

FALL WORKSHOP

The Fall Workshop topic is Elemental Mass Spectrometry, and is being organized by Willard Harrison, University of Florida, and Gary Hieftje, Indiana University. The workshop will be held at the San Francisco Hilton Hotel, November 14 and 15.

Elemental analysis by mass spectrometry shows rapidly increasing interest. Numerous recent symposia have focused on the advantages of such techniques, new commercial instrumentation has appeared, and many analysts are finding mass spectrometry to be the preferred method for rapid, sensitive multielement analysis. This workshop will address both solution and solids analysis by ICPMS and solids analysis using GDMS.

NEW BOARD MEMBERS ELECTED

The following have been elected to the ASMS Board of Directors: Sanford P. Markey, Vice President for Arrangements, Brian Chait, Secretary, and Alan G. Marshall, Member at Large. Their two-year terms begin on July 1, 1991. They will replace Robert P. Lattimer, Veronica M. Bierbaum, and Richard Caprioli, all of whom made major contributions to ASMS through their service on the Board.

As Vice President for Arrangements, Bob Lattimer selected sites for the 1994 through 1997 conferences. He standardized the site selection process with a ranking procedure that quantifies factors of importance to ASMS in choosing a site. This greatly simplified the ability of the Board to evaluate potential sites.

Veronica Bierbaum served as ASMS Secretary, bringing to this responsibility tremendous efficiency in recording the proceedings of the Board. She also served on the Asilomar Conference Board, conducted the Board elections, and coordinated the selection of student travel stipends and insurance matters for the Society.

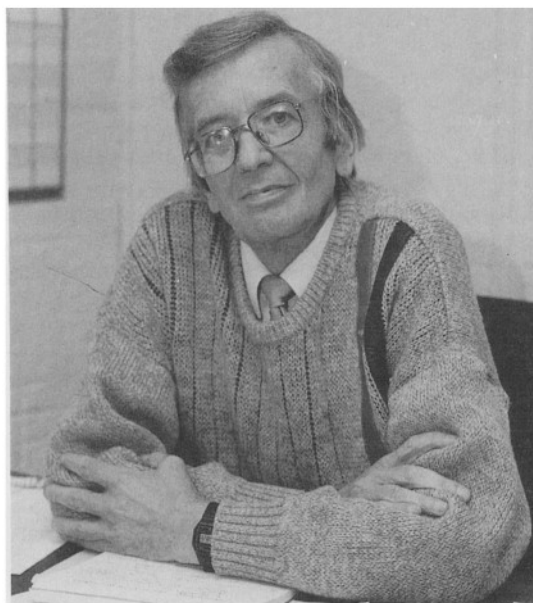
Richard M. Caprioli, who is retiring as Member at Large, not only served as Editor of the Proceedings, but also organized the 1989 Fall Workshop and the 1991 Sanibel Conference. He was the first coordinator of the Distinguished Contribution Award. This involved developing the guidelines for the program and coordinating the selection committee.

FORMER PRESIDENT HONORED

Gerry G. Meisels, Past President of ASMS, has begun his term as 1991 Chair of the Council of Scientific

Society Presidents. CSSP plays a significant role in influencing national science and technology policy, including science education. One of Gerry's goals with CSSP is to advance the agenda of the scientific community rather than being driven by legislation someone has introduced. He also believes that more attention needs to be focused on state support to scientific programs, which in total exceeds the support provided by the federal government. He hopes to begin state-by-state initiatives to broaden support to scientific education and research.

1991 AWARD FOR DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY



Professor Michael Barber

The 1991 Award for Distinguished Contributions in Mass Spectrometry honors Professor Michael Barber, University of Manchester Institute of Science and Technology, for his pioneering work in the development of fast atom bombardment mass spectrometry. Fast atom bombardment (FAB) has undoubtedly been one of the most important advances in mass spectrometric techniques of the past two decades.

It was only 10 years ago that Professor Barber and co-workers first published their results on the devel-

opment of FAB in the journal of the Chemical Society (*Chem. Commun.* 1981, 325). This work was an outgrowth of studies of secondary ion mass spectrometry on metal surfaces, an area of research of several groups who thus collectively laid the groundwork that later developed into FAB ionization.

