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: shelx

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Bond precision:   P- O = 0.0028 A          Wavelength=0.71073

Cell:              a=25.944(5)      b=5.1426(10)         c=13.870(3)
                   alpha=90         beta=111.60(3)       gamma=90
Temperature:       293 K
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	Calculated	Reported
Volume	1720.6(7)	1720.4(7)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	Fe20 H40 Mg3.04 Mn0.96 O96 P16, 0.72(Ca), 3.28(Na)	?
Sum formula	Ca0.72 Fe20 H40 Mg3.04 Mn0.96 Na3.28 O96 P16	Ca0.19 H10 Fe5 Mg0.76 Mn0.24 Na0.81 O24 P4
Mr	3419.75	855.19
Dx,g cm-3	3.300	3.312
Z	1	4
Mu (mm-1)	4.895	4.939
F000	1679.0	1685.0
F000'	1689.08	
h,k,lmax	28,5,15	26,5,14
Nref	1221	1060
Tmin,Tmax	0.888,0.952	0.396,0.429
Tmin'	0.841	

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Correction method= # Reported T Limits: Tmin=0.396 Tmax=0.429
AbsCorr = ?

Data completeness= 0.868           Theta(max)= 23.148
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R(reflections)= 0.0197(1057)

wR2(reflections)= 0.0533(1060)

S = 1.258 Npar= 182

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

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5531
PLAT005_ALERT_5_B No Embedded Refinement Details Found in the CIF Please Do !
PLAT088_ALERT_3_B Poor Data / Parameter Ratio ..... 6.71 Note
PLAT964_ALERT_2_B SHELXL WEIGHT Par. Values in CIF & RES Differ .. Please Check

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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 !
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

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Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum Ca0.19 H10 Fe5 Mg0.76 Mn0.24 Na0.8
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Ca	0.76	0.72	0.04
H	40.00	40.00	0.00
Fe	20.00	20.00	0.00
Mg	3.04	3.04	0.00
Mn	0.96	0.96	0.00
Na	3.24	3.28	-0.04
O	96.00	96.00	0.00
P	16.00	16.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 9 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.250 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.86 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a 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 Mn2 Constrained at 0.24 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mg2 Constrained at 0.76 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca Constrained at 0.18 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na Constrained at 0.82 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 6% 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
PLAT480_ALERT_4_G Long H...A H-Bond Reported H12A ..O1 . 2.61 Ang.

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PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          4 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............          5 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL     2019/3 Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ          2 Units
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  22 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  11 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
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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 10/05/2023; check.def file version of 10/05/2023

Datablock shelx - ellipsoid plot