UNIVERSITY OF RHODE ISLAND
Department of Chemistry

SEMINAR

Room 105 Beaupre Center
3:00 p.m, Monday, Jan. 23, 2017

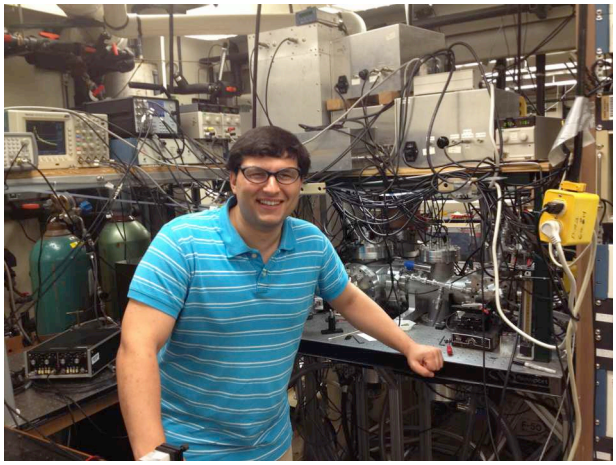
Dr. Andrew DeBlase

Department of Chemistry
Purdue University
West Lafayette, IN

"Advances in Cold Ion Spectroscopy"

HOST

David Freeman
Department of Chemistry
401-874-5093



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Advances in Cold Ion Spectroscopy

We all learn in general and/or organic chemistry that UV/Vis spectroscopy is mostly used for quantification, infrared (IR) spectroscopy tells us the functional group of a molecule, and NMR spectroscopy or x-ray crystallography are required to learn the finer details of molecular structure. If the infrared spectrum gives us a "fingerprint" of the molecule, why then is it not used more regularly to determine structure? There are three main reasons: (1) the vibrational frequencies are sensitive to the specific solvation environment, which fluctuates at room temperature, (2) vibrational transitions are broadened by the thermal population of rotations and low frequency vibrations at 298 K, and (3) multiple conformations of a molecule may exist at room temperature, which convolute the spectra. The situation becomes even more complicated in UV/Vis spectroscopy because electronic, vibrational, and rotational degrees of freedom can all be coupled together. In this seminar, I will describe several experimental methods that I have helped to develop as a Ph.D. student and a postdoctoral researcher to glean detailed structural insight using IR and UV spectroscopy. The general strategy is to remove solute ions from solution by electrospray ionization and to cool the molecules into their vibrational zero-point levels (10 K). At such cold temperatures, we can obtain spectra of individual conformers by applying double resonance laser spectroscopies. The infrared spectra are directly comparable to *ab initio* or DFT vibrational frequency calculations in a vacuum at 0 K, providing a "training set" by which to improve theory as we study progressively larger molecules. I will describe the details of these techniques and comment on the future of this field, which includes the isolation and elucidation of transient reactive intermediates.