

Nuclear magnetic resonance and infrared spectroscopic study of excess-boron olenite from Koralpe, Styria, Austria

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ABSTRACT

Significant amounts of boron in both trigonal and tetrahedral coordination have been found through ¹¹B magic-angle-spinning (MAS) nuclear magnetic resonance (NMR) spectroscopy of natural olenite (aluminum-rich tourmaline) from Stoffhütte, Koralpe, Styria, Austria. The ¹¹B MAS NMR spectrum consists of a superposition of two quadrupolar MAS peaks. A broad peak with $\delta_{\text{iso}} = 18.3$ ppm, $\nu_{\text{Q}} = 1410$ KHz, and $\eta = 0.11$ demonstrates the trigonal-planar environment of the BO₃ group (relative area ratio = 80%). The narrow symmetrical peak ($\delta_{\text{iso}} = 0.0$ ppm, $\nu_{\text{Q}} = 300$ KHz, $\eta = 0.00$) represents tetrahedral BO₄ groups (relative area ratio = 20%). An infrared spectrum shows hydroxyl stretching bands at low wavenumbers indicating that underbonded O atoms of the hexagonal ring (due to a partial replacement of [⁴Si⁴⁺ by ⁴B³⁺]) form relatively strong hydrogen bonds with the protons of the hydroxyl groups. A ²⁹Si MAS NMR spectrum shows a peak consisting of a main signal at –90 ppm and a shoulder at about –85 ppm. The main signal originates from Si atoms connected (via oxygen bridges) to two other Si atoms in the hexagonal ring, and the minor signal is from Si atoms connected to one Si and one B atom. No signal corresponding to ¹⁶Si was detected in this natural olenite sample.