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Tourmaline chemistry and the ^{III}B site

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Abstract

Based on a large database of tourmaline crystal-structure refinements and associated electron microprobe analyses, the <B-O> bond length in the triangular (BO_3) groups was found to be reasonably constant for all tourmaline species, but the B-O2 and B-O8 are variable as a function of the crystal chemistry. Tourmalines, such as elbaite, tend to have B-O2 distances significantly shorter than the B-O8 distances, whereas others, like povondraite, tend to have B-O2 distances that are longer than their B-O8 bonds. Statistical analysis of the bond-valence contributions for the nine-coordinated X-O2, and the six-coordinated Y-O2, Z-O8, and Z'-O8 bonds—as they relate to the B-O2/B-O8 bond valence—suggest that the Z'-O8 bond has the most influence over the geometry of the (BO_3) triangle. This study highlights variations in what has otherwise been assumed to be a static site in the crystal structure of tourmaline-group minerals.

Keyword: Tourmaline, boron, stereochemistry, crystal-structure, statistical analysis