checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1_sphaerisch

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_sphaerisch

Bond precision: C-C = 0.0132 A Wavelength=0.71073

Cell: a=15.9933(7) b=28.0507(12) c=27.0409(11)
alpha=90 beta=90.246(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	12131.1(9)	12131.1(9)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C54 H78 Bi3 La3 Sn2, 2(C18 H36 K N2 O6), 0.667(C7 H8) [+ solven	C54 H78 Bi3 La3 Sn2, 2(C18 H36 K N2 O6), 0.667(C7 H8)
Sum formula	C94.67 H155.33 Bi3 K2 La3 N4 O12 Sn2 [+ solvent]	C94.67 H155.33 Bi3 K2 La3 N4 O12 Sn2
Mr	2900.85	2900.81
Dx,g cm-3	1.588	1.588
Z	4	4
Mu (mm-1)	5.888	5.888
F000	5621.3	5621.0
F000'	5568.10	
h,k,lmax	20,35,34	20,35,34
Nref	25911	25636
Tmin,Tmax	0.932,0.943	0.006,0.010
Tmin'	0.029	

Correction method= # Reported T Limits: Tmin=0.006 Tmax=0.010
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 26.788

R(reflections)= 0.0454(14660)

wR2(reflections)= 0.1097(25636)

S = 0.900 Npar= 1196

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 C

PLAT214_ALERT_2_C	Atom C1_1 (Anion/Solvent) ADP max/min Ratio	4.8	prolat
PLAT234_ALERT_4_C	Large Hirshfeld Difference C55 --C56 .	0.23	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C67 --C68 .	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N3 --C79 .	0.17	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C61	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C85	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	3.4	Note
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01315	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	25	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H44C .	-0.31	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H82B .	-0.32	eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	14	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	9	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	6	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	10	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	4	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C1_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C7_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C6_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1A_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1B_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1C_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4_1 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1_2 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5_2 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C7_2 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2_2 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C6_2 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3_2 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4_2 Constrained at	0.3333	Check

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PLAT300_ALERT_4_G Atom Site Occupancy of H1A_2      Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1B_2      Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1C_2      Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5_2       Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7_2       Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6_2       Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3_2       Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4_2       Constrained at     0.3333 Check
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
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         30 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        319 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        249 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         25 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  49 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
  46 ALERT type 4 Improvement, methodology, query or suggestion
   0 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.

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

Datablock 1_sphaerisch - ellipsoid plot