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.

Datablock: cubothioplumbite

```
S-O=0.0080 A
                                            Wavelength=0.71075
Bond precision:
Cell:
                  a=14.9179(13)
                                    b=14.9179(13)
                                                       c=14.9179(13)
                                    beta=90
                  alpha=90
                                                       gamma=90
                  293 K
Temperature:
                 Calculated
                                             Reported
Volume
                 3319.9(9)
                                             3319.9(9)
Space group
                P a -3
                                             P a -3
Hall group
                -P 2ac 2ab
                                             -P 2ac 2ab
Moiety formula H4 O13 Pb5 S6
Sum formula
                H4 O13 Pb5 S6
                                             H1.33 O4.33 Pb1.67 S2
Mr
                 1440.39
                                             480.11
                 5.764
                                             5.763
Dx,g cm-3
                                             24
Mu (mm-1)
                 51.355
                                             51.355
                 4912.0
F000
                                             4912.0
F000'
                 4798.82
h, k, lmax
                 19,19,19
                                             19, 19, 19
Nref
                 1265
                                             1274
Tmin, Tmax
                 0.000,0.001
                                             0.486,1.000
Tmin'
                 0.000
Correction method= # Reported T Limits: Tmin=0.486 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 1.007
                                    Theta (max) = 27.432
                                                       wR2 (reflections) =
R(reflections) = 0.0353(1090)
                                                        0.0813 ( 1274)
S = 1.104
                           Npar= 79
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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 B

PLAT420_ALERT_2_B D-H Bond Without Acceptor Oh5 --H5 . Please Check

Alert level G

 ${\tt CELLZ01_ALERT_1_G~Difference~between~formula~and~atom_site~contents~detected.} \\ {\tt CELLZ01_ALERT_1_G~ALERT:~check~formula~stoichiometry~or~atom~site~occupancies.} \\ {\tt CELLZ01_ALERT_1_G~ALERT_1_G$

From the CIF: _cell_formula_units_Z 24
From the CIF: _chemical_formula_sum H1.33 04.33 Pb1.67 S2
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif site	es diff
H	31.92	32.00	-0.08
0	103.92	104.00	-0.08
Pb	40.08	40.00	0.08
S	48.00	48.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note 3 Info PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.33 Check PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 15.50 Why ? PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 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 2 Note PLAT794_ALERT_5_G Tentative Bond Valency for Pb3 (II) 1.64 Info (II) PLAT794_ALERT_5_G Tentative Bond Valency for Pb4 1.34 Info PLAT860_ALERT_3_G Number of Least-Squares Restraints 2 Note PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do ! PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 3 Note PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check

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0 ALERT level A = Most likely a serious problem - resolve or explain
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- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
- 1 ALERT type 3 Indicator that the structure quality may be low
- 2 ALERT type 4 Improvement, methodology, query or suggestion
- 3 ALERT type 5 Informative message, check

¹ ALERT level ${\bf B}$ = A potentially serious problem, consider carefully

⁰ 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

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 13/07/2021; check.def file version of 13/07/2021

