checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelxl

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: shelxl

```
Bond precision:  C-C = 0.0059 A          Wavelength=0.71073

Cell:          a=12.3211(16)     b=14.0300(16)    c=15.1473(19)
               alpha=70.485(6)   beta=79.212(6)   gamma=68.642(6)
Temperature:   296 K
```

	Calculated	Reported
Volume	2292.1(5)	2292.1(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40 H54 O4 P2 S4 Sn	C40 H54 O4 P2 S4 Sn
Sum formula	C40 H54 O4 P2 S4 Sn	C40 H54 O4 P2 S4 Sn
Mr	907.76	907.76
Dx,g cm-3	1.315	1.315
Z	2	2
Mu (mm-1)	0.845	0.845
F000	940.0	940.0
F000’	940.37	
h,k,lmax	16,18,19	16,18,19
Nref	10981	10817
Tmin,Tmax	0.904,0.935	0.635,0.746
Tmin’	0.896	

```
Correction method= MULTI-SCAN

Data completeness= 0.985          Theta(max)= 27.920

R(reflections)= 0.0330( 8608)     wR2(reflections)= 0.0973( 10817)

S = 0.986                 Npar= 470
```

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

```
PLAT220_ALERT_2_B Large Non-Solvent    C     Ueq(max)/Ueq(min) ...        4.7 Ratio
PLAT241_ALERT_2_B High      Ueq as Compared to Neighbors for .....       C35 Check
```

Alert level C

```
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uiso(min) ..        5.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C33    --  C34'    ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C34'   --  C35     ..       0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C35    --  C36'    ..       0.24 Ang.
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         C5 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C19 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C21 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C39 Check
PLAT334_ALERT_2_C Small Average Benzene  C-C Dist. C1     -C6           1.37 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H35B   ..  H36C    ..       1.82 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.504
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600         10
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          1
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Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         6 Note
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..........    0.00600 Deg.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Sn1    --  S1      ..        7.7 su
PLAT301_ALERT_3_G Main Residue  Disorder ............ Percentage =         4 Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C7 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C8 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C15 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C16 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C24 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C31 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C32 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         6 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       158
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  13 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  11 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*, 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 18/09/2013; check.def file version of 12/09/2013

Datablock shelxl - ellipsoid plot