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Supplement of

**Pleysteinrite, [(H\textsubscript{2}O\textsubscript{0.5}K\textsubscript{0.5})\textsubscript{2}Mn\textsubscript{2}Al\textsubscript{3}(PO\textsubscript{4})\textsubscript{4}F\textsubscript{2}(H\textsubscript{2}O)\textsubscript{10} \cdot 4H\textsubscript{2}O, the Al analogue of benyacarite, from the Hagendorf-Süd pegmatite, Oberpfalz, Bavaria, Germany**

Ian E. Grey 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: Mn–O = 0.0042 Å

Cell: a=10.4133(8) b=20.5242(17) c=12.2651(14)
alpha=90 beta=90 gamma=90

Temperature: 294 K

Volume
Calculated 2621.4(4) Reported 2621.4(4)

Space group P b c a P b c a
Hall group -P 2ac 2ab -P -2xab;-2

Moiety formula P16 Ti1.75, 20.216(O), 3.784(K)

Sum formula A17.73 F8 Fe2.52 Mn8 O104
O124.22 P16 Ti1.75

Mr 3655.56 456.90
Dx, g cm⁻³ 2.316 2.316
Z 1 8
Mu (mm⁻¹) 2.021 2.021
F000 1782.2 1778.0
F000’ 1790.36

h,k,lmax 14,29,17 13,26,16
Nref 3895 3310
Tmin,Tmax 0.836,0.939 0.929,1.000
Tmin’ 0.801

Correction method= # Reported T Limits: Tmin=0.929 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.850 Theta(max) = 30.190
R(reflections) = 0.0545 (1692)  
wR2(reflections) = 0.0682 (3310)  
S = 1.410  
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**

<table>
<thead>
<tr>
<th>ALERT</th>
<th>Description</th>
<th>Alert level</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT306_ALERT_2_B</td>
<td>Isolated Oxygen Atom (H-atoms Missing ?)</td>
<td>0014 Check</td>
</tr>
<tr>
<td>PLAT306_ALERT_2_B</td>
<td>Isolated Oxygen Atom (H-atoms Missing ?)</td>
<td>0015 Check</td>
</tr>
</tbody>
</table>

**Alert level C**

<table>
<thead>
<tr>
<th>ALERT</th>
<th>Description</th>
<th>Alert level</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSTY02_ALERT_1_C</td>
<td>An <code>_exptl_absorpt_correction_type</code> has been given without a literature citation. This should be contained in the <code>_exptl_absorpt_process_details</code> field.</td>
<td>0014 Check</td>
</tr>
<tr>
<td>PLAT041_ALERT_1_C</td>
<td>Calc. and Reported SumFormula Strings Differ</td>
<td>Please Check</td>
</tr>
<tr>
<td>PLAT068_ALERT_1_C</td>
<td>Reported F000 Differs from Calcd (or Missing)</td>
<td>Please Check</td>
</tr>
<tr>
<td>PLAT077_ALERT_4_C</td>
<td>Unitcell Contains Non-integer Number of Atoms</td>
<td>Please Check</td>
</tr>
<tr>
<td>PLAT127_ALERT_1_C</td>
<td>Implicit Hall Symbol Inconsistent with Explicit -P -2xab;</td>
<td>Please Check</td>
</tr>
</tbody>
</table>

