

Raman Observations of the OH Stretching Region in Hydrous β -Mg₂SiO₄ (Wadsleyite) to 50 GPa

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β -Mg₂SiO₄ (wadsleyite) is presumed to be one of the most abundant minerals in the mantle transition zone at depths of 400-500 km. The presence of water as OH in such nominally anhydrous minerals could significantly affect phase relations and the bulk-elastic properties in the mantle transition zone. Much recent work including IR, Raman and NMR spectroscopies as well as bond-strength systematics has provided evidence for protonation at the O1 site, although O2 protonation has also been suggested. The pressure dependence of the Raman spectrum has not been well characterized above 21 GPa. We report high-pressure Raman observations on single crystals (polished to 0.020x0.010 mm) in the diamond-anvil cell in the range 100-4000 cm⁻¹ including the OH stretch region up to 50 GPa, pressures far beyond the stability field of the phase. The hydrous wadsleyite was synthesized at 16 GPa and 1300°C in a 1000-ton multi-anvil press from mixtures of MgO, Mg(OH)₂ and SiO₂ in welded platinum capsules and has been well characterized by NMR techniques, giving a water

content of up to a maximum of 2.5 wt%. The experiments in the DAC to 50 GPa were performed with a helium pressure medium and 514.5 nm excitation. A baseline structural check on the sample was obtained from Rietveld refinement of powder diffraction data measured with image-plate techniques at beamline ID9 of the European Synchrotron Radiation Facility. It is consistent with the orthorhombic symmetry, space group *Imma*, of previous studies, with no mixed impurities. The 1 bar Raman spectra showed a broad asymmetric doublet comprising two components at 3329 and 3373 cm⁻¹ and a single mode at 3586 cm⁻¹. These components may be associated with differences in the H environment at this high water content. The doublet frequencies decrease linearly with pressure ($\gamma_1 = -0.36$ and $\gamma_2 = -0.39$ respectively). The highest frequency mode observed remains nearly constant up to 24 GPa before decreasing at higher pressures ($\gamma_{3a} = -0.01$ and $\gamma_{3b} = -0.17$ respectively). Further work is required to reconcile both the Raman and NMR results.