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Tourmaline crystal chemistry

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Abstract

Tourmalines form the most important boron rock-forming minerals on Earth. They belong to the cyclosilicates with a structure that may be regarded as a three-dimensional framework of octahedra ZO_6 that encompass columns of structural "islands" made of XO_9, YO_6, BO_3, and TO_4 polyhedra. The overall structure of tourmaline is a result of short-range and long-range constraints resulting, respectively on the charge and size of ions. In this study, published data are reviewed and analyzed to achieve a synthesis of relevant experimental results and to construct a crystal-chemical model for describing tourmalines and their compositional miscibility over different length scales. Order-disorder substitution reactions involving cations and anions are controlled by short-range structural constraints, whereas order-disorder intracrystalline reaction involving only cations are controlled by long-range structural constraints. The chemical affinity of a certain cation to a specific structural site of the tourmaline structure has been established on the basis of structural data and crystal-chemical considerations. This has direct implications for the tourmaline nomenclature, as well as on petrogenetic and provenance information. Some assumptions behind the classification scheme of tourmaline have been reformulated, revealing major agreement and significant improvements compared to earlier proposed scheme.

Keywords: Tourmaline, order-disorder, crystal structure, nomenclature