**Alert level G**

<table>
<thead>
<tr>
<th>ALERT</th>
<th>Description</th>
<th>Alert level</th>
</tr>
</thead>
<tbody>
<tr>
<td>FORMU01_ALERT_2_G</td>
<td>There is a discrepancy between the atom counts in the <code>_chemical_formula_sum</code> and the formula from the <code>_atom_site*</code> data.</td>
<td>0014 Check</td>
</tr>
<tr>
<td>CELLZ01_ALERT_1_G</td>
<td>Difference between formula and atom_site contents detected.</td>
<td>0014 Check</td>
</tr>
<tr>
<td>CELLZ01_ALERT_1_G</td>
<td>ALERT: check formula stoichiometry or atom site occupancies.</td>
<td>0014 Check</td>
</tr>
<tr>
<td>From the CIF:</td>
<td>_cell_formula_units_Z</td>
<td>8</td>
</tr>
<tr>
<td>From the CIF:</td>
<td><code>_chemical_formula_sum</code></td>
<td>K 0.47 Mn Fe0.32 Ti0.22 Al0.97 P2 O</td>
</tr>
<tr>
<td>TEST: Compare cell contents of formula and atom_site data</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>atom</th>
<th>Z*formula</th>
<th>cif sites</th>
<th>dif</th>
</tr>
</thead>
<tbody>
<tr>
<td>K</td>
<td>3.76</td>
<td>3.78</td>
<td>-0.02</td>
</tr>
<tr>
<td>Mn</td>
<td>8.00</td>
<td>8.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Fe</td>
<td>2.56</td>
<td>2.52</td>
<td>0.04</td>
</tr>
<tr>
<td>Ti</td>
<td>1.76</td>
<td>1.75</td>
<td>0.01</td>
</tr>
<tr>
<td>Al</td>
<td>7.76</td>
<td>7.73</td>
<td>0.03</td>
</tr>
<tr>
<td>P</td>
<td>16.00</td>
<td>16.00</td>
<td>0.00</td>
</tr>
<tr>
<td>O</td>
<td>124.00</td>
<td>124.22</td>
<td>-0.22</td>
</tr>
<tr>
<td>F</td>
<td>8.00</td>
<td>8.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ALERT</th>
<th>Description</th>
<th>Alert level</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT004_ALERT_5_G</td>
<td>Polymeric Structure Found with Maximum Dimension</td>
<td>2 Info</td>
</tr>
<tr>
<td>PLAT005_ALERT_5_G</td>
<td>No Embedded Refinement Details Found in the CIF</td>
<td>Please Do !</td>
</tr>
<tr>
<td>PLAT017_ALERT_1_G</td>
<td>Check Scattering Type Consistency of M1</td>
<td>MN</td>
</tr>
<tr>
<td>PLAT017_ALERT_1_G</td>
<td>Check Scattering Type Consistency of M2A</td>
<td>AL</td>
</tr>
<tr>
<td>PLAT017_ALERT_1_G</td>
<td>Check Scattering Type Consistency of M2B</td>
<td>FE</td>
</tr>
<tr>
<td>PLAT017_ALERT_1_G</td>
<td>Check Scattering Type Consistency of M3A</td>
<td>AL</td>
</tr>
<tr>
<td>PLAT017_ALERT_1_G</td>
<td>Check Scattering Type Consistency of M3B</td>
<td>TI</td>
</tr>
<tr>
<td>PLAT045_ALERT_1_G</td>
<td>Calculated and Reported Z Differ by a Factor ...</td>
<td>0.125 Check</td>
</tr>
<tr>
<td>PLAT301_ALERT_3_G</td>
<td>Main Residue Disorder ................(Resid 1 )</td>
<td>11% Note</td>
</tr>
<tr>
<td>PLAT302_ALERT_4_G</td>
<td>Anion/Solvent/Minor-Residue Disorder (Resid 2 )</td>
<td>100% Note</td>
</tr>
</tbody>
</table>
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 21 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!
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)

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

13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
4 ALERT type 4 Improvement, methodology, query or suggestion
5 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.

```bash
# start Validation Reply Form
_vrf_ABSTY02_I
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT306_I
;
PROBLEM: Isolated Oxygen Atom (H-atoms Missing?) Ow Check
RESPONSE: ...
;
_vrf_PLAT041_I
;
PROBLEM: Calc. and Reported SumFormula Strings Differ Please Check
RESPONSE: ...
;
_vrf_PLAT068_I
;
PROBLEM: Reported F000 Differs from Calcd (or Missing)... Please 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.

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**PLATON version of 18/05/2022; check.def file version of 17/05/2022**