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Thermal equation of state of Li-rich schorl up to 15.5 GPa and 673 K: Implications for lithium and boron transport in slab subduction

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Abstract

The thermal equation of state (EoS) of a natural schorl has been determined at high temperatures up to 673 K and high pressures up to 15.5 GPa using in situ synchrotron X-ray diffraction combined with a diamond-anvil cell. The pressure-volume (*P*-*V*) data were fitted to a third-order Birch-Murnaghan EoS with V_0 = 1581.45 ± 0.25 Å^3, K_0 = 111.6 ± 0.9 GPa, and K'_0 = 4.4 ± 0.2; additionally, when K'_0 was fixed at a value of 4, V_0 = 1581.04 ± 0.20 Å^3, and K_0 = 113.6 ± 0.3 GPa. The V_0 (1581.45 ± 0.25 Å^3) obtained by the third-order Birch-Murnaghan EoS agrees well with the V_0 (1581.45 ± 0.05 Å^3) measured at ambient conditions. Furthermore, the axial compression data of schorl at room temperature were fitted to a "linearized" third-order Birch-Murnaghan EoS, and the obtained axial moduli for the *a*- and *c*-axes are K_a = 621 ± 9 GPa and K_c = 174 ± 2 GPa, respectively. Consequently, the axial compressibilities are $\beta_a = 1.61 \times 10^{-3}$ GPa^{-1} and $\beta_c = 5.75 \times 10^{-3}$ GPa^{-1} with an anisotropic ratio of β_a:β_c = 0.28:1.00, indicating axial compression anisotropy. In addition, the compositional effect on the axial compressibilities of tourmalines was discussed. Fitting our pressure-volume-temperature (*P*-*V*-*T*) data to a high-temperature third-order Birch-Murnaghan EoS yielded the following thermal EoS parameters: V_0 = 1581.2 ± 0.2 Å^3, K_0 = 110.5 ± 0.6 GPa, K'_0 = 4.6 ± 0.2, $(\partial K_T/\partial T)_P$ = –0.012 ± 0.003 GPa K^{-1} and $\alpha_{V0} = (2.4 \pm 0.2) \times 10^{-5}$ K^{-1}. These parameters were compared with those of previous studies on other tourmalines, and the potential factors influencing the thermal EoS parameters of tourmalines were further discussed.

Keywords: Schorl, equation of state, high pressure and high temperature, X-ray diffraction, diamond-anvil cell