Two novel aspects of Professor Barber's landmark contribution were the use of glycerol as a matrix to protect the analyte and the use of an atom gun as a source of fast moving neutral particles. These made possible the ionization and analysis of relatively high molecular weight polar or ionic compounds. In that first paper, the original FAB mass spectrum of the undecapeptide met-lys-bradykinin, $(M + H)^+ = m/z$ 1319, was reproduced and immediately drew everyone's attention.

Because FAB could be readily adapted to existing sector and quadrupole mass spectrometers with minimal modifications, the method's use grew rapidly. The intervening decade witnessed a revolution in the application of mass spectrometry to problems in chemistry and biology as a direct result of this discovery.

We are greatly saddened by the death of Professor Barber, on May 8, following a long illness. He was looking forward to attending the Nashville Conference and to presenting a Plenary Lecture. We deeply regret that he was unable to do this. His scientific contributors will continue to advance the discipline of mass spectrometry.

ASMS CALENDAR

May 18-19	ASMS Short Courses
May 19-24	39th ASMS Conference
September	Proceedings of the 39th ASMS Conference
November 14-15	Fall Workshop: Elemental Mass Spectrometry

THE SANIBEL CONFERENCE

January 29-February 1, 1991

Report prepared by Robert P. Lattimer,
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Gray sandy beaches. Warm salt air and sunny skies. Gently waving palm trees and surf. What a pleasant setting for a meeting of mass spectrometrists in January (especially for us Northerners!). The third Sanibel Conference, sponsored by ASMS, was held at the Sundial Beach and Tennis Resort, located on the Gulf coast in southwest Florida. This year's conference, *Ion Activation and Dissociation*, was organized by Richard Caprioli (University of Texas Health Science Center) and Robert Boyd (National Research Council-Canada). Over a 4-day period (January 29-February 1) 67 conferees listened to 14 invited speakers and viewed 19 contributed posters. By all indications the meeting was a great success.

The concept of the Sanibel Conference was developed about 3 years ago by Mark Ross (Naval Research Laboratory) in discussions with other colleagues. It was felt that a conference with limited attendance on a narrowly focused "special topic" in mass spectrometry should be started in the eastern United States. The format was envisioned to be similar to the well-established Asilomar Conference on Mass Spectrometry (ACMS), which is based in California. Ross suggested the Sanibel Island location and made a proposal to the ASMS Board of Directors, with sponsorship by then Board member Gary Glish (Oak Ridge National Laboratory). Ross, Robert Cotter (Johns Hopkins University), and Kenneth Busch (Georgia Institute of Technology) organized the first conference in 1989; the topic was *Mechanisms in Desorption Ionization*. The second conference in 1990 was organized by Gary Glish and Michelle Buchanan (Oak Ridge National Laboratory); the topic was *Ion Trapping in Mass Spectrometry*. In 1990 the ASMS Board established a Sanibel Committee to provide long-term leadership and stability. This committee currently consists of Mark Ross (Chair), Robert Cotter (ASMS Board representative), Richard Caprioli, Jeanette Adams (Emory University), and Vernon Reinhold (Harvard University). The committee members are appointed by the ASMS President and Board with 3-year rotating terms. The Sanibel Committee is responsible for general oversight of the meeting, site selection, budgeting, and the selection of conference topics and organizers. The committee's intent is to schedule a variety of topics from year to year and to strike a balance between fundamentals and applications. The ASMS Executive Director, Judith Watson, works with the committee and handles the registration and detailed physical arrangements for the meeting.

The conference has adopted a semi-Gordon Conference format that seems to work well for this type of small, informal meeting. Sessions are held in the morning and evening, with the afternoons free for informal discussions and/or local recreation. At this year's conference, 14 invited speakers gave talks during the morning sessions, and in general their presentations were excellent. Interaction among conferees was promoted by the informal evening poster sessions and the general discussion held on the final evening of the conference. Some highlights from the invited lectures are given below.

CONFERENCE LECTURES

Scott McLuckey (Oak Ridge National Laboratory) began the conference with an excellent overview of mechanisms in collisional activation (CA). CA is by far the most widely used method for inducing fragmentation in the tandem mass spectrometry (MS/MS) experiment. McLuckey traced the development of collision-induced dissociation (CID) from its origins in mass-analyzed ion kinetic energy spectrometry

(MIKES) in the late 1960s, through the development of the numerous instruments currently used for MS/MS: triple quadrupoles, quadrupole ion traps, Fourier transform mass spectrometers (FT-MS), four-sector magnetic systems, and various hybrids. McLuckey outlined the main phenomena occurring in ion-molecule reactions, of which three general types of collisions can be envisioned. One is a "sticky" collision, which results in the formation of a reasonably long-lived collision complex. The second type is an "impulsive" collision, which results in rapid dissociation to yield product ions (fragments). This is the type of collision most commonly observed in typical MS/MS experiments. The third possibility is "electronic excitation," which is most likely for light ions with high collision energy.

