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

Bond precision: C-C = 0.0218 A Wavelength=1.34143

Cell: a=27.2073(14) b=27.2073(14) c=35.229(2)
alpha=90 beta=90 gamma=120
Temperature: 150 K

	Calculated	Reported
Volume	22584(3)	22584(3)
Space group	R -3	R -3
Hall group	-R 3	-R 3
Moiety formula	C60, 2(C24 H20 S6 Sn4) [+ solvent]	2(C24 H20 S6 Sn4), C60, 1.2[C7H8], 1.2[C4H8O]
Sum formula	C108 H40 S12 Sn8 [+ solvent]	C108 H40 S12 Sn8
Mr	2671.80	2671.64
Dx,g cm-3	1.768	1.768
Z	9	9
Mu (mm-1)	12.436	12.267
F000	11520.0	11520.0
F000'	11577.95	
h,k,lmax	32,32,41	32,32,41
Nref	8708	8688
Tmin,Tmax	0.165,0.293	0.165,0.293
Tmin'	0.057	

Correction method= # Reported T Limits: Tmin=0.165 Tmax=0.293
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 52.498

R(reflections)= 0.0757(5356) wR2(reflections)= 0.2046(8688)

S = 1.056 Npar= 687

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

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02179 Ang.

Author Response: This is due to a slightly limited quality of the crystal and the diffraction data.

Alert level C

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RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.129
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .....      0.129 Report
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.609 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.591         20 Report
               0  3  0,  -2  4  0,  -7 13  1,  11 19  1,  -5 30  1, -19 30  2,
               1  3  4,   0  7  5,  12 19  5,  12 18  6, -20 31  6,   2 13 10,
             -14 12 13, -22 15 17,  -9 24 18, -11 20 20,  -1  4 22,  -1 10 25,
              -9 24 27, -11  7 39,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.41Ang From S6              1.52 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Sn4       1.30 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Sn4       1.28 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Sn1       1.19 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Sn3       1.09 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.87Ang From C3      .      -0.95 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H32       .      -0.80 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H34       .      -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H38       .      -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H40       .      -0.41 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H45       .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H53B      .      -0.32 eA-3
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Alert level G

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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:   C108 H40 S12 Sn8
           Atom count from _chemical_formula_moiety:C116.4 H49.6 S12 Sn8
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        32 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms         66 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
             Calc: C60, 2(C24 H20 S6 Sn4)
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              Rep.: 2(C24 H20 S6 Sn4), C60, 1.2[C7H8], 1.2[C4H8O]
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       1.38 %
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.12 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         42 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
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)        35% Note
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C1 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C3 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C4 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C5 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C13 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C14 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C15 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C16 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C18 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C20 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C22 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C23 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C24 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C27 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C30 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        869 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        32% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         11 Note
               -7 13  1,   2 13 10, -11 20 20,  -1  4 22,  -2  4  0, -22 15 17,
               -1 10 25,   0  7  5,   0  3  0, -14 12 13,   1  3  4,
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..      105.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..........      3.741 Note
              Predicted wR2: Based on SigI**2  5.47 or SHELX Weight 19.37
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
PLAT984_ALERT_1_G The Sn-f'=    0.1615 Deviates from the B&C-Value     0.1164 Check
PLAT985_ALERT_1_G The Sn-f"=    4.3614 Deviates from the B&C-Value     4.3256 Check
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  1 ALERT level B = A potentially serious problem, consider carefully
 16 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 56 ALERT level G = General information/check it is not something unexpected

  7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 32 ALERT type 2 Indicator that the structure model may be wrong or deficient
 24 ALERT type 3 Indicator that the structure quality may be low
  7 ALERT type 4 Improvement, methodology, query or suggestion
  3 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 13/05/2024; check.def file version of 04/05/2024

Datablock 1 - ellipsoid plot