Mass Spectrometry

Jürgen H. Gross

Mass Spectrometry

A Textbook

Third Edition

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Jürgen H. Gross
Institute of Organic Chemistry
Heidelberg University
Heidelberg, Germany

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Preface

When non-mass spectrometrists are talking about mass spectrometry, it rather often sounds as if they were telling a story out of Poe's *Tales of Mystery and Imagination*. Indeed, mass spectrometry appears to be regarded as a mysterious method, just good enough to supply some molecular weight information. Unfortunately, this rumor about the dark side of analytical methods may reach students way before their first contact with mass spectrometry. Possibly, some of this may have been bred by some mass spectrometrists who used to celebrate each mass spectrum they obtained from the very first gigantic machines of the early days. Of course, there were also those who enthusiastically started in the 1950s toward developing mass spectrometry out of the domain of physics to become a new analytical tool for chemistry. Within the more than a hundred years since J. J. Thomson's seminal work, there has been a lot that has happened and a lot now to be known and learned about mass spectrometry.

How All This Began

Back in the late 1980s, J. J. Veith's mass spectrometry laboratory at the Technical University of Darmstadt was bright and clean, had no noxious odors, and thus presented a nice contrast to a preparative organic chemistry laboratory. Numerous stainless steel flanges and electronics cabinets were tempting to be explored and – whoops – infected me with CMSD (chronic mass spectrometry disease). Staying with Veith's group slowly transformed me into a mass spectrometrist. Inspiring books such as *Fundamental Aspects of Organic Mass Spectrometry* or *Metastable Ions*, out of stock even in those days, did help me very much during my metamorphosis. Having completed my doctoral thesis on fragmentation pathways of isolated immonium ions in the gas phase, I assumed my current position. Since 1994, I have been head of the mass spectrometry laboratory at the Chemistry Department of Heidelberg University where I teach introductory courses and seminars on mass spectrometry.

When students then asked what books to read on mass spectrometry, there were various excellent monographs, but the ideal textbook still seemed to be missing – at least in my opinion. Finally, 2 years of writing began.

A Third Edition

Now, *Mass Spectrometry – A Textbook* is here in its third edition. For me, the author, preparing the third edition meant an obligation to update and further improve the content of this book. The extent of overall coverage and global organization has not changed as much for this edition as in the transition from the first to the second edition – nonetheless, many new sections have been added to adequately present the recent innovations in this ever-developing field of mass spectrometry. No chapter has remained untouched. Each of the 15 chapters has carefully been reworked and augmented with hundreds of additions, changes, and corrections.

What's New?

Since the second edition, new techniques have gained importance, and some instrumentation has received notable attention and attained considerable commercial success. To keep pace with recent developments, Chap. 4 now includes TOF instruments with folded flight paths, the dynamically harmonized FT-ICR cell, more on hybrid instruments, and ion mobility spectrometry–mass spectrometry. The increasing relevance of high-resolution and accurate mass measurements is even strongly reflected in Chap. 3. The five chapters dedicated to soft ionization methods (CI, APCI, APPI, FAB, LSIMS, FI, FD, LIFDI, ESI, LDI, MALDI) as well as those on ambient desorption/ionization (DESI, DART, REIMS, etc.) and on tandem mass spectrometry have been substantially updated and upgraded. There is also much more on chromatographic techniques (GC, LC) and their coupling to mass spectrometry in Chap. 14.

The way we are using books and literature in general has dramatically changed during the last decade. Back in 2001, when I started preparing the first edition of this book, regular visits to the libraries of several institutions in the area were on my schedule to collect some vast amount of literature. Today, almost all journal articles are electronically available within seconds, and even textbooks are now being extensively used in their e-book versions. This had also some impact on the layout and production process of this book.

In the light of an ever-growing abundance of methods, instruments, tools, and rules in mass spectrometry, the ease of how a complex field of analytical science can be grasped mentally certainly deserves attention. Therefore, the emphasis of my work was on refinement in terms of presentation, convenience of use, and ease of learning. Obviously, a textbook ranging around 900 pages may deter the novice, and thus, my focus was on a didactic and educational approach. Although the actual number of pages has notably increased once again, you will find the textbook easier to read, and you will benefit when transferring theory in actual practice such as spectral interpretation and method selection.

