



Monday, April 2, 2018, 12:00 pm
Seaver Science Library, Room 150
SSC Auditorium next to the library

Professor Anne McCoy

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Understanding spectral signatures of large amplitude vibrations and hydrogen-bonding through studies of the vibrational spectroscopy of solvated ion complexes

In this talk, I will discuss recent work in our group in which we made connections between proton transfer processes and hydrogen bonding and vibrational frequencies and intensities. Due to the large amplitude motions associated with proton transfer along a hydrogen bond, the vibrational spectra of these systems contain features that cannot be understood by the usual harmonic description of molecular vibrations. The breakdown reflects both the anharmonicity along this coordinate and coupling between this mode and other low frequency modes in these systems. It also reflects changes in the electronic structure as molecules vibrate. The presentation will draw from reported vibrational spectra for systems either containing intra- or intermolecular hydrogen bonds. Both the theoretical approaches used to study these systems and the insights gained from the studies will be described, with a particular emphasis on understanding the spectral signatures of proton transfer in aqueous systems. The theoretical approaches range from the introduction of higher order terms to the harmonic analysis to adiabatic treatments in which the high- and low-frequency modes are treated at different levels of approximation and diffusion Monte Carlo studies in the full dimensionality of the system of interest.

Anne B. McCoy, Timothy L. Guasco, Christopher M. Leavitt, Solveig G. Olesen and Mark A. Johnson. Vibrational manifestations of strong non-Condon effects in the $\text{H}_3\text{O}^+\text{X}^-$ ($\text{X} = \text{Ar}, \text{N}_2, \text{CH}_4, \text{H}_2\text{O}$) complexes: A possible explanation for the intensity in the "association band" in the vibrational spectrum of water. *Phys. Chem. Chem. Phys.*, 2012, 14, 7205–7214.

Conrad T. Wolke, Joseph A. Fournier, Laura C. Dzugan, Matias R. Fagiani, Tuguldur T. Odbadrakh, Harald Knorke, Kenneth D. Jordan, Anne B. McCoy, Knut R. Asmis, Mark A. Johnson. Spectroscopic snapshots of the proton-transfer mechanism in water. *SCIENCE*, 2016, 351, 1131.

Hosted by Professor Anna Krylov

The scientific community is invited

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