SEMINAR ANNOUNCEMENT

Molecular structure of hydrogen bonded systems in liquid phase

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Wednesday, 14 Dec. 2016, 11:00-12:00 PM, ROOM No. 2308

In life science, the hydrogen-bonds contribute in establishing and preserving the protein secondary and higher order structures as well as playing a key role in the solvation of protein surfaces. Moreover, these bio-molecular systems are solvated by water molecules to form extended hydrogen-bond networks. Many biologically significant processes, such as protein folding and denaturation, involve the formation or the breaking of hydrogen bonds in aqueous solution. The microscopic description of solute-solvent interactions in aqueous solutions of amides is then of particular interest for many reasons. First, simple amide systems have been investigated extensively as models of peptide bonds because of its presence as a repeating unit in biological macromolecules and some polymers. Second, N-H and C=O groups can form hydrogen bonds in pure and aqueous solutions which gives rise to a short-range order in these media. Therefore, understanding how these groups can interact with each other and with the surrounding solvent molecules can give information explaining the formation of the native structure of proteins and some mechanisms involving the formation of new hydrogen bonds.
To investigate the molecular structure of hydrogen bonded systems in aqueous solutions, we have performed experimental measurements by several techniques (X-ray and neutron scattering, IR spectroscopy) and theoretical calculations (DFT, NBO, and AIM). In my talk, I present the latest results of my studies of molecular associations in N-methylformamide (NMF) and Urea in solutions.

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