

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: zincochenite

Bond precision: S- O = 0.0250 A

Wavelength=0.71075

Cell: a=5.883(4) b=7.938(5) c=7.948(5)
 alpha=110.511(12) beta=98.497(10) gamma=100.152(8)
Temperature: 293 K

	Calculated	Reported
Volume	333.2(4)	333.2(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	O14 Pb4 S2 Zn	?
Sum formula	O14 Pb4 S2 Zn	H6 O14 Pb4 S2 Zn
Mr	1182.31	1188.30
Dx, g cm ⁻³	5.892	5.922
Z	1	1
Mu (mm ⁻¹)	52.515	52.514
F000	502.0	508.0
F000'	490.69	
h, k, lmax	6, 9, 9	6, 9, 9
Nref	1162	1152
Tmin, Tmax	0.092, 0.350	0.470, 1.000
Tmin'	0.037	

Correction method= # Reported T Limits: Tmin=0.470 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.991

Theta(max)= 24.961

R(reflections)= 0.0874(936)

wR2(reflections)=
0.2558(1152)

S = 1.067

Npar= 97

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

PLAT213_ALERT_2_A Atom Oh2 has ADP max/min Ratio 8.6 oblate

Alert level B

PLAT213_ALERT_2_B Atom Oh1 has ADP max/min Ratio 4.6 prolat

Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -7.576
Test value = -6.150

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.145

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.145 Report

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 5.99 Check

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

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.26 Report

PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 8.21 eA-3

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -7.58 eA-3

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:H6 O14 Pb4 S2 Zn1
Atom count from the _atom_site data: O14 Pb4 S2 Zn1

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 1
From the CIF: _chemical_formula_sum H6 O14 Pb4 S2 Zn
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
H	6.00	0.00	6.00
O	14.00	14.00	0.00
Pb	4.00	4.00	0.00
S	2.00	2.00	0.00
Zn	1.00	1.00	0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 3 Note

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.0 Low

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

10 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
4 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

PLATON version of 19/02/2022; check.def file version of 19/02/2022

