

Matrix Isolation Spectroscopy of Hydrogen-Bonded Molecules: Ionic Liquids and Water

Adam H Turner, Woongmo Sung, Soo Ryeon Ryu, Sunghyun Huh, and Doseok Kim
Sogang University, Seoul, Korea

The vibrational spectrum of a single molecule is typically investigated in the gas phase, however, the spectrum is crowded by combination bands with rotational transitions and not all molecules can be prepared in the gas phase. Room-temperature matrix isolation spectroscopy (MIS) is a tool that utilizes the weak interactions of the probe molecule with the CCl_4 solvent. CCl_4 has a large transparency window in the infrared and shows potential as an analytical tool to give information on single molecules in a nearly isolated and inert environment. Ionic liquids ([OMIM]I and [OMIM]Cl) and water (H_2O and D_2O) molecules were loaded on top of CCl_4 , and the in-situ inclusion process was monitored in the CCl_4 phase with time by infrared absorption spectroscopy. Spectral signatures indicate that the [OMIM] (1-octyl-3-methyl imidazolium) cations exist in CCl_4 as monomers without the influence of anions. Inclusion into CCl_4 is more than an order of magnitude larger for [OMIM]I than [OMIM]Cl. The water in-situ spectra showed small non-linear deviations from the monomer spectrum attributed to formation of the water dimer by systematically increasing the water concentration in in-situ inclusion process. The water dimer spectrum was extracted from the monomer spectrum with 2D correlation spectroscopy and principal component analysis (PCA). Changes from the monomer spectrum to the dimer spectrum as well as the difference between H_2O and D_2O dimer spectra are discussed in terms of the hydrogen bonding.