

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kenoargentotetrahedrite-Zn

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 Å

Wavelength=0.71073

Cell: a=10.4624(4) b=10.4624(4) c=10.4624(4)

 alpha=90

 beta=90

 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	Ag7.56 As0.56 Cu12.24 Fe1.68 S24.74 Sb7.44 Zn2.52	Ag3.78 As0.28 Cu6.12 Fe0.84 S12.372 Sb3.72 Zn1.26
Sum formula	Ag7.56 As0.56 Cu12.24 Fe1.68 S24.74 Sb7.44 Zn2.52	Ag3.78 As0.28 Cu6.12 Fe0.84 S12.37 Sb3.72 Zn1.26
Mr	3592.97	1796.36
Dx, g cm ⁻³	5.210	5.209
Z	1	2
Mu (mm ⁻¹)	16.332	16.332
F000	1623.3	1623.3
F000'	1620.85	
h, k, lmax	13, 13, 13	11, 10, 13
Nref	284[164]	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 = MULTII-SCAN

Data completeness= 1.79/1.04

Theta(max)= 28.235

R(reflections)= 0.0310(274)

wR2(reflections)=
0.0595(294)

S = 1.103

Npar= 18

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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.60Ang From Cu2	-1.51 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.60Ang From Cu2	-1.51 eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on Ag2	1.14 eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on Cu2	1.14 eA-3



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	19.97 Why ?
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	3 Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Sb1 Constrained at	0.93 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ag2 Constrained at	0.63 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of As1 Constrained at	0.07 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cu1 Constrained at	0.65 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Zn1 Constrained at	0.21 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cu2 Constrained at	0.37 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fe1 Constrained at	0.14 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	85% 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 !
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
PLAT996_ALERT_1_G	Non-Standard SHELXL LIST 4 Style FCF Supplied ..	! Check

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
10 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.

