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: haywoodite

```
Bond precision:    S- O = 0.0045 A           Wavelength=0.71075

Cell:          a=8.35298(19)      b=13.2769(7)      c=18.2744(13)
               alpha=92.427(8)    beta=90.419(6)   gamma=108.214(4)
Temperature:   293 K

               Calculated                  Reported
Volume         1922.94(18)                 1922.94(18)
Space group    P -1                        P -1
Hall group     -P 1                        -P 1
Moiety formula H40 O72 Pb2.17 S6 Zn24,     ?
               13.778(O)
Sum formula    H40 O85.78 Pb2.17 S6 Zn24   H20 O42.89 Pb1.08 S3 Zn12
Mr             3623.57                     1810.86
Dx,g cm-3      3.129                       3.128
Z              1                           2
Mu (mm-1)      12.349                      12.333
F000           1720.0                      1719.0
F000'          1721.51
h,k,lmax       10,17,23                    10,17,23
Nref           8782                        8748
Tmin,Tmax      0.275,0.477                 0.668,1.000
Tmin'          0.219

Correction method= # Reported T Limits: Tmin=0.668 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996              Theta(max)= 27.451


R(reflections)= 0.0372( 6880)                      wR2(reflections)=
                                                   0.1002( 8748)
S = 1.051                    Npar= 641
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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
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PLAT430_ALERT_2_A Short Inter D...A Contact  W3        ..W12      .      2.45 Ang.
                                             x,y,z  =      1_555 Check
```

Alert level B
```
PLAT220_ALERT_2_B NonSolvent    Resd 1  O   Ueq(max)/Ueq(min) Range      9.8 Ratio
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......      W5 Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor  Oh13    --H13      .    Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor  Oh15    --H15      .    Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor  Oh18    --H18      .    Please Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O1      ..W10B     .      2.55 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O1      ..W12      .      2.63 Ang.
                                            1-x,1-y,1-z  =      2_666 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O7      ..W9B      .      2.83 Ang.
                                             x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O10     ..W9A      .      2.76 Ang.
                                             x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  W1      ..W6       .      2.79 Ang.
                                            1+x,y,z  =      1_655 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  W2      ..W8       .      2.82 Ang.
                                             x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  W3      ..W12      .      2.79 Ang.
                                            1-x,2-y,1-z  =      2_676 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  W5      ..W11      .      2.72 Ang.
                                             x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  W6      ..W11      .      2.68 Ang.
                                            1-x,1-y,1-z  =      2_666 Check
```

Alert level C
```
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..    Please Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       S2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       S3 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       W6    0.117 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       W11   0.225 Check
PLAT430_ALERT_2_C Short Inter D...A Contact  O2      ..W4       .      2.87 Ang.
                                            -1+x,-1+y,z  =      1_445 Check
PLAT430_ALERT_2_C Short Inter D...A Contact  O7      ..W9A      .      2.86 Ang.
                                             x,y,z  =      1_555 Check
PLAT430_ALERT_2_C Short Inter D...A Contact  O9      ..W6       .      2.89 Ang.
                                            x,y,1+z  =      1_556 Check
PLAT430_ALERT_2_C Short Inter D...A Contact  W9A     ..W11      .      2.89 Ang.
                                            1-x,1-y,1-z  =      2_666 Check
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Alert level G
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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      40 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension       3 Info
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PLAT017_ALERT_1_G Check Scattering Type Consistency of W1        as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W2        as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W3        as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W4        as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W5        as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W6        as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W7        as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W8        as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W9A       as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W9B       as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W10A      as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W10B      as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W11       as        O
PLAT017_ALERT_1_G Check Scattering Type Consistency of W12       as        O
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     0.50 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...  Please Check
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem      sub       94 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem        R       94 %Fit
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records      3 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)    293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)     293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )      2% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2 )    100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3 )    100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4 )    100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5 )    100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6 )    100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7 )    100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8 )    100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9 )    100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10 )    100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 11 )    100% Note
PLAT303_ALERT_2_G Full Occupancy Atom H1       with # Connections    1.96 Check
PLAT303_ALERT_2_G Full Occupancy Atom H5       with # Connections    1.96 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....    W4 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....    W6 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....    W7 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....    W8 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   W9A Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....  W10A Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   W11 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   W9B Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....  W10B Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   W12 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........     34 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............     20 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .  Please Do !
PLAT933_ALERT_2_G Number of 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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   1 **ALERT level A** = Most likely a serious problem – resolve or explain
  14 **ALERT level B** = A potentially serious problem, consider carefully
   9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  51 **ALERT level G** = General information/check it is not something unexpected

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

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40 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
13 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 13/07/2021; check.def file version of 13/07/2021

Datablock haywoodite - ellipsoid plot