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Crystal chemical relationships in the tourmaline group: Structural constraints on chemical variability

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Abstract

This paper explores some aspects of the crystal chemistry and structural constraints on tourmaline by examining 127 samples from the literature. According to the bond-valence model, the tourmaline structure shows lattice-induced strain at each polyhedron. The overall effect is an expansion of the triangular (BO_3) group and compression of the tetrahedron. The X polyhedron can be either compressed or expanded: compression increases with vacancy content, whereas expansion is typical of Ca-rich tourmaline. The Y octahedron changes extensively from compressed through an unstrained to expanded state as a function of increasing Li content. The Z octahedron is almost unstrained in crystals with $\Sigma^{Z}R^{2+} < 0.40$ apfu, whereas it is compressed in crystals with $\Sigma^{Z}R^{2+} > 0.40$ apfu.

The configuration of the six-membered tetrahedral ring is strongly affected by <Y-O>, which is the most important parameter linked to the deviation of the tetrahedral ring from hexagonal symmetry. The whole structure is stable when the channels through the Z octahedron framework are able to accommodate the Y cations. As <Y-O> becomes larger, the less puckered the tetrahedral ring and the more the O7 atom is displaced away from Z. Consequently, the difference between <Y-O> and <Z-O> cannot be too large, otherwise <Z-O> will be too small to be commensurate with shifting of the O7 atom. One possible mechanism to reduce the difference between <Y-O> and <Z-O>, is the disordering reaction $^{Y}Al + {}^{Z}R \rightarrow {}^{Y}R + {}^{Z}Al$, which increases <Z-O> and decreases <Y-O>. In ideal dravite, schorl, and "tsilaisite," <Y-O> and <Z-O> are incommensurate.

Keywords: Order-disorder, crystal structure, tourmalina, XRD data