Effects of hydration on the structure and compressibility of wadsleyite, β-(Mg₂SiO₄)

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ABSTRACT

A suite of pure magnesian wadsleyite (β-Mg₂SiO₄) samples containing 0.005, 0.38, 1.18, and 1.66 wt% H_2O was studied by single-crystal X-ray diffraction to determine the effects of hydration on cation ordering and crystal symmetry. Separate compressibility experiments were carried out to 9.6 GPa to determine the effects of hydration on isothermal equations of state. Crystal-structure refinements at ambient conditions show cation vacancies order onto the M3 site. The most hydrous sample (1.6 wt% H_2O) displayed monoclinic symmetry with β = 90.090(7)°, whereas the samples with lower content were statistically orthorhombic. The density of wadsleyite decreases with increasing water content at STP according to the empirical relation, $\rho = 3.470(2) - 0.046(2)\ C_{H_2O}$ g/cm³ (with C_{H_2O} in wt% H_2O). Bulk moduli and pressure derivatives of wadsleyite are $K_{T0} = 173(5)$ GPa, $K_0' = 4.1(15)$ for 0.005 wt% H_2O; $K_{T0} = 161(4)$ GPa, $K_0' = 5.4(11)$ for 0.38 wt% H_2O; $K_{T0} = 158(4)$ GPa, $K_0' = 4.2(9)$ for 1.18 wt% H_2O; and $K_{T0} = 154(4)$ GPa, $K_0' = 4.9(11)$ for 1.66 wt% H_2O. Variation of the bulk modulus of wadsleyite with water content is non-linear, which may be attributable to softening of the structure by ordering of vacancies onto two non-equivalent M3 sites (M3a and M3b) and an accompanying dilution of orthorhombic symmetry.

Keywords: Wadsleyite, bulk modulus, equation of state, nominally anhydrous minerals, mantle Transition Zone