

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) HR514_0m

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: HR514_0m

Bond precision:	Sn- O = 0.0023 A	Wavelength=0.71073	
Cell:	a=7.8788 (1) alpha=90	b=7.8788 (1) beta=90	c=9.0582 (2) gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	562.292 (19)	562.292 (19)	
Space group	P -4 21 c	P -4 21 c	
Hall group	P -4 2n	P -4 2n	
Moiety formula	H4 O8 Sn6	?	
Sum formula	H4 O8 Sn6	H4 O8 Sn6	
Mr	844.29	844.17	
Dx, g cm ⁻³	4.987	4.986	
Z	2	2	
Mu (mm ⁻¹)	13.133	13.133	
F000	736.0	736.0	
F000'	728.47		
h, k, lmax	12, 12, 14	12, 12, 14	
Nref	1241 [724]	1242	
Tmin, Tmax	0.388, 0.383	0.414, 0.545	
Tmin'	0.359		

Correction method= # Reported T Limits: Tmin=0.414 Tmax=0.545
AbsCorr = MULTI-SCAN

Data completeness= 1.72/1.00 Theta(max)= 34.963

R(reflections)= 0.0127 (1221)	wR2(reflections)= 0.0278 (1242)
S = 1.332	Npar= 35

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 G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT019_ALERT_1_G	_diffn_measured_fraction_theta_full/*_max < 1.0	0.998	Report
PLAT794_ALERT_5_G	Tentative Bond Valency for Sn1 (II) .	1.97	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sn2 (II) .	1.92	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	70.0	Degree

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
0 **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

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

