The crystal structure of meurigite

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ABSTRACT

The crystal structure of meurigite, ideally $[[\text{K(H}_2\text{O)}_{2.5}]\text{[Fe}^3+)\text{PO}_4\text{]}\text{[O(OH)}\text{]}\text{[H}_2\text{O)}_4\text{]},$ monoclinic, $C2/c,$ $a = 29.018(5), b = 5.1892(6), c = 19.695(3) \AA, \beta = 106.987(1)^\circ, Z = 4,$ from the Santa Rita mine, New Mexico, has been solved and refined to $R_I = 4.69\%,$ $wR_2 = 12.6\%$ 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 Fe$^{3+}$O$_6$ dimers, which are linked by sharing corners with corner-sharing dimers and isolated Fe$^{3+}$O$_6$ octahedra to form thick slabs of octahedra parallel to the $a$-c plane. 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 H$_2$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 (K + Na + O = 38.5 per formula unit), which for the chemical analysis provided in the original description yields [(K$_{0.91}$Na$_{0.03}$)PO$_4$]$_{0.82}$(Fe$^{3+}$)$_{0.75}$Cu$_{0.17}$O$^{\mu}$$_{3.52}$H$_2$O$^{\mu}$$_{3.96}$]. 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 phosphofibrate are isomorphous, phosphofibrate 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, phosphofibrate, crystal structure, crystal chemistry, fibrous iron phosphates

INTRODUCTION

Meurigite was first described by Birch et al. (1996) from the Santa Rita mine, Grant Co., New Mexico, where it occurs as tabular, elongated crystals forming spherical and hemispherical clusters to 2 mm across. The authors noted that the fibrous nature of meurigite made single crystal X-ray diffraction study and crystal structure determination impossible. From TEM studies and indexed X-ray powder diffraction patterns, Birch et al. (1996) derived probable space groups $C2, Cm,$ and $C2/m,$ and unit-cell parameters $a = 29.52(4), b = 5.249(6), c = 18.26(1) \AA, \beta = 109.27(7)^\circ.$ Meurigite and its Na analog have been noted at several other localities (Birch et al. 1996; Walenta and Theye 2001; Kolitsch 1999; Kolitsch pers. comm.); however, crystals at these localities have generally been smaller and even less suitable for single-crystal X-ray diffraction work.

Birch et al. (1996) noted meurigite to be a member of the group of fibrous ferric phosphates with a discrete 5 Å fiber axis (which corresponds to the sum of the edges of one octahedron and one tetrahedron). They pointed out that compositionally meurigite is most closely related to kidwellite and phosphofibrate; however, the structural relationships between these minerals were at that time unclear, because none of their structures were known. Kolitsch (2004) determined the structure of kidwellite, as well as that of the “laubmannite” of Moore (1970).

Kolitsch (1999) using transmission electron microscopy and X-ray powder diffraction concluded that meurigite and phosphofibrate were the same mineral species; however, phosphofibrate type material was not examined in this study. A proposal to discredit one of these species has never been submitted to the Commission on New Minerals and Mineral names.

Continuing efforts to unravel the structural relationships and crystal chemistry among the fibrous ferric iron phosphates led to the present study in which synchrotron radiation has been successfully employed to collect single-crystal X-ray diffraction data from a small crystal fragment of meurigite from the type specimen and to finally determine the structure of this mineral.

STRUCTURE DETERMINATION

For structure data collection a $100 \times 40 \times 5 \mu$m crystal fragment of meurigite from the type specimen was mounted on the tip of a glass fiber. Data were collected at GSECARS and...