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: boojumite

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Bond precision:   S- O = 0.0200 A          Wavelength=0.71075

Cell:              a=14.0103(8)      b=20.5529(10)      c=7.2668(5)
                   alpha=90          beta=90            gamma=90
Temperature:       293 K

                 Calculated                 Reported
Volume           2092.5(2)                  2092.5(2)
Space group      P n m a                    P n m a
Hall group       -P 2ac 2n                  -P 2ac 2n
Moiety formula   O15 Pb8 S6                 ?
Sum formula      O15 Pb8 S6                 H2 O15 Pb8 S6
Mr               2089.96                    2091.90
Dx,g cm-3        6.634                      6.640
Z                4                          4
Mu (mm-1)        64.780                     64.780
F000             3488.0                     3496.0
F000'            3397.09
h,k,lmax         16,24,8                    16,24,8
Nref             1907                       1878
Tmin,Tmax        0.015,0.198                0.240,1.000
Tmin'            0.008

Correction method= # Reported T Limits: Tmin=0.240 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.985           Theta(max)= 25.023

R(reflections)= 0.0570( 1538)                wR2(reflections)=
                                             0.1477( 1878)
S = 1.052                  Npar= 135
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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

PLAT031_ALERT_4_A Refined Extinction Parameter Within Range of ... 0.750 Sigma

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.203

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT213_ALERT_2_C Atom O2 has ADP max/min Ratio ..... 3.1 prolat
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S1 Check

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:H2 O15 Pb8 S6
Atom count from the _atom_site data: O15 Pb8 S6
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 4
From the CIF: _chemical_formula_sum H2 O15 Pb8 S6
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
H	8.00	0.00	8.00
O	60.00	60.00	0.00
Pb	32.00	32.00	0.00
S	24.00	24.00	0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.203 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 ..... 1 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.12 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb5 (II) . 1.67 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 ..... 4.8 Low

1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  4 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
  2 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 19/02/2022; check.def file version of 19/02/2022

Datablock boojumite - ellipsoid plot