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Jasonsmithite, a new phosphate mineral with a complex microporous framework, from the Foote mine, North Carolina, U.S.A.

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Abstract

Jasonsmithite (IMA2019-121), $Mn_4^{2+}ZnAl(PO_4)_4(OH)(H_2O)_7 \cdot 3.5H_2O$, is a pegmatite-phosphate mineral from the Foote Lithium Company mine, Kings Mountain district, Cleveland County, North Carolina, U.S.A. It is interpreted as having formed by late-stage, low-temperature hydrothermal alteration. Crystals are colorless to light brown, slightly flattened prisms to about 1 mm in length with wedge-shaped terminations. The mineral is transparent with vitreous luster, white streak, Mohs hardness 2, brittle tenacity, irregular fracture, and perfect {001} cleavage. The density is 2.63(2) g/cm^3. Jasonsmithite is biaxial (–), with $\alpha = 1.561(2)$, $\beta = 1.580(2)$, $\gamma = 1.581(2)$, measured in white light. The $2V$ is 25(5)° and dispersion is $r < v$ moderate. The optical orientation is $Y = \mathbf{b}$, $X \wedge \mathbf{c} = 18°$ in obtuse β. The Raman spectrum is dominated by vibrational modes of PO_4 and ZnO_4 tetrahedra, AlO_6 and MnO_6 octahedra, and OH groups. Electron microprobe analyses gave the empirical formula $(Mn_{3.09}Fe_{0.87})_{\Sigma 3.96}Zn_{1.05}Al_{0.98}(PO_4)_4(OH)(H_2O)_7 \cdot 3.5H_2O$. The mineral is monoclinic, $P2_1/c$, $a = 8.5822(3)$, $b = 13.1770(6)$, $c = 20.3040(14)$ Å, $\beta = 98.485(7)°$, $V = 2271.0(2)$ Å^3, and $Z = 4$. The structure ($R_1 = 0.0443$ for 3685 $I > 2\sigma I$ reflections) contains zigzag chains of edge-sharing MnO_6 octahedra that corner-link to adjacent chains and to PO_4 tetrahedra to form sheets, which are decorated by ZnO_4 tetrahedra. The sheets are linked to one another via dimers of AlO_6 octahedra, forming a framework with large channels containing H_2O groups. With H_2O groups removed, the framework has a void space of 70.2% per unit cell, and a framework density of 14.5 polyhedral atoms/1000 Å^3, which would place jasonsmithite among the most porous minerals.

Keywords: Jasonsmithite, new mineral, phosphate, microporous framework structure, Raman spectroscopy, Foote mine, Kings Mountain, North Carolina, U.S.A.; Microporous Materials: Crystal-Chemistry, Properties, and Utilizations