Mass Spectrometry: A Textbook

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The purpose of this book is clearly reflected in its title. The author's stated reason for writing the book was to create an "ideal textbook" for his duties involving the teaching of mass spectrometry courses and seminars at Heidelberg University. Dr. Gross has spent the last 10 years in the chemistry department's mass spectrometry service laboratory, where he is the head. He has held this position since the completion of his doctoral thesis on fragmentation pathways of isolated immonium ions in the gas phase in J. J. Veith's mass spectrometry laboratory at Darmstadt University. Dr. Gross professes to be infected with *CMSD* (chronic mass spectrometry disease). This is probably a misinterpretation of the enthusiasm for the use of mass spectrometry that he exhibits throughout this book. This book has a single author; however, he had each of the 12 chapters undergo critical review by people he refers to as "leading experts in the field." These 12 people are mentioned by name in the Preface and include a very impressive group from the literature of mass spectrometry. The first paragraph in the *Introduction* chapter of this book makes it clear that this is an organic mass spectrometry book. Readers should not think that other disciplines that use mass spectrometry, such as geology, environmental speciation of inorganic ions by ICP-MS, and so forth, are going to be covered because there was never any intention to do that.

In addition to the 12 chapters, there is a 10-page Appendix containing the usual information found in a mass spectrometry text's Appendix such as a list of impurities, common fragments, isotopic composition of elements, and so forth. The book has an 11-page Index that is very useful. Of the 494 pages of text, 72 are references (almost 15%); and, when these references are to journal articles, the tile of the article is included. A quick read through the 12 chapter titles can be somewhat misleading. This list gives the appearance that the book is primarily about electron ionization mass spectrometry, and some important topics such as electron capture ionization, collisionally activated dissociation, and accurate mass measurement to determine elemental composition, and so forth, have been omitted; but they are all there and probably exactly where they should be for introducing these concepts in a beginning course on mass spectrometry.

Part of the reason for some possible misunderstandings of the entire contents of the book is the brief chapter titles used: 1 *Introduction* (one-and-a-half pages of references and another one-and-a-half pages of suggested books); 2 *Gas Phase Ion Chemistry*, where tandem mass spectrometry is introduced (43 pages plus 6 pages of references); 3 *Isotopes*, which includes accurate mass measurements and an introduction to multiple-charge ions that is revisited in the mathematical charge deconvolution part of the electrospray chapter (42 pages plus 2 pages of references); 4 *Instrumentation* (71 pages plus 11 pages of references); 5 *Electron Ionization* (25 pages plus 5 pages of references); 6 *Fragmentation of Organic Ions and Interpretation of EI Mass Spectra* (97 pages plus 11 pages of references); 7 *Chemical Ionization*, which includes details on resonance electron capture ionization (20 pages plus 4 pages of references); 8 *Field Ionization and Field Desorption* (21 pages plus 5 pages of references); 9 *Fast Atom Bombardment* (23 pages plus 7 pages of references); 10 *Matrix-Assisted Laser Desorption/Ionization* (23 pages plus 7 pages of references); 11 *Electrospray Ionization* (27 pages plus 7 pages of references); 12 *Hyphenated Methods* (16 pages plus 4 pages of references). The organization of these chapters clearly follows a logical approach to teaching a course in organic mass spectrometry: Theory → Instrumentation → Data → Ionization techniques → Hyphenated techniques (GC/MS and LC/MS).

The author is clearly of the opinion that an understanding of mass spectrometry requires both an understanding of an ion's behavior in the evacuated gas phase and how ions break apart regardless of their origin. A lay mass spectrometrist who read this book commented that until he had read the *Gas Phase Ion Chemistry* chapter in this book, he had never had a very good understanding of the subject. This is one of the better chapters in the book and makes the teaching of this particular aspect of the subject very easy. Another very good chapter is the one on instrumentation, especially with respect to the different types of *m/z* analyzers. The chapter has details and the latest technology that includes the linear quadrupole ion trap. The chapter is weak in the area of ion detection and vacuum system. There is no mention of the photomultiplier systems used in preference to electron multipliers by some commercial manufacturers, and the treatment of mechanical pumps omits the new scroll pump technology now appearing on commercial instruments. Most of the subjects in the book have very good illustrations (which is one of the important attributes of this book) associated with them; however, the section on vacuum has no illustrations. At the end of the *Instrumentation*

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chapter, there is a sort of afterthought on *Buying an Instrument*. At first, this paragraph with a six-bullet list appeared to be slim; however, for a first-time purchaser of a mass spectrometer, it is very thought-provoking.

This book is truly a modern book on mass spectrometry and is easy to recognize as having its origins in Europe. All such previous texts discussed the pressure in the mass spectrometer in terms of Torr or millibar (depending on which side of the Pond the book was written). This book uses only the pascal (Pa) as the unit of pressure. In the above-mentioned *Buying an Instrument* section, the prices are in *Euros* (€).

Some may consider that devoting more than 20% of the book to the *Fragmentation of Organic Ions and Interpretation of EI Mass Spectra* limits the book in the so-called area of "Modern Mass Spectrometry." I contend that it is easier to get an understanding of how ions fragment, regardless of the way they were formed, through the extensive studies that have been carried out on ions produced by electron ionization and then apply this understanding to ions that come from other sources. The author agrees with the following statement that appears at the beginning of this interpretation chapter:

> "Although the discussion of common fragmentation pathways of organic ions is imbedded here in the context of EI mass spectrometry, their occurrence is not restricted to this technique. The reactions of isolated gaseous ions do not directly depend on the ionization method, but are almost exclusively governed by intrinsic properties of the respective ion and by its internal energy (Chap. 2)."

