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Book Review

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BOOK REVIEW

Mass Spectrometry/Mass Spectrometry, K. L. Bush, G. L. Glish and S. A. McLuckey, VCH Publishers, Inc., 1988.

This is an extraordinary book.

At the first glance, the book looks like others for some experts in the field. But looking a bit more closely reveals that a discussion of MS/MS needs far more than simply to cover one aspect of today's mass spectrometry. The technique—or better: the strategy—of MS/MS is so intimately embedded into almost every aspect of mass spectrometry that essentially the authors had to deal with mass spectrometry itself. And so they did. They reviewed and evaluated every significant facet in such a well organized manner that it does not need much more to complete a full bodied view on today's most powerful detection method—mass spectrometry.

The book comprises seven chapters of very different lengths, a list of 900!! references (up to the beginning of 1988, almost complete) one quite useful and necessary appendix for the large number of MS/MS scan modes available for the various instrument configurations, a second appendix for symbols and abbreviations, a *conditio sine qua non* in all scientific texts in instrumental analytical chemistry, and an index, well balanced and sufficiently detailed for the need of most readers, I presume.

The first, short chapter leads the reader into the history and the philosophy of MS/MS which is a necessary basis for the following discussions. Since the idea of MS/MS came up at the same time as mass spectrometry was invented, it appears almost logical that its influence on the development of mass spectrometry was great and an understanding of today's situation needs the historical view. In addition, a thorough explanation of the nomenclature used in the book is given in that chapter.

The second chapter, devoted to MS/MS instrumentation, discusses briefly the principles of charged particles analysis and their realizations in sectorfield, quadrupole and ion-trapping instruments for MS/MS applications including the required reaction regions for high and low energy collisions. This chapter convinced the reviewer that with some additional support by primary literature—some is provided already—this text could serve to teach mass spectrometry on an advanced level and not only MS/MS.

The third chapter, dealing with reactions of ions in MS/MS, supports this view; most of the topics—unimolecular reactions, collisional activation, photodissociations, electron excitation and surface induced excitation—are (should be) basic knowledge in mass spectrometry, not only in MS/MS. Again, the thorough discussion is backed up by an extensive list of references.

The fourth chapter reviews on the basis of examples the applications of MS/MS for fundamental aspects in theoretical studies in organic and physical chemistry and some of the contents is of key interest to most mass spectrometrists-to-be.

The fifth, rather short chapter explains the characteristics of MS/MS for analytical applications. This presentation makes evident that the content is common knowledge in analytical chemistry, which is by no means common place to all mass spectroscopists. Therefore, this chapter serves very well as a very timely introduction to analytical chemistry for mass spectrometrists.

The sixth chapter, with just over 100 pages the longest one, identifies in a comprehensive list nearly all fields of applications (and possible applications) for MS/MS in environmental analysis, in natural and industrial products, for food analysis and in forensic sciences, in geological and geochemical research and, last but not least, in bioorganic and pharmaceutical studies. The examples are well chosen and the reader becomes a realistic impression of the merits as well as of the limitations of MS/MS, namely with respect to sensitivity, specificity and quantitation, e.g. of drugs and metabolites.

Finally, the seventh and last chapter summarizes and updates shortly and gives an outlook in the future with special emphasis on the influence of data systems for instrument control and automation as well as data handling and interpretations; indeed, the development of computers will be crucial for a more extensive acceptance and further distribution of MS/MS instruments, although it is conceivable that due to the cost of such an instrument the way to routine analysis is long.

Overall, it is a real pleasure to read this book and at no stage one gets the impression that the authors are advertising "their" method; instead they have placed it right where it belongs. I have found only one error. It is stated in the preface, the applications of MS/MS were so diverse and development so rapid that an update of this book could be written every other year. This is certainly not true, because new applications and even new instruments make the list longer, but don't change the principles, which are discussed here clear and convincing, considering the puzzling diversity of the matter.

In conclusion: The book is a must to every mass spectroscopist and analytical chemist considering an application of the MS/MS strategy. It is recommended as a textbook for graduate courses in mass spectrometry, since it is, aside from being a formidable text on MS/MS, a valuable source for short and clear information as well as for important primary literature. The price (154.00 DM, £51.00) appears to be acceptable, since it is not only well written, but also well made; one may ask, whether this and similar books could not be produced in a second, affordable version for students, though.

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NUCLEAR MAGNETIC RESONANCE (Vol. 2 in the Series "Modern Methods of Plant Analysis"), edited by H. F. Linskens, Nijmegen and J. F. Jackson, Adelaide, 196 pages (including 69 figures), hard cover, format 170 × 250 mm, ISBN 3-540-15910-X, Springer, Berlin-Heidelberg-New York-Tokyo (1986), DM 139.00.

