# 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: pohlite

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```
Bond precision:   I- O = 0.0083 A          Wavelength=0.71075

Cell:           a=7.3366(5)        b=9.5130(9)       c=16.2434(15)
                alpha=81.592(7)    beta=84.955(7)    gamma=89.565(6)
Temperature:    293 K

                Calculated                 Reported
Volume          1117.13(17)                1117.13(17)
Space group     P -1                       P -1
Hall group      -P 1                       -P 1
Moiety formula  Cl9 H I O7 Pb7             ?
Sum formula     Cl9 H I O7 Pb7             Cl9 H4 I O7 Pb7
Mr              2009.36                    2012.31
Dx,g cm-3       5.974                      5.982
Z               2                          2
Mu (mm-1)       55.027                     55.027
F000            1674.0                     1680.0
F000'           1634.36
h,k,lmax        8,11,19                    8,11,19
Nref            3952                       3941
Tmin,Tmax       0.017,0.012                0.603,1.000
Tmin'           0.009

Correction method= # Reported T Limits: Tmin=0.603 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997           Theta(max)= 25.028

R(reflections)= 0.0328( 3394)                wR2(reflections)=
                                             0.0709( 3941)
S = 1.107                  Npar= 221
```

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 C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       2.95 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT213_ALERT_2_C Atom O3              has ADP max/min Ratio .....        3.1 oblate
```

## 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:H4 Cl9 I1 O7 Pb7
           Atom count from the _atom_site data:  H1 Cl9 I1 O7 Pb7
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  Cl9 H4 I O7 Pb7
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          Cl        18.00     18.00    0.00
          H          8.00      2.00    6.00
          I          2.00      2.00    0.00
          O         14.00     14.00    0.00
          Pb        14.00     14.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       8.75 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT303_ALERT_2_G Full Occupancy Atom H7        with # Connections       2.00 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          4 Note
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          4 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.0 Low
```

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

8 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
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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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**PLATON version of 19/02/2022; check.def file version of 19/02/2022**

**Datablock pohlite** - ellipsoid plot