

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Pb2SO5\_Cu3P\_925du24h\_20230811\_S1

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\_925du24h\_20230811\_S1

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Bond precision:	P- O = 0.0063 A	Wavelength=0.71073	
Cell:	a=9.8327(3) alpha=90	b=9.8327(3) beta=90	c=7.3846(3) gamma=120
Temperature:	300 K		
	Calculated	Reported	
Volume	618.31(5)	618.31(5)	
Space group	P 63/m	P 63/m	
Hall group	-P 6c	-P 6c	
Moiety formula	Cu1.05 O25.48 P6 Pb8.95	?	
Sum formula	Cu1.05 O25.48 P6 Pb8.95	Cu0.26 O6.38 P1.50 Pb2.24 S0	
Mr	2513.71	628.61	
Dx, g cm-3	6.751	6.753	
Z	1	4	
Mu (mm-1)	62.033	62.041	
F000	1057.8	1058.0	
F000'	1032.32		
h,k,lmax	12,12,9	12,12,9	
Nref	511	512	
Tmin,Tmax	0.034,0.084	0.166,0.746	
Tmin'	0.000		

Correction method= # Reported T Limits: Tmin=0.166 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 1.002      Theta(max)= 27.488

R(reflections)= 0.0209( 486)

wR2(reflections)=  
0.0440( 512)

S = 1.276

Npar= 47

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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.

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### Alert level B

PLAT220_ALERT_2_B	NonSolvent	Resd 1	O	Ueq(max)/Ueq(min)	Range	6.5	Ratio
PLAT250_ALERT_2_B	Large U3/U1	Ratio for <U(i,j)>	Tensor(Resd	1)		5.0	Note

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### Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings	Differ	Please	Check
	Calc: Cu1.05 O25.48 P6 Pb8.95				
	Rep.: Cu0.26 O6.38 P1.50 Pb2.24 S0				
PLAT077_ALERT_4_C	Unit Cell Contains Non-integer Number of Atoms	.		Please	Check
PLAT213_ALERT_2_C	Atom O1A	has ADP max/min Ratio	.....	3.7	prolat
PLAT213_ALERT_2_C	Atom O1B	has ADP max/min Ratio	.....	3.7	prolat
PLAT218_ALERT_3_C	Constrained U(i,j) Components(s) for Cu2			2	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....		4.155	Check
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	1.06Ang From O4	.	0.50	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	1.05Ang From O4	.	0.48	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.96Ang From O2	.	0.45	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.87Ang From O2	.	0.45	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	1.01Ang From O4	.	-0.40	eA-3

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### 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 Cu0.26 O6.38 P1.50 Pb2.24 S0

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
Cu	1.04	1.05	-0.01
O	25.52	25.48	0.04
P	6.00	6.00	0.00
Pb	8.96	8.95	0.01
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	6.02	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 .....	3.409	Note
	Predicted wr2: Based on SigI**2 1.29 or SHELX Weight	3.45	

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
2 **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  
12 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.

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