

Single-crystal X-ray study of K-tourmaline crystal structure up to 20 GPa

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The structure behaviour of K-rich tourmaline ($\text{Na}_{0.5}\text{K}_{0.5}(\text{Mg}_{1.5}\text{Fe}_{1.5})\text{Al}_6[\text{Si}_6\text{O}_{18}](\text{BO}_3)_3(\text{OH})_3(\text{OH})$) from the ultrahigh-pressure metamorphic rocks of Kokchetav massif was studied using synchrotron-based single crystal diffraction up to 20 GPa.

Within the whole pressure range the compression is regular (Fig.1); fitting the PV -data with the 2nd and 3rd order Birch-Murnaghan equations of state gives: $V_0 = 1587.2 \text{ \AA}^3$, $K_0 = 115.6 \text{ GPa}$ at fixed $K' = 4$, and $V_0 = 1587.7 \text{ \AA}^3$, $K_0 = 112.7 \text{ GPa}$, $K' = 4.4$. The bulk modulus values are slightly higher as compared to those found for pure Na-variety (dravite): 112.0 and 109.6 GPa, respectively (O'Bannon *et al.* 2018). This is due to the presence of a larger cation (K^+) in the X site which controls greatly the compressibility of tourmaline.

The absence of the structure anomalies found in dravite at 15.4 GPa (symmetry reduction from $R3m$ to $R3$) is also apparently a consequence of stabilizing function of potassium cation. On the other hand, the overall structure behaviour, including the compression anisotropy (Fig.1) and the evolution of the main structure parameters, is very much similar to that of dravite. This indicates a predominant role in the compression behaviour of tourmaline to belong to a octahedral-tetrahedral framework, rather than the X site polyhedra which comprise a relatively small part of the structure.

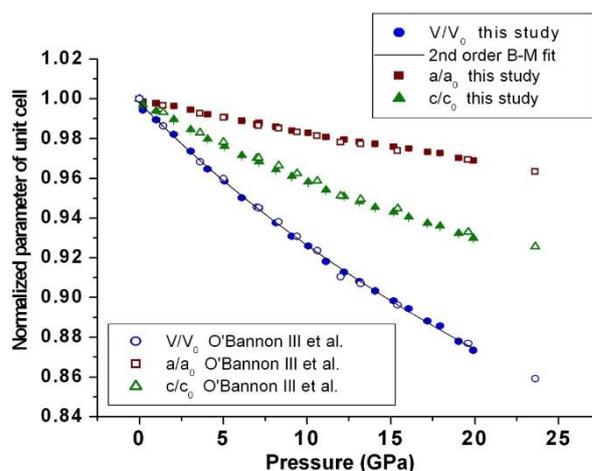


Figure 1. Normalized axial and volume compression curves of K-bearing tourmaline, in comparison with the data of O'Bannon *et al.* (2018) for Na-tourmaline (dravite)

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[1] E. O'Bannon, C.M. Beavers, M. Kunz, Q. Williams, *American Mineralogist* 2018, **103**, 1622.