checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Compound1

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: Compound1

```
Bond precision:   C-C = 0.0250 A          Wavelength=0.71073

Cell:             a=14.3357(2)      b=14.3357(2)      c=53.4365(8)
                  alpha=90          beta=90           gamma=120
Temperature:      100 K

                 Calculated                Reported
Volume           9510.6(3)                 9510.6(3)
Space group      R -3 c                    R -3 c
Hall group       -R 3 2"c                  -R 3 2"c
Moiety formula   C18 H7 N9 O22 Pb5         C18 H9 N9 O23 Pb5
Sum formula      C18 H7 N9 O22 Pb5         C18 H9 N9 O23 Pb5
Mr               1737.33                   1755.31
Dx,g cm-3        3.640                     3.640
Z                12                        12
Mu (mm-1)        26.573                    26.573
F000             9168.0                    9168.0
F000'            8985.18
h,k,lmax         17,17,64                  17,17,64
Nref             1942                      1944
Tmin,Tmax        0.004,0.033               0.013,0.134
Tmin'            0.002

Correction method= # Reported T Limits: Tmin=0.013 Tmax=0.134
AbsCorr = GAUSSIAN

Data completeness= 1.001          Theta(max)= 25.350

R(reflections)= 0.0521( 1926)                wR2(reflections)=
                                             0.1170( 1944)
S = 1.260                 Npar= 164
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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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.92Ang From Pb1 4.87 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre. This unaccounted residual density may be due to the non-bondin electron pair of the metal atom.

Alert level B

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 17.98 Check

Author Response: The difference between the calculated and reported molecular weight is due to the presence of a lattice water molecule contained in the voids of the structure. Although the water molecule has been confirmed to be complete by thermogravimetry, the residual density did not account for a whole molecule. Moreover, given that the molecule does not show a clear hydrogen bonding scheme, this molecule was not refined.

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.025 Ang.

Author Response: The presence of a heavy atom and a partially disordered water molecule occupying the voids causes some mismatches in the structure.

PLAT420_ALERT_2_B D-H Bond Without Acceptor O1 --H1 . Please Check

Author Response: The acceptor of this bond is the lattice water molecule that could not be properly refined.

PLAT601_ALERT_2_B Unit Cell Contains Solvent Accessible VOIDS of . 122 Ang**3

Author Response: The difference between the calculated and reported molecular weight is due to the presence of a lattice water molecule contained in the voids of the structure. Although the water molecule has been confirmed to be complete by thermogravimetry, the residual density did not account for a whole molecule. Moreover, given that the molecule does not show a clear hydrogen bonding scheme, this molecule was not refined.

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PLAT971_ALERT_2_B Check Calcd Resid. Dens.  0.92Ang From Pb1            2.53 eA-3
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Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre. This unaccounted residual density may be due to the non-bondin electron pair of the metal atom.

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PLAT972_ALERT_2_B Check Calcd Resid. Dens.  0.72Ang From Pb1           -3.47 eA-3
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Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre.

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PLAT975_ALERT_2_B Check Calcd Resid. Dens.  1.09Ang From O1      .      1.52 eA-3
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Author Response: Such unaccounted electron density corresponds to the lattice water molecule that could not be properly refined.

Alert level C

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DENSD01_ALERT_1_C  The ratio of the submitted crystal density and that
           calculated from the formula is outside the range 0.99 <> 1.01
           Crystal density given    =      3.640
           Calculated crystal density =      3.677
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT046_ALERT_1_C Reported Z, MW and D(calc) are Inconsistent ....      3.678 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O22 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Pb1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Pb3 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.915 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.92Ang From Pb1             2.22 eA-3
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Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre. This unaccounted residual density may be due to the non-bondin electron pair of the metal atom.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.92Ang From Pb1            1.89 eA-3
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Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre. This unaccounted residual density may be due to the non-bondin electron pair of the metal atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From Pb2 1.77 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre. This unaccounted residual density may be due to the non-bondin electron pair of the metal atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From Pb2 1.71 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre. This unaccounted residual density may be due to the non-bondin electron pair of the metal atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.93Ang From Pb1 1.66 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre. This unaccounted residual density may be due to the non-bondin electron pair of the metal atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.97Ang From Pb1 1.60 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre. This unaccounted residual density may be due to the non-bondin electron pair of the metal atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.22Ang From Pb1 1.58 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre. This unaccounted residual density may be due to the non-bondin electron pair of the metal atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.24Ang From Pb3 1.53 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre. This unaccounted residual density may be due to the non-bondin electron pair of the metal atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.24Ang From Pb3 1.53 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre. This unaccounted residual density may be due to the non-bondin electron pair of the metal atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.09Ang From O1 1.52 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre. This unaccounted residual density may be due to the non-bondin electron pair of the metal atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.48Ang From C15 -1.80 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.56Ang From Pb1 -1.75 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.84Ang From C17 -1.71 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.55Ang From Pb1 -1.67 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.55Ang From Pb1 -1.67 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.04Ang From C18   -1.67 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.04Ang From C18   -1.66 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.78Ang From C12   -1.56 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.44Ang From O171   -1.54 eA-3

Author Response: Although careful absorption correction has been applied to the data reduction, the Fourier map contains some substantially high maxima close to the metal centre.

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.85Ang From O1   .   1.47 eA-3

Author Response: Such unaccounted electron density corresponds to the lattice water molecule that could not be properly refined.

Alert level G

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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:C18 H9 N9 O23 Pb5
           Atom count from the _atom_site data:  C18 H7 N9 O22 Pb5
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   12
          From the CIF: _chemical_formula_sum  C18 H9 N9 O23 Pb5
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        216.00    216.00    0.00
          H        108.00     84.00   24.00
          N        108.00    108.00    0.00
          O        276.00    264.00   12.00
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           Pb        60.00     60.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    2663.02 Why ?
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.00 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       2.17 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.63 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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  1 ALERT level A = Most likely a serious problem - resolve or explain
  7 ALERT level B = A potentially serious problem, consider carefully
 28 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
 32 ALERT type 2 Indicator that the structure model may be wrong or deficient
  2 ALERT type 3 Indicator that the structure quality may be low
  1 ALERT type 4 Improvement, methodology, query or suggestion
  5 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 06/07/2023; check.def file version of 30/06/2023

Datablock Compound1 - ellipsoid plot