American Mineralogist, Volume 104, pages 1005–1015, 2019

Compressibility of synthetic Mg-Al tourmalines to 60 GPa

ELEANOR J. BERRYMAN[1,*], DONGZHOU ZHANG[2], BERND WUNDER[3], AND THOMAS S. DUFFY[1]

[1]Department of Geosciences, Princeton University, Princeton, New Jersey 08544, U.S.A.
[2]Hawai'i Institute of Geophysics and Planetology, University of Hawai'i at Manoa, Honolulu, Hawai'i 96822, U.S.A. Orcid 0000-0002-6679-892X
[3]Chemistry and Physics of Earth Materials, GFZ German Research Centre for Geosciences, 14473 Potsdam, Germany

ABSTRACT

High-pressure single-crystal X-ray diffraction patterns on five synthetic Mg-Al tourmalines with near end-member compositions [dravite $NaMg_3Al_6Si_6O_{18}(BO_3)_3(OH)_3OH$, K-dravite $KMg_3Al_6Si_6O_{18}(BO_3)_3(OH)_3OH$, magnesio-foitite $\square(Mg_2Al)Al_6Si_6O_{18}(BO_3)_3(OH)_3OH$, oxy-uvite $CaMg_3Al_6Si_6O_{18}(BO_3)_3(OH)_3O$, and olenite $NaAl_3Al_6Si_6O_{18}(BO_3)_3O_3OH$, where $\square$ represents an *X*-site vacancy] were collected to 60 GPa at 300 K using a diamond-anvil cell and synchrotron radiation. No phase transitions were observed for any of the investigated compositions. The refined unit-cell parameters were used to constrain third-order Birch-Murnaghan pressure-volume equation of states with the following isothermal bulk moduli (K_0 in GPa) and corresponding pressure derivatives ($K_0' = \partial K_0/\partial P)_T$: dravite $K_0 = 97(6)$, $K_0' = 5.0(5)$; K-dravite $K_0 = 109(4)$, $K_0' = 4.3(2)$; oxy-uvite $K_0 = 110(2)$, $K_0' = 4.1(1)$; magnesio-foitite $K_0 = 116(2)$, $K_0' = 3.5(1)$; olenite $K_0 = 116(6)$, $K_0' = 4.7(4)$. Each tourmaline exhibits highly anisotropic behavior under compression, with the **c** axis 2.8–3.6 times more compressible than the **a** axis at ambient conditions. This anisotropy decreases strongly with increasing pressure and the **c** axis is only ~14% more compressible than the **a** axis near 60 GPa. The octahedral *Y*- and *Z*-sites' composition exerts a primary control on tourmaline's compressibility, whereby Al content is correlated with a decrease in the **c**-axis compressibility and a corresponding increase in K_0 and K_0'. Contrary to expectations, the identity of the *X*-site-occupying ion (Na, K, or Ca) does not have a demonstrable effect on tourmaline's compression curve. The presence of a fully vacant *X* site in magnesio-foitite results in a decrease of K_0' relative to the alkali and Ca tourmalines. The decrease in K_0' for magnesio-foitite is accounted for by an increase in compressibility along the **a** axis at high pressure, reflecting increased compression of tourmaline's ring structure in the presence of a vacant *X* site. This study highlights the utility of synthetic crystals in untangling the effect of composition on tourmaline's compression behavior.

Keywords: Tourmaline, synthetic, single-crystal X-ray diffraction, equation of state, diamond-anvil cell