

Elucidation of the dynamics of water clusters generated in hydrophobic solvents

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Recently, metal nanoparticles attract much attention. Understanding certain behaviors of water, e.g., its dynamics, is extremely important in various fields. Recently, using ¹H nuclear magnetic resonance spectroscopy, we have identified a metastable state of water molecules, i.e., water clusters, in hydrophobic solvents in addition to dissolved water molecules and a small bulk water domain. However, the low abundance of water clusters made observing their dynamics challenging. In this study, the dynamics of water clusters in benzene-*d*₆ were investigated by quasi-elastic neutron scattering measurements using the AGNES time-of-flight spectrometer of

the Japan Research Reactor JRR-3. From the measurements as shown in Fig. 1, the diffusion dynamics of the hydrogen atoms were much slower than those of bulk water (with a self-diffusion coefficient of 1.15×10^{-9} m²/s at 273 K) and even slower than the upper-limit dynamics at the observable scale (10^{-10} m²/s). The dynamics of water clusters are slow, “like ice”, even at 283–303 K, which is above the freezing point of water (273 K). This report is published in [1].

[1] K. Oka *et al.*, J. Phys. Chem. Lett. **15**, 267-271 (2024).

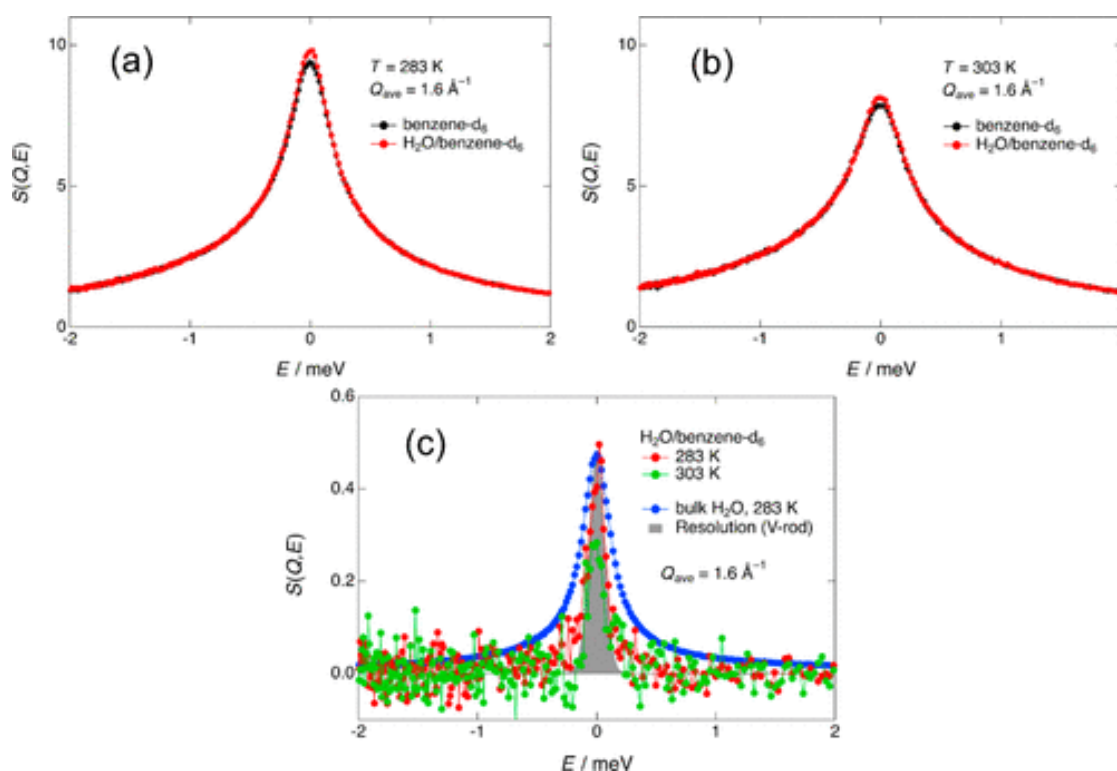


Fig. 1. Quasi-elastic neutron scattering spectra of benzene-*d*₆ and H₂O/benzene-*d*₆ samples acquired at (a) 283 and (b) 303 K. (c) Quasi-elastic neutron scattering spectra were obtained by subtracting the spectrum of benzene-*d*₆ from that of H₂O/benzene-*d*₆. The wavelength of the incident neutron is 4.22 Å.