

氷 VII 相の高温高圧下でのプロトンネリングーホッピング転移の可能性について Near-infrared spectra of ice under high pressure and high temperature

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The physical properties of ice VII under high pressure and high temperature (HP-HT) conditions are important to planetary science. Ice VII is considered a primary constituent of the interior of giant icy satellites and planets (e.g., Podolak et al. 1998). Thus, understanding the physical properties of ice VII will contribute to better knowledge about the structure and dynamics of other satellite and planetary interiors. In particular, the ionic conductivity of ice VII, which affects the magnetic fields of these bodies (Stevenson 2003), is controlled by ionic and rotational defects in the ices (Jaccard 1959); moreover, ionic defects have two types: OH⁻ and H₃O⁺. The probability of forming defects in ice VII under the HP - HT conditions that typify the interiors of icy satellites and planets is surely increased by thermal activation.

In the near-infrared (NIR) region, the spectrum of ice VII shows absorption bands of the bending-stretching combination ($\nu_2 + \nu_3$) and stretching overtone ($2\nu_3$) modes of the normal vibration of water molecules (Larsen and Williams 1998). These modes correspond to the high vibrational energy level of the potential well, and provide information regarding the potential barrier along the O...O axis. To determine the probability of forming ionic defects in the ice VII structure at elevated temperatures, the NIR spectra of ice VII must be measured. The aim of this study is to investigate the state of protons in ice VII under HP-HT conditions. Thus, we measured the NIR absorption spectra of water at pressures up to 16 GPa and temperatures up to 368 °C using an external heating diamond anvil cell and synchrotron NIR radiation of BL43IR at SPring-8.

The absorption band of the first OH stretching overtone mode divided into doublet peaks above 5 GPa at room temperature, suggesting that proton tunneling occurs at the overtone level. As the temperature increased, the doublet peaks gradually reduced to a singlet. This result implies that thermally activated protons hop between the two potential minima along the oxygen-oxygen axis. A P-T diagram for the proton state was constructed from the changing band shape of the overtone mode.

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