

## Looking through the Mass-to-Charge Ratio: Past, Present and Future Perspectives

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**Abstract :** The mass spectrometry (MS) provides the mass-to-charge ratios of atoms, molecules, stable/metastable complexes, and their fragments. I have taken a long journey with MS to address outstanding issues and problems by experiments and theory and gain insights into underlying principles in chemistry. By looking through the mass-to-charge ratio, I have studied thermochemical problems in silicon chemistry, the infrared multiphoton dissociation spectroscopy of organometallic intermediates, unimolecular dissociations of halotoluene radical cations, and the kinetics of association/dissociation of alkali halide triple ions with Lewis bases. Various MS platforms have been used to characterize non-covalent interactions between porphyrins and fullerenes and those between the group IIB ions and trioctylchalcogenides, and to examine the binding of the group IA, IIA and porphyrin ions to G-quadruplex DNA. Recently, I have focused on mass-balanced H/D isotope dipeptide tags for MS-based quantitative proteomics, a simple chemical modification method for MS-based lipase assay, and the kinetics and dynamics of energy-variable collision-induced dissociation of chemically modified peptides. Now, I see an important role of MS in global issues in the post-COVID era, as the society demands high standards for indoor air quality to contain the airborne-pathogen transmission as well as in-situ monitoring and tracking of carbon emissions to reduce global warming.

**Keywords :** silicenium ion chemistry, IRMPD spectroscopy, triple ions, MS-based quantitation tags

During my BS and MS courses at Seoul National University, I studied double resonance in NMR as a BS thesis topic and examined the effects of internal rotation of methyl group in liquid toluene on  $^{13}\text{C}$  nuclear spin relaxation as a MS thesis work. I realized that the principles of NMR were applicable to ion cyclotron resonance (ICR): The Lorentz force equation of the charged particle in the presence of external magnetic field with collisional cooling is analogous to the Bloch equation of nuclear magnetization with spin relaxation. A nuclear magnetic moment undergoes a precession around the field axis, whereas a charged particle undergoes a cyclotron motion around the field axis. The spin relaxation induces a magnetization decay in NMR,

while the collisional cooling induces an image charge decay in ICR. I got interested in ICR spectroscopy and decided to join the ICR laboratory at Caltech.

A newer Fourier transform (FT)-ICR data system was installed at the ICR lab in 1985. My first PhD work using FT-ICR was to determine the proton affinity of silylene ( $\text{SiH}_2$ ),<sup>1</sup> a reference molecule in hydrosilicon like methylene ( $\text{CH}_2$ ) in hydrocarbon, by examining proton-transfer reactions of  $\text{SiH}_3^+$  with a series of n-donor bases. This work led to a revision of the heat of formation of  $\text{SiH}_2$ . The proton affinities of methylsilylene ( $\text{CH}_3\text{SiH}$ ) and silaethylene ( $\text{CH}_2=\text{SiH}_2$ ) were also determined to see the difference in thermal stability between the two compounds, a hot topic of theoretical debate at that time.<sup>2</sup> Reactions of  $\text{CH}_3\text{SiD}_2^+$  with various n-donor bases yielded either silaethylene from proton transfer or methylsilylene from deuterium transfer as a neutral product. Then, the hydride-transfer reactions of methyl-substituted silicenium ions with various hydrocarbons were studied to determine their heats of formation.<sup>3</sup> To carry out these silicenium ion works, I synthesized silane, silane- $d_4$ , methylsilane, methylsilane- $d_3$ , dimethylsilane and trimethylsilane using a vacuum line in a wet lab by running reactions of chlorosilane and methyl-substituted chlorosilanes with lithium aluminum hydride or lithium aluminum deuteride. Moreover, both photoelectron spectroscopy and mass spectrometry were used to characterize gas-phase reactive intermediates formed by heterogeneous processes in chlorosilane chemical vapor deposition.<sup>4</sup> Ab initio theoretical

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calculations were also performed to corroborate experimental findings.<sup>5,6</sup> During this period, I worked both in the ICR lab and in the computational chemistry lab to look beyond  $m/z$  and find answers relevant to my project.

