tl1B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C91 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C92 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C93 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C94 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C95 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C96 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C97 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C98 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C99 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H91A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H91B Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H93A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H93B Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H93C Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H95A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H95B Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H95C Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H97A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H97B Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H97C Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H99A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H99B Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H99C Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C100 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C101 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C103 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10B Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10C Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10D Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10E Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10F Constrained at 0.25 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of H10G       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Bi4A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Bi4B       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         2% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  4  )       5.75 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  6  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  7  )       0.50 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C9 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C39 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.50 Dev...       1.50 Degree
             C98     -C99     -H99C       1_555  1_555  1_555     #  974 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
             H99A    -C99     -H99B       1_555  1_555  1_555     #  975 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          2 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
             C18 H36 K N2 O6
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          2 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        18 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        52% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          4 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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2 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
28 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
68 **ALERT level G** = General information/check it is not something unexpected

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

PLATON version of 06/07/2023; check.def file version of 30/06/2023

Datablock 1 - ellipsoid plot