

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: kenoargentotetrahedrite-zn

Bond precision:	= 0.0000 A	Wavelength=0.71073	
Cell:	a=10.4624 (4) alpha=90	b=10.4624 (4) beta=90	c=10.4624 (4) gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1145.23 (13)	1145.23 (13)	
Space group	I -4 3 m	I -4 3 m	
Hall group	I -4 2 3	I -4 2 3	
Moiety formula	Ag6.74 As0.58 Cu13.06 Fe1.80 S24 Sb7.42 Zn2.40, 0.876(S)	Ag3.371 As0.288 Cu6.529 Fe0.9 S12.438 Sb3.712 Zn1.2	
Sum formula	Ag6.74 As0.58 Cu13.06 Fe1.80 S24.88 Sb7.42 Zn2.40	Ag3.38 As0.30 Cu6.53 Fe0.90 S12.43 Sb3.71 Zn1.20	
Mr	3559.27	1779.22	
Dx, g cm-3	5.161	5.160	
Z	1	2	
Mu (mm-1)	16.345	16.347	
F000	1610.0	1610.0	
F000'	1608.60		
h, k, lmax	13, 13, 13	11, 10, 13	
Nref	295 [170]	294	
Tmin, Tmax	0.892, 0.922	0.911, 1.000	
Tmin'	0.892		
Correction method=	# Reported T Limits: Tmin=0.911 Tmax=1.000		
AbsCorr =	MULTI-SCAN		
Data completeness=	1.73/1.00	Theta (max)= 28.235	

R(reflections)= 0.0247(274)

wR2(reflections)=
0.0389(294)

S = 1.111

Npar= 22

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

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

Calc: Ag3.37 As0.29 Cu6.53 Fe0.90 S12.44 Sb3.71 Zn1.20

Rep.: Ag3.38 As0.30 Cu6.53 Fe0.90 S12.43 Sb3.71 Zn1.

20

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: Ag6.74 As0.58 Cu13.06 Fe1.80 S24 Sb7.42 Zn2.40, 0.876(S)

Rep.: Ag3.371 As0.288 Cu6.529 Fe0.9 S12.438 Sb3.712

Zn1.2

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) 7.73 Note



Alert level G

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: Ag3.38 As0.3 Cu6.53 Fe0.9 S12

Atom count from _chemical_formula_moiety: Ag3.371 As0.288 Cu6.529 Fe0.9

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: Ag3.38 As0.3 Cu6.53 Fe0.9 S12.43

Atom count from the _atom_site data: Ag3.372 As0.288 Cu6.528 Fe0.9 S1

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 Ag3.38 As0.30 Cu6.53 Fe0.90 S12.43

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
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Ag	6.76	6.74	0.02
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As	0.60	0.58	0.02
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Cu	13.06	13.06	0.00
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Fe	1.80	1.80	-0.00
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S	24.86	24.88	-0.02
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Sb	7.42	7.42	-0.00
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Zn	2.40	2.40	0.00
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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

PLAT017_ALERT_1_G Check Scattering Type Consistency of M2A as

AG

PLAT017_ALERT_1_G Check Scattering Type Consistency of M2B as

CU

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...

0.500 Check

PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	2	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffraction_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of M1CU Constrained at	0.65	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of M1ZN Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of M1FE Constrained at	0.15	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	81%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	7	Note
	M2A M2B M1CU M1ZN M1FE X3SB X3AS		
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 !
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2	Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	3	Units

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
 23 **ALERT level G** = General information/check it is not something unexpected

13 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
 2 ALERT type 3 Indicator that the structure quality may be low
 8 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.

