



PHYSICAL CHEMISTRY  
**McELVAIN  
SEMINAR**

**Mark A. Johnson**  
*Yale University*

*From water clusters to structural metabolomics:  
A chemical road trip on a cryogenic ion  
photofragmentation mass spectrometer*

The coupling between ambient ionization sources, developed for mass spectrometric analysis of biomolecules, and cryogenic ion processing, originally designed to study interstellar chemistry, creates a new and general way to capture transient chemical species and elucidate their structures with vibrational spectroscopy. Advances in non-linear optics over the past decade allow single-investigator, table top laser access to IR bands from 550 to 4000  $\text{cm}^{-1}$ , essentially covering the same range as a typical FTIR instrument. When vibrational spectra are acquired using predissociation of weakly bound rare gas “tags,” the resulting spectra are equivalent to absorption spectra and correspond to target ions at 10K or less. Taken together, what emerges is a new way to add a structural component to mass spectrometric analysis. Moreover, because the spectral features of the cold ions are sharp, the evolution of bond-specific transitions can be used to shed new light on everything from the nature of the hydrated proton to the structures of metabolites. Examples will be chosen from applications to catalytic intermediates and the microscopic mechanics underlying the dissolution of salts.

**Tuesday, April 7, 2015**

**11:00 AM**

**Seminar Hall 1315**

*Refreshments will be available prior to the seminar  
at 10:45 a.m. outside room 1315*

