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In-situ infrared spectra of hydroxyl in wadsleyite and ringwoodite at high pressure and high temperature

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ABSTRACT

The infrared spectra of hydroxyl in synthetic hydrous wadsleyite (β-Mg_2SiO_4) and ringwoodite (γ-Mg_2SiO_4) were measured at room temperature up to ~18.8 GPa for wadsleyite and up to ~21.5 GPa for ringwoodite. High-temperature spectra were measured in an externally heated diamond-anvil cell up to 650 °C at ~14.2 GPa for wadsleyite and up to 900 °C at ~18.4 GPa for ringwoodite. The synthetic samples reproduce nearly all the important OH bands previously observed at ambient conditions. Only subtle changes were observed in the infrared spectra of both minerals, both upon compression at room temperature and upon heating at high pressure. For wadsleyite, upon compression to ~18.8 GPa, the frequencies of the bands at ~3600 cm^{-1} remain almost unchanged, while the main bands at 3200–3400 cm^{-1} shift to lower frequencies. During heating at 14.2 GPa to 650 °C the bands at 3200–3400 cm^{-1} broaden and shift to slightly lower frequencies. For ringwoodite, upon compression to ~21.5 GPa, the main bands at 3115 cm^{-1} progressively shift to lower frequencies. During heating at 18.4 GPa to 900 °C, no frequency shift was observed for the band at ~3700 cm^{-1}, but the band initially at ~3115 cm^{-1} shifts very slightly to higher frequencies, which should yield almost the same band positions at 1300–1400 °C as those measured at ambient conditions. Our data suggest that water speciation in hydrous wadsleyite and ringwoodite at ambient conditions may be comparable to that under mantle conditions, except perhaps for subtle changes in hydrogen bonding. The low OH-stretching frequencies in wadsleyite and ringwoodite under transition zone conditions imply a large H/D fractionation during degassing of the deep mantle. This may explain the apparent disequilibrium between the hydrogen isotopic composition of the upper mantle and the ocean.

Keywords: Hydroxyl, wadsleyite, ringwoodite, infrared spectra, high-pressure, high-temperature, diamond-anvil cell