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Rossmanite, $\square(LiAl_2)Al_6(Si_6O_{18})(BO_3)_3(OH)_4$, a new alkali-deficient tourmaline: Description and crystal structure

Julie B. Selway,[1] Milan Novák,[1,*] Frank C. Hawthorne,[1,†] Petr Černý,[1] Luisa Ottolini,[2] and T. Kurtis Kyser[3]

[1] Department of Geological Sciences, University of Manitoba, Winnipeg, Manitoba R3T 2N2, Canada
[2] CNR Centro di Studio per la Cristallochimica e la Cristallografia via Abbiategrasso 209, 27100 Pavia, Italy
[3] Department of Geological Sciences, Queen's University, Kingston, Ontario K7L 3N6, Canada

Abstract

Rossmanite is a new tourmaline species from near Rožná, western Moravia, Czech Republic. It forms pale pink columnar crystals about 25 mm long and 5 mm thick, elongated along *c* with striations parallel to *c* on the prism faces. It is brittle, $H = 7$, $D_{meas} = 3.00$ g/cm^3, $D_{calc} = 3.06$ g/cm^3. In plane-polarized light, it is colorless. Rossmanite is uniaxial negative, $\omega = 1.645(1)$, $\epsilon = 1.624(1)$, trigonal, space group $R3m$, in the hexagonal setting $a = 15.770(2)$, $c = 7.085(1)$ Å, $V = 1525.8(4)$ Å^3, $Z = 3$. The strongest six X-ray diffraction lines in the powder pattern are at $d = 3.950$ Å with $I = 100\%$ for $(hkl) =$ (220); 2.552 Å, 93%, (051); 1.898 Å, 72%, (342); 4.181 Å, 58%, (211); 2.924 Å, 56%, (122); and 3.434 Å, 53%, (012). Analysis by a combination of electron microprobe, SIMS, H-line extraction, and crystal-structure refinement gave SiO_2 38.10 wt%, Al_2O_3 44.60, Na_2O 1.43, $Li_2O = 1.13$, $B_2O_3 = 10.88$, $H_2O = 3.70$, F = 0.20, O ≡ F 0.08, sum = 99.96 wt%, Fe, Mg, Ca, Mn, Ti, F, K not detected. The formula unit (31 anions) is $^X(\square_{0.57}Na_{0.43})^Y(Li_{0.71}Al_{2.17})^ZAl_6(Si_{5.92}O_{18})(B_{2.92}O_9)(OH)_{3.83}F_{0.10}O_{0.07}$, with the ideal end-member formula $\square(LiAl_2)Al_6(Si_6O_{18})(BO_3)_3(OH)_4$; thus rossmanite can be derived from elbaite $[Na(Al_{1.5}Li_{1.5})(Si_6O_{18})(BO_3)_3(OH)_4]$ by the substitution $^X\square_2 + {}^Y\!Al \rightarrow {}^X\!Na_2 + {}^Y\!Li$, where $\square$ = vacancy. The crystal structure of rossmanite was refined to an *R* index of 1.7% using 1094 observed (5σ) reflections collected with Mo$K\alpha$ X-radiation from a single crystal. The structure refinement confirmed the low occupancy of the X site and the presence of Li at the Y site. There is considerable positional disorder at the O1 and O2 sites induced by the local variations in bond-valence distribution associated with □-Na disorder at X and Li-Al disorder at Y.