checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

```
Bond precision:    Si- O = 0.0009 A          Wavelength=0.71075

Cell:              a=10.7811(2)     b=9.7836(1)            c=7.0348(1)
                   alpha=90         beta=108.0722(16)      gamma=90
Temperature:       293 K

                   Calculated                 Reported
Volume             705.410(19)                705.410(19)
Space group        P 21/a                     P 1 21/a 1
Hall group         -P 2yab                    -P 2yab
Moiety formula     F4 Fe2.60 O32 Si8 Ti4.11,  ?
                   4.82(Ca), 4.576(Na)
Sum formula        Ca4.82 F4 Fe2.60 Na4.58 O32 Ca2.411 F2 Fe1.301 Na2.287
                   Si8 Ti4.11                 O16 Si4 Ti2.056
Mr                 1453.38                    726.60
Dx,g cm-3          3.421                      3.421
Z                  1                          2
Mu (mm-1)          3.857                      3.857
F000               708.9                      709.0
F000'              713.18
h,k,lmax           18,16,12                   18,16,12
Nref               3809                       3692
Tmin,Tmax          0.820,0.908
Tmin'              0.778

Correction method= Not given

Data completeness= 0.969              Theta(max)= 37.880


R(reflections)= 0.0206( 3214)                      wR2(reflections)=
                                                   0.0798( 3692)
S = 1.040                   Npar= 139
```

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

PLAT075_ALERT_1_A Occupancy   1.028 Greater Than 1.0 for ......   TI_TI

🟡 Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ    Please Check
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given    Please Do !
PLAT057_ALERT_3_C Correction for Absorption Required   RT(exp) ...      1.11 Do !
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..    Please Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..         1 Check
```

⚪ Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF    Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...    0.500 Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  P21/a    P21/c Note
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  )        5% 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  5  )      100% Note
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O1       .    163.6 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         6 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       117 Note
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of       3.0 Sig(I)
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by         4 Check
```

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

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 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
   7 ALERT type 4 Improvement, methodology, query or suggestion
   4 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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT075_I
;
PROBLEM: Occupancy     1.028 Greater Than 1.0 for ......        TI_TI
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 12/09/2022; check.def file version of 09/08/2022