After getting familiar with FT-ICR, I was attracted to the spectroscopy of molecular ions. Using an ICR cell as a magnetic bottle to trap molecular ions of interest, I explored the infrared multiphoton dissociation (IRMPD) spectroscopy. There was a grating tuned CW CO<sub>2</sub> laser with a spectrum analyzer in the lab. The CO<sub>2</sub> laser was combined with FT-ICR to study the IRMPD spectroscopy of organometallic compounds containing the trifluoromethyl group, because the C-F stretching vibration was known to be IR-active in the CO<sub>2</sub> laser wavelength range (917–1100 cm<sup>-1</sup>).<sup>7–9</sup> I learned from the organometallic chemistry course about the migratory insertion of methyl group on the manganese carbonyl compounds. To check the migratory insertion of trifluoromethyl group on the manganese compounds in the gas phase, I synthesized CF<sub>3</sub>COMn(CO)<sub>5</sub> by reactions of NaMn(CO)<sub>5</sub> with trifluoroacetic anhydride and obtained CF<sub>3</sub>Mn(CO)<sub>5</sub> by heating CF<sub>3</sub>COMn(CO)<sub>5</sub>. The dissociative electron attachment of manganese carbonyl compounds in the ICR cell was used to generate ions of interest, both CF<sub>3</sub>COMn(CO)<sub>4</sub><sup>-</sup> and CF<sub>3</sub>Mn(CO)<sub>4</sub><sup>-</sup>.<sup>7</sup> In addition, ligand-displacement reactions of CF<sub>3</sub>Mn(CO)<sub>4</sub><sup>-</sup> with nitric oxide yielded CF<sub>3</sub>Mn(CO)<sub>3</sub>(NO)<sup>-</sup> and iodine atom-transfer reactions of CF<sub>3</sub>Mn(CO)<sub>4</sub><sup>-</sup> with CF<sub>3</sub>I resulted in CF<sub>3</sub>Mn(CO)<sub>4</sub>I.<sup>8,9</sup> The IRMPD spectra of CF<sub>3</sub>Mn(CO)<sub>4</sub><sup>-</sup>, CF<sub>3</sub>Mn(CO)<sub>3</sub>(NO)<sup>-</sup> and CF<sub>3</sub>Mn(CO)<sub>4</sub>I were recorded by monitoring the CO-loss products as a function of wavelength at all possible CO<sub>2</sub> laser lines. Although CF<sub>3</sub>COMn(CO)<sub>4</sub><sup>-</sup> did not undergo IRMPD, its CO-loss product from collision-induced dissociation (CID) underwent IRMPD, indicating that the CID product was CF<sub>3</sub>Mn(CO)<sub>4</sub><sup>-</sup> and the CF<sub>3</sub> migration took place after a loss of CO on the manganese center.<sup>7</sup> These IRMPD studies contributed to broaden the vibrational spectroscopy field of gas-phase ions as a variety of versatile IR light sources became available.

To expand the scope of my research, I joined the molecular dynamics group at USC in 1989 and looked into photoinitiated reactions in weakly-bonded complexes. I studied the reaction dynamics of hydrogen atom with carbon dioxide in CO<sub>2</sub>-HI/DI and CO<sub>2</sub>-HBr/DBr complexes<sup>10–13</sup> and with nitrous oxide in N<sub>2</sub>O-HI/DI complexes.<sup>14,15</sup> The supersonic expansion through a pulsed nozzle was used to prepare weakly-bonded complexes. The pulsed laser photolysis was employed to initiate the hydrogen-atom reactions with oxygen-containing molecules pre-aligned in close proximity within the complex. Laser-induced fluorescence of the OH product was monitored as a function of photolysis energy. The rovibrational state distribution of OH was characterized to see the effects of precursor alignment on the reaction dynamics. I learned the importance of synchronized operations of a pulsed molecular beam, a pump (inducing photolysis) laser beam,

a probe (inducing fluorescence) laser beam, and a gated photomultiplier tube (PMT). To synchronize them, I used a quadrupole mass analyzer to monitor the pulsed molecular beam and tweaked the pulsed valve to maximize the intensity of a weakly-bonded complex on an oscilloscope. Then, photodiode signals from the pump and probe laser beams were monitored to synchronize triggers for the pump and probe lasers as well as the gated PMT. The clock on the pump laser was utilized as a master clock to eliminate the time jitter as much as possible. This time-synchronization exercise was useful in setting up an instrument at UCSB later.

