checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Pb2SO5_Cu3P_925du12h_20230814_S2

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: Pb2SO5_Cu3P_925du12h_20230814_S2

Bond precision: P- O = 0.0060 A Wavelength=0.71073

Cell: a=9.8193(1) b=9.8193(1) c=7.3743(2)
alpha=90 beta=90 gamma=120
Temperature: 300 K

	Calculated	Reported
Volume	615.76(2)	615.76(2)
Space group	P 63/m	P 63/m
Hall group	-P 6c	-P 6c
Moiety formula	Cu1.09 O25.50 P6 Pb8.90	?
Sum formula	Cu1.09 O25.50 P6 Pb8.90	Cu0.27 O6.37 P1.50 Pb2.23 S0
Mr	2507.71	626.99
Dx,g cm-3	6.763	6.763
Z	1	4
Mu (mm-1)	62.027	62.053
F000	1055.6	1056.0
F000'	1030.28	
h,k,lmax	12,12,9	12,12,9
Nref	507	507
Tmin,Tmax	0.004,0.024	0.243,0.746
Tmin'	0.000	

Correction method= # Reported T Limits: Tmin=0.243 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 27.502

R(reflections)= 0.0196(486) wR2(reflections)= 0.0429(507)

S = 1.322 Npar= 48

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 B

PLAT213_ALERT_2_B Atom O1A has ADP max/min Ratio ..... 4.2 prolat
PLAT213_ALERT_2_B Atom O1B has ADP max/min Ratio ..... 4.2 prolat
PLAT250_ALERT_2_B Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 5.9 Note

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Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: Cu1.09 O25.50 P6 Pb8.90
Rep.: Cu0.27 O6.37 P1.50 Pb2.23 S0
PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check
PLAT213_ALERT_2_C Atom P1 has ADP max/min Ratio ..... 3.1 prolat
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for Cu2 2 Check
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 4.7 Ratio
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.026 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.90Ang From O4 . 0.69 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.87Ang From O2 . 0.62 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.08Ang From O4 . 0.48 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.98Ang From O3 . -0.43 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.95Ang From O2 . -0.42 eA-3

Alert level G

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 4
From the CIF: _chemical_formula_sum Cu0.27 O6.37 P1.50 Pb2.23 S0
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Cu	1.08	1.09	-0.01
O	25.48	25.50	-0.02
P	6.00	6.00	0.00
Pb	8.92	8.90	0.02
S	4.00	0.00	4.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.250 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.04 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 63% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) ..... O1A Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) ..... O1B Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.582 Note
Predicted wR2: Based on SigI**2 1.20 or SHELX Weight 3.24

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  0 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

  6 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
  3 ALERT type 3 Indicator that the structure quality may be low
  3 ALERT type 4 Improvement, methodology, query or suggestion
  3 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 19/12/2024; check.def file version of 19/12/2024

Datablock Pb2SO5_Cu3P_925du12h_20230814_S2 - ellipsoid plot