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The 2*H* and 3*R* polytypes of sabieite, $NH_4Fe^{3+}(SO_4)_2$, from a natural fire in an oil-bearing shale near Milan, Ohio

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Abstract

The mineral sabieite, $NH_4Fe^{3+}(SO_4)_2$, was found in 2011 along the banks of the Huron River near Milan, Ohio, where it formed as the result of a natural fire in an oil-bearing shale. The mineral is directly associated with pyracmonite, tschermigite, and voltaite and occurs as colorless, pale pink, tan, and yellow hexagonal tablets. The streak is white. Crystals are transparent with vitreous luster. Mohs hardness is 2½, tenacity is brittle, fracture is irregular, and cleavage is perfect on {001}. The measured density is 2.65(2) g/cm^3. The mineral is optically uniaxial (–) with indices of refraction $\omega = 1.657(3)$ and $\varepsilon = 1.621(5)$ (white light). The empirical formula (based on 2 S apfu) is $[(NH_4)_{0.73}(H_3O)_{0.22}K_{0.04}Na_{0.01}]_{\Sigma 1.00}(Fe^{3+}_{0.95}Al_{0.02}Mg_{0.01})_{\Sigma 0.98}(SO_4)_2$. Powder diffraction showed crystals to be combinations of the 2*H* and 3*R* polytypes. The structure of the 2*H* polytype was solved and refined from single-crystal data yielding $R_1 = 0.0694$ for 509 $F_o > 4\sigma(F)$ reflections. The 2*H* polytype has space group $P6_3$ and cell parameters $a = 4.83380(17)$, $c = 16.4362(9)$ Å, $V = 332.59(2)$ Å^3, and $Z = 2$ and the 3*R* polytype has space group $R\overline{3}$ and cell parameters $a = 4.835(2)$, $c = 24.496(15)$ Å, $V = 495.9(5)$ Å^3, and $Z = 3$. The sabieite polytypes (including the original sabieite from Sabie, South Africa, which is the 1*T* polytype) have glaserite-like structures with layers consisting of $Fe^{3+}O_6$ octahedra that share each of their vertices with SO_4 tetrahedra. NH_4 groups occupy 12-coordinated sites in the interlayer region, bonding to 6 O atoms in each of the adjacent layers. In the 1*T* polytype, successive layers have identical configuration and orientation, providing a one-layer repeat sequence. In the 2*H* polytype, alternate layers are flipped (or rotated), in a two-layer repeat sequence. In the 3*R* polytype, successive layers are shifted relative to one another, in a three-layer repeat sequence. The different orientations of adjacent layers in the structures of the 2*H* and 3*R* polytypes result in significant changes in the linkages between the $(NH_4)O_{12}$ and $Fe^{3+}O_6$ polyhedra.

Keywords: Sabieite; crystal structure; polytype; glaserite-like structure; Huron Shale burn site, Milan, Ohio