checkCIF/PLATON report

Structure factors have been supplied for datablock(s) linhuishi_TB_jinghuashangmao_20230803_S1

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: linhuishi_TB_jinghuashangmao_20230803_S1

```
Bond precision:   P- O = 0.0023 A          Wavelength=0.71073

Cell:               a=9.3731(4)      b=9.3731(4)      c=6.8769(3)
                    alpha=90         beta=90          gamma=120
Temperature:        300 K

                 Calculated                  Reported
Volume           523.23(5)                   523.23(5)
Space group      P 63/m                      P 63/m
Hall group       -P 6c                       -P 6c
Moiety formula   3(O4 P), H O, 5(Ca)         ?
Sum formula      Ca5 H O13 P3                Ca10 H2 O26 P6
Mr               502.32                      1004.63
Dx,g cm-3        3.188                       3.188
Z                2                           1
Mu (mm-1)        3.097                       3.097
F000             500.0                       500.0
F000'            503.15
h,k,lmax         12,12,8                     12,12,8
Nref             438                         438
Tmin,Tmax        0.805,0.857                 0.695,0.746
Tmin'            0.805

Correction method= # Reported T Limits: Tmin=0.695 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000            Theta(max)= 27.503

                                                    wR2(reflections)=
R(reflections)= 0.0220( 388)                        0.0492( 438)
S = 1.125                  Npar= 42
```

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

```
SHFSU01_ALERT_2_A  The absolute value of parameter shift to su ratio > 0.20
           Absolute value of the parameter shift to su ratio given   3.238
           Additional refinement cycles may be required.
```

Author Response: This is caused by the "vibration" of the O4 atom.

```
PLAT080_ALERT_2_A Maximum Shift/Error ..........................       3.24 Why ?
```

Author Response: This is caused by the "vibration" of the O4 atom.

Alert level B

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PLAT420_ALERT_2_B D-H Bond Without Acceptor  O4       --H1       .     Please Check
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Author Response: This problem may arise from the disordered nature of O4 and H1 atoms.

Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: Ca5 H O13 P3
             Rep.: Ca10 H2 O26 P6
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Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          2 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms          1 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...          2 Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at ............        0.5 Check
             O4      H1
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)        100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       0.33 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    3)       0.33 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)       0.50 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          7 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      5.067 Note
             Predicted wR2: Based on SigI**2  0.97 or SHELX Weight  4.38
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2 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully

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  1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 13 ALERT level G = General information/check it is not something unexpected

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  5 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
```

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 19/12/2024; check.def file version of 19/12/2024

Datablock linhuishi_TB_jinghuashangmao_20230803_S1 - ellipsoid plot