No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: shelx

Bond precision: = 0.0000 A   Wavelength=0.71073

Cell: a=9.8270(7)   b=18.0300(8)   c=5.316(4)
             alpha=90   beta=104.63(4) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	911.4(7)	911.4(6)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	Al3.08 Fe5.68 H2.80 Mg3.39 O48 Si13.20 Ti0.64, 0.12(K4), 0.357(	H2.88 Al3.17 Ca2.20 Fe5.67 K0.46 Mg3.32 Na3.23 O148 Si5.60 Si7.
Sum formula	Al3.08 Ca2.20 Fe5.68 H2.80 K0.48 Mg3.39 Na3.23 O48 Si13.20 Ti0.	H2.88 Al3.17 Ca2.20 Fe5.67 K0.46 Mg3.32 Na3.23 O148 Si5.60 Si7.
Mr	1835.90	1835.51
Dx,g cm-3	3.345	3.344
Z	1	2
Mu (mm-1)	3.471	0.049
F000	902.6	890.0
F000'	907.22	
h,k,lmax	13,24,7	13,24,7
Nref	1253	1266
Tmin,Tmax	0.995,0.996	0.995,0.996
Tmin'	0.990	

Correction method= # Reported T Limits: Tmin=0.995
Tmax=0.996 AbsCorr = REFDELF

Data completeness= 1.010   Theta(max)= 29.000

R(reflections)= 0.0277(1064)   wR2(reflections)= 0.0714(1266)

 S = 1.071   Npar= 116

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

ATOM007_ALERT_1_A _atom_site_aniso_label is missing
       Unique label identifying the atom site.
ABSMU01_ALERT_1_A The ratio of given/expected absorption coefficient lies
       outside the range 0.90 <> 1.10
       Calculated value of mu =   7.648
       Value of mu given   =   0.049
CHEMW01_ALERT_1_A The ratio of given/expected molecular weight as calculated
       from the _chemical_formula_sum lies outside
       the range 0.90 <> 1.10
       Calculated formula weight = 3435.4998
       Formula weight given   = 1835.5100

DENSD01_ALERT_1_A The ratio of the submitted crystal density and that
        calculated from the formula is outside the range 0.90 <> 1.10
        Crystal density given   =   3.344
        Calculated crystal density =   6.688
PLAT043_ALERT_1_A Calculated and Reported Mol. Weight Differ by ..   1835.12 Check
PLAT046_ALERT_1_A Reported Z, MW and D(calc) are Inconsistent ....   6.689 Check
PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .   6982.65 %

● Alert level C
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ   Please Check
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
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ....   1 Check
        Ca1
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) ....   O1 Check

● Alert level G
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   2 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of PT   as   SI
And 7 other PLAT017 Alerts
More ...
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.500 Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical   ? Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records   8 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   9 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 Ti1   Constrained at   0.16 Check
And 4 other PLAT300 Alerts
More ...
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   45% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)   100% Note
And 3 other PLAT302 Alerts
More ...
PLAT396_ALERT_2_G Deviating Si-O-Si Angle From 150 for O6   .   138.2 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   8 Note
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters   5 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....   ! Info
PLAT881_ALERT_1_G No Datum for _diffrn_reflns_av_R_equivalents ...   Please Do !
PLAT982_ALERT_1_G The Al-f'=   0.0056 Deviates from IT-value =   0.0645 Check
And 8 other PLAT982 Alerts
More ...
PLAT983_ALERT_1_G The Al-f"=   0.0052 Deviates from IT-Value =   0.0514 Check
PLAT983_ALERT_1_G The Si-f"=   0.0071 Deviates from IT-Value =   0.0704 Check

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

 34 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  2 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
 14 ALERT type 4 Improvement, methodology, query or suggestion
  2 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.

Response to the A alerts

For some reason, which we have been unable to find, there seems to be a problem with the way that WINGX and CheckCIF calculate some values, as results do not coincide. Some of the affected results are calculated density, absorption coefficient, molecular weight and Z.

start Validation Reply Form
_vrf_ATOM007_shelx
;
PROBLEM: _atom_site_aniso_label is missing
RESPONSE: ...
;
_vrf_ABSMU01_shelx
;
PROBLEM: The ratio of given/expected absorption coefficient lies
RESPONSE: ...
;
_vrf_CHEMW01_shelx
;
PROBLEM: The ratio of given/expected molecular weight as calculated
RESPONSE: ...
;
_vrf_DENSD01_shelx
;
PROBLEM: The ratio of the submitted crystal density and that
RESPONSE: ...

;
_vrf_PLAT043_shelx
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..   1835.12 Check
RESPONSE: ...
;
_vrf_PLAT046_shelx
;
PROBLEM: Reported Z, MW and D(calc) are Inconsistent ....   6.689 Check
RESPONSE: ...
;
_vrf_PLAT051_shelx
;
PROBLEM: Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .   6982.65 %
RESPONSE: ...
;
_vrf_PLAT041_shelx
;
PROBLEM: Calc. and Reported SumFormula   Strings Differ   Please Check
RESPONSE: ...
;
_vrf_PLAT042_shelx
;
PROBLEM: Calc. and Reported MoietyFormula Strings Differ   Please Check
RESPONSE: ...
;
_vrf_PLAT068_shelx
;
PROBLEM: Reported F000 Differs from Calcd (or Missing)...   Please Check
RESPONSE: ...
;
_vrf_PLAT077_shelx
;
PROBLEM: Unitcell Contains Non-integer Number of Atoms ..   Please Check
RESPONSE: ...
;
_vrf_PLAT202_shelx
;
PROBLEM: Isotropic non-H Atoms in Anion/Solvent ....   1 Check
RESPONSE: ...
;
_vrf_PLAT313_shelx
;
PROBLEM: Oxygen with Three Covalent Bonds (rare) ....   O1 Check
RESPONSE: ...
;
end Validation Reply Form