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Supplement of

Fluormacraeite, $[(H_2O)K]Mn_2(Fe_2Ti)(PO_4)_4[OF](H_2O)_{10} \cdot 4H_2O$, the first type mineral from the Plößberg pegmatite, Upper Palatinate, Bavaria, Germany

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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 = 0.0030 A Wavelength=0.71070

Cell: a=10.546(2) b=20.655(1) c=12.405(1)
alpha=90 beta=90.09(1) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2702.2(6)	2702.1(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ycb
Moiety formula	Fe10.71 H88 K0.53 Mn7.41 O115.07 P16, 12(H2 O), 4(H O), 0.824(O	?
Sum formula	Fe10.71 H116 K3.70 Mn7.41 O131.90 P16	H29 O32.973 Mg0 P4 K0.927 Ti0 Mn1.853 Fe2.678
Mr	3872.98	968.30
Dx,g cm-3	2.380	2.380
Z	1	4
Mu (mm-1)	2.760	2.760
F000	1945.3	1945.0
F000'	1955.11	
h,k,lmax	15,31,18	14,28,18
Nref	9568	6313
Tmin,Tmax	0.871,0.921	0.570,0.750
Tmin'	0.871	

Correction method= # Reported T Limits: Tmin=0.570 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.660 Theta(max)= 32.240

R(reflections)= 0.0559(5646)

wR2(reflections)=
wR= 0.0710(6313)

S = 2.430 Npar= 488

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 ..... 22.42 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
PLAT417_ALERT_2_B Short Inter D-H..H-D H12A1 ..H14A1 . 1.87 Ang.
x,y,z = 1_555 Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O12B --H12B2 . Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O15A --H15A1 . 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
GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 2.430
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: Fe2.68 H29 K0.93 Mn1.85 O32.97 P4
Rep.: H29 O32.973 Mg0 P4 K0.927 Ti0 Mn1.853 Fe2.678
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 <U(i,j)> Tensor(Resd 1) 2.2 Note

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Alert level G

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 H29 O32.973 Mg0 P4 K0.927 Ti0 Mn1.
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
H	116.00	116.00	0.00
O	131.89	131.90	-0.00

```
          Mg         4.00      0.00    4.00
          P         16.00     16.00    0.00
          K          3.71      3.70    0.00
          Ti         4.00      0.00    4.00
          Mn         7.41      7.41    0.00
          Fe        10.71     10.71    0.00
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      as         MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1B      as         MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2A      as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2B      as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3A      as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3B      as         FE
PLAT017_ALERT_1_G Check Scattering Type Consistency of A1       as         K
PLAT017_ALERT_1_G Check Scattering Type Consistency of A2       as         K
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
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         A          88 %Fit
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        16% 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
PLAT303_ALERT_2_G Full Occupancy Atom H10A2     with # Connections       1.13 Check
PLAT303_ALERT_2_G Full Occupancy Atom H12B2     with # Connections       1.13 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        Ow2 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         41 Note
              M1A     M1B     M2A     M2B     M3A     M3B     A1      A2
              Ow1     Ow2     X1      X2      H9B1    H11B1   H11B2   H12A1
              H9B2    H10A1   H12B1   H11A1   H9A1    Ha1A    H10A2   H9A2
              H12B2   H10B1   H13B1   H12A2   H13A1   H13B2   H11A2   H14A1
              H15A1   H15B1   H14B1   H15B2   H10B2   H14A2   H14B2   Ha1B
              H13A2
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         43 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           3 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
6 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
30 **ALERT level G** = General information/check it is not something unexpected

19 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 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
4 ALERT type 4 Improvement, methodology, query or suggestion
5 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_PLAT027_I
;
PROBLEM: _diffrn_reflns_theta_full value (too) Low ......      22.42 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_PLAT417_I
;
PROBLEM: Short Inter D-H..H-D       H12A1    ..H14A1    .       1.87 Ang.
RESPONSE: ...
;
_vrf_PLAT420_I
```

;
PROBLEM: D-H Bond Without Acceptor O12B   --H12B2   .   Please Check
RESPONSE: ...
;
end Validation Reply Form

PLATON version of 13/05/2024; check.def file version of 04/05/2024

Datablock I - ellipsoid plot