

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2

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: 2

Bond precision:	C-C = 0.0194 Å	Wavelength=1.34143
Cell:	a=23.0469(19) alpha=90	b=19.2279(18) beta=101.982(6) c=24.3732(18) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	10565.5(15)	10565.5(15)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	3(C60), 4(C24 H20 S6 Sn4), 2(C7 H8)	C31 H28 S6 Sn4, C24 H20 S6 Sn4, 1.5(C60)
Sum formula	C290 H96 S24 Sn16	C145 H48 S12 Sn8
Mr	6248.47	3124.07
Dx, g cm ⁻³	1.964	1.964
Z	2	4
Mu (mm ⁻¹)	11.895	11.895
F000	6040.0	6040.0
F000'	6067.30	
h, k, lmax	28, 23, 30	28, 23, 29
Nref	20815	19768
Tmin, Tmax	0.593, 0.788	0.593, 0.788
Tmin'	0.467	

Correction method= # Reported T Limits: Tmin=0.593 Tmax=0.788
AbsCorr = MULTI-SCAN

Data completeness= 0.950 Theta(max)= 55.883

R(reflections)= 0.0562(12746)

wR2(reflections)=
0.1605(19768)

S = 1.026

Npar= 1709

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

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
reddish

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.976 Why?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: 3(C60), 4(C24 H20 S6 Sn4), 2(C7 H8)
Rep.: C31 H28 S6 Sn4, C24 H20 S6 Sn4, 1.5(C60)
PLAT234_ALERT_4_C Large Hirshfeld Difference C01K --C01M . 0.23 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C042 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2) 2.4 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C1A 0.130 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C1 --C0 . 1.37 Ang.
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C00M --C03P . 1.37 Ang.
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C00R --C03N . 1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01939 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C025 - C030 . 1.53 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C02P - C030 . 1.56 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C038 - C045 . 1.53 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -1.380 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 456 Report
2 1 0, 3 0 0, 3 2 0, 3 16 0, 4 2 0, 5 0 0,
6 3 0, 7 0 0, 7 15 0, 9 0 0, 11 0 0, 13 0 0,
15 0 0, 17 0 0, 17 7 0, 19 0 0, 21 0 0, 23 0 0,
25 0 0, 27 0 0, -5 3 1, -4 2 1, -4 3 1, -4 16 1,
-3 2 1, -3 16 1, -2 1 1, -2 2 1, -1 1 1, 0 2 1,
3 1 1, 17 7 1, 18 7 1, -27 0 2, -25 0 2, -23 0 2,
-21 0 2, -19 0 2, -17 0 2, -15 0 2, -13 0 2, -11 0 2,
-9 0 2, -7 0 2, -5 0 2, -5 4 2, -4 3 2, -4 16 2,
-3 0 2, -3 2 2, -3 3 2, -2 2 2, -1 0 2, -1 2 2,
0 2 2, 0 3 2, 1 0 2, 2 0 2, 3 0 2, 4 0 2,
5 0 2, 7 0 2, 9 0 2, 9 10 2, 9 16 2, 11 0 2,
13 0 2, 13 11 2, 15 0 2, 17 0 2, 19 0 2, 21 0 2,
23 0 2, 25 0 2, -18 3 3, -10 14 3, -5 21 3, -4 2 3,
-4 3 3, -4 4 3, -3 3 3, -3 4 3, -2 3 3, -1 2 3,
0 3 3, 4 1 3, 10 10 3, 17 6 3, -27 0 4, -25 0 4,
-23 0 4, -21 0 4, -19 0 4, -17 0 4, -16 5 4, -15 0 4,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.65Ang From ClB 1.93 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.11Ang From ClB 1.54 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.11Ang From ClB 1.54 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.46Ang From ClB 1.51 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.96Ang From Sn08 -1.82 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.91Ang From Sn07 -1.82 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H1D . -0.33 eA-3



Alert level G

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

59 Note

[illegible]

[illegible]