The book consists of 8 chapters dealing with different aspects of plant analysis.

¹³C-NMR in Metabolic Studies (T. J. Simpson). This chapter is the largest one. Methods are discussed to assign ¹³C-NMR spectra, including some of the newer techniques like two-dimensional C,H-correlation. Subsequent sections are concerned with incorporation of singly labelled (¹³C) and doubly labelled (¹³C, ¹³C) precursors to investigate biosynthetic pathways by ¹³C-NMR. In addition methods of incorporating both ¹³C and ²H (or ¹⁵N; ¹⁸O), giving answer to the origin of hydrogen (nitrogen, oxygen) are also discussed. Several examples are presented referring to the biosynthesis of plant metabolites like colchicine, naphthoquinones, anthraquinones, vitamin B₁₂, flavones, triterpenes, cholesterol, etc.

Determination of the Energy Status of Plant Cells by ³¹P-Nuclear Magnetic Resonance Spectroscopy (J. K. M. Roberts). The concentration of phosphate-containing *in vivo* compounds (ATP, glucose-6-phosphate, inorganic phosphate, uridine diphospho-glucose) is determined by ³¹P-NMR. Experimental details regarding the *in vivo* NMR investigation of plant tissues under condition of perfusion (with a solution containing sugar and oxygen) as well as quantitative considerations are given.

The Use of NMR Spectroscopy to Follow Deuterium in Studies of Fungal Metabolism (C. Abell). This review describes experiments to trace the fate of hydrogen in oxidation processes, hydride shifts, substitution reactions, pathways of aromatization, etc. The investigations are mainly performed by ²H-NMR, in some cases by ¹³C-NMR exploiting upfield shifts caused by deuterium. The excellent NMR properties of tritium (no quadrupolar line broadening) have not been fully exploited so far because of the need to use high levels of radioactivity in precursors.

Proton NMR Studies on DNA Structure (P. Bendal). Theoretical background and examples are given. ¹H-NMR is the most powerful tool to determine details of DNA structure in solution. Comparison of NOE and X-ray results reveals that structure in solution and in fibres or crystals in most cases is the same. Interaction between DNA and other molecules, particularly intercalating drugs and proteins, may also be studied by ¹H-NMR.

NMR Methods for Determination of Intracellular pH (J. K. M. Roberts). A variety of nuclei in compounds belonging to the cytoplasm or vacuoles of plant tissues can be used to measure the pH. Most measurements were performed with pH-sensitive ³¹P-NMR signals for naturally occurring inorganic and sugar phosphate. Concerning the accuracy a lot of pitfalls exist. However, changes of pH (for instance under condition of hypoxia) can be monitored with considerable precision and accuracy. Heterogeneity in pH over the sample is also discussed.

Orientation of Chloroplasts in Leaves by ¹H-NMR Spectroscopy (D. C. McCain). The ¹H-NMR spectra of leaves display in some cases one signal, in other cases up

to three signals. The signals result from water molecules belonging to different compartments of the leaf. The chemical shift of the signals depends on the orientation of the leaf surface relative to the magnetic field thus giving insight into the orientation of the magnetically anisotropic compartments (e.g., chloroplasts). Experimental details (sample holders, sample preparation), a computer program to calculate the spectrum, and applications are given.

¹³C-NMR Determination of Rubber Content in Guayale Bushes (J. Visintainer, R. C. Hirst). Guayale Bushes are an alternative natural source of natural rubber. The content of the latter can be quickly determined by ¹³C-NMR. Portions of the bush are milled, dried, pressed into pellet and measured by liquid (not solid-state) NMR. The weight percentage of rubber is obtained by comparing the area of one distinct ¹³C-NMR signal of polyisopren with a calibration curve obtained from polyisopren standards. Detailed experimental conditions are given.

Nuclear Magnetic Resonance and Pollen Quality (C. Kerhoas, C. Dumas). The necessity to appreciate pollen quality arises in several contexts (e.g., fertilization, induction of hay fever). NMR provides information in term of water content and membrane state. The water content is determined by ¹H-NMR demonstrating two types of water: free water with high transversal relaxation time T_2 and bound water with low T_2 . The membrane state is investigated by ³¹P-NMR, which, however, cannot discriminate between membranes of different cellular compartments.

All chapters are carefully written and display a well of information. This book is a must for all those involved in plant analysis. It can also be highly recommended to everybody interested in new applications of nuclear magnetic resonance.

J. BUDDRUS