

## The crystal structure of meurigite

ANTHONY R. KAMPF,<sup>1,\*</sup> JOSEPH J. PLUTH,<sup>2</sup> AND YU-SHENG CHEN<sup>3</sup>

<sup>1</sup>Mineral Sciences Department, Natural History Museum of Los Angeles County, 900 Exposition Blvd., Los Angeles, California 90007, U.S.A.

<sup>2</sup>Department of Geophysical Sciences, Center for Advanced Radiation Sources and Materials Research Science and Engineering Center, University of Chicago, 5734 S. Ellis Avenue, Chicago, Illinois 60637-1434, U.S.A.

<sup>3</sup>Center for Advanced Radiation Sources, University of Chicago, 5640 S. Ellis Avenue, Chicago, Illinois 60637-1434, U.S.A.

### ABSTRACT

The crystal structure of meurigite, ideally  $[\text{K}(\text{H}_2\text{O})_{2.5}][\text{Fe}_8^{3+}(\text{PO}_4)_6(\text{OH})_7(\text{H}_2\text{O})_4]$ , monoclinic,  $C2/c$ ,  $a = 29.018(5)$ ,  $b = 5.1892(6)$ ,  $c = 19.695(3)$  Å,  $\beta = 106.987(1)^\circ$ ,  $Z = 4$ , from the Santa Rita mine, New Mexico, has been solved and refined to  $R_1 = 4.69\%$ ,  $wR_2 = 12.6\%$  using 3325 unique [ $F_o > 4\sigma(F_o)$ ] reflections collected using a Bruker 6000 SMART CCD diffractometer and synchrotron radiation of wavelength 0.41328 Å. The structure of meurigite is a framework consisting of face-sharing octahedral  $\text{Fe}_2^{3+}\text{O}_9$  dimers, which are linked by sharing corners with corner-sharing dimers and isolated  $\text{Fe}^{3+}\text{O}_6$  octahedra to form thick slabs of octahedra parallel to the **a-c** plane.  $\text{PO}_4$  tetrahedra further link octahedra within the slabs and also link slabs to one another perpendicular to the **a-c** plane. Relatively large channels through the framework along the **b** axis contain disordered K atoms and  $\text{H}_2\text{O}$  molecules, which take part in two overlapping arrays. Partial vacancies in the Fe and P sites may account for discrepancies between the empirical and ideal chemical formulas. Packing considerations suggest that the empirical formula should be based on the total number of large ions ( $\text{K} + \text{Na} + \text{O} = 38.5$  per formula unit), which for the chemical analysis provided in the original description yields  $[(\text{K}_{0.91}\text{Na}_{0.03})_{\Sigma 0.94}(\text{H}_2\text{O})_{2.56}]_{\Sigma 3.50}[(\text{Fe}_{7.52}\text{Al}_{0.17}\text{Cu}_{0.03})_{\Sigma 7.72}(\text{PO}_4)_{5.48}(\text{CO}_3)_{0.21}(\text{OH})_{7.20}(\text{H}_2\text{O})_{5.23}]$ . The meurigite structure is related to those of other fibrous ferric phosphates with 5 Å fiber axes and shows a particularly close relationship with the structure of dufrénite. Crystal chemical evidence suggests that, even if meurigite and phosphofibrite are isostructural, phosphofibrite may qualify as a distinct species based upon its low K content (<0.5 apfu based on a recalculation of the original chemical analysis).

**Keywords:** Meurigite, phosphofibrite, crystal structure, crystal chemistry, fibrous iron phosphates