Probing Molecular Interaction in Ionic Liquids by Low Frequency Spectroscopy: Coulomb Energy, Hydrogen Bonding and Dispersion Forces

TCI SEMINAR

Wednesday, August 27, 2014
3:00 p.m. Room 9341

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Ionic liquids are defined as salts composed solely of ions with melting points below 100°C. These remarkable liquids have unique and fascinating properties and offer new opportunities for science and technology. New combinations of ions provide changing physical properties and thus novel potential applications for this class of liquid material. To a large extent, the structure and properties of ionic liquids are determined by the intermolecular interaction between anions and cations. In this talk we show that far infrared and terahertz spectroscopy are suitable methods for studying the cation-anion interaction in these Coulomb fluids. The interpretation of the measured low frequency spectra is supported by density functional theory calculations and molecular dynamics simulations. We present results for selected aprotic and protic ionic liquids and their mixtures with molecular solvents. In particular, we focus on the strength and type of intermolecular interaction and how both parameters are influenced by the character of the ions and their combinations. We show that the total interaction between cation and anion is a result of a subtle balance between Coulomb forces, hydrogen bonds and dispersion forces. For protic ionic liquids we could measure distinct vibrational modes in the low frequency spectra indicating clearly the cation-anion interaction characterized by linear and medium to strong hydrogen bonds. Using isotopic substitution we have been able to dissect frequency shifts related to pure interaction strength between cation and anion and to different reduced masses only. In this context we also show how these different types of interaction may influence the physical properties of ionic liquids such as melting point, viscosity or enthalpy of vaporization.

Theoretical Chemistry Institute Seminar Series