Additions and Corrections

The Anomalous Infrared Amide I Intensity Distribution in ^{13}C Isotopically Labeled Peptide β-Sheets Comes from Extended, Multiple-Stranded Structures. An ab Initio Study
[*J. Am. Chem. Soc.* **2001**, *123*, 6142−6150]. JAN KUBELKA AND TIMOTHY A. KEIDERLING*

Page 6146, column 1, lines 16 and 18 and page 6147 in captions for Figures 6 and 8:

Ac-AA*AA*A_8-NH-CH_3 should be Ac-AAA*AA*A_7-NH-CH_3.

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Book Reviews *

Principles and Practice of Biological Mass Spectrometry. By Chhabil Dass (University of Memphis). J. Wiley & Sons, Inc.: New York. 2001. xxviii + 416 pp. $99.95. ISBN 0-471-33053-1.

According to the author, the purpose of this book is to provide an up-to-date examination of the basic principles of instrumentation, technique, and application of the expanding field of biological mass spectrometry (MS) in a single volume. Written for professionals in the biological sciences, this book provides some fundamentals of contemporary mass spectrometry for assistance in choosing the best instrumentation and technique for solving daily problems. The book is composed of 16 chapters.

Due to the advent of electrospray ionization (ESI) and matrix-assisted laser desorption/ionization (MALDI) techniques in the past two decades, mass spectrometry has revolutionized the field of biological sciences. In the past, MS was mainly limited to small molecules (<3000 Da) using gas chromatography−mass spectrometry (GC−MS), high-performance liquid chromatography−mass spectrometry (HPLC−MS), and capillary electrophoresis−mass spectrometry (CE−MS) for the analysis of biological mixtures. Since most biological compounds are thermally labile, GC−MS analysis required derivatization—a time-consuming process. On the other hand, ionization techniques available for LC−MS analysis (thermospray, continuous-flow fast-atom bombardment (CF−FAB), and particle beam) were not as robust and required continuous maintenance, which meant that "experts" were needed to keep them operational. The ESI and MALDI techniques changed all that. In addition to enhancing the mass range capability of the mass spectrometers, ESI and MALDI instruments are sensitive, robust, and easy to operate. The drawback of these turnkey systems is that they appear as black boxes to their "nonexpert" operators, which hinders them from being used to their full capability. These ionization techniques are now available on a variety of mass analyzers, have been applied to a variety of applications in almost every field of biological sciences, and have almost eliminated the need for older ionization techniques for the analysis of biological mixtures. In this regard, books that can explain these ionization techniques, instrumentation, and their applications are much needed. The book by Dass is an attempt to bring the readers in the field of biological sciences up-to-date with these current techniques and applications. However, it is a daunting challenge to include the vast amount of information that is available today regarding MS technology and its applications in a one-book volume having some 400 pages. To accomplish this, the author had to sacrifice the details, which resulted in a format that makes this book similar to a short encyclopedia or a descriptive dictionary. Thus, the information provided in some areas is somewhat choppy and has little elaboration. This is especially true for the first two sections of the book that deal with instrumentation and techniques.

The book begins with a general introduction to MS and a review of the fundamentals and the recent developments in biological mass spectrometry instrumentation, including ionization modes, mass analyzers, ion detectors, and MS/MS. Some concepts relevant to MS, such as the importance of high resolution and high mass accuracy, the role of calibration standards for accurate mass measurement of biological compounds, and factors that can affect mass accuracy, are also explained. In addition, the role of MS for quantitative analysis, including the use of internal standards that incorporate stable isotopes and the application of a variety of scanning modes for achieving a high level of precision and accuracy, is discussed. The last part of this section briefly discusses the coupling of separation techniques, including GC, HPLC, and CE, with MS.

The major advantage of this section is that the author tries to cover a large number of the MS techniques that are available. Some of these techniques (such as electron impact (EI) and CF−FAB) are rarely used by professionals in the biological sciences, however. Thus, in my opinion, it would have been better to reference these techniques than to discuss them. Also, more information could have been provided in this section regarding the mechanism of ESI, and the advantages and disadvantages of different CE-to-MS interfaces could have been explained. In addition, the one-page discussion of MS/MS in ion trap and ion cyclotron resonance (ICR), which these days are among the most commonly used mass spectrometers for MS/MS of biological samples, could have replaced the several pages that are dedicated to MS/MS in sector instruments which, due to their long scan time, are not often used for the analysis of complex biological mixtures.

