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: cuprocherokeeite

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Bond precision:   S- O = 0.0550 A          Wavelength=0.71075

Cell:             a=12.6828(5)     b=9.4629(5)         c=14.7876(8)
                  alpha=90         beta=94.798(4)      gamma=90
Temperature:      293 K
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	Calculated	Reported
Volume	1768.53(15)	1768.53(15)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	Cu O34 Pb8 S4 Zn3, 2(O)	?
Sum formula	Cu O36 Pb8 S4 Zn3	Cu H12 O36 Pb8 S4 Zn3
Mr	2621.56	2633.51
Dx,g cm-3	4.923	4.945
Z	2	2
Mu (mm-1)	40.854	40.855
F000	2254.0	2278.0
F000'	2209.70	
h,k,lmax	12,9,14	12,9,14
Nref	1649	3226
Tmin,Tmax	0.390,0.442	0.995,1.000
Tmin'	0.011	

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Correction method= # Reported T Limits: Tmin=0.995 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.956           Theta(max)= 20.021

R(reflections)= 0.0746( 2411)                    wR2(reflections)=
                                                 0.2072( 3226)
S = 1.153                  Npar= 150
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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 = 0.4817

Alert level B

PLAT031_ALERT_4_B Refined Extinction Parameter Within Range of ... 1.563 Sigma
PLAT220_ALERT_2_B NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 10.0 Ratio
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of O6 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow2 Check

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Alert level C

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 11.95 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 1 Check
Ow2
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pb1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pb3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S2 Check

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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:H12 Cu1 O36 Pb8 S4 Zn3
Atom count from the _atom_site data: Cu1 O36 Pb8 S4 Zn3
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 2
From the CIF: _chemical_formula_sum Cu H12 O36 Pb8 S4 Zn3
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Cu	2.00	2.00	0.00
H	24.00	0.00	24.00
O	72.00	72.00	0.00
Pb	16.00	16.00	0.00
S	8.00	8.00	0.00
Zn	6.00	6.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 13 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 37.96 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 10 Report
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 ..... 10 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 10 Note

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PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         13 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.0 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 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
   4 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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 18/05/2022; check.def file version of 17/05/2022

Datablock cuprocherokeeite - ellipsoid plot