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Supplement of

Hochleitnerite, $[K(H_2O)]Mn_2(Ti_2Fe)(PO_4)_4O_2(H_2O)_{10} \cdot 4H_2O$, a new paulkerrite-group mineral, from the Hagendorf-Süd pegmatite, Oberpfalz, 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 = 0.0040 A Wavelength=0.71073

Cell: a=10.5513(3) b=20.6855(7) c=12.4575(4)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	2718.96(15)	2718.96(15)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P -2xab;-2
Moiety formula	Al0.80 Fe6.32 Mn6 O112 P16 Ti6.88, ***(O), 3.5(K)	?
Sum formula	Al0.80 Fe6.32 K3.50 Mn6 O132.50 P16 Ti6.88	K Mn1.5 Fe1.67 Al0.13 Ti1.61 P4 O33
Mr	3786.00	951.60
Dx,g cm-3	2.312	2.325
Z	1	4
Mu (mm-1)	2.490	2.463
F000	1842.6	1843.0
F000'	1852.38	
h,k,lmax	15,30,18	15,30,18
Nref	4707	4268
Tmin,Tmax	0.744,0.801	0.800,0.900
Tmin'	0.726	

Correction method= # Reported T Limits: Tmin=0.800 Tmax=0.900
AbsCorr = GAUSSIAN

Data completeness= 0.907 Theta(max)= 31.950

R(reflections)= 0.0651(2242)

wR2(reflections)=
wR= 0.0866(4268)

S = 1.850 Npar= 199

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

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.214
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O14 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O15 Check

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Alert level C

ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies
outside the range 0.99 <> 1.01
Calculated value of mu = 2.522
Value of mu given = 2.463
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 gaussian
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 20.40 Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -P -2xab;- 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:Al0.13 Fe1.67 K1 Mn1.5 O33 P4 Ti
Atom count from the _atom_site data: Al0.2 Fe1.58 K0.876 Mn1.5 O33.12
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 K Mn1.5 Fe1.67 Al0.13 Ti1.61 P4 O3
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
K	4.00	3.50	0.50
Mn	6.00	6.00	0.00
Fe	6.68	6.32	0.36
Al	0.52	0.80	-0.28
Ti	6.44	6.88	-0.44
P	16.00	16.00	0.00
O	132.00	132.50	-0.50

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT017_ALERT_1_G Check Scattering Type Consistency of F as O
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.214 Report

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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
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 Mn1        Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe1        Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Al2        Constrained at       0.1 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       16% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )      100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        Ow Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         2 Note
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 !
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of       3.0 Sig(I)
PLAT982_ALERT_1_G The Al-f'=    0.0659 Deviates from  IT-value =      0.0645 Check
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 Al-f"=    0.0527 Deviates from  IT-Value =      0.0514 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
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
   6 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

  25 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 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
   7 ALERT type 4 Improvement, methodology, query or suggestion
   4 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_RINTA01_I
;
PROBLEM: The value of Rint is greater than 0.18
RESPONSE: ...
;
_vrf_ABSMU01_I
;
PROBLEM: The ratio of given/expected absorption coefficient lies
RESPONSE: ...
;
```

```
_vrf_ABSTY02_I
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT306_I
;
PROBLEM: Isolated Oxygen Atom (H-atoms Missing ?) .......        O14 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 ..      20.40 Check
RESPONSE: ...
;
_vrf_PLAT077_I
;
PROBLEM: Unitcell Contains Non-integer Number of Atoms ..     Please Check
RESPONSE: ...
;
_vrf_PLAT127_I
;
PROBLEM: Implicit Hall Symbol  Inconsistent with Explicit -P -2xab;- Check
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 28/11/2022; check.def file version of 28/11/2022

Datablock I - ellipsoid plot