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Nonequilibrium Mixed Quantum-Classical simulations of Hydrogen-bond Structure and Dynamics in Methanol-d Carbon tetrachloride liquid mixtures and its spectroscopic signature KIJEONG KWAC, EITAN GEVA — Liquid mixtures of methanol-d and carbon tetrachloride provide attractive model systems for investigating hydrogen-bond structure and dynamics. The hydrogen-bonded methanol oligomers in these mixtures give rise to a very broad hydroxyl stretch IR band ($\sim$150 cm^{-1}). We have employed mixed quantum-classical molecular dynamics simulations to study the nature of hydrogen- bond structure and dynamics in this system and its spectroscopic signature. In our simulations, the hydroxyl stretch mode is treated quantum mechanically. We have found that the absorption spectrum is highly sensitive to the type of force fields used. Obtaining absorption spectra consistent with experiment required the use of corrected polarizabile force fields and a dipole damping scheme. We have established mapping relationships between the electric field along the hydroxyl bond and the hydrogen-stretch frequency and bond length thereby reducing the computational cost dramatically to simulate the complex nonequilibrium dynamics underlying pump-probe spectra.

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