Keith Jennings (University of Warwick) followed with a lecture on experimental aspects of CID, particularly with regard to modern four-sector magnetic instruments. Jennings compared the relative merits of commonly used collision gases (helium, argon, xenon). He noted that argon is more efficient than helium for cleaving peptide side chains and for generally effecting fragmentation of higher mass (≈ 1500 – 2500 u) ions.

Graham Cooks (Purdue University) discussed various charge exchange processes, using tungsten hexacarbonyl as his principal example. The charge exchange experiments were performed at both high (keV) and low (eV) kinetic energies. Internal energy deposition was considered as a function of translational energy, the nature of the target (collision) gas, the cell pressure, and in some cases the scattering angle. The results were interpreted in terms of vibrational and electronic excitation.

Simon Gaskell (Baylor College of Medicine) presented a talk on the features of a hybrid (BEqQ) instrument for MS/MS. CID in the "collision quadrupole" is characterized by relatively long residence times (many microseconds) and multiple collisions. Product ions typically have high yields and may result from multiple bond cleavages and rearrangement processes. Gaskell gave several illustrations from various biomedical analyses.

Michael Gross (University of Nebraska) discussed the features of high energy CID in a four-sector tandem mass spectrometer. A principal advantage of high energy CID is its generality, i.e., the required experimental set-up is minimal and useful data can be obtained for nearly all compound types. A recent innovation that greatly improves the sensitivity of beam instruments is the array detector. Gross proposed a new CAD set-up for FT-MS in which ions are activated by acceleration in the Z-direction of an FT-MS cell. Gross concluded his talk by showing interesting CID spectra of Buckminsterfullerene (C_{60}), which loses consecutive C_2 units upon dissociation.

Richard Smith (Pacific Northwest Laboratory) considered the activation and dissociation of large, multi-

ply charged ions produced by electrospray ionization (ESI). Smith showed that "preheating" the ions during transport through the atmosphere/vacuum interface is effective in inducing dissociation. It was shown that either CID or "thermal activation" promotes relatively more dissociation the higher the charge state of the ion. Also, theoretical calculations indicate that cleavage should be more facile near the center of the molecule. Smith was mainly concerned about methods for activation/dissociation of ESI-produced ions; the interpretation of spectra of product ions from multiply charged precursors was not discussed in detail.

Gary Glish (Oak Ridge National Laboratory) discussed ion activation in the quadrupole ion trap (QIT). He particularly compared MS/MS in the QIT to that of low energy CID in beam instruments (i.e., triple quadrupoles and hybrid systems). Among the features of the QIT are its relatively long time scale and path length for CID, the ability to isolate specific ions for activation, and the possibility of carrying out several stages of mass spectrometry analysis (MS^n). Glish emphasized that several different types of ion activation are possible in the QIT.

Michael Bowers (University of California, Santa Barbara) gave the first in a series of talks on photoinduced dissociation (PID). Bowers nicely illustrated the wealth of detailed information that can be obtained on small molecules and cluster ions using PID. The dynamics of photodissociation of small cluster ions (e.g., $C_2H_2 \cdot OCS^+$ and $N_2O \cdot H_2O^+$) was discussed in detail. A beam (BE) instrument was used in which laser photodissociation occurs between the magnetic and electric sectors.

David Russell (Texas A&M University) discussed the design and features of a novel tandem (EB/TOF) mass spectrometer. Ions mass-selected in the double-focusing section (EB) are decelerated to ≈ 10 – 100 eV and then collisionally activated or else photoactivated by using a laser. The product ions are then reaccelerated into a reflectron time of flight (TOF-MS) for mass analysis. This tandem system offers high sensitivity at high resolution, with very fast data acquisition. The system is compatible with matrix-assisted, pulsed-laser desorption ionization. Protonated or sodiated peptide ions, for example, can be formed and subsequently dissociated and analyzed at the picomole level.

