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Supplement of

Whiteite-(CaMnFe), a new jahnsite-group mineral from the Hagendorf-Süd pegmatite, Oberpfalz, Bavaria

Rupert Hochleitner et al.

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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: Fe- O = 0.0055 A Wavelength=0.71073

Cell: a=14.925(5) b=7.0100(14) c=10.053(2)
alpha=90 beta=111.31(2) gamma=90
Temperature: 294 K

	Calculated	Reported
Volume	979.9(4)	979.9(4)
Space group	P 2/a	P 1 2/a 1
Hall group	-P 2ya	-P 2ya
Moiety formula	Al3.20 Fe4.80 Mn2.60 O52 P8, 1.4(Ca)	?
Sum formula	Al3.20 Ca1.40 Fe4.80 Mn2.60 O52 P8	Ca Mn Fe2 Al2 P4 O26 H18
Mr	1633.13	800.50
Dx,g cm-3	2.767	2.713
Z	1	2
Mu (mm-1)	3.277	0.000
F000	795.4	787.0
F000'	799.74	
h,k,lmax	20,9,14	20,9,13
Nref	2851	2354
Tmin,Tmax		0.817,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.817 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.826 Theta(max)= 29.960

R(reflections)= 0.0704(1613)

wR2(reflections)=
wR= 0.0556(2354)

S = 2.130 Npar= 149

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

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 32.13 Check
O10 O11 O12 O13

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 gaussian
CHEMW01_ALERT_1_C The ratio of given/expected molecular weight as calculated
from the _chemical_formula_sum lies outside
the range 0.99 <> 1.01
Calculated formula weight = 818.6968
Formula weight given = 800.5000
GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 2.130
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O4 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O6 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O7 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O8 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of P1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of P2 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:H18 Al2 Ca1 Fe2 Mn1 O26 P4
Atom count from the _atom_site data: Al1.6 Ca0.7 Fe2.4 Mn1.3 O26 P4
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 Ca Mn Fe2 Al2 P4 O26 H18
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Ca	2.00	1.40	0.60
Mn	2.00	2.60	-0.60
Fe	4.00	4.80	-0.80
Al	4.00	3.20	0.80
P	8.00	8.00	0.00

```
           O         52.00     52.00    0.00
           H         36.00      0.00   36.00
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 !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  P2/a          P2/n Note
PLAT300_ALERT_4_G Atom Site Occupancy of Fe3A       Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe3B       Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mn         Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Al3A       Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Al3B       Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca         Constrained at        0.7 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         12% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2A      (II)      .       2.16 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2B      (II)      .       2.08 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1       (II)      .       1.84 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 !
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of        3.0 Sig(I)
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  21 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   9 ALERT type 4 Improvement, methodology, query or suggestion
   7 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_ABSTY02_I
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_CHEMW01_I
;
PROBLEM: The ratio of given/expected molecular weight as calculated
RESPONSE: ...
;
_vrf_GOODF01_I
;
PROBLEM: The least squares goodness of fit parameter lies
RESPONSE: ...
;
_vrf_PLAT043_I
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..      32.13 Check
```

```
RESPONSE: ...
;
_vrf_PLAT041_I
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT077_I
;
PROBLEM: Unitcell Contains Non-integer Number of Atoms ..     Please Check
RESPONSE: ...
;
_vrf_PLAT241_I
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of         O4 Check
RESPONSE: ...
;
_vrf_PLAT242_I
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of         P1 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 18/05/2022; check.def file version of 17/05/2022

Datablock I - ellipsoid plot