

Infrared study of OH sites in tourmaline from the elbaite-schorl series

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ABSTRACT

Two different behaviors controlled by local lattice environment of crystallization are observed in the IR spectra of polycrystalline natural tourmalines from the elbaite-schorl series in the O-H stretching region (3800–3100 cm⁻¹). The first case is characterized by the presence of three O-H stretching bands, and is observed in elbaite [Na(Li,Al)₃Al₆(BO₃)₃Si₆O₁₈(OH)₄], schorl [NaFe³⁺Al₆(BO₃)₃Si₆O₁₈(OH)₄] and Fe-elbaite. The second case is observed in Li-rich schorl and is marked by four O-H stretching bands. This behavior is due to the presence of Li-rich and Fe-rich domains in schorl crystallized in Li-bearing-pegmatites. Band assignments are discussed using the results of the factor group analysis for a C_{3v}⁵ crystal structure and considering the interactions between the O-H and the atoms in the Y and Z sites in the crystal. The interpretation presented differs from previous conclusions.