Focus on Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

The editors of the *Journal of the American Society for Mass Spectrometry (JASMS)* are pleased to organize focus sections that commemorate the achievements of members of our society. A few years ago, we decided to use the two scientific awards of the society as a starting point for focus sections. In this way, the society's journal leaves behind a permanent record of research related to its awards and instructs its members in the state of research in a given field. The editorial staff usually arranges articles published in a focus section, but at least two and sometimes three experts review each contribution.

We are pleased to present a focus section honoring Mel Comisarow and Alan Marshall for their creative invention of Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS) in 1974. Their efforts were recognized in at the 1999 ASMS Conference, and they received the Distinguished Contribution Award. At the time of the invention, ion cyclotron resonance mass spectrometry was principally a tool for a few dozen mass spectrometrists and ion chemists who were investigating gas-phase ion-molecule reactions and ion spectroscopy. Although the significance of their invention took a few years to be recognized, the subject of analytical mass spectrometry and ion chemistry has been changed immeasurably. An exciting feature of FT-ICR-MS is that its capabilities have not been exhausted, and new developments continue apace.

After the few-year induction period, the inventors as well as other analytical mass spectrometrists persisted to carry on research in FT-ICR-MS, inspired by the opportunities they recognized to develop new methods, new measurement strategies, and new combinations of this instrument with others (e.g., separation methods, lasers, other mass spectrometers). They were challenged by the need to have a mass spectrometer with ultra high mass resolving power, unprecedented mass accuracy and precision, high sensitivity and speed owing to the multichannel advantage of the instrument, and high mass range. Additional challenges were to couple the instrument with separation methods, to utilize established and new ionization methods, to explore advantages of MS/MS in time rather than space, and to exploit remeasurement of mass spectra by using the ion-trapping and nondestructive-detection methods to improve the signal-to-noise ratio of ion detection. Comisarow and Marshall foresaw some of these advantages and predicted their utility in their early articles.

We see in the early advances in FT-ICR-MS a foreshadowing of the development of the Paul or ion trap. Many ideas demonstrated earlier with FT-ICR-MS apply to the Paul method of trapping, and their successful implementation in FT-ICR-MS certainly promoted and expedited the development of the ion trap. A few devotees who were fascinated by opportunities in ion chemistry and instrumentation kept interest in the ion trap, like that in FT-ICR-MS, alive.

In parallel with the analytical advances, ion chemists found the FT-ICR method to be invaluable in their research. Rapid measurement of the rates of ion-molecule reactions and elucidation of reaction pathways by using multiple resonance, ion activation, and reagent gas pulsing provided capabilities that so exceeded those of ion cyclotron resonance (ICR) that the connection between the two instruments became obscure, and ICR disappeared. Even ion chemistry at pressures as high as 10^{-2} torr became possible with the introduction of an ion-trapping event in FT-ICR-MS sequence.

JASMS is proud to present this focus to honor Alan and Mel. After speaking with the awardees, we decided to organize a focus section that emphasized chemistry: gas-phase ion chemistry and solution chemistry. The article by McLafferty and coworkers demonstrates a large step forward in utilizing ion trapping to effect electron capture dissociation for "far larger molecules (42 kDa) than previously observed (< 1kDa)." This article illustrates both exciting ion chemistry and method development.

A classic use of ion trapping is the study of ion-molecule reactions. Williams and Rodriguez-Cruz show the reactions of hydrated divalent alkaline earth meal ions and benzene as a function of the number of solvating water molecules on the metal ion. The work begins to build a bridge between chemistry in the gas phase and in solution. Kenttämaa and coworkers provide another example in the third article. They use the features of ion trapping and sustained off-resonance irradiation to sort out reaction pathways and ion structures in organic ion-molecule reactions.

Limbach and Marshall show in the fourth article the beauty of FT-ICR-MS for investigating H/D exchange of mononucleotides in the gas phase. Lebrilla and his students demonstrate how ion trapping can be used for

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chiral recognition in the gas phase, contradicting those who hold the view that mass spectrometry is too energetic to reveal such subtle differences in molecular structure. The final chemistry example is work from Marshall, Gaskell, and coworkers, who give us an example of the use of FT-ICR to do peptide sequencing in the gas phase in a manner that is analogous to the Edman degradation in solution. They report utilizing the method for the direct analysis of a mixture of 25 tryptic peptides.

The final contribution to the focus reminds us of the opportunities in instrument development. My co-worker, Don Rempel, and I present the theoretical foundation for capturing the high-translational-energy ions produced by matrix assisted laser desorption in ICR trap. We predict that the method will capture ions having a velocity range of two decades and a mass of three decades, opening the door for higher sensitivity for MALDI in FT-ICR.

We extend our congratulations to Mel Comisarow and Alan Marshall, and we hope that this small collection of articles will show our readers the continuing excitement of their invention.

Michael L. Gross
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