Study of Solvated Ion by Classical Molecular Dynamics Simulations

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Cyanide ion (CN^-) solvated in water is investigated computationally for the study of the influence of intermolecular interactions, as the simulations can be carried out easily due to the small size of the system and detailed experimental results are available. In this work, we compute the vibrational relaxation time, two-dimensional infrared spectra, and solvation free energy of CN^- ion in water from the classical molecular dynamics (MD) simulations. They all depend very sensitively on intermolecular interactions. Two kinds of intermolecular interactions are considered in the simulations: van der Waals and electrostatic interactions. The van der Waals interactions are described by the Lennard-Jones potential. For a more accurate description of the electrostatic interactions, point multipoles are included in addition to point charges. The inclusion of multipoles is found to be important for the reproduction of some properties. It is noted that one single physically motivated force field parameterization can capture nuclear dynamics, spectroscopy, and thermodynamics in quantitative agreement with experiments.