checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Aluminotaipingite-CeCa

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: Aluminotaipingite-CeCa

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Bond precision:    Si- O = 0.0160 A           Wavelength=0.71073

Cell:              a=10.658(3)        b=10.658(3)        c=37.865(9)
                   alpha=90           beta=90            gamma=120
Temperature:       293 K

                   Calculated                 Reported
Volume             3725(2)                    3725(2)
Space group        R 3 c                      R 3 c :H
Hall group         R 3 -2"c                   R 3 -2"c
Moiety formula     Al3.36 Ce45.22 F12 Fe2.64  ?
                   O174 Si42
Sum formula        Al3.36 Ce45.22 F12 Fe2.64  Al0.56 Ce7.54 F2 Fe0.44 O29
                   O174 Si42                  Si7
Mr                 10765.54                   1794.30
Dx,g cm-3          4.799                      4.799
Z                  1                          6
Mu (mm-1)          14.260                     14.260
F000               4822.8                     4823.0
F000'              4818.74
h,k,lmax           15,15,55                   15,15,54
Nref               2813[ 1410]                2640
Tmin,Tmax          0.604,0.652                0.766,1.000
Tmin'              0.560

Correction method= # Reported T Limits: Tmin=0.766 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 1.87/0.94        Theta(max)= 31.656
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R(reflections)= 0.0306( 2297)          wR2(reflections)=
                                       0.0669( 2640)

S = 1.124              Npar= 153
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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 C**
```
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..    Please Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.72Ang From Ce2          1.58 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.08Ang From F11          1.53 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.91Ang From Oh13   .     0.99 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.73Ang From Oh1    .     0.86 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.60Ang From Oh1    .     0.86 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.82Ang From O9     .    -0.80 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.75Ang From O9     .    -0.80 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.51Ang From Oh13   .    -0.71 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.94Ang From O9     .    -0.69 eA-3
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⚪ **Alert level G**
```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension        3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...    0.167 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...    Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    35.87 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
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )       19% Note
PLAT431_ALERT_2_G Short Inter HL..A Contact  F11       ..O2        .     2.75 Ang.
                              1/3-x+y,1/3-x,1/3+z  =      9_455 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  F11       ..O2        .     2.75 Ang.
                              2/3-y,1/3+x-y,1/3+z  =      8_555 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  F11       ..O2        .     2.75 Ang.
                              -1/3+x,-2/3+y,1/3+z  =      7_445 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  F12       ..O7        .     2.67 Ang.
                              1/3-x+y,-2/3+y,-1/6+z  =    11_444 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  F12       ..O7        .     2.67 Ang.
                              2/3-y,1/3-x,-1/6+z  =      10_554 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  F12       ..O7        .     2.67 Ang.
                              -1/3+x,1/3+x-y,-1/6+z  =    12_454 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       3 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600       57 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
   0 ALERT level B = A potentially serious problem, consider carefully
  10 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
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 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
17 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
 5 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.

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