# INTEGRATING CRYOGENIC ION CHEMISTRY AND OPTICAL SPECTROSCOPY: CAPTURING THE MOLECULAR LEVEL MECHANICS DRIVING BULK CHEMICAL BEHAVIORS FROM CATALYSIS TO THE SPECTRAL DYNAMICS OF WATER

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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 optical spectroscopies. Advances in non-linear optics over the past decade allow single-investigator, table top lasers to access radiation from 550 cm-1 in the infrared to the vacuum ultraviolet. When spectra are acquired using predissociation of weakly bound rare gas "tags," the resulting patterns are directly equivalent to absorption spectra of target ions at temperatures below 10 K, and quenched close to their global minimum energy geometries. Taken together, what emerges is a new and powerful structural capability that augments the traditional tools available in high resolution mass spectrometry. Currently, these methods are being exploited to monitor chemical and physical processes in assemblies with well-defined temperatures and compositions. Recent applications, ranging from the mechanisms of small molecule activation by homogeneous catalysts to the microscopic mechanics underlying the ultrafast spectral diffusion in water, emphasize the generality and utility of the methods in contemporary chemistry.