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Mn-rich tourmaline from Austria: structure, chemistry, optical spectra, and relations to synthetic solid solutions

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ABSTRACT

Yellow-brown to pink Mn-rich tourmalines with MnO contents in the range 8–9 wt% MnO (~0.1 wt% FeO) from a recently discovered locality in Austria, near Eibenstein an der Thaya (Lower Austria), have been characterized by crystal structure determination, by chemical analyses (EMPA, SIMS), and by optical absorption spectroscopy. Qualitatively, the optical spectra show that Mn^{2+} is present in all regions of the crystals, and that there is more Mn^{3+} in the pink regions (~8% of the total Mn is Mn^{3+}) than in the yellow-brown regions. A gamma-ray irradiated crystal fragment is distinctly pink compared to the yellow-brown color of the sample before irradiation, but it still has hints of the yellow-brown color, which suggests that the natural pink color in Mn-rich tourmaline from this locality is due to natural irradiation of the initial Mn^{2+}. For these Mn-rich and Li-bearing olenite samples, crystal structure refinements in combination with the chemical analyses give the optimized formulae $^{X}(Na_{0.80}Ca_{0.01}\square_{0.19})\ ^{Y}(Al_{1.28}Mn^{2+}_{1.21}Li_{0.37}Fe^{2+}_{0.02}\square_{0.12})\ ^{Z}Al_6\ ^{T}(Si_{5.80}Al_{0.20})\ B_3O_{27}[(OH)_{3.25}F_{0.43}O_{0.32}]$, with a = 15.9466(3) Å, c = 7.1384(3) Å, and R = 0.036 for the sample with ~9 wt% MnO, and $^{X}(Na_{0.77}Ca_{0.03}\square_{0.20})\ ^{Y}(Al_{1.23}Mn^{2+}_{1.14}Li_{0.48}Fe^{2+}_{0.02}Ti_{0.01}\square_{0.12})^{Z}Al_6^{T}(Si_{5.83}Al_{0.17})\ B_3O_{27}\ [(OH)_{3.33}F_{0.48}O_{0.19}]$ for a sample with a = 15.941(1) Å, c = 7.136(1) Å, R = 0.025 and ~8 wt% MnO. The refinements show 1.22–1.25 Al at the Y site. As the Mn content increases, the Li and the F contents decrease. The Li content (0.37–0.48 apfu) is similar to, or lower than, the Li content of olenite (rim-composition) from the type locality, but these Mn-rich tourmalines do not contain $^{[4]}B$. Like the tourmaline from Eibenstein an der Thaya, synthetic Mn-rich tourmaline (in a Li + Mn-bearing system), containing up to ~0.9 apfu Mn (~6.4 wt% MnO), is aluminous but not Li-rich. This study demonstrates that although a positive correlation exists between Mn and Li (elbaite) in tourmaline samples from some localities, this coupling is not required to promote compatibility of Mn in tourmaline. The a parameter in Mn-rich tourmalines (MnO: ≥3 wt%) is largely a function of the cation occupancy of the Y site (r^2 = 0.97).