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: 2019xy497a_a

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Bond precision:    = 0.0000 A                 Wavelength=0.71073

Cell:          a=10.3377(5)      b=10.3377(5)      c=10.3377(5)
               alpha=90          beta=90           gamma=90
Temperature:   293 K

               Calculated                Reported
Volume         1104.77(16)               1104.77(16)
Space group    F d -3 m                  F d -3 m
Hall group     -F 4vw 2vw                -F 4vw 2vw
Moiety formula Fe5.34 O48 Pb8.06 W10.68, Fe0.667 O6.62 Pb1.008
               4.96(O)                   W1.334
Sum formula    Fe5.34 O52.96 Pb8.06      Fe0.667 O6.62 Pb1.008
               W10.68                    W1.334
Mr             4778.85                   613.87
Dx,g cm-3      7.183                     7.382
Z              1                         8
Mu (mm-1)      60.062                    60.878
F000           2013.7                    2074.0
F000'          1985.07
h,k,lmax       14,14,14                  14,14,14
Nref           94                        94
Tmin,Tmax      0.308,0.296               0.613,1.000
Tmin'          0.285

Correction method= # Reported T Limits: Tmin=0.613 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000        Theta(max)= 29.088

R(reflections)= 0.0459( 80)     wR2(reflections)= 0.1269( 94)

S = 1.322                  Npar= 11
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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
PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by ..   132.11 Check

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🟡 Alert level C
ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies
                outside the range 0.99 <> 1.01
            Calculated value of mu =   60.053
            Value of mu given   =   60.878
ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as multi-scan
CHEMW01_ALERT_1_C The ratio of given/expected molecular weight as calculated
            from the _chemical_formula_sum lies outside
            the range 0.99 <> 1.01
            Calculated formula weight =   597.2795
            Formula weight given   =   613.8700
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .   1.34 %
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..   Please Check
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ....   8.55 Note
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ....   1 Check
                O2

⚪ Alert level G
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   1 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.13 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   39.59 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records   1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   1 Report
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 Pb1   Constrained at   0.504 Check
PLAT300_ALERT_4_G Atom Site Occupancy of W1   Constrained at   0.6672 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe1   Constrained at   0.3336 Check
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   83% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)   100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 1)   20.65 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 2)   0.03 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O2 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....   ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !

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

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

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3 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
9 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 05/12/2020; check.def file version of 05/12/2020