

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: O- C = 0.0050 A Wavelength=0.71073

Cell: a=10.9403(10) b=12.7296(11) c=10.5843(9)
 alpha=90 beta=103.353(7) gamma=90

Temperature: 200 K

| | Calculated | Reported |
|----------------|-----------------|-----------------|
| Volume | 1434.2(2) | 1434.2(2) |
| Space group | P 21/c | P 21/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C6 H18 O8 P2 Sn | C6 H18 O8 P2 Sn |
| Sum formula | C6 H18 O8 P2 Sn | C6 H18 O8 P2 Sn |
| Mr | 398.85 | 398.83 |
| Dx,g cm-3 | 1.847 | 1.847 |
| Z | 4 | 4 |
| Mu (mm-1) | 2.028 | 2.028 |
| F000 | 792.0 | 792.0 |
| F000' | 790.59 | |
| h,k,lmax | 13,15,12 | 13,15,12 |
| Nref | 2515 | 2516 |
| Tmin,Tmax | 0.647,0.922 | 0.779,0.923 |
| Tmin' | 0.406 | |

Correction method= # Reported T Limits: Tmin=0.779 Tmax=0.923
AbsCorr = INTEGRATION

Data completeness= 1.000 Theta(max)= 24.991

R(reflections)= 0.0227(1793) wR2(reflections)= 0.0534(2516)

S = 0.918 Npar= 160

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 BPLAT019_ALERT_1_B _diffn_measured_fraction_theta_full/_max < 1.0 0.969 Report

Alert level CPLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for P1 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 3.590 Check

Alert level GPLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.11 Ratio
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still 51 %
PLAT953_ALERT_1_G Reported (CIF) and Actual (FCF) Hmax Differ by . 1 Units
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check

-
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
1 ALERT type 4 Improvement, methodology, query or suggestion
2 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*, 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 29/01/2015; check.def file version of 29/01/2015

Datablock shelx - ellipsoid plot

