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Celleriite, $\square(Mn_2^{2+}Al)Al_6(Si_6O_{18})(BO_3)_3(OH)_3(OH)$, a new mineral species of the tourmaline supergroup

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Abstract

Celleriite, $\square(Mn_2^{2+}Al)Al_6(Si_6O_{18})(BO_3)_3(OH)_3(OH)$, is a new mineral of the tourmaline supergroup. It was discovered in the Rosina pegmatite, San Piero in Campo, Elba Island, Italy (holotype specimen), and in the Pikárec pegmatite, western Moravia, Czech Republic (co-type specimen). Celleriite in hand specimen is violet to gray-blue (holotype) and dark brownish-green (co-type) with a vitreous luster, conchoidal fracture, and white streak. Celleriite has a Mohs hardness of ~7 and a calculated density of 3.13 and 3.14 g/cm^3 for holotype and its co-type, respectively. In plane-polarized light in thin section, celleriite is pleochroic (O = pale violet and E = light gray-blue in holotype; O = pale green and E = colorless in co-type) and uniaxial negative. Celleriite has trigonal symmetry: space group $R3m$, $Z = 3$, $a = 15.9518(4)$ and $15.9332(3)$ Å, $c = 7.1579(2)$ and $7.13086(15)$ Å, $V = 1577.38(9)$ and $1567.76(6)$ Å^3 for holotype and co-type, respectively (data from single-crystal X-ray diffraction). The crystal structure of the holotype specimen was refined to $R1 = 2.89\%$ using 1696 unique reflections collected with Mo$K\alpha$ X-ray intensity data. Structural, chemical, and spectroscopic analyses resulted in the formulas:

$^{X}(\square_{0.58}Na_{0.42})_{\Sigma 1.00}{}^{Y}(Mn^{2+}_{1.39}Fe^{2+}_{0.16}Mg_{0.01}Al_{1.14}Fe^{3+}_{0.01}Li_{0.28}Ti_{0.01})_{\Sigma 3.00}{}^{Z}Al_6[{}^{T}(Si_{5.99}Al_{0.01})_{\Sigma 6.00}O_{18}](BO_3)_3(OH)_3{}^{W}[(OH)_{0.65}F_{0.03}O_{0.32}]_{\Sigma 1.00}$ (for holotype)

and

$^{X}(\square_{0.51}Na_{0.49})_{\Sigma 1.00}{}^{Y}(Mn^{2+}_{0.90}Fe^{2+}_{0.50}Al_{1.36}Fe^{3+}_{004}Li_{0.17}Zn_{0.04})_{\Sigma 3.00}{}^{Z}Al_6[{}^{T}(Si_{5.75}B_{0.25})_{\Sigma 6.00}O_{18}](BO_3)_3(OH)_3{}^{W}[(OH)_{0.35}F_{0.17}O_{0.48}]_{\Sigma 1.00}$ (for co-type)

Celleriite is a hydroxy species belonging to the *X*-site vacant group of the tourmaline supergroup. The new mineral was approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association, proposal no. 2019-089.

In the Rosina pegmatite, celleriite formed an overgrowth at the analogous pole of elbaite–fluor-elbaite–rossmanite crystals during the latest stage of evolution of pegmatite cavities after an event of a pocket rupture. In the Pikárec pegmatite, celleriite occurs as an intermediate growth sector of elbaite, princivalleite, and fluor-elbaite.

Keywords: Celleriite, tourmaline, crystal-structure refinement, electron microprobe, Mössbauer spectroscopy, laser-induced breakdown spectroscopy, laser-ablation inductively coupled plasma mass-spectroscopy, Raman spectroscopy; Lithium, Beryllium, and Boron: Quintessentially Crustal