Michael Duncan (University of Georgia) described photodissociation in a reflectron TOF mass spectrometer. A pulsed-nozzle laser vaporization ion source is used to prepare a variety of metal cluster and metal-organic ions. A pulsed gate in the reflectron is used to mass-select ions of interest. Numerous examples were given in the area of metal-organic complexes. In some cases dissociation results in charge retention on the metal, while in other cases charge is transferred to the organic component.

A. L. Burlingame (University of California, San

Francisco) discussed applications of MS/MS in biological chemistry. Burlingame's main theme was that mass spectrometric developments within the past 2-4 years are providing unprecedented advances in structural biochemistry research. The two key areas are (1) the use of laser desorption and ESI for accurate molecular weight measurement of intact biomolecules, and (2) the use of four-sector tandem instruments to derive sequence information via MS/MS. These modern mass spectrometric methods are more rapid and have better sensitivity than micro-Edman degradation, crystallography, and two-dimensional magnetic resonance imaging. Burlingame gave examples in which MS/MS has been indispensable for the rapid resolution of some very difficult problems in structural biology.

Robert Cotter (Johns Hopkins University) discussed the novel use of endothermic ion-molecule reactions to produce reaction-induced dissociation (RID) of complex biomolecules. Reactions between protonated peptides and ammonia lead, for example, to dissociation of the amide bond. For peptides containing more basic residues, dimethylamine provides a better target gas. These reactions are believed to proceed via an intermediate "collision complex." An advantage of RID is that efficient fragmentation can be achieved at very low beam energies (≈ 10 eV). In addition, it is interesting that charge-remote fragmentations are observed under these low beam energy conditions.

Hilkka Kenttamaa (Purdue University) discussed the use of CID to investigate problems involving the structures of small organic ions. A dual-cell Fourier transform-ion cyclotron resonance (FT-ICR or FT-MS) instrument was used; this is especially advantageous in that ions may be isolated in one cell or transferred between cells. Kenttamaa showed how different ion structures can be distinguished by using energy-resolved CID, functional group selective ion-molecule reactions, and H/D exchange reactions.

Steven Buckner (University of Arizona) discussed the use of FT-MS to activate and dissociate ions via multiphoton absorption. FT-MS spectrometers are particularly useful for studying multiphoton processes due to the possibility of long irradiation times and ion manipulation in trapping cells. The use of FT-MS to study relaxation kinetics and ion dissociation reactions was considered. Various transition metal carbonyl complexes were used as examples.

SUMMARY

Many attendees of the 1991 Sanibel Conference were concerned with finding the "best" method for activation/dissociation of large molecules, particularly

biomolecules, in the mass range ≈ 1000 - 3000 u (or even higher). The basic difficulty with larger molecules is that, when activated, they tend to dissipate energy quickly via isomerization and radiative loss. The trick to induce bond dissociation would seem to be to get energy into specific sites where bonds can be broken quickly (before other relaxation processes can occur). This task should provide a challenge to theoreticians and experimentalists for years to come.

At the present time CID is the method of choice for most MS/MS applications, especially with larger molecules. CID is applicable to almost any molecule, and the technique can be carried out with a wide variety of mass spectrometer types. Also, CID parameters such as choice of target gas, collision energy, and collision residence time can be varied to produce the desired results.

PID is capable of producing a wealth of detailed kinetic and thermodynamic information on small molecular and cluster ions. It is questionable, however, whether PID will ever be as effective as CID for large molecules. Surface-induced dissociation (SID), another promising alternative, was discussed very little at this conference (which is a disappointment!). SID is a relatively new technique that has yet to prove its worth with larger molecules. RID, while still in its infancy, looks promising for certain classes of molecules. However, its future use is likely to be more selective than universal.

Conference organizer Robert Boyd, in his concluding remarks, stated that it is no longer proper to say that we just don't understand ion activation/dissociation processes. Scientists are indeed gaining knowledge about these processes, and this understanding will lead to better instrumentation and experimental designs to optimize MS/MS experiments. MS/MS has emerged, after only a dozen years or so, to become an integral part of modern mass spectrometry. The challenge is still there, however, to optimize and control the experimental conditions to best achieve the goals of various applications.

1992 CONFERENCE

The fourth Sanibel Conference is scheduled for January 26-29, 1992, at the Sundial Resort. The topic will be *Lasers in Mass Spectrometry*, and the organizers are Tomas Baer (University of North Carolina) and Klaus Biemann (Massachusetts Institute of Technology).

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