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: hayelasdiite

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Bond precision:   Cu- O = 0.0170 A         Wavelength=0.71075

Cell:           a=7.52089(15)       b=14.9345(3)      c=17.9895(13)
                alpha=106.727(8)    beta=90.965(6)    gamma=90.031(6)
Temperature:    293 K

                 Calculated                 Reported
Volume           1934.79(17)                1934.79(16)
Space group      P -1                       P -1
Hall group       -P 1                       -P 1
Moiety formula   Cu5 O29 Pb8 S12, 2(O)      ?
Sum formula      Cu5 O31 Pb8 S12            Cu5 H17 O31 Pb8 S12
Mr               2856.07                    2873.07
Dx,g cm-3        4.903                      4.932
Z                2                          2
Mu (mm-1)        38.091                     38.092
F000             2482.0                     2516.0
F000'            2440.02
h,k,lmax         9,19,23                    9,19,23
Nref             8885                       8835
Tmin,Tmax        0.036,0.218                0.256,1.000
Tmin'            0.000

Correction method= # Reported T Limits: Tmin=0.256 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994           Theta(max)= 27.474

R(reflections)= 0.0550( 5636)                wR2(reflections)=
                                             0.1741( 8835)
S = 1.098                  Npar= 505
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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

PLAT213_ALERT_2_A Atom Ow27 has ADP max/min Ratio ..... 15.1 prolat

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Alert level B

PLAT220_ALERT_2_B NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 6.2 Ratio
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow30 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow31 Check

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Alert level C

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 0.125
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 17.00 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.44 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 6.63 eA-3
PLAT213_ALERT_2_C Atom S6A has ADP max/min Ratio ..... 4.0 prolat
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O16 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cu1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S6 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:H17 Cu5 O31 Pb8 S12
Atom count from the _atom_site data: Cu5 O31 Pb8 S12
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 Cu5 H17 O31 Pb8 S12
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Cu	10.00	10.00	0.00
H	34.00	0.00	34.00
O	62.00	62.00	0.00
Pb	16.00	16.00	0.00
S	24.00	24.00	0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.125 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 33.34 Why ?
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem B 85 %Fit
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 ..... 12 Note

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PLAT794_ALERT_5_G Tentative Bond Valency for Cu3       (I)       .       1.09 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          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........        4.9 Low
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  14 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 19/02/2022; check.def file version of 19/02/2022

Datablock hayelasdiite - ellipsoid plot