American Mineralogist, Volume 106, pages 1009–1015, 2021

Zhanghuifenite, $Na_3Mn_4^{2+}Mg_2Al(PO_4)_6$, a new mineral isostructural with bobfergusonite, from the Santa Ana mine, San Luis province, Argentina

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Abstract

A new mineral species, zhanghuifenite, ideally $Na_3Mn_4^{2+}Mg_2Al(PO_4)_6$, has been found in the Santa Ana mine, San Luis province, Argentina. It occurs in irregular veinlets or patches, 5 mm thick, in a nodule of beusite interlaminated with lithiophilite. Broken pieces of zhanghuifenite are blocky or tabular. Single crystals are up to 0.8 × 0.5 × 0.5 mm. No twinning or parting is observed macroscopically. The mineral is deep green, transparent with pale green streak and vitreous luster. It is brittle and has a Mohs hardness of ~5 with good cleavage on {010}. The measured and calculated densities are 3.63(2) and 3.62 g/cm^3, respectively. Optically, zhanghuifenite is biaxial (+), with α = 1.675(2), β = 1.680(2), γ = 1.690(2) (white light), $2V$ (meas) = 74(2)°, and $2V$ (calc) = 71°. The calculated compatibility index based on the empirical formula is 0.020 (excellent). An electron microprobe analysis yields an empirical formula (based on 24 O apfu) $(Na_{2.80}Ca_{0.11})_{\Sigma 2.91}(Mn_{3.09}^{2+}Fe_{0.47}^{2+}Mg_{0.36})_{\Sigma 3.92}(Mg_{1.31}Fe_{0.69}^{2+})_{\Sigma 2.00}(Al_{0.81}Fe_{0.19}^{3+})(PO_4)_6$. Zhanghuifenite is insoluble in water or hydrochloric acid.

Zhanghuifenite is isostructural with bobfergusonite, a member of the alluaudite supergroup. It is monoclinic, with space group $P2_1/n$, Z = 4, and unit-cell parameters a = 12.8926(3), b = 12.4658(3), c = 10.9178(2) Å, β = 97.9200(10)°, and V = 1737.93(7) Å^3. The crystal structure of zhanghuifenite contains six octahedral M (= Mn, Fe, Mg, Al) sites and five X (= Na, Mn, Ca) sites with coordination numbers between 6 and 8. The six M octahedra share edges to form two types of kinked chains extending along [101], with one consisting of $M1$-$M4$-$M5$ and the other $M2$-$M3$-$M6$. These chains are joined by PO_4 tetrahedra to form sheets parallel to (010), which are linked together through corner-sharing between PO_4 tetrahedra and MO_6 octahedra in the adjacent sheets, leaving open channels parallel to a, where the large X cations are situated. Zhanghuifenite differs from bobfergusonite in two major aspects. One is that the $M4$ and $M5$ sites in the former are mainly occupied by Mg, but by Fe^{2+} and Fe^{3+}, respectively, in the latter. The other is that the $X2$-$X5$ sites in zhanghuifenite are all nearly or fully filled with Na, resulting in 3 Na apfu in the ideal formula, but $X4$ and $X5$ are merely half-occupied in bobfergusonite, giving rise to 2 Na apfu.

Keywords: Zhanghuifenite, wyllieite, alluaudite, crystal structure, X-ray diffraction, Raman spectra