This book has many attributes that make it good to use as a text for an introductory course. In addition to the extensive illustrations (some new and some borrowed from classic sources with permission), the book uses the concept of "Note" boxes throughout to bring focus on salient topics on various pages. The use of a double-column format for the reference makes reading them very easy even though they are in a smaller font than the rest of the text. The Table of Contents uses a three-level format, which gives a much better view of the book than just a quick review of the chapter titles. Another interesting concept for a book intended as a textbook is the lack of exercises and answer keys for the student. The author points out in the *Introduction* chapter that they were purposely omitted and are available at the book's Web site http://www.ms-textbook.com. This site is very well done and can be useful to anyone using this book as a text for a course.

The book is not without areas that elicit criticism. In addition to the omissions on vacuum and ion detection already mentioned, some areas such as the chapters on FAB and FD/FI could have been more abbreviated and included in the MALDI and Electrospray chapters. More space could have been devoted to the latter techniques along with the *Hyphenated Methods* chapter.

The author has done a very thorough job of trying to make sure that the terminology used throughout the book is correct and not misleading. There are some questionable inclusions such as the use of *quasi-molecular* ion (as Maurice Bursey would say, "Show me a *quasi-molecule* and I'll show you a *quasi-molecular ion*.") Another potential problem is the use of the term "charge exchange" instead of, what I believe today is the more common term, "charge transfer." The author even makes a point in one of his "Note:" boxes that the use of CE as an abbreviation for charge exchange can be confused with CE also used as an abbreviation for capillary electrophoresis, but goes ahead and uses charge exchange. I presume the author is using charge exchange rather than charge transfer because this is the terminology used by Alex Harrison in his classic monograph *Chemical Ionization Mass Spectrometry, 2nd ed.* (CRC Press: Boca Raton, FL, 1992). The author makes another very common mistake in terminology when (in the Note: box on page 109 in the *Isotopes* chapter) he uses the symbol u (unified atomic mass unit) as a synonymy for *m/z*. He says, ". . .distance between the peaks is reduced to 1/2 u. . ." when it should have read ". . .distance between the two peaks is reduced to 1/2 *m/z* units. . ." This may seem a little nitpicky, but the author emphasizes in the *Introduction* chapter the importance of proper terminology. Along the same lines of terminology, the author makes a statement about how the use of *electron impact ionization* or *electron impact* has been discontinued in the recent past and then uses the term in the 5.1 heading title.

Other problems are in the *Isotopes* chapter. The differentiation among X, X+1, and X+2 elements is cloudy at best. The concept of an X−1 element is introduced, which is good because of the presence of boron and lithium in organic mass spectrometry. However, even with the introduction of copper and silver as X+2 elements and sodium as an X element, there is no mention of potassium as an X−2 element. The isotope pattern of peaks representing ions containing potassium is extremely significant for electrospray. There is also a reversal in the definitions of *resolution* and *resolving power*. The author states that the *resolution* is defined as $m/\Delta m$ and signified by the symbol R; and that, ". . .Δm the *resolving power* as defined by the peak width. . .at a specific fraction of the peak height." The citation for these definitions is the John Todd paper on IUPAC nomenclature for mass spectrometry that appeared in the *Int. J. Mass Spectrom. Ion Processes* in 1995. Some care will be necessary in keeping students straight in the *Isotopes* chapter. The term "nominal mass" is clearly defined in the *Isotopes* chapter (page 71); but on page 239 in the *Fragmentation of Organic Ions and Interpretation of EI Mass Spectra* chapter, the author says, "If a compound contains an even number of nitrogen atoms (0, 2, 4. . .), its monoisotopic molecular ion will be detected at an even-number *m/z* (integer value)." Of course, this is only true after a correction for mass defect

has been applied and should have been stated as ". . .its nominal *m/z* value will be even."

Although the overall production of the book is very good and the presentation of figures and schemes is incomparably superior to many recently published books, the publisher could have done a better job of copy editing. The book is well written but, from time to time, the German grammar structure shows through; as this is an English-language book, this could make it difficult for those who do not have either German or English as a first language. The author introduces a lot of abbreviations throughout the book. The inside front and back covers, which are bare, could be used to provide a glossary of these abbreviations. Until the next edition, this glossary would be a good thing to put on the book's Web site.

One last point about the book's production (and/or organization) is the fact that at the bottom of page 374 in the *Field Ionization and Field Desorption* chapter, there is a "Note:" box that says in part, "One alkali adduct ion almost never occurs exclusively, i.e., $[M + H]^+$, $[M + Na]^+$, and $[M + K]^+$ [sic] (M + 1, M + 23, and M + 39 [sic]) are observed with varying relative intensities at. . ." It would appear that this "Note:" box should have been in the *Electrospray Ionization* chapter. This "Note:" box also exhibited the error of using u as a synonym for *m/z*. It is true that these adduct ions are seen in field desorption, but they are of more significance in electrospray.

Overall, this is an excellent textbook. It will serve any introductory class on mass spectrometry well, whether that class is a group of students in a formal setting or is a directed study for an individual entering a research group. I used this book as a reference resource in my Fall 2004 "Introduction to Mass Spectrometry" class. The reaction of my students was such that it will become the required textbook next Fall (2005). This is also a reasonably priced book. At US$ 79.95, the value far surpasses the price. The author has promised future editions, and I look forward to them. Again, his passion for the topic and his intensity of study shows throughout his manuscript.