

# Chemistry Seminar

**"Solvent Effects at the Molecular Level"**

**Dr. Ken Leopold**  
U. of Minnesota

**Wednesday, Oct. 6**

**12:00 p.m.**

**WSB-122**

Solvation plays an enormous role in aqueous phase chemistry, impacting thermodynamics and reactivity in a wide range of environments from living cells to cloud droplets. A thorough understanding of solute-solvent interactions, therefore, is an important goal of chemistry. In this talk, we focus on the effects of hydration on reactive systems, with special attention paid to those that undergo the simplest of chemical reactions, namely proton transfer. Rotational spectroscopy and computational methodologies are used to investigate the sequential hydration of nitric acid and to explore the effects of individual solvent molecules on its proton transfer to water. While nitric acid ionizes in bulk aqueous solution, the ionization is not fully realized in small molecular clusters. However, the extent of proton transfer can be defined and tracked by two distinct methods, one based on molecular structure and the other based on nuclear hyperfine interactions. Additional work on the  $\text{HNO}_3\text{-N}(\text{CH}_3)_3$  complex utilizes these hyperfine interactions to address the question of whether the acid and base can (and should) agree on the extent of proton transfer. Finally, as time permits, progress on new experiments aimed at studying the hydration of simple ion pairs will be presented.

**Dr. Leopold will meet with students at 1:00 p.m. in WSB-344**