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 = 0.0033 A Wavelength=0.71090

Cell: a=10.547(2) b=20.577(4) c=12.373(2)
alpha=90 beta=90.09(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2685.3(8)	2685.3(8)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ycb
Moiety formula	Fe4.84 Mn8 O112 P16 Ti7.16, 18.188(O), 3.572(K)	?
Sum formula	Fe4.84 K3.57 Mn8 O130.19 P16 Ti7.16	O32.759 P4 K0.841 Ti1.785 Mn2.041 Fe1.215
Mr	3770.79	946.30
Dx,g cm-3	2.332	2.341
Z	1	4
Mu (mm-1)	2.566	2.515
F000	1832.7	1833.0
F000'	1842.68	
h,k,lmax	15,30,18	13,28,17
Nref	9401	7459
Tmin,Tmax	0.913,0.963	0.340,0.430
Tmin'	0.904	

Correction method= # Reported T Limits: Tmin=0.340 Tmax=0.430
AbsCorr = MULTI-SCAN

Data completeness= 0.793 Theta(max)= 32.090

R(reflections)= 0.0583(6718)

wR2(reflections)=
wR= 0.0722(7459)

S = 2.720 Npar= 357

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 ..... 24.06 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
WARNING: Disordered Atoms Excluded from Analysis
Check Model Parameter Symmetry for Reflection Data Support
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O14A Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O14B Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O15A Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O15B Check

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Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -2.490
Test value = -1.950
DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 2.720
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: Fe1.21 K0.89 Mn2 O32.55 P4 Ti1.79
Rep.: O32.759 P4 K0.841 Ti1.785 Mn2.041 Fe1.215
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 14.41 Check
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 2.04 %
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -2.49 eA-3
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -P 2ycb Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for P2A . 5 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for P2B . 5 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for P1A . 5 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for P1B . 5 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:Fe1.215 K0.841 Mn2.041 O32.75899
Atom count from the _atom_site data: Fe1.2105 K0.893 Mn2 O32.54699 P4
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu

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                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  O32.759 P4 K0.841 Ti1.785 Mn2.041
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           O        131.04    130.19    0.85
           P         16.00     16.00    0.00
           K          3.36      3.57   -0.21
           Ti         7.14      7.16   -0.02
           Mn         8.16      8.00    0.16
           Fe         4.86      4.84    0.02
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         O
PLAT017_ALERT_1_G Check Scattering Type Consistency of X2       as         O
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.250 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        11% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    6)       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 ?) .....        Ow1 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        Ow2 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          4 Note
              Ow1     Ow2     X1      X2
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1A      (I)       .       0.65 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1B      (II)      .       2.25 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 !
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ           2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           2 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of        3.0 Sig(I)
PLAT982_ALERT_1_G The Fe-f'=    0.3486 Deviates from  IT-value =       0.3463 Check
PLAT982_ALERT_1_G The  K-f'=    0.2025 Deviates from  IT-value =       0.2009 Check
PLAT982_ALERT_1_G The Mn-f'=    0.3394 Deviates from  IT-value =       0.3368 Check
PLAT982_ALERT_1_G The  P-f'=    0.1041 Deviates from  IT-value =       0.1023 Check
PLAT982_ALERT_1_G The Ti-f'=    0.2808 Deviates from  IT-value =       0.2776 Check
PLAT983_ALERT_1_G The Fe-f"=    0.8535 Deviates from  IT-Value =       0.8444 Check
PLAT983_ALERT_1_G The  K-f"=    0.2536 Deviates from  IT-Value =       0.2494 Check
PLAT983_ALERT_1_G The Mn-f"=    0.7370 Deviates from  IT-Value =       0.7283 Check
PLAT983_ALERT_1_G The  P-f"=    0.0961 Deviates from  IT-Value =       0.0942 Check
PLAT983_ALERT_1_G The Ti-f"=    0.4522 Deviates from  IT-Value =       0.4457 Check
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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
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
35 **ALERT level G** = General information/check it is not something unexpected

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

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 13 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
  6 ALERT type 4 Improvement, methodology, query or suggestion
  8 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.

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_DIFMN02_I
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_DIFMN03_I
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_GOODF01_I
;
PROBLEM: The least squares goodness of fit parameter lies
RESPONSE: ...
;
```

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_vrf_PLAT027_I
;
PROBLEM: _diffrn_reflns_theta_full value (too) Low ......      24.06 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 ?) .......       O14A Check
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 ..      14.41 Check
RESPONSE: ...
;
_vrf_PLAT051_I
;
PROBLEM: Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       2.04 %
RESPONSE: ...
;
_vrf_PLAT077_I
;
PROBLEM: Unitcell Contains Non-integer Number of Atoms ..     Please Check
RESPONSE: ...
;
_vrf_PLAT098_I
;
PROBLEM: Large Reported Min.  (Negative) Residual Density      -2.49 eA-3
RESPONSE: ...
;
_vrf_PLAT127_I
;
PROBLEM: Implicit Hall Symbol  Inconsistent with Explicit    -P 2ycb Check
RESPONSE: ...
;
_vrf_PLAT218_I
;
PROBLEM: Constrained U(ij) Components(s) for P2A        .          5 Check
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock I - ellipsoid plot