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: a

Bond precision: In- S = 0.0055 A Wavelength=0.71073

Cell: a=7.764(3) b=7.764(3) c=39.41(2)
alpha=90 beta=90 gamma=90
Temperature: 566 K

	Calculated	Reported
Volume	2376(2)	2375.6(19)
Space group	I 41/a m d	I4(1)/amd
Hall group	-I 4bd 2	?
Moiety formula	In S2	C2N2H9InS2
Sum formula	In S2	C2N2H9InS2
Mr	178.94	240.05
Dx,g cm-3	2.001	2.685
Z	16	16
Mu (mm-1)	4.508	4.554
F000	1296.0	1856.0
F000’	1288.51	
h,k,lmax	9,9,47	9,9,47
Nref	646	606
Tmin,Tmax	0.365,0.761	0.194,1.000
Tmin’	0.370	

Correction method= # Reported T Limits: Tmin=0.194 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.938 Theta(max)= 25.450

R(reflections)= 0.2593(481) wR2(reflections)= 0.7481(606)

S = 1.000 Npar= 43

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

```
CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
            calculated from the _atom_site* data lies outside
            the range 0.90 <> 1.10
           From the CIF: _cell_formula_units_Z                  16
           From the CIF: _chemical_formula_weight           240.05
           TEST: Calculate formula weight from _atom_site_*
           atom     mass    num     sum
           C        12.01    0.00    0.00
           H         1.01    0.00    0.00
           N        14.01    0.00    0.00
           S        32.07    2.00   64.13
           In      114.82    1.00  114.82
           Calculated formula weight              178.95
RFACG01_ALERT_3_A  The value of the R factor is > 0.20
            R factor given   0.259
RFACR01_ALERT_3_A  The value of the weighted R factor is > 0.45
            Weighted R factor given   0.748
RINTA01_ALERT_3_A  The value of Rint is greater than 0.25
            Rint given   0.371
PLAT020_ALERT_3_A The value of Rint is greater than 0.12 .........      0.371 Report
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low .......      0.938 Note
PLAT043_ALERT_1_A Calculated and Reported Mol. Weight Differ by ..      61.11 Check
PLAT082_ALERT_2_A High R1 Value ..................................       0.26 Report
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ...................       0.75 Report
PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of .        290 Ang3
```

Alert level B

```
CHEMS01_ALERT_1_B  The sum formula contains elements in the wrong order.
            N  precedes H
            Sequence must be C, H, then alphabetical.
CRYSS01_ALERT_1_B  The magnitudes of the crystal dimensions do not
                match the min, mid and max definitions
SHFSU01_ALERT_2_B  The absolute value of parameter shift to su ratio > 0.10
            Absolute value of the parameter shift to su ratio given   0.123
            Additional refinement cycles may be required.
PLAT080_ALERT_2_B Maximum Shift/Error ............................       0.12 Why ?
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X)  In1    --  S2      ..       11.0 s.u.
```

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as Multi-scan
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       1.02 %
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT234_ALERT_4_C Large Hirshfeld Difference In1    --  S1      ..       0.16 Ang.
```

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:C2 H9 In1 N2 S2
            Atom count from the _atom_site data:  In1 S2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z   16
```

```
          From the CIF: _chemical_formula_sum  C2N2H9InS2
          TEST: Compare cell contents of formula and atom_site data
          WARNING: Unexpected atom type is in site list: In
          WARNING: Unexpected atom type is in site list: S
          WARNING: Formula and atom_type_symbol element names mismatch.

          atom    Z*formula  cif sites diff
          C         32.00      0.00   32.00
          N         32.00      0.00   32.00
          H        144.00      0.00  144.00
          InS       32.00      0.00   32.00
           WARNING: Site labels do not match formula elements
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF      Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.99 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  In1    --  S3      ..        5.6 s.u.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.75 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for In1     (III)   .....       2.87 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

```
  10 ALERT level A = Most likely a serious problem - resolve or explain
   5 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   3 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 19/11/2015; check.def file version of 17/11/2015

Datablock a - ellipsoid plot