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Foreword

Spectroscopy in its various forms is a critical tool for scientists interested in understanding molecular structure, dynamics, and reactivity. Infrared absorption spectroscopy provides information about functional groups in molecules, and a spectrum can serve as a "fingerprint" for molecular identification. X-ray spectroscopies can provide information about elemental composition, surface structure, protein conformation, and local environments of atoms. Spectroscopies at lower frequency are used for molecular structure elucidation, remote sensing, imaging, etc. Additional information can be obtained from non-linear and multi-dimensional spectroscopies that can be used to probe the structures of molecules at surfaces or at other interfaces and to measure how structure, excitations, or reactions evolve with time. Dynamics as short as a few femtoseconds can be probed, and new methods have made attosecond experiments possible. While many spectroscopic methods are routinely used to investigate condensed phase and some gaseous samples, more general applications of various spectroscopies to investigating the structures of ions have been more limited owing in part to the low ion density, restricted ion access, or short lifetime typical of many ion beam or trapping experiments. Despite the many challenges associated with obtaining spectra of ions, the high information content associated with many spectroscopies motivates the application of these methods to ion structural characterization. Absorption and fluorescence measurements can provide unique and detailed information about ion structure that is not readily available from more conventional tandem mass spectrometry experiments where ions are dissociated typically by collisions with gaseous atoms or molecules, or by capture of electrons. While these dissociation experiments provide extensive information about bond connectivity, more subtle information about ion structure, such as how a metal ion binds or the conformation of the ion, can be more challenging to obtain. With the increasing use of mass spectrometry for investigating intact protein and macromolecular assemblies, questions arise concerning how the structure of an ion changes as it transitions from its native environment in solution to that in isolation in vacuum. How does solvent change molecular structure, and how do ions change the structure of the solvent itself? There is evidence from many different techniques that ion structures can be kinetically trapped and thus ions can retain a "memory" of their solution-phase structure. What elements of structure are retained in the gas phase, and what elements are lost? Recent ion spectroscopy experiments are providing new insights into these and many other fundamental questions about ion structures. The detailed structural information that is being obtained from these experiments also provides challenging benchmarks that can be used to improve the accuracy of theory.

This special issue on ion spectroscopy comes at a time when new methods and applications of various spectroscopies to ion structure are rapidly increasing. The 21 articles in this issue are just a sampling of some of the excellent work that is currently being done in this area and no attempt was made to make this special issue comprehensive. Many groups have taken advantage of the capabilities of the free electron laser facilities at the Centre Laser Infrarouge d'Orsay (CLIO) and at the FOM Institute for Plasma Physics Rijnhuizen (FELIX) to measure infrared multiple photon dissociation spectra of a wide variety of ions, and the high productivity of these facilities is reflected by the relatively large number of papers from users of these facilities. I thank each of the authors for their contributions and for their timely submissions and revisions. I also thank each of the anonymous reviewers who generously donated their time and efforts to play such a vital role in making this high-quality publication possible. I hope that you will enjoy this special issue.

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