PLAT367_ALERT_2_G	Long?	C(sp?)	-C(sp?)	Bond	C01T	-	C02Z	.	1.58	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)	-C(sp?)	Bond	C01T	-	C03L	.	1.52	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)	-C(sp?)	Bond	C01Y	-	C02R	.	1.54	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)	-C(sp?)	Bond	C027	-	C029	.	1.58	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)	-C(sp?)	Bond	C02J	-	C032	.	1.55	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)	-C(sp?)	Bond	C02K	-	C02X	.	1.51	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)	-C(sp?)	Bond	C02V	-	C03Y	.	1.51	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)	-C(sp?)	Bond	C02Y	-	C03F	.	1.56	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)	-C(sp?)	Bond	C033	-	C04A	.	1.58	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)	-C(sp?)	Bond	C036	-	C03U	.	1.56	Ang.
PLAT411_ALERT_2_G	Short	Inter	H...H	Contact	H03K	..	H04U	.	2.10	Ang.
						-x,1-y,-z	=		3_565	Check
PLAT411_ALERT_2_G	Short	Inter	H...H	Contact	H1F	..	H7	.	2.04	Ang.
						-x,-1/2+y,1/2-z	=		2_545	Check
PLAT411_ALERT_2_G	Short	Inter	H...H	Contact	H1F	..	H04U	.	1.73	Ang.
						-x,-1/2+y,1/2-z	=		2_545	Check
PLAT432_ALERT_2_G	Short	Inter	X...Y	Contact	C1E	..	C04U	.	2.77	Ang.
						-x,-1/2+y,1/2-z	=		2_545	Check
PLAT432_ALERT_2_G	Short	Inter	X...Y	Contact	C1E	..	C7	.	3.11	Ang.
						-x,-1/2+y,1/2-z	=		2_545	Check
PLAT432_ALERT_2_G	Short	Inter	X...Y	Contact	C1F	..	C04U	.	1.92	Ang.
						-x,-1/2+y,1/2-z	=		2_545	Check
PLAT432_ALERT_2_G	Short	Inter	X...Y	Contact	C1F	..	C7	.	2.15	Ang.
						-x,-1/2+y,1/2-z	=		2_545	Check
PLAT432_ALERT_2_G	Short	Inter	X...Y	Contact	C1F	..	C8	.	2.89	Ang.
						-x,-1/2+y,1/2-z	=		2_545	Check
PLAT432_ALERT_2_G	Short	Inter	X...Y	Contact	C1G	..	C7	.	2.78	Ang.
						-x,-1/2+y,1/2-z	=		2_545	Check
PLAT432_ALERT_2_G	Short	Inter	X...Y	Contact	C1G	..	C04U	.	2.99	Ang.
						-x,-1/2+y,1/2-z	=		2_545	Check
PLAT432_ALERT_2_G	Short	Inter	X...Y	Contact	C01W	..	C04L	.	3.07	Ang.
						x,y,z	=		1_555	Check
PLAT432_ALERT_2_G	Short	Inter	X...Y	Contact	C01W	..	C04T	.	3.15	Ang.
						x,y,z	=		1_555	Check
PLAT432_ALERT_2_G	Short	Inter	X...Y	Contact	C03B	..	C04P	.	3.19	Ang.
						x,y,z	=		1_555	Check
PLAT650_ALERT_4_G	SWAT	Instruction Used to Model Solvent Disorder							! Report	
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels								210 Note	
	Sn01	Sn02	Sn03	Sn04	Sn05	Sn06	Sn07	Sn08		
	S009	S00A	S00B	S00C	S00D	S00E	S00F	S00G		
	S00H	S00I	S00J	S00K	C00L	H00L	C00M	C00N		
	C00O	C00P	H00P	C00Q	H00Q	C00R	C00S	C00T		
	H00T	C00U	C00V	H00V	C00W	C00X	C00Y	C00Z		
	C010	C011	H011	C012	C013	C014	C015	C016		
	C017	H017	C018	C019	C01A	C01B	H01B	C01C		
	C01D	C01E	C01F	C01G	C01H	C01I	C01J	C01K		
	C01L	C01M	C01N	C01O	C01P	C01Q	C01R	C01S		
	C01T	C01U	C01V	C01W	C01X	H01X	C01Y	C01Z		
	C020	C021	C022	C023	H023	C024	C025	C026		
	C027	C028	C029	C02A	C02B	C02C	C02D	C02E		
	H02E	C02F	C02G	C02H	C02I	C02J	C02K	C02L		
	H02L	C02M	C02N	C02O	C02P	C02Q	C02R	C02S		
	C02T	H02T	C02U	C02V	C02W	C02X	C02Y	C02Z		
	C030	C031	C032	C033	C034	C035	H035	C036		
	C037	C038	C039	H039	C03A	C03B	C03C	H03C		
	C03D	C03F	C03G	H03G	C03H	C03I	C03J	H03J		
	C03K	H03K	C03L	C03M	H03M	C03N	H03N	C03O		

C03P	H03P	C03Q	H03Q	C03R	H03R	C03S	C03U
C03V	C03W	C03Y	C03Z	H03Z	C041	C042	H042
C045	C046	H046	C049	H049	C04A	C04B	H04B
C04D	H04D	C04F	H04F	C04G	H04G	C04H	H04H
C04J	H04J	C04K	H04K	C04L	H04L	C04O	H04O
C04P	H04P	C04S	H04S	C04T	H04T	C0	C04I
H04I	C04Q	H04Q	C04U	H04U	C04E	H04E	H1AA
H1AB	H1AC						

PLAT773_ALERT_2_G Check long C-C Bond in CIF: C04U --CIF 1.92 Ang.
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 2467 Note
 PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
 1 0 0,
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 583 Note
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.2 Low
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 6.439 Note
 Predicted wR2: Based on SigI**2 2.49 or SHELX Weight 15.63
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 24 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 148 **ALERT level G** = General information/check it is not something unexpected

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

Datablock 2 - ellipsoid plot

