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Orientational relaxation of OH-bond in water over short to intermediate timescales PING-HAN TANG, SUAN-JEN LIN, TEN-MING WU, Natl Chiao Tung Univ — By simulating the rigid simple point charge extended model at $300K$, the orientational relaxation of the OH-bond in water was investigated over short to intermediate timescales, within which molecules undergo inertial rotation and libration and then enter the rotational diffusion regime. Simulated molecules were classified into subensembles according to their H-bond connections. For global molecules and classified subensembles of molecules, the simulation results of the orientational time correlation functions (TCFs) were compared with the second-cumulant predictions obtained using the rotational stable instantaneous-normal-mode (INM) spectra and the power spectra of angular velocity autocorrelation functions (AVAFs). On short timescales, the OH-bond in water behaves similar to an inertial rotor and its anisotropy is lower than that of a water molecule. For molecules connected with three or more H-bonds, the OH-bond orientational TCFs are characterized by a recurrence, which is an indication for OH-bond libration. By contrast, the OH-bond orientational TCFs of molecules initially connected with one or two H-bonds decay monotonically or exhibit a weak recurrence, indicating rapid relaxation into the rotational diffusion regime after the initial Gaussian decay.

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