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: I

Bond precision: P- O = 0.0027 A Wavelength=0.71073

Cell: a=10.444(2) b=20.445(2) c=12.269(1)
alpha=90 beta=90.17(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2619.8(6)	2619.8(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ycb
Moiety formula	Al5.68 Fe1.76 Mg2.62 Mn5.38 O112 P16 Ti4.56, 21.068(O), 2.932(K	?
Sum formula	Al5.68 Fe1.76 K2.93 Mg2.62 Mn5.38 O133.07 P16 Ti4.56	O33.65 Mg0.64 Al1.51 P4 K0.77 Ti1.06 Mn0.83 Fe0.86
Mr	3568.18	893.00
Dx,g cm-3	2.262	2.264
Z	1	4
Mu (mm-1)	1.777	1.752
F000	1746.0	1745.0
F000'	1753.66	
h,k,lmax	15,30,18	12,28,16
Nref	9155	6549
Tmin,Tmax	0.969,0.974	
Tmin'	0.932	

Correction method= Not given

Data completeness= 0.715 Theta(max)= 32.080

R(reflections)= 0.0582(5893)

wR2(reflections)=
wR= 0.0686(6549)

S = 3.310 Npar= 382

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

PLAT027_ALERT_3_A _diffrn_reflns_theta_full value (too) Low ..... 20.21 Degree

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Alert level B

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem a 100 %Fit
PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem b 100 %Fit
PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Pbca Check
Check Model Parameter Symmmetry for Reflection Data Support
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O014_1 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O014_2 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O015_1 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O015_2 Check

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Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 3.310
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.970 Why?
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.82 Check
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
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
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -P 2ycb Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.8 Note
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) ..... Oh1 Check
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) ..... Oh2 Check

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Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:Al1.51 Fe0.86 K0.77 Mg0.64 Mn0.8
Atom count from the _atom_site data: Al1.4205 Fe0.44 K0.733 Mg0.656 M
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum O33.65 Mg0.64 Al1.51 P4 K0.77 Ti1.
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
O	134.60	133.07	1.53
Mg	2.56	2.62	-0.06
Al	6.04	5.68	0.36
P	16.00	16.00	0.00
K	3.08	2.93	0.15
Ti	4.24	4.56	-0.32
Mn	3.32	5.38	-2.06
Fe	3.44	1.76	1.68

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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 !
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1A_1    as         MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1A_2    as         MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1B_1    as         MG
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1B_2    as         MG
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2A_1    as         AL
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2C_1    as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2A_2    as         AL
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2C_2    as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2B_1    as         TI
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2B_2    as         TI
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3A_1    as         AL
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3C_1    as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3A_2    as         AL
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3C_2    as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3B_1    as         TI
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3B_2    as         TI
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.250 Check
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         A         91 %Fit
PLAT300_ALERT_4_G Atom Site Occupancy of M2C_1      Constrained at       0.17 Check
PLAT300_ALERT_4_G Atom Site Occupancy of M2C_2      Constrained at       0.17 Check
PLAT300_ALERT_4_G Atom Site Occupancy of M3C_1      Constrained at        0.1 Check
PLAT300_ALERT_4_G Atom Site Occupancy of M3C_2      Constrained at        0.1 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        16% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9  )       100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow_2 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       Ow_1 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         56 Note
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ           3 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           2 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.          2 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of        3.0 Sig(I)
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1 **ALERT level A** = Most likely a serious problem - resolve or explain
7 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
42 **ALERT level G** = General information/check it is not something unexpected

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

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 15 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
 10 ALERT type 4 Improvement, methodology, query or suggestion
  7 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_GOODF01_I
;
PROBLEM: The least squares goodness of fit parameter lies
RESPONSE: ...
;
_vrf_PLAT027_I
;
PROBLEM: _diffrn_reflns_theta_full value (too) Low ......      20.21 Degree
RESPONSE: ...
;
_vrf_PLAT112_I
;
PROBLEM: ADDSYM Detects New (Pseudo) Symm. Elem         a        100 %Fit
RESPONSE: ...
;
```

```
_vrf_PLAT113_I
;
PROBLEM: ADDSYM Suggests Possible Pseudo/New  Space Group       Pbca Check
RESPONSE: ...
;
_vrf_PLAT306_I
;
PROBLEM: Isolated Oxygen Atom (H-atoms Missing ?) .......     O014_1 Check
RESPONSE: ...
;
_vrf_PLAT029_I
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .      0.970 Why?
RESPONSE: ...
;
_vrf_PLAT041_I
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT043_I
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..       3.82 Check
RESPONSE: ...
;
_vrf_PLAT052_I
;
PROBLEM: Info on Absorption Correction Method   Not Given     Please Do !
RESPONSE: ...
;
_vrf_PLAT068_I
;
PROBLEM: Reported F000 Differs from Calcd (or Missing)...     Please Check
RESPONSE: ...
;
_vrf_PLAT077_I
;
PROBLEM: Unitcell Contains Non-integer Number of Atoms ..     Please Check
RESPONSE: ...
;
_vrf_PLAT127_I
;
PROBLEM: Implicit Hall Symbol  Inconsistent with Explicit    -P 2ycb Check
RESPONSE: ...
;
_vrf_PLAT250_I
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.8 Note
RESPONSE: ...
;
_vrf_PLAT313_I
;
PROBLEM: Oxygen with Three Covalent Bonds (rare) ........        Oh1 Check
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock I - ellipsoid plot