

Raman spectroscopic quantification of tetrahedral boron in synthetic aluminum-rich tourmaline

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ABSTRACT

The Raman spectra of five ¹⁴B-bearing tourmalines of different composition synthesized at 700 °C/4.0 GPa (including first-time synthesis of Na-Li-¹⁴B-tourmaline, Ca-Li-¹⁴B-tourmaline, and Ca-bearing □-¹⁴B-tourmaline) reveal a strong correlation between the tetrahedral boron content and the summed relative intensity of all OH-stretching bands between 3300–3430 cm⁻¹. The band shift to low wavenumbers is explained by strong O3-H···O5 hydrogen bridge bonding. Applying the regression equation to natural ¹⁴B-bearing tourmaline from the Koralpe (Austria) reproduces the EMPA-derived value perfectly [EMPA: 0.67(12) ¹⁴B pfu vs. Raman: 0.66(13) ¹⁴B pfu]. This demonstrates that Raman spectroscopy provides a fast and easy-to-use tool for the quantification of tetrahedral boron in tourmaline. The knowledge of the amount of tetrahedral boron in tourmaline has important implications for the better understanding and modeling of B-isotope fractionation between tourmaline and fluid/melt, widely used as a tracer of mass transfer processes.

Keywords: Tourmaline, high pressure, synthesis, tetrahedral boron, Raman, SIMS; Lithium, Beryllium and Boron: Quintessentially Crustal