American Mineralogist, Volume 95, pages 1765–1772, 2010

Crystal structure of hydrous wadsleyite with 2.8% H_2O and compressibility to 60 GPa

Yu Ye,[1,*] Joseph R. Smyth,[2] Anwar Hushur,[3] Murli H. Manghnani,[3] Dayana Lonappan,[3] Przemyslaw Dera,[4] and Daniel J. Frost[5]

[1]Department of Physics, University of Colorado, Boulder, Colorado 80309, U.S.A.
[2]Department of Geological Sciences, University of Colorado, Boulder, Colorado 80309, U.S.A.
[3]Hawaii Institute of Geophysics, University of Hawaii, Honolulu, Hawaii 96822, U.S.A.
[4]Center for Advanced Radiation Sources, University of Chicago, Argonne National Laboratory, Argonne, Illinois 60439, U.S.A.
[5]Bayerisches Geoinstitut, Universität Bayreuth, Bayreuth D95440, Germany

Abstract

Hydrous wadsleyite (β-Mg_2SiO_4) with 2.8 wt% water content has been synthesized at 15 GPa and 1250 °C in a multi-anvil press. The unit-cell parameters are: a = 5.6686(8), b = 11.569(1), c = 8.2449(9) Å, β = 90.14(1)°, and V = 540.7(1) Å^3, and the space group is $I2/m$. The structure was refined in space groups *Imma* and $I2/m$. The room-pressure structure differs from that of anhydrous wadsleyite principally in the increased cation distances around O1, the non-silicate oxygen. The compression of a single crystal of this wadsleyite was measured up to 61.3(7) GPa at room temperature in a diamond anvil cell with neon as pressure medium by X-ray diffraction at Sector 13 at the Advanced Photon Source, Argonne National Laboratory. The experimental pressure range was far beyond the wadsleyite-ringwoodite phase-transition pressure at 525 km depth (17.5 GPa), while a third-order Birch-Murnaghan equation of state (EoS) [V_0 = 542.7(8) Å^3, K_{T0} = 137(5) GPa, K' = 4.6(3)] still fits the data well. In comparison, the second-order fit gives V_0 = 542.7(8) Å^3, K_T = 147(2) GPa. The relation between isothermal bulk modulus of hydrous wadsleyite K_{T0} and water content C_{H_2O} is: K_{T0} = 171(1)–12(1) C_{H_2O} (up to 2.8 wt% water). The axial-compressibility β_c is larger than both β_a and β_b, consistent with previous studies and analogous to the largest coefficient of thermal expansion along the c-axis.

Keywords: Compressibility, hydrous wadsleyite, neon, orthorhombic