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Fluor-elbaite, $Na(Li_{1.5}Al_{1.5})Al_6(Si_6O_{18})(BO_3)_3(OH)_3F$, a new mineral species of the tourmaline supergroup

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Abstract

Fluor-elbaite, $Na(Li_{1.5}Al_{1.5})Al_6(Si_6O_{18})(BO_3)_3(OH)_3F$, is a new mineral of the tourmaline supergroup. It is found in miarolitic cavities in association with quartz, pink muscovite, lepidolite, spodumene, spessartine, and pink beryl in the Cruzeiro and Urubu mines (Minas Gerais, Brazil), and apparently formed from late-stage hydrothermal solutions related to the granitic pegmatite. Crystals are blue-green with a vitreous luster, sub-conchoidal fracture and white streak. Fluor-elbaite has a Mohs hardness of approximately 7.5, and has a calculated density of about 3.1 g/cm^3. In plane-polarized light, fluor-elbaite is pleochroic (O = green/bluish green, E = pale green), uniaxial negative. Fluor-elbaite is rhombohedral, space group *R*3*m*, *a* = 15.8933(2), *c* = 7.1222(1) Å, *V* = 1558.02(4) Å^3, *Z* = 3 (for the Cruzeiro material). The strongest eight X-ray-diffraction lines in the powder pattern [*d* in Å(*I*)(*hkl*)] are: 2.568(100)(051), 2.939(92)(122), 3.447(67)(012), 3.974(58)(220), 2.031(57)(152), 4.200(49)(211), 1.444(32)(642), and 1.650(31)(063). Analysis by a combination of electron microprobe, secondary ion mass spectrometry, and Mössbauer spectroscopy gives SiO_2 = 37.48, Al_2O_3 = 37.81, FeO = 3.39, MnO = 2.09, ZnO = 0.27, CaO = 0.34, Na_2O = 2.51, K_2O = 0.06, F = 1.49, B_2O_3 = 10.83, Li_2O = 1.58, H_2O = 3.03, sum 100.25 wt%. The unit formula is: $^{X}(Na_{0.78}\square_{0.15}Ca_{0.06}K_{0.01})^{Y}(Al_{1.15}Li_{1.02}Fe^{2+}_{0.46}Mn^{2+}_{0.28}Zn_{0.03})$ $^{Z}Al_6{}^{T}(Si_{6.02}O_{18})^{B}(BO_3)_3{}^{V}(OH)_3{}^{W}(F_{0.76}OH_{0.24})$.

The crystal structure of fluor-elbaite was refined to statistical indices *R*1 for all reflections less then 2% using Mo$K\alpha$ X-ray intensity data. Fluor-elbaite shows relations with elbaite and tsilaisite through the substitutions $^{W}F \leftrightarrow {}^{W}OH$ and $^{Y}(Al + Li) + {}^{W}F \leftrightarrow 2{}^{Y}Mn^{2+} + {}^{W}OH$, respectively.

Keywords: Fluor-elbaite, tourmaline, new mineral species, crystal-structure refinemnet, electron microprobe, ion microprobe, Mössbauer spectroscopy