Overall, the third edition of *Mass Spectrometry – A Textbook* comes with lots of didactical improvements:

- Numerous passages have been rewritten and improved while remaining short and concise. Care has been taken not only to explain *how* but also *why* things are done a particular way.
- The number of figures has been notably increased, and about one third of them are now in full color. More photographs and schematics mean easier comprehension of contents, often providing valuable insight into the practical aspects of instrumentation and according procedures.
- Flowcharts have been introduced to describe procedures and approaches to mass spectral interpretation or aid in decision making.
- Bulleted enumerations have been introduced wherever a larger number of features, arguments, assumptions, or properties regarding a subject warrant a clear presentation.
- More examples, especially of methods and applications, are given and some *how-to-style* paragraphs provide practical guidance.
- Examples and notes now come with a short subheading that immediately tells what the particular section is all about.
- All chapters conclude with a concise summary that is subdivided into compact sections highlighting the basic concepts of the subject area, its figures of merit, typical applications, and its role in current MS. Chapter 4 ("Instrumentation") provides summaries of all types of mass analyzers.
- Digital object identifiers (DOIs) are included in the lists of references to facilitate the retrieval of references for e-book users. For those of you who, like me, still prefer a hardbound book, the DOIs offer an additional level of comfort. So, I am pretty convinced that the tedious work of collecting DOIs was very much worth the effort.
- The book's website has been updated providing new exercises and supplementary material (www.ms-textbook.com).

Deepest Gratitude

To all readers of the previous editions of *Mass Spectrometry – A Textbook*, I would like to express my deepest gratitude. Without their interest in wanting to learn more about mass spectrometry by the use of this book, all the efforts in writing it would have been a mere waste of time, and moreover, without their demand for updates, there would be no next edition. I also would like to thank the instructors all over the world who adopted and recommended this book for their own mass spectrometry courses.

Being an author of a textbook means to retrieve, collect, compile, sort, and balance knowledge, findings, and inventions of others. Most of what is written here relies on the intelligence, skill, integrity, and devotion of hundreds of researchers who have contributed to mass spectrometry each in their own way.

Many kind people have supported me in the process of compiling this and the previous editions. I appreciate the detailed knowledge and great thoroughness allocated by Kenzo Hiraoka, Yasuhide Naito, Takemichi Nakamura, and Hiroaki Sato to the translation of the first edition into Japanese. The valuable and welcome comments from readers from all over the world and, in particular, from book reviewers and colleagues have revealed some shortcomings, which now could be adequately addressed.

For the second edition, several competent and renowned colleagues had contributed by carefully checking the according contents in their fields of expertise. I want to express my special thanks to Jürgen Grotemeyer, University of Kiel, for checking Chap. 2 (“Principles of Ionization and Ion Dissociation”); Alexander Makarov, Thermo Fisher Scientific, Bremen (Chap. 4, “Instrumentation”); Christoph A. Schalley, Freie Universität Berlin (Chap. 9, “Tandem Mass Spectrometry”); Belá Paizs, German Cancer Research Center, Heidelberg (Chap. 11, “Matrix-Assisted Laser Desorption/Ionization”); Zoltán Takáts, Universität Gießen (Chap. 13, “Ambient Mass Spectrometry”); and Detlef Günther, ETH Zürich (Chap. 15, “Inorganic Mass Spectrometry”).

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Again, many manufacturers of mass spectrometers and mass spectrometry supply are gratefully acknowledged for generously providing schemes and photographs. The author wishes to express his thanks to those scientists, many of them from Heidelberg University, who allowed to use material from their research as examples and to those publishers, who granted the numerous copyrights for the use of figures from their publications. The generous permission of the National Institute of Standards and Technology (S. Stein, G. Mallard, J. Sauerwein) to use a large set of electron ionization mass spectra from the NIST/EPA/NIH Mass Spectral Library is also gratefully acknowledged.

Permission to prepare this third edition alongside my official professional duties, granted by Oliver Trapp, former director of OCI, and Heinfried Schöler, former dean of the Faculty of Chemistry and Earth Sciences, is sincerely acknowledged. Many thanks to my team Doris Lang, Iris Mitsch, and Norbert Nieth for smoothly running the routine analyses in our MS facility. Once more, Theodor C. H. Cole accomplished a great job in polishing up my English. Finally, I am again grateful to my family for their patience and solidarity in times when I had to come home late or needed to vanish on Saturdays during the writing of this book.

Have a good time studying, learning, and enjoying the world of mass spectrometry!

Jürgen H. Gross

Institute of Organic Chemistry (OCI)
Heidelberg University
Im Neuenheimer Feld 270
69120 Heidelberg, Germany
email: author@ms-textbook.com

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