

In-situ synchrotron infrared spectroscopic studies of hydroxyl in mantle phases at high pressure

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The effect of water (OH⁻) within the crystalline structure of deep Earth minerals influences bulk properties including melting temperatures, rheology, electrical conductivity, and atomic diffusivity. In addition, hydrogen bond symmetrization in hydrous minerals may influence the response of bulk properties to pressure, for example increasing bulk modulus by as much as ~20%. Combining infrared spectroscopy with diamond anvil cells allows for the direct detection of the O-H bond stretching frequency within a hydrogen bond (O-H...O) as it changes with pressure. In this study, room temperature infrared spectra of both natural and synthetic hydrous phases were collected at 1 bar and at pressure intervals up to 65 GPa, allowing a detailed assessment of the evolution of hydroxyl band frequencies as a function of pressure. Combining these new high-resolution infrared data, in conjunction with the findings of previous high-pressure studies, reveals systematics in the pressure dependence of hydroxyl bands in various mineral phases. For example, within the amphibole group the starting 1-bar hydroxyl band frequency linearly correlates with the hydroxyl pressure-dependence, while composition plays a secondary role. By examining a wider suite of hydrous minerals it is possible to better understand the complex interplay between local hydroxyl bonding environment, initial hydrogen bond frequency, pressure, and OH-band pressure-evolution, augmenting ab initio computational predictions concerning hydrogen bond symmetrization in a range of hydrous deep Earth phases.