Some specific comments on this section are required. On page 47, paragraph 4, the duty cycle given for time-of-flight mass spectrometry (TOF-MS) is 3%, but no explanation of duty cycle or the value of 3% is provided. In the final paragraph of this page, the author writes, "Some modifications are made to the ESI interface. For example, additional differential pumping and vacuum baffles are added to the interface to prevent electrical discharge." This statement is not accompanied by any discussion about vacuum systems or discharge zones and therefore does not help the novice reader to understand what the author is talking about. The author also states (page 135) that, "In magnetic sector instruments, a convenient way to record the ion current at different m/z values is to change the accelerating voltage rather than magnetic field strength", but does not explain why (it is actually a question of mass accuracy rather than convenience, since now both adjustments are made with clicks of a button). In addition, the abbreviations used on page 139 seem to be erratic: for example, HPLC/ESI−MS/MS (the correct notation), LC/MS/MS, and LC−ESIMS/MS are all used interchangeably. The same inconsistency also occurs for CE interface to MS notation on page 161. Also, when a mass measurement is presented, the isotope pattern (page 117), which is also referred to as the *isotopic distribution profile* (page 119), *isotopic cluster* (page 119), and *molecular ion distribution* (page 118), is not defined, and the difference between it and the isotopic fine structure (page 121) is not discussed. Finally, in Table 5.1 it is stated that the useful mass ranges—which should be referred to as the *m*/*z* range to cover its

*Unsigned book reviews are by the Book Review Editor.

usefulness for multiply charged ions—of the calibration standard Ultramark 1621 are <3000 for EI and chemical ionization (CI), <6000 for ESI, and <1500 for EI, but they are incorrect. In actuality, the better range for CI, FAB, and ESI is >800 and <2000 and only <2000 for EI (reference 50, Chapter 5, which is listed in the References but not referenced in the text, and Jiang, L.; Moini, M. *J. Am. Soc. Mass Spectrom.* **1992**, *3*, 842−846).

The second half of the book, starting with Chapter 8, includes the analysis of biological compounds. In this section, the MS-based protocols for the analysis of proteins, lipids, and oligonucleotides are given for both MALDI analysis and HPLC/ESI−MS analysis. Protocols for peptide and oligonucleotide sequencing using MS/MS are provided for both MALDI−MS and ESI−MS analysis. For MALDI analysis, useful matrixes and their applications are conveniently provided in a table. A variety of examples for different compounds are given, and many references are provided. The book concludes with a very interesting chapter titled "Application to Real-World Problems", which includes analyses of biological tissues, single neurons, single mast cells, bacteria and viruses, etc. From my point of view, this section is the most interesting part of the book. Several examples are provided to discuss the characterization of biological compounds and to clearly illustrate the importance and advantages of MS in the analysis of complex biological mixtures. However, the real-world analysis of biological samples focused mostly on MALDI analysis, with very little emphasis on ESI−MS analysis. For example, CE/ESI−MS of single intact cells is not discussed.

In general, the book is well written and has only a few minor errors. Many up-to-date references are provided at the end of each chapter, although they mostly represent the author's preference in each area and do not necessarily represent all the new developments in that area. There are a few missing reference numbers in the text. In my opinion, the scope of the book is overly broad, and the field of mass spectrometry would have been better served if the author could have focused on modern techniques, where comprehensive information is limited, and referenced older techniques that are not widely used for biological analysis. The second half of the book, in which applications to complex biological mixtures are discussed, is the more interesting part of the book and makes reading it worthwhile.

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Molecular Magnetism: New Magnetic Materials. By Koichi Itoh (Osaka City University) and Minoru Kinoshita (Science University of Tokyo in Yamaguchi). Kodansha and Gordon & Breach: Tokyo and Amsterdam. xvi + 348 pp. $120.00. ISBN 4-06-209070-1 (Kondansha) and 90-5699-307-0 (Gordon & Breach).

