DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE

SPRING 2017 SEMINAR SERIES

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FRIDAY, FEBRUARY 3, 2017 **TIERNAN HALL**
10:00 AM **ROOM 373**

GUEST SPEAKER

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TOPIC

Advances in Cold Ion Spectroscopy

ABSTRACT

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.

BIOGRAPHY

Andrew DeBlase is a postdoctoral researcher at Purdue University, who uses vibrational and electronic spectroscopy to determine the gas-phase conformational preferences of biological ions at 10 K. He works under the advisement of Professors Scott McLuckey and Timothy Zwier. Andrew received his Ph.D. in physical chemistry at Yale University in 2014. At Yale, he was advised by Professor Mark Johnson and he studied charge accommodation in organic motifs using vibrational predissociation spectroscopy. Andrew graduated Marist College in 2009 with a B.S. in Chemistry. Recently, he was awarded the postdoctoral research award by the American Society of Mass Spectrometry.

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