American Mineralogist, Volume 82, pages 270–275, 1997

Crystal structure of monoclinic hydrous wadsleyite [β-$(Mg,Fe)_2SiO_4$]

JOSEPH R. SMYTH,[1] TATSUHIKO KAWAMOTO,[2] STEPHEN D. JACOBSEN,[1] R. JEFFREY SWOPE,[1] RICHARD L. HERVIG,[2,3] AND JOHN R. HOLLOWAY[2,4]

[1]Department of Geological Sciences University of Colorado, Boulder, Colorado 80309-0250, U.S.A.
[2]Department of Geology, Arizona State University, Tempe, Arizona 85287, U.S.A.
[3]Center for Solid State Science, Arizona State University, Tempe, Arizona 85287, U.S.A.
[4]Department of Chemistry, Arizona State University, Tempe, Arizona 85287, U.S.A.

ABSTRACT

Wadsleyite [β-$(Mg,Fe)_2SiO_4$] is known to accept variable amounts of H and may be an important reservoir of H in the transition zone of the mantle. The crystal structure of $Fo_{94.6}$ hydrous wadsleyite ($Mg_{1.730}Fe_{0.098}Al_{0.008}Si_{0.991}H_{0.355}O_4$) synthesized at 1400 °C and 17 GPa was refined in space group *I*2/*m* from 1784 measured intensities of which 830 were unique, and, of these, 650 were of intensity greater than 4σ. Unit cell parameters are a = 5.6715(7), b = 11.582(2), c = 8.258(1) Å, and β = 90.397(9)°. The final $R(F)$ for all reflections was 0.026 (R_w = 0.024); goodness of fit was 1.68. An H position was located on the nonsilicate O atom (O1). Partial occupancy of a normally vacant tetrahedral site adjacent to M3 was observed. This is postulated to be the result of Si moving from M3 to the adjacent tetrahedral void on decompression. Deviation from orthorhombic symmetry appears to result from ordering of H, (Mg, Fe), and possibly Si, within the two nonequivalent M3 sites.