

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	= 0.0000 A	Wavelength=0.71073
Cell:	a=10.6975 (16)	b=10.6975 (16) c=10.6975 (16)
	alpha=90	beta=90 gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	1224.2 (5)	1224.2 (5)
Space group	I -4 3 m	I -4 3 m
Hall group	I -4 2 3	I -4 2 3
Moiety formula	Cu ₄ S _{0.52} Se _{7.48} , 0.027 (Cu ₂₄), 2.568 (Te), 0.16 (Se), 0.099 (As),	?
Sum formula	As _{0.10} Cu _{7.96} S _{1.03} Se _{7.64} Te _{2.57}	As _{0.15} Cu ₁₂ S _{1.54} Se _{11.46} Te _{3.85}
Mr	1477.10	2215.65
Dx, g cm ⁻³	6.011	6.011
Z	3	2
Mu (mm ⁻¹)	31.999	31.999
F000	1931.5	1931.5
F000'	1935.01	
h, k, lmax	13, 13, 13	13, 12, 13
Nref	284 [164]	283
Tmin, Tmax	0.469, 0.619	0.562, 0.746
Tmin'	0.323	

Correction method= # Reported T Limits: Tmin=0.562 Tmax=0.746
AbsCorr = MULTII-SCAN

Data completeness= 1.73/1.00 Theta (max)= 27.407

R(reflections)= 0.0191(267)

wR2(reflections)=
0.0358(283)

S = 1.174

Npar= 24

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

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) 6.83 Note



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: As0.15 Cu12 S1.54 Se11.46 Te3.85
Atom count from the _atom_site data: As0.148 Cu11.94 S1.54 Se11.46 Te
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 2
From the CIF: _chemical_formula_sum As0.15 Cu12 S1.54 Se11.46 Te3.85
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
As	0.30	0.30	0.00
Cu	24.00	23.88	0.12
S	3.08	3.08	0.00
Se	22.92	22.92	0.00
Te	7.70	7.70	-0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2A as CU
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2B as CU
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 1.500 Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 3 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 4 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder (Resd 1) 62% Note
PLAT301_ALERT_3_G Main Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 7) 100% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact X3TE ..Se1 . 2.53 Ang.
z,y,x = 14_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact X3TE ..Se1 . 2.53 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact X3TE ..Se1 . 2.53 Ang.
y,z,x = 9_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 5 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note

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

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
10 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.

