

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 021bvi24

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: 021bvi24

Bond precision:	C-C = 0.0060 Å	Wavelength=1.54184	
Cell:	a=17.0537(3) alpha=90	b=9.2728(1) beta=111.898(2)	c=20.2706(3) gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	2974.22(9)	2974.22(8)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C36 H30 Sn2	2(C18 H15 Sn)	
Sum formula	C36 H30 Sn2	C36 H30 Sn2	
Mr	700.02	699.98	
Dx, g cm-3	1.563	1.563	
Z	4	4	
Mu (mm-1)	13.510	13.510	
F000	1384.0	1384.0	
F000'	1387.39		
h, k, lmax	21, 11, 25	21, 11, 25	
Nref	6231	6166	
Tmin, Tmax	0.087, 0.195	0.965, 0.982	
Tmin'	0.011		

Correction method= # Reported T Limits: Tmin=0.965 Tmax=0.982
AbsCorr = ANALYTICAL

Data completeness= 0.990 Theta (max)= 76.151

R(reflections)= 0.0370(5819)	wR2(reflections)= 0.1003(6166)
S = 1.035	Npar= 343

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

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.70Ang From Sn02 3.33 eA-3

Author Response: Residual electron density is observed around the heavy Sn atom.



Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C36 H30 Sn2
Rep.: 2(C18 H15 Sn)

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.58 Report

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.39Ang From Sn01 1.67 eA-3

Author Response: Residual electron density is observed around the heavy Sn atom.



Alert level G

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 68 Note

Sn01	Sn02	C003	C004	C005	H005	C006	C007
C008	C009	H009	C00A	H00A	C00B	H00B	C00C
H00C	C00D	C00E	H00E	C00F	H00F	C00G	H00G
C00H	H00H	C00I	H00I	C00J	H00J	C00K	H00K
C00L	H00L	C00M	H00M	C00N	H00N	C00O	H00O
C00P	H00P	C00Q	H00Q	C00R	H00R	C00S	H00S
C00T	H00T	C00U	H00U	C00V	H00V	C00W	H00W
C00X	H00X	C00Y	H00Y	C00Z	H00Z	C010	H010
C011	H011	C012	H012				

PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C36 H30 Sn2

PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
-1 0 1,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 64 Note

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.6 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.925 Note
Predicted wR2: Based on SigI**2 3.43 or SHELX Weight 9.69

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

4 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
3 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.

PLATON version of 19/12/2024; check.def file version of 19/12/2024

