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: Mn- O = 0.0026 A Wavelength=0.71073

Cell: a=15.024(3) b=6.9470(14) c=9.999(2)
alpha=90 beta=110.71(3) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	976.2(4)	976.2(4)
Space group	P 2/a	P 1 2/a 1
Hall group	-P 2ya	-P 2ya
Moiety formula	Al4 Mn7.20 O52 P8, 0.8(Ca)	?
Sum formula	Al4 Ca0.80 Mn7.20 O52 P8	Al2 Ca0.38 Fe0.78 H18 Mg0.08 Mn2.61 O26 P4 Zn0.15
Mr	1615.31	825.90
Dx,g cm-3	2.748	2.810
Z	1	2
Mu (mm-1)	2.936	3.061
F000	784.0	784.0
F000’	788.14	
h,k,lmax	22,10,14	21,9,14
Nref	3399	2626
Tmin,Tmax	0.929,0.941	
Tmin’	0.736	

Correction method= Not given

Data completeness= 0.773 Theta(max)= 32.010

R(reflections)= 0.0519(2014) wR2(reflections)= wR= 0.0588(2626)

S = 2.150 Npar= 170

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 B

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 36.49 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 = 2.150
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 4.08 %
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O3 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.1 Note

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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:H18 Al2 Ca0.38 Fe0.78 Mg.08 Mn2.
Atom count from the _atom_site data: Al2 Ca0.4 Mn3.6 O26 P4
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 2
From the CIF: _chemical_formula_sum Al2 Ca0.38 Fe0.78 H18 Mg0.08 Mn2.6
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Al	4.00	4.00	0.00
Ca	0.76	0.80	-0.04
Fe	1.56	0.00	1.56
H	36.00	0.00	36.00
Mg	0.16	0.00	0.16
Mn	5.22	7.20	-1.98
O	52.00	52.00	0.00
P	8.00	8.00	0.00
Zn	0.30	0.00	0.30

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 X1 as MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of X2as CA
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1 as MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3A as AL
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3B as AL
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group P2/a P2/n Note
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 X1 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of X2 Constrained at 0.4 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 3% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 5 Note

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PLAT794_ALERT_5_G Tentative Bond Valency for Mn2A      (I)       .       0.71 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mn2B      (II)      .       2.35 Info
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 !
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  24 ALERT level G = General information/check it is not something unexpected

  16 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 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
   6 ALERT type 4 Improvement, methodology, query or suggestion
   5 ALERT type 5 Informative message, check
```

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_PLAT043_I
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..      36.49 Check
RESPONSE: ...
;
_vrf_PLAT041_I
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT051_I
;
PROBLEM: Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       4.08 %
RESPONSE: ...
;
_vrf_PLAT052_I
;
PROBLEM: Info on Absorption Correction Method   Not Given     Please Do !
RESPONSE: ...
;
_vrf_PLAT077_I
;
PROBLEM: Unitcell Contains Non-integer Number of Atoms ..     Please Check
RESPONSE: ...
;
_vrf_PLAT241_I
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of         O3 Check
RESPONSE: ...
;
_vrf_PLAT250_I
;
```

```
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
RESPONSE: ...
;
# end Validation Reply Form
```

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 22/03/2021; check.def file version of 19/03/2021

Datablock I - ellipsoid plot