Fast molecular transport in hydrogen-filled ices by high-resolution diamond-anvil cell NMR

Takuo Okuchi[1]; Masashi Takigawa[2]; Takehiko Yagi[2]

[1] Inst. Adv. Res., Nagoya Univ.; [2] Inst. Solid State Phys, Univ. Tokyo

We report NMR spectra and relaxation times of filled-ice II and Ic hydrogen hydrates [1]. These were measured in situ at pressures to 3.6 GPa using a novel high-resolution diamond-anvil-cell NMR method which has become available recently [2]. Guest H2 gave a narrow resonance indicating their fast transport between ice cavity sites. The hopping frequency was estimated from their relaxation times, giving a liquid-like diffusion coefficient that was not much sensitive to pressure. The framework H2O gave a broad resonance due to dipolar interaction. However, the observed line-width was smaller than pure ice, indicating some mobility of their protons. Curiously enough, the filled-ice II has a fully proton-ordered framework, within which the protons must be immobile. The logical consequence is framework-guest interexchange of protons, revealing chemically very active nature of the filled-ice hydrate.

[1] Vos, W. L. et al., Phys. Rev. Lett. 71, 3150 (1993)
[2] Okuchi, T. et al., J. Chem. Phys. 122, 244509 (2005)