checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3

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: 3

Bond precision: C-C = 0.0115 A Wavelength=1.34143

Cell: a=18.6432(11) b=25.1311(15) c=28.9919(17)
alpha=90 beta=90 gamma=90
Temperature: 180 K

	Calculated	Reported
Volume	13583.4(14)	13583.4(14)
Space group	P b n b	P b n b
Hall group	-P 2bc 2ab	-P 2bc 2ab
Moiety formula	2(C60), 2(C24 H20 Se6 Sn4), 2(C7 H8), C4 H8 O	C24 H20 Se6 Sn4, C7 H8, 0.5(C4 H8 O), 1(C60)
Sum formula	C186 H64 O Se12 Sn8	C93 H32 O0.50 Se6 Sn4
Mr	4211.57	2105.70
Dx,g cm-3	2.059	2.059
Z	4	8
Mu (mm-1)	10.627	10.627
F000	7984.0	7984.0
F000'	7946.98	
h,k,lmax	22,30,35	22,30,35
Nref	13304	12910
Tmin,Tmax	0.397,0.588	0.397,0.588
Tmin'	0.300	

Correction method= # Reported T Limits: Tmin=0.397 Tmax=0.588
AbsCorr = MULTI-SCAN

Data completeness= 0.970 Theta(max)= 55.716

R(reflections)= 0.0344(6521) wR2(reflections)= 0.0469(12910)

S = 0.875 Npar= 1547

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

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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C60), 2(C24 H20 Se6 Sn4), 2(C7 H8), C4 H8 O
             Rep.: C24 H20 Se6 Sn4, C7 H8, 0.5(C4 H8 O), 1(C60)
PLAT088_ALERT_3_C Poor Data / Parameter Ratio .....................       8.35 Note
PLAT213_ALERT_2_C Atom C4A             has ADP max/min Ratio .....        3.6 prolat
PLAT213_ALERT_2_C Atom C7A             has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom C27A            has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom C28A            has ADP max/min Ratio .....        3.4 prolat
PLAT213_ALERT_2_C Atom C29A            has ADP max/min Ratio .....        3.2 oblate
PLAT213_ALERT_2_C Atom C53A            has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C3B             has ADP max/min Ratio .....        3.3 oblate
PLAT213_ALERT_2_C Atom C7B             has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C31B            has ADP max/min Ratio .....        3.7 oblate
PLAT213_ALERT_2_C Atom C38B            has ADP max/min Ratio .....        3.6 oblate
PLAT234_ALERT_4_C Large Hirshfeld Difference C79      --C84      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C82      --C83      .       0.17 Ang.
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C90 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       C85      0.125 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01148 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H89      ..H91B     .       1.89 Ang.
                                                    x,y,z  =      1_555 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.464 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         91 Report
                2  0  0,   4  0  0,   0  2  0,   2  2  0,   3  2  0,   4  2  0,
                0  6  0,   0 20  0,  11 24  0,   3  0  1,   2  1  1,   3  1  1,
                4  1  1,   3  2  1,   4  2  1,   3  3  1,   4  3  1,   2  0  2,
                4  0  2,   3  1  2,   4  1  2,   5  1  2,   4  2  2,   3  3  2,
                4  3  2,   3  4  2,   4  4  2,   3  0  3,   3  1  3,   4  1  3,
                0 16  3,   1 16  3,   0 18  3,   4  0  4,   3  1  4,   4  1  4,
                0  2  4,   0 16  4,   0 18  4,   3 19  5,   4 19  5,   9 27  5,
                0  4  6,   9 27  6,   1  5  7,   0 16  7,   3 29  8,   1 29  9,
                1 18 12,   8 26 12,   7 26 13,   0 10 14,  12 18 14,   6 14 16,
               13 20 16,   0 26 16,  10 20 17,  11 21 17,  18  0 18,  19  1 18,
                5 13 18,   3 14 18,   2 18 18,   9 21 18,  10 21 18,  11 21 18,
               15 13 19,   9 21 19,   9 22 19,  10 10 20,  14 11 20,  13 13 20,
               14 13 20,  14 14 20,  13 17 20,   5 21 20,   8  2 21,  13 14 21,
               13 15 21,   5 22 21,   7  1 22,   3 23 22,   5  0 23,  11 17 23,
                0 22 23,   1 22 23,  13 13 24,   8 17 25,   0  0 26,  14  0 26,
                0  0 32,
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Alert level G

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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        116 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms         144 Report
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PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          3 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         78 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          7 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         11 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par     0.0100 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar     0.0200 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
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
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C86      --C87      .        6.0 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C90      --C91      .       14.8 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O1         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C92        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C93        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C94        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C95        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H92A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H92B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H93A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H93B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H94A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H94B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H95A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H95B       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)       100% Note
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    2)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)        18% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    5)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    1)      35.70 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)      24.30 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    5)       6.50 Check
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O1       .      133.1 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  Se1      ..C1A      .       3.38 Ang.
                                          1/2-x,1/2+y,z  =      7_665 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         13 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............        4539 Note
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PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
                1  0  1,   0  0  2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        301 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
                0  0  2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........        4.0 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..........      0.887 Note
             Predicted wR2: Based on SigI**2  5.30 or SHELX Weight  5.36
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 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
  21 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  65 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 ALERT type 2 Indicator that the structure model may be wrong or deficient
  29 ALERT type 3 Indicator that the structure quality may be low
  33 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 3 - ellipsoid plot