This book is an English language version of one previously published in Japanese. It covers a broad variety of topics in the growing area of molecular magnetism. The two editing authors acknowledge contributions from a number of colleagues in assembling the final selection of material.

The book does a good job in covering a breadth of subtopics that are useful to those interested in molecular magnetism. The coverage of each area is variable. Very detailed coverage is given to the basic theory of exchange interactions within molecules (Chapter 1), within polymeric polyradical chains and networks (Chapters 1 and 4.1), and between molecules (mostly in Chapter 1). Similarly strong coverage is given to treatment of advanced methods for electron spin resonance investigations (Chapter 3.2) of open-shell molecules. There is also extensive referencing of the methodology and literature for computational studies of exchange interactions within and between pairs of molecules. Overall, throughout the book there is a strong concentration on understanding spin density distributions, spin alignment, and spin wave behavior within individual molecules and polymer chains as well as within dimeric models for crystal packing.

Methods of analyzing molecular magnetic materials are similarly subject to some variability in depth of treatment. Chapter 3.1, on magnetic susceptibility measurements, is one of the larger chapters in the book and includes listings of some of the fundamental equations in magnetism. Chapter 3.3, on heat capacity studies, is shorter, though clearly written. There is virtually no treatment of the important area of neutron diffraction for investigation of spin density distributions in crystalline arrays. Overall, the treatment of the methods—other than magnetic susceptibility—for investigating bulk magnetic properties in materials is useful but somewhat scattered. Much of the information on such studies is placed in the context of studies of specific systems, rather than in methodology sections. This works out reasonably well for a chemist's approach to classifying the studies by molecule type rather than by magnetism type.

The book contains quite a bit of information and numerous examples of charge-transfer and hybrid behavior electronic materials, such as molecule-based systems that simultaneously exhibit conductive and magnetic behavior. Chapter 4.4 is a useful reminder of the promise of molecular complexes as materials that also exhibit metallic behavior. Recent results that have appeared after the production of the book (such as Coronado, E., et al. *Nature* **2000**, *408*, 447−449) demonstrate the timeliness and importance of this topic. The latter chapters that cover magnetic behavior of organic systems give plenty of detail and tables of results. The last chapter of the book ("Molecular Design and Synthesis for Inorganic Molecular Magnetism") includes vignettes of very important future areas of interest, such as photoinduced molecular magnetism, hybrid organic−inorganic systems (both with and without spin-bearing organic building blocks), and metal clusters. They provide a useful reminder to the reader about how vital inorganic chemical approaches are to many strategies in the area, although they are much less detailed than the chapters on organic systems.

Overall, the book is a survey of most of the important topic areas in the field of molecular magnetism. Its strength is its depth of coverage of qualitative molecular (particularly organic molecular) aspects of molecular magnetism. It is less strong in terms of covering the various areas to equal extents. The selectivity of topics and depth of topics is influenced by the fact that all of those contributing to the book were from institutions near the authors. This reflects the original, Japanese language version of the book. The contributors are all strong in various aspects of molecular magnetism, but the overall effect is to restrict a more international viewpoint of the state-of-the-art in molecular magnetism. In fairness, one must remember that to try to cover the full sweep of areas in molecular magnetism to the extent that has been done for many of the book chapters, one would have produced a much larger book.

I think that this book stands best in combination with others that fill in some of the important areas that it was not able to cover in detail. I found it to be a good introduction and useful background resource for those looking to pursue the area of molecular magnetism, especially in a wide variety of areas as described above.

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Associative Polymers in Aqueous Media. Edited by J. Edward Glass (North Dakota State University). American Chemical Society: Washington, DC (Distributed by Oxford University Press). 2000. xii + 418 pp. $145.00. ISBN 0-8412-3659-3.

This book, a volume in the ACS Symposium Series, contains 22 chapters on the title subject. The topics are organized under the following two subheadings: Block Copolymers and Dendrimers, and Surfactant-Modified, Water-Soluble Polymers. The latter category is further divided into the sections: HMPAM and HEUR Polymers; Adsorption Studies: POE, HEUR and HMPAM; HMHEC and HMEHEC Polymers; and HASE Thickeners.

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