



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: erzwiesite

Bond precision:	Pb- S = 0.0110 Å	Wavelength=0.71073	
Cell:	a=4.085 (5)	b=13.462 (15)	c=33.92 (4)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1865 (4)	1866 (4)	
Space group	C m c m	C m c m	
Hall group	-C 2c 2	-C 2c 2	
Moiety formula	Ag8.64 Bi16.32 Pb11.04 S40	?	
Sum formula	Ag8.64 Bi16.32 Pb11.04 S40	Ag8.23 Bi16.31 Pb11.43 S40	
Mr	7912.44	7946.82	
Dx, g cm-3	7.045	7.074	
Z	1	1	
Mu (mm-1)	66.477	67.207	
F000	3305.9	3318.0	
F000'	3210.77		
h, k, lmax	4, 13, 33	4, 13, 34	
Nref	583	352	
Tmin, Tmax	0.037, 0.095	0.050, 0.110	
Tmin'	0.002		

Correction method= # Reported T Limits: Tmin=0.050 Tmax=0.110
AbsCorr = EMPIRICAL

Data completeness= 0.604

Theta(max)= 20.842

R(reflections)= 0.0524(308)

wR2(reflections)=
0.1232(352)

S = 1.138

Npar= 51

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

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5006

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 empirical

PLAT018_ALERT_1_C _diffn_measured_fraction_theta_max .NE. *_full ! Check

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

Calc: Ag8.64 Bi16.32 Pb11.04 S40

Rep.: Ag8.23 Bi16.31 Pb11.43 S40

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 34.38 Check

PLAT051_ALERT_1_C Mu(calc) and Mu(cif) Ratio Differs from 1.0 by . 1.09 %

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT077_ALERT_4_C Unit-Cell Contains Non-integer Number of Atoms . Please Check

PLAT148_ALERT_3_C s.u. on the a - Axis is (Too) Large 0.005 Ang.

PLAT148_ALERT_3_C s.u. on the b - Axis is (Too) Large 0.0150 Ang.

PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large 0.040 Ang.

S2 S3 S4 S5 S6

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours S1 Check

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 3.3 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: Ag8.23 Bi16.31 Pb11.43 S40

Atom count from the _atom_site data: Ag8.64 Bi16.32 Pb11.04 S40

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 1

From the CIF: _chemical_formula_sum Ag8.23 Bi16.31 Pb11.43 S40

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Ag	8.23	8.64	-0.41
Bi	16.31	16.32	-0.01
Pb	11.43	11.04	0.39
S	40.00	40.00	0.00

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	63.32	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
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	44%	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Bi1 (III)	2.91	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb2 (II)	1.96	Info
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	7	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	150	Note
	2 6 5, 2 2 1, 2 0 8, 2 4 7, 1 1 17,	3	1 22,
	2 2 2, 1 11 1, 2 2 3, 0 6 15, 1 7 9,	2	6 14,
	4 2 4, 2 10 12, 1 1 16, 2 2 7, 1 9 21,	2	4 4,
	1 1 22, 2 2 0, 3 1 12, 0 4 14, 0 6 29,	1	5 15,
	3 5 3, 1 7 23, 2 4 13, 1 11 0, 1 9 0,	1	7 13,
	0 4 15, 0 2 20, 0 6 7, 3 1 9, 1 5 14,	0	8 25,
	0 0 20, 3 7 9, 2 2 9, 3 7 11, 2 10 0,	3	9 3,
	3 7 4, 1 11 17, 2 4 9, 2 6 2, 4 2 1,	3	1 7,
	3 3 9, 2 4 15,		
	(100 More NOT listed: see .ckf listing file)		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.1	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT994_ALERT_1_G	SHELXL .ins Contains no or MERG 0 Instruction ..		! Note

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
18 **ALERT level G** = General information/check it is not something unexpected
- 12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_THETM01_erzwiesite
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.550
RESPONSE: ...
;
_vrf_ABSTY02_erzwiesite
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;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT018_erzwiesite
;
PROBLEM: _diffn_measured_fraction_theta_max .NE. *_full           ! Check
RESPONSE: ...
;
_vrf_PLAT041_erzwiesite
;
PROBLEM: Calc. and Reported SumFormula      Strings      Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT043_erzwiesite
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..        34.38 Check
RESPONSE: ...
;
_vrf_PLAT051_erzwiesite
;
PROBLEM: Mu(calc) and Mu(cif) Ratio Differs from 1.0 by .        1.09 %
RESPONSE: ...
;
_vrf_PLAT068_erzwiesite
;
PROBLEM: Reported F000 Differs from Calcd (or Missing)...        Please Check
RESPONSE: ...
;
_vrf_PLAT077_erzwiesite
;
PROBLEM: Unit-Cell Contains Non-integer Number of Atoms .        Please Check
RESPONSE: ...
;
_vrf_PLAT148_erzwiesite
;
PROBLEM: s.u. on the          a          - Axis is (Too) Large ....    0.005 Ang.
RESPONSE: ...
;
_vrf_PLAT241_erzwiesite
;
PROBLEM: High MainResAtom Ueq as Compared to Neighbours          S1 Check
RESPONSE: ...
;
_vrf_PLAT250_erzwiesite
;
PROBLEM: Large U3/U1 Ratio for <U(i,j)> Tensor(Resd      1)        3.3 Note
RESPONSE: ...
;
# end Validation Reply Form

```

duplicate check

A reduced cell check using CCDC's cellCheckCSD service has found that one or more structures in this CIF are similar to those previously published in the CSD or the ICSD.

DATABLOCK: erzwiesite

- ICSD number: 169940



[Cell Parameters for 169940: 4.084,13.453,33.932(90,90,90)]

Datablock erzwiesite - ellipsoid plot

