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Hydrogen bonding motifs in hydroxy- and carboxy-functionalized ionic liquids

Ralf Ludwig

Physical and Theoretical Chemistry, University of Rostock, 18059 Rostock, Germany
ralf.ludwig@uni-rostock.de

The unique properties of ionic liquids (ILs) result from the tunable mélange of Coulomb interactions, hydrogen bonding, and dispersion interactions among the constituent ions. In hydroxy-functionalized ILs, local and directional hydrogen bonds (H-bonds) lead to the anticipated formation of ion pairs but also to the elusive formation of cationic clusters. Here, we report how hydrogen-bonding motifs in the bulk liquid and gas phase of hydroxy-functionalized ILs shed light on the general nature of hydrogen bonding. Infrared spectroscopy, nuclear magnetic resonance, neutron diffraction, and molecular dynamics simulations provide information about the structure, strength, and dynamics of cationic clusters in the bulk liquid ILs. Cryogenic ion vibrational predissociation (CIVP) spectroscopy along with density functional theory calculations has established a clear picture about the specific contacts within isolated H-bonded cationic clusters formed in the gas phase. For carboxy-functionalized ILs we provide experimental evidence for doubly H-bonded cationic dimers in the solid, liquid, and gaseous phases. This information from experiment, simulation, and theory provides a fundamental understanding of hydrogen bonding between the ions in ILs.