In 1991, I started up my own research group in the chemistry department at UCSB. To study photoinitiated reactions in ion-molecule complexes,<sup>16</sup> we built a 5-T FT-ICR instrument. A large bore 5-Tesla superconducting magnet was used to accommodate a differentially pumped ultrahigh vacuum chamber equipped with a 2-inch cubic ICR cell. The calcium fluoride and sapphire windows were mounted at the ends of the chamber to pass the counter-propagating photoionization pump and photodissociation probe laser beams. A pulsed valve was installed to deliver gaseous samples into the ICR cell. This instrument was used in combination with various laser spectroscopic techniques to explore unimolecular dissociations of halotoluene radical cations<sup>16–19</sup> and the formation of the silacycloheptatrienyl cation from phenylsilane.<sup>20</sup> The halotoluene and phenylsilane radical cations were generated by multiphoton ionization (MPI) using a 266 nm pump laser and then they were thermalized for 1 s in the ICR cell by charge-transfer reactions with parent neutrals in the chamber. Thermalized ions were irradiated with a pulsed probe laser to induce unimolecular dissociation and the product appearance was monitored as a function of time delay from the photoexcitation. Here, it was critical to synchronize various things: a pulsed valve, pump and probe lasers, an impulse excitation pulse and the gated transient digitizer in the ICR data system. A proper synchronization not only minimizes the time jitter but also improves the signal-to-noise ratio by the square root of the number of scans for the real-time detection and accumulation of ion signals. Lastly, ions of interest trapped in the ICR cell were characterized by examining their reactivities with neutral molecules. This state-of-the-art instrument enabled gas-phase reactions of thermalized radical cations as well as their time- and product-resolved photodissociation.

With halotoluene radical cations, the low-energy photodissociation product was identified as the benzyl cation, not the tropylium ion.<sup>21</sup> However, the portion of the tropylium ion gradually increased with an increase in energy. Since then, my group collaborated with a theory group to gain insights into the reaction dynamics of the halotoluene radical cations and came up with a coupled multi-barrier reaction mechanism.<sup>22–25</sup> As a result, a debate around the formation of C<sub>7</sub>H<sub>7</sub><sup>+</sup> (benzyl vs. tropylium) was

finally settled: Although the tropylium ion is thermodynamically more stable than the benzyl cation, the benzyl channel is kinetically favored because it involves a lower entrance barrier with fewer rearrangements than the tropylium channel.<sup>25</sup>

While taking time to build a 5-Tesla FT-ICR instrument, we worked on nonlinear oscillations in ICR to explain satellite peaks,<sup>26</sup> examined space-charge effects on image-charge signals,<sup>27</sup> investigated the heterodyne detection of ICR signals and radial separation of ions using off-resonance burst irradiation as an exploratory study for double resonance,<sup>28-29</sup> and applied FT-ICR to MPI spectroscopy.<sup>30,31</sup> In addition, we rebuilt a 1.2-Tesla electromagnet ICR instrument with a 1.85-inch cubic cell to carry out MALDI-FT-ICR experiments using a XeCl laser. Ions were desorbed from the matrix pasted on a Teflon substrate by the pulsed XeCl laser and they were trapped by cyclotron motion caused by the orthogonal magnetic field. Trapped ions were reacted with neutral molecules flowing into the ICR cell and thermal ion-molecule reactions were set to reach equilibria by extending the trapping time in the temperature range 15–85°C. Lithium halide triple ions were generated by MALDI and their reactions with several Lewis bases were studied to obtain the binding energy of Li<sup>+</sup> with Lewis bases from temperature-dependent equilibrium constants.<sup>32-34</sup>

In 1999, my lab was moved from UCSB to POSTECH and both 5-Tesla and 1.2-Tesla FT-ICR instruments were installed back on track. However, the delicate data system was not cooperative and it showed trouble-after-trouble due to frequent power outages and severe voltage sags. After numerous downtimes, I lost my faith on the resurrection of the data system and looked for user facilities around the country. Since then, I switched the gear from building up an instrument for the state-of-the-art experiments to developing a ditopic ion receptor<sup>35</sup> and an electrospray MALDI apparatus<sup>36</sup> as well as using commercial instruments for the target-oriented experiments.<sup>37-50</sup> For instance, a gas handling manifold was added to a QSTAR ESI-QTOF instrument to use Xe as a collision gas and some parameters were adjusted to enable energy-variable CID.<sup>37-41</sup> Energy-variable CID was used to characterize the binding of cadmium and zinc ions to trioctylphosphine chalcogenides,<sup>37</sup> noncovalent interactions between protonated porphyrins and fullerenes,<sup>38</sup> endo- and exo-binding modes of doubly-protonated jaws porphyrin to fullerenes,<sup>39,40</sup> and collision-activated reactions of cadmium ions with bifunctional thiols.<sup>41</sup> In addition, 12-T ESI-FT-ICR was employed to examine the binding constants of alkali metal, alkaline-earth metal and various porphyrin ions to G-quadruplexed DNA and characterize their binding sites by IRMPD.<sup>42,43</sup> Moreover, mass-balanced H/D isotope dipeptide tags (MBITs) were developed for simultaneous identification and quantification of proteins.<sup>44</sup> MBITs are amine-reactive 2-plex isobaric tags derived from N-acetyl-Xaa-Ala dipeptide,

