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Ferro-papikeite, ideally $NaFe^{2+}_2(Fe^{2+}_3Al_2)(Si_5Al_3)O_{22}(OH)_2$, a new orthorhombic amphibole from Nordmark (Western Bergslagen), Sweden: Description and crystal structure

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Abstract

Ferro-papikeite, ideally $NaFe^{2+}_2(Fe^{2+}_3Al_2)(Si_5Al_3)O_{22}(OH)_2$, is a new mineral of the amphibole supergroup from the Filipstad Municipality, Värmland County, Central Sweden, where it occurs in a medium-grade felsic metavolcanic rock. Ferro-papikeite is pale brown with a translucent luster, has a colorless to very pale-brown streak, and shows no fluorescence under long-wave or short-wave ultraviolet light. Grains are subhedral, 0.4–3.0 mm in size, and show well-developed {210} cleavage. It has a Mohs hardness of ~6 and is brittle with a splintery fracture, has the characteristic perfect {210} cleavage of orthorhombic amphiboles, intersecting at ~56°, and the calculated density is 3.488 g/cm^3. In transmitted plane-polarized light, ferro-papikeite is moderately pleochroic X = very pale brown, Y = Z = honey brown; X < Y = Z. Ferro-papikeite is biaxial (+), α = 1.674(2), β = 1.692(2), γ = 1.716(2), $2V_{meas}$ = 86.2(9) and $2V_{calc}$ = 88.3°, dispersion is r < v, weak. The orientation is: X ∥ a, Y ∥ b, Z ∥ c.

Ferro-papikeite is orthorhombic, space group *Pnma*, *a* = 18.628(4), *b* = 17.888(4), *c* = 5.3035(11) Å, *V* = 1767.2(6) Å^3, *Z* = 4. The strongest ten X-ray diffraction lines in the powder pattern are [*d* in Å(*I*)(*hkl*)]: 8.255(100)(210), 3.223(39)(440), 3.057(68)(610), 2.824(28)(251), 2.674(41)(351), 2.572(56)(161,621), 2.549(38)(202), 2.501(50)(261,451), 2.158(25)(502), and 1.991(31)(661). Chemical analysis by electron microprobe gave SiO_2 36.50, Al_2O_3 22.24, TiO_2 0.09, FeO 31.54, MnO 0.65, MgO 5.48, CaO 0.08, Na_2O 2.35, F 0.22, H_2O_{calc} 1.85, O=F –0.09, sum 100.91 wt%. The formula unit, calculated on the basis of 24 (O+OH+F) with (OH) = 2 apfu and Fe^{3+} = 0.13 apfu (determined from the <*M*2–O> distance) is $^{A}(Na_{0.70}Ca_{0.01})^{B+C}(Mg_{1.25}Fe^{2+}_{3.90}Mn^{2+}_{0.08}Al_{1.62}Fe^{3+}_{0.13}Ti^{4+}_{0.01})_{\Sigma 6.99}{}^{T}(Si_{5.60}Al_{2.40})_{\Sigma 8}O_{22}(OH_{1.89}F_{0.11})_2$. The crystal structure of ferro-papikeite was refined to an R-index of 3.60% using 2335 unique observed reflections collected with Mo*K*a X-radiation. $^{[4]}Al^{3+}$ is ordered over the four *T* sites as follows: *T*1B > *T*1A > *T*2B >> *T*2a, $^{[6]}Al^{3+}$ is completely ordered at *M*2, and Fe^{2+} is strongly ordered at *M*4. The *A* site is split with Na^+ strongly ordered at *A*1. End-member ferro-papikeite is related to end-member gedrite, $\square Mg_2(Mg_3Al_2)(Si_6Al_2)O_{22}(OH)_2$, by the substitutions $Na^+ \rightarrow \square$, $Fe^{2+} \rightarrow Mg$, and $Al^{3+} \rightarrow Si^{4+}$. The description of ferro-papikeite as a new species further emphasizes the compositional similarities between the monoclinic calcium amphiboles and the orthorhombic magnesium-iron-manganese amphiboles.

Keywords: Ferro-papikeite, new amphibole, electron-microprobe analysis, optical properties, crystal-structure refinement, Bergslagen, Sweden