checkCIF/PLATON report

Structure factors have been supplied for datablock(s) KP2002_0m_d

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: KP2002_0m_d

```
Bond precision:   Pb- O = 0.0090 A         Wavelength=0.71073

Cell:               a=7.9693(3)      b=7.9693(3)      c=9.2741(3)
                    alpha=90         beta=90          gamma=90
Temperature:        100 K

                 Calculated                 Reported
Volume           589.00(5)                  589.00(5)
Space group      P 4/m n c                  P 4/m n c
Hall group       -P 4 2n                    -P 4 2n
Moiety formula   O8 Pb6                     ?
Sum formula      O8 Pb6                     H4 O8 Pb6
Mr               1371.20                    1375.17
Dx,g cm-3        7.732                      7.754
Z                2                          2
Mu (mm-1)        85.453                     85.455
F000             1112.0                     1120.0
F000'            1077.68
h,k,lmax         12,12,14                   12,12,14
Nref             688                        689
Tmin,Tmax        0.373,0.425                0.381,0.587
Tmin'            0.174

Correction method= # Reported T Limits: Tmin=0.381 Tmax=0.587
AbsCorr = MULTI-SCAN

Data completeness= 1.001           Theta(max)= 34.939

R(reflections)= 0.0217( 651)                    wR2(reflections)=
                                                0.0427( 689)
S = 1.090                  Npar= 20
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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

```
PLAT213_ALERT_2_A Atom O1              has ADP max/min Ratio .....        5.9 prolat
PLAT971_ALERT_2_A Check Calcd Resid. Dens.  0.45Ang From O1              4.45 eA-3
PLAT972_ALERT_2_A Check Calcd Resid. Dens.  0.13Ang From O1             -3.93 eA-3
PLAT975_ALERT_2_A Check Calcd Resid. Dens.  0.45Ang From O1      .       4.45 eA-3
PLAT976_ALERT_2_A Check Calcd Resid. Dens.  0.81Ang From O1      .      -2.01 eA-3
```

Alert level B

```
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  0.29Ang From O1              3.17 eA-3
PLAT976_ALERT_2_B Check Calcd Resid. Dens.  0.75Ang From O1      .      -1.90 eA-3
```

Alert level C

```
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       3.97 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.81Ang From O1             -2.01 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.75Ang From O1             -1.90 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.72Ang From Pb1            -1.73 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.62Ang From Pb1            -1.72 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.37Ang From O1             -1.62 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.63Ang From Pb1            -1.55 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.79Ang From O1      .       1.08 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.05Ang From O1      .       0.90 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.90Ang From O1      .      -0.89 eA-3
```

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 O8 Pb6
           Atom count from the _atom_site data:  O8 Pb6
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  H4 O8 Pb6
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          H          8.00      0.00    8.00
          O         16.00     16.00    0.00
          Pb        12.00     12.00    0.00
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      26.97 Why ?
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  1  )      12.25 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       1.94 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       1.98 Info
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       70.0 Degree
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  5 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
  8 ALERT level G = General information/check it is not something unexpected

  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 19 ALERT type 2 Indicator that the structure model may be wrong or deficient
  0 ALERT type 3 Indicator that the structure quality may be low
  1 ALERT type 4 Improvement, methodology, query or suggestion
  3 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.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock KP2002_0m_d - ellipsoid plot