where Xaa was a natural amino acid and H/D isotopes were differentially encoded in the methyl groups on N-acetyl and alanine.<sup>45</sup> 2-Plex MBIT-linked peptides co-migrated in reversed-phase liquid chromatography. Replacing Xaa with an artificial amino acid containing an alkyl side chain (C<sub>n</sub>H<sub>2n+1</sub>, n = 1-8) offered a series of 2-plex quantitation signals separated by 14 Da, which allowed multi 2-plex quantifications of proteins derived from several different physiological states.<sup>46</sup> Various instruments (TOF/TOF, Q-TOF, Q-TRAP, LTQ and HCT) were used to characterize the performance of MBITs on different MS platforms. MBITs yielded both low-mass b-type and high-mass y-type signals for protein quantification without sacrificing the relative abundance of sequence ions.<sup>47</sup> Besides, MBIT variants containing an alkyl side chain on the N-acyl group, N-acyl-Ala-Ala dipeptide tags, were developed as the internal standards for ion temperature to assign a temperature to the peptide fragment spectra.<sup>48</sup> Thus, MBITs can be generally applied to diverse quantitative proteomics in all types of MS platforms. A one-step chemical derivatization method was also developed for label-free quantification of lipase reaction products, a mixture of triacylglycerol (TAG), diacylglycerol (DAG) and monoacylglycerol (MAG), using ESI-Q-TRAP.<sup>49</sup>

My group members have used the following instruments on many occasions and I am grateful to the hosts at various departments and institutions for their generosity and good spirit: ESI-triple quadrupole time-of-flight (TOF) MS (QSTAR Pulsar-i), MALDI-TOF/TOF MS (4700 Proteomics Analyzer), ESI-triple quadrupole-ion trap MS (2000 Q-TRAP), and ESI-linear ion trap MS (LTQ XL) at POSTECH; ESI triple quadrupole time-of-flight (Q-TOF Premiere) at Korea Basic Science Institute; ESI-high capacity ion trap (HCT) at Ulsan National Institute of Science and Technology; 12-T ESI-FT-ICR at Korea Research Institute of Science and Standards.

Lately, we began to examine hydrogen-bonding environments in chemically modified peptides<sup>50</sup> and take a thermochemical approach to energy-variable CID of the protonated peptide ion.<sup>51</sup> Collisional activation increases an internal energy of a peptide and the extent of temperature rise varies with heat capacity. Since the unimolecular dissociation rate depends on the temperature, the ion temperature is an important parameter in the analysis of energy-variable CID curves. The thermochemical approach takes the temperature and heat capacity of peptide into account to simulate energy-variable CID curves obtained from experiments.

Over the last two years, the COVID-19 pandemic has become an outstanding global issue that challenges every corner of our society. In the past, when the diseases like cholera and malaria propagated through water and insects, respectively, the public health efforts successfully contained their outbreaks by renovating a sewage system and by installing window screens, respectively. At present,

COVID-19 and other respiratory diseases spread through air and/or solid surface,<sup>52</sup> which offers a unique opportunity to the MS community. The MS community should prepare for the post-COVID era to address the problems associated with air-borne transmission of the pathogens in the form of droplets and/or aerosols as well as surface-adsorbed pathogens. An innovative and robust MS tool is needed to enable the real-time detection of airborne viruses to guide indoor air-quality standards. The drone technology can be combined with the compact MS instruments to enable in-situ detection of air pollutants, carbon emissions and hazardous substances, which allows to draw 2D aerial maps for real-time tracking and to make 3D spatial maps for airborne-transmission monitoring. Looking beyond the mass-to-charge ratios will be fun and worth practicing, because the mass spectrometry can address the current issues in airborne-virus detection, air-quality control, and climate change.

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