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 = 0.0100 A         Wavelength=0.71073

Cell:               a=7.8788(1)      b=7.8788(1)      c=9.0582(2)
                    alpha=90         beta=90          gamma=90
Temperature:        100 K

                 Calculated                  Reported
Volume           562.292(19)                 562.292(19)
Space group      P 4/m n c                   P 4/m n c
Hall group       -P 4 2n                     -P 4 2n
Moiety formula   O8 Sn6                      ?
Sum formula      O8 Sn6                      H4 O8 Sn6
Mr               840.26                      844.17
Dx,g cm-3        4.963                       4.986
Z                2                           2
Mu (mm-1)        13.132                      13.133
F000             728.0                       736.0
F000'            720.48
h,k,lmax         12,12,14                    12,12,14
Nref             657                         657
Tmin,Tmax        0.388,0.383                 0.454,0.712
Tmin'            0.359

Correction method= # Reported T Limits: Tmin=0.454 Tmax=0.712
AbsCorr = MULTI-SCAN

Data completeness= 1.000           Theta(max)= 34.963

R(reflections)= 0.0400( 654)                wR2(reflections)=
                                            0.0841( 657)
S = 1.263                  Npar= 20
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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 A

```
PLAT213_ALERT_2_A Atom O1              has ADP max/min Ratio .....        5.6 prolat
PLAT975_ALERT_2_A Check Calcd Resid. Dens.  0.43Ang From O1      .       3.46 eA-3
PLAT975_ALERT_2_A Check Calcd Resid. Dens.  0.51Ang From O1      .       3.16 eA-3
PLAT976_ALERT_2_A Check Calcd Resid. Dens.  0.93Ang From O1      .      -2.50 eA-3
PLAT976_ALERT_2_A Check Calcd Resid. Dens.  0.80Ang From O1      .      -2.17 eA-3
```

Alert level B

```
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  0.43Ang From O1              3.46 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  0.51Ang From O1              3.16 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens.  0.13Ang From O1             -3.34 eA-3
```

Alert level C

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       3.91 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       3.87 eA-3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.885 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.94Ang From Sn1             2.11 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  2.03Ang From Sn1             1.65 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.79Ang From Sn1             1.60 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.45Ang From Sn1             1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.93Ang From O1             -2.50 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.80Ang From O1             -2.17 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.40Ang From Sn1            -1.97 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.70Ang From Sn1            -1.94 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  2.09Ang From O1             -1.55 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.93Ang From O1      .       0.92 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.07Ang From O1      .       0.90 eA-3
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:H4 O8 Sn6
           Atom count from the _atom_site data:  O8 Sn6
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  H4 O8 Sn6
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          H          8.00      0.00    8.00
          O         16.00     16.00    0.00
          Sn        12.00     12.00    0.00
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```
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0      0.998 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      24.97 Why ?
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  1  )      12.25 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Sn1       (II)      .       1.94 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sn2       (II)      .       1.94 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
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       70.0 Degree
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   5 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  16 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  12 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  24 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
   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.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock HR514_0m - ellipsoid plot