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Estimation and testing of standard molar thermodynamic properties of tourmaline end-members using data of natural samples

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ABSTRACT

Different estimation methods have been combined with calorimetric data for a natural Mg-rich tourmaline and dumortierite, a structurally similar borosilicate, to estimate thermodynamic properties of five tourmaline end-members (dravite, schorl, alkali-free dravite, aluminofoitite, and ferrifoitite). The results were tested by predicting the solubility of Fe-rich tourmaline in natural, low-variance hydrothermal mineral assemblages, for which the B concentration was independently known from Laser Ablation-ICP-MS analysis of coexisting fluid inclusions. Agreement within the uncertainty of experimental and thermodynamic data supports the validity of the estimation methods that used the fictive properties of the $^{III}B_2O_3$ polyhedron for calculating standard enthalpy and entropy, and reactions involving dumortierite to estimate the heat-capacity functions. This study indicates more generally that the development of new microanalytical techniques for measuring the composition of natural fluid inclusions in well-constrained mineral assemblages represents a promising approach to estimating or testing thermodynamic data for complex silicates.