

Thermal expansion of minerals in the tourmaline supergroup

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ABSTRACT

The thermal behavior of 15 natural tourmaline samples has been measured by X-ray powder diffraction from room temperature to ~930 °C. Axial thermal expansion is generally greater along the **c** crystallographic axis (α_c 0.90–1.05 $\times 10^{-5}$ /K) than along the **a** crystallographic axis and the symmetrically equivalent **b** axis (α_a 0.47–0.60 $\times 10^{-5}$ /K). Ferro-bearing samples show lower expansion along **a** than in other tourmalines. In povondraite the thermal expansion along the **c** axis is higher than in other tourmalines, whereas along **a** it is lower [$\alpha_a = 0.31(2)$ and $\alpha_c = 1.49(3) \times 10^{-5}$ /K]. Volume expansion in the tourmaline-supergroup minerals is relatively low compared with other silicates such as pyroxenes and amphiboles. Volume also exhibits a relatively narrow range of thermal expansion coefficients (1.90–2.05 $\times 10^{-5}$ /K) among the supergroup members. An interpretation for the small changes in thermal expansion in a compositionally heterogeneous group like tourmaline is that all members, except povondraite, share a framework of dominantly ²AlO₆ polyhedra that limit thermal expansion. Povondraite, with a framework dominated by ²Fe³⁺O₆ polyhedra, displays thermal expansion that is different from other members of the group.

Unit-cell dimensions of tourmalines having significant Fe²⁺ deviate from linearity above 400 °C on plots against temperature (*T*); along with the resulting substantial reduction in unit-cell volume, these effects are likely the result of deprotonation/oxidation processes. Lithium-rich and Fe²⁺-free tourmalines deviate similarly at *T* > 600 °C. In Li- and Fe²⁺-free tourmalines, no such deviation is observed up to the highest temperatures of our experiments. It is not clear whether this is due to cation order-disorder over *Y* and *Z* sites that occurs during the highest temperature measurements, a phenomenon that is apparently inhibited (at least in the short term) in Li-free/Mg-rich samples. If so, this must occur at a relatively rapid rate, as no difference in unit-cell values was detected at 800 °C after heating in both one- and 12-h experiments on Na-rich rossmanite.

Keywords: Tourmaline, thermal expansion, modeling, systematics, unit-cell parameters, X-ray diffraction