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: dinilawiite

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Bond precision:    S- O = 0.0233 A           Wavelength=0.71075

Cell:              a=17.4100(5)     b=9.2191(2)          c=21.6980(15)
                   alpha=90         beta=107.276(8)      gamma=90
Temperature:       293 K

                   Calculated                Reported
Volume             3325.5(3)                 3325.5(3)
Space group        I 2/a                     I 2/a
Hall group         -I 2ya                    -I 2ya
Moiety formula     Al4 O40 Pb16 S8, 2(O4 S), ?
                   12(O0.50)
Sum formula        Al4 O58 Pb16 S10          Al2 H0 O29 Pb8 S5
Mr                 4671.72                   2335.78
Dx,g cm-3          4.666                     4.665
Z                  2                         4
Mu (mm-1)          40.807                    40.807
F000               3976.0                    3976.0
F000'              3883.66
h,k,lmax           22,11,28                  22,11,28
Nref               3814                      3776
Tmin,Tmax          0.099,0.294               0.463,1.000
Tmin'              0.015

Correction method= # Reported T Limits: Tmin=0.463 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.990             Theta(max)= 27.485


R(reflections)= 0.0363( 3190)                     wR2(reflections)=
                                                  0.0846( 3776)

S = 1.070                     Npar= 201
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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**
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   Ow11 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   Ow12 Check

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🟡 **Alert level C**
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.46 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ....   1 Check
               O14
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   S1 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of   S Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   S   0.211 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   Ow11   0.274 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   Ow12   0.216 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   Ow13   0.154 Check

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⚪ **Alert level G**
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 Al2 H0 O29 Pb8 S5
          TEST: Compare cell contents of formula and atom_site data

          atom   Z*formula   cif sites diff
          Al   8.00   8.00   0.00
          H   4.00   0.00   4.00
          O   116.00   116.00   0.00
          Pb   32.00   32.00   0.00
          S   20.00   20.00   0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   1 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.500 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   162.50 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K)   293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O15   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O16   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow13   Constrained at   0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)   40% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5)   100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   Ow13 Check
PLAT395_ALERT_2_G Deviating X-O-Y   Angle From 120 for O15   .   68.8 Degree
PLAT395_ALERT_2_G Deviating X-O-Y   Angle From 120 for O16   .   61.5 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   9 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   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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 2 ALERT level B = A potentially serious problem, consider carefully
 8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
19 ALERT level G = General information/check it is not something unexpected

 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 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
 7 ALERT type 4 Improvement, methodology, query or suggestion
 1 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 10/05/2023; check.def file version of 10/05/2023

Datablock dinilawiite - ellipsoid plot