checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 20181115-sns-1

```
Bond precision:   Sn- S = 0.0037 A          Wavelength=0.71073

Cell:             a=11.1935(15)       b=3.9833(4)       c=4.3293(5)
                  alpha=90            beta=90           gamma=90
Temperature:      295 K

                  Calculated                  Reported
Volume            193.03(4)                   193.03(4)
Space group       P n m a                     P n m a
Hall group        -P 2ac 2n                   -P 2ac 2n
Moiety formula    S Sn                        0.25(S4 Sn4)
Sum formula       S Sn                        S Sn
Mr                150.77                       150.75
Dx,g cm-3         5.188                        5.187
Z                 4                            4
Mu (mm-1)         13.764                      13.764
F000              264.0                        264.0
F000'             261.94
h,k,lmax          13,4,5                       13,4,5
Nref              224                          224
Tmin,Tmax         0.150,0.290                 0.300,1.000
Tmin'             0.116

Correction method= # Reported T Limits: Tmin=0.300 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000         Theta(max)= 26.370

R(reflections)= 0.0448( 200)     wR2(reflections)= 0.1135( 224)

S = 1.196                  Npar= 13
```

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

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension        2 Info
PLAT012_ALERT_1_G No        _shelx_res_checksum Found in CIF ......   Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ   Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     5.07 Why ?
PLAT794_ALERT_5_G Tentative Bond Valency for Sn1         (II)       .   1.90 Info
```

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   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
   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
   0 ALERT type 3 Indicator that the structure quality may be low
   0 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* 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 19/10/2018; check.def file version of 15/10/2018