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: final

Bond precision: Si- O = 0.0014 A Wavelength=0.71073

Cell: a=9.9533(4) b=18.1440(7) c=5.2970(2)
alpha=90 beta=103.948(4) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	928.39(6)	928.39(6)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	H3.04 Mg5.04 Mn5.74 O48 Si16, 0.527(Na4), 0.047(Na4), 3.224(Na)	?
Sum formula	H3.04 Mg5.04 Mn5.74 Na5.52 O48 Si16	Al0.03 H1.52 Ca0.24 Fe0.26 K0.24 Mg2.54 Mn2.40 Na2.26 O24 Si7.9
Mr	1785.19	891.22
Dx,g cm-3	3.193	3.188
Z	1	2
Mu (mm-1)	2.728	2.743
F000	875.7	876.0
F000'	879.68	
h,k,lmax	13,24,7	13,24,7
Nref	1189	1182
Tmin,Tmax	0.715,0.903	0.575,1.000
Tmin'	0.549	

Correction method= # Reported T Limits: Tmin=0.575 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 28.281

R(reflections)= 0.0264(1001)

wR2(reflections)= 0.0684(1182)

S = 1.030 Npar= 111

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

PLAT420_ALERT_2_B D-H Bond Without Acceptor O3 --H3 . Please Check

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Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 2.75 Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please 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:H1.52 Al.03 Ca0.24 Fe0.26 K0.24
Atom count from the _atom_site data: H1.52 Mg2.518 Mn2.87 Na2.76 O24
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 Al0.03 H1.52 Ca0.24 Fe0.26 K0.24 M
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Al	0.06	0.00	0.06
H	3.04	3.04	0.00
Ca	0.48	0.00	0.48
Fe	0.52	0.00	0.52
K	0.48	0.00	0.48
Mg	5.08	5.04	0.04
Mn	4.80	5.74	-0.94
Na	4.52	5.52	-1.00
O	48.00	48.00	0.00
Si	15.94	16.00	-0.06
Ti	0.08	0.00	0.08

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1 as MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2 as MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3 as MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of T2 as SI
PLAT017_ALERT_1_G Check Scattering Type Consistency of T1 as SI
PLAT017_ALERT_1_G Check Scattering Type Consistency of M4as NA

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PLAT017_ALERT_1_G Check Scattering Type Consistency of        AMas         NA
PLAT017_ALERT_1_G Check Scattering Type Consistency of        A2as         NA
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records          4 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX 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
PLAT300_ALERT_4_G Atom Site Occupancy of H3         Constrained at       0.76 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         28% 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  4  )        100% Note
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O5       .      137.1 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O6       .      136.7 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O7       .      137.7 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          8 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         1 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          6 Note
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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
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
33 **ALERT level G** = General information/check it is not something unexpected

18 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
9 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.

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

Datablock final - ellipsoid plot