checkCIF/PLATON report

Structure factors have been supplied for datablock(s) alet_0m_a

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: alet_0m_a

Bond precision: C-C = 0.0042 A Wavelength=1.54178

Cell: a=12.7424(6) b=7.3373(3) c=15.3561(7)
alpha=90 beta=114.107(1) gamma=90
Temperature: 143 K

	Calculated	Reported
Volume	1310.50(10)	1310.50(10)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C9 H18 Cl In N2 S2	0.33(C9 H18 Cl In N2 S2)
Sum formula	C9 H18 Cl In N2 S2	C3 H6 Cl0.33 In0.33 N0.67 S0.67
Mr	368.64	122.88
Dx,g cm-3	1.868	1.868
Z	4	12
Mu (mm-1)	19.030	19.030
F000	736.0	736.0
F000’	741.78	
h,k,lmax	15,9,18	15,9,18
Nref	2589	2567
Tmin,Tmax	0.153,0.149	0.377,0.754
Tmin’	0.015	

Correction method= # Reported T Limits: Tmin=0.377 Tmax=0.754
AbsCorr = NONE

Data completeness= 0.992 Theta(max)= 72.423

R(reflections)= 0.0275(2556) wR2(reflections)= 0.0720(2567)

S = 1.198 Npar= 137

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 C

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ABSTY03_ALERT_1_C  The _exptl_absorpt_correction_type has been given as none.
           However values have been given for Tmin and Tmax. Remove
           these if an absorption correction has not been applied.
  From the CIF: _exptl_absorpt_correction_T_min   0.377
  From the CIF: _exptl_absorpt_correction_T_max   0.754
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        18 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....         4 Note
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....         1 Check
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C3 H6 Cl0.33 In0.33 N0.67 S0.
           Atom count from _chemical_formula_moiety:C2.97 H5.94 Cl0.33 In0.33 N0.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
          From the CIF: _cell_formula_units_Z   12
          From the CIF: _chemical_formula_sum  C3 H6 Cl0.33 In0.33 N0.67 S0.67
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         36.00     36.00    0.00
          H         72.00     72.00    0.00
          Cl         3.96      4.00   -0.04
          In         3.96      4.00   -0.04
          N          8.04      8.00    0.04
          S          8.04      8.00    0.04
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.33 Check
PLAT793_ALERT_4_G Model has Chirality at N1          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at N2          (Centro SPGR)          R Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         4 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         3 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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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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 03/05/2019; check.def file version of 29/04/2019

Datablock alet_0m_a - ellipsoid plot