Interpretation Of Mass Spectra Of Organic Compounds

Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is the most versatile of the surface analysis techniques that have been developed during the last 30 years. This is the Second Edition of the first book ToF-SIMS: Surface analysis by Mass Spectrometry to be dedicated to the subject and the treatment is comprehensive

Understanding Mass Spectra: A Basic Approach, Second Editioncombines coverage of the principles underlying mass spectralanalysis with clear guidelines on how to apply them in a laboratorysetting. Completely revised from the first edition, an updated andunified approach to mass spectral interpretation emphasizes theapplication of basic principles from undergraduate organic,analytical, and physical chemistry courses. A detailed overview of theory and instrumentation, this usefulguide contains step-by-step descriptions of interpretativestrategies and convenient lists and tables detailing theinformation needed to solve unknowns. Other features includereal-world case studies and examples, skill-building problems withclearly explained answers, and easy-to-follow explanations of theimportant mathematical derivations.

The second edition of Gas Chromatography and Mass Spectrometry: A Practical Guide follows the highly successful first edition by F.G. Kitson, B.S. Larsen, and C.N. McEwen (1996), which was designed as an indispensible resource for GC/MS practitioners regardless of whether they are a novice or well experienced. The Fundamentals section has been extensively reworked from the original edition to give more depth of an understanding of the techniques and science involved with GC/MS. Even with this expansion, the original brevity and simple didactic style has been retained. Information on chromatographic peak deconvolution has been added along with a more in-depth understanding of the use of mass spectral databases in the identification of unknowns. Since the last edition, a number of advances in GC inlet systems and sample introduction techniques have occurred, and they are included in the new edition. Other updates include a discussion on fast GC and options for combining GC detectors with mass spectrometry. The section regarding GC Conditions, Derivatization, and Mass Spectral Interpretation of Specific Compound Types has the same number of compound types as the original edition, but the information in each section has been expanded to not only explain some of the spectra but to also explain why certain fragmentations take place. The number of Appendices has been increased from 12 to 17. The Appendix on Atomic Masses and Isotope Abundances has been expanded to provide tools to aid in determination of elemental composition from isotope peak intensity ratios. An appendix with examples on "Steps to follow in the determination of elemental compositions based on isotope peak intensities" has been added. Appendices on whether to

use GC/MS or LC/MS, third-party software for use in data analysis, list of information required in reporting GC/MS data, X+1 and X+2 peak relative intensities based on the number of atoms of carbon in an ion, and list of available EI mass spectral databases have been added. Others such as the ones on derivatization, isotope peak patterns for ions with Cl and/or Br, terms used in GC and in mass spectrometry, and tips on setting up, maintaining and troubleshooting a GC/MS system have all been expanded and updated. Covers the practical instruction necessary for successful operation of GC/MS equipment Reviews the latest advances in instrumentation, ionization methods, and quantitation Includes troubleshooting techniques and a variety of additional information useful for the GC/MS practitioner A true benchtop reference A guide to a basic understanding of the components of a Gas Chromatograph-Mass Spectrometer (GC-MS) Quick References to data interpretation Ready source for information on new analyses

With more than 20 years of experience in the teaching of mass tral interpretation to chemists in the health, environmental, and forensic fields, R. Martin Smith has done an excellent job (with the help of Prof. Ken Busch as technical editor) with this introductory book on mass spectrometry (MS) and spectral interpretation. Rather than attempt to cover the entire field, he focuses on electron ionization (EI), instruments that use this ionization technique, and the spectra that result. In writing a book on EIIMS, it is very difficult to not be, in some way, derivative of Fred McLaffeity's Interpretation of Mass Spectra, historically the most important book in this field to date. Smith covers the basics, creates new "basics," and offers a text that will be conlpetitive with the best. Understanding Mass Spectra contains chapters on "Isotopic Abundances," "Ionization, Fragmentation and Electron Accounting," "Neutral es and Ion Series," "Alpha-Cleavage," and "Important Mass tral Reairangements," the key topics of this field. However, h's work also offers unique and important chapters such as riting Mass Spectral Fragmentation Mechanisms" and "Structure Determination in Complex Molecules Using Mass trometry".

This is the first modern book to treat inorganic and organometallic mass spectrometry simultaneously. It is textbook and handbook in one; as a textbook it introduces the techniques and gives hints on how to apply the various techniques, as a handbook it lists all available ionization techniques for just about any given compound. The book also includes non-mathematical explanations of how modern MS instruments work Mass Spectrometry of Inorganic and Organometallic Compounds will inspire the synthetic inorganic and organometallic chemist with the confidence to apply some of the new techniques to their characterization problems.

This thoroughly updated second edition of the ACOL text on Mass Spectrometry gives a modern approach to those beginning to use or study mass spectrometry. Self assessment questions and solutions are included. Fundamentals and modern instrumental techniques are also covered in this book.

Introduction -- Elemental formulas -- Radical ions -- General appearance of the spectrum -- Series of even-electron ions -- Identification of neutral fragments -- Postulation of ion structures -- Mechanisms of unimolecular ion decomposition reactions -- Molecular structure postulations -- Solutions to unknowns -- Appendix : Standard interpretation procedure -- Elemental composition -- Molecular ion abundances versus compound type -- Series of common fragment ions -- Common neutral fragments -- Metastable ion nomograph -- Common odd-electron fragment ions.

During the last decade, mass spectrometry has become a powerful tool in understanding the various aspects of molecular processes occurring in biological systems. This paves the way to the understanding of complicated life processes that are among the greatest challenges in the contemporary bioscience. Sample preparation is a critical area in elemental speciation analysis and it is important that techniques used to extract elemental species are efficient yet correctly reflecting the chemical species present in native sample. However, with all respect to sample preparation, data analysis and critical evaluation of experimental observations based on the molecular-level explanation is becoming a major obstacle in transferring the experimental knowledge into valid conclusions. Many problems in the context of mass spectrometry can be solved using techniques of computer sciences, graph theory, and discrete mathematics. The aim of this dissertation is to recollect several essays that demonstrate the power and the need for developing skills in mass spectrometry data interpretation. These include the study of chemical behavior of selenium bio-volatiles using mass spectrometry, element-specific fingerprinting of mass spectra using isotope patterns, data analysis for accurate isotope ratio measurements and isotope pattern analysis as an extension of isotope dilution analysis.

This book presents an overview of computational and statistical design and analysis of mass spectrometry-based proteomics, metabolomics, and lipidomics data. This contributed volume provides an introduction to the special aspects of statistical design and analysis with mass spectrometry data for the new omic sciences. The text discusses common aspects of design and analysis between and across all (or most) forms of mass spectrometry, while also providing special examples of application with the most common forms of mass spectrometry. Also covered are applications of computational mass spectrometry not only in clinical study but also in the interpretation of omics data in plant biology studies. Omics research fields are expected to revolutionize biomolecular research by the ability to simultaneously profile many compounds within either patient blood, urine, tissue, or other biological samples. Mass spectrometry is one of the key analytical techniques used in these new omic sciences. Liquid chromatography mass spectrometry, time-of-flight data, and Fourier transform mass spectrometry are but a selection of the measurement platforms available to the modern analyst. Thus in practical proteomics or metabolomics, researchers will not only be confronted with new high dimensional data types—as opposed to the familiar data structures in more classical genomics—but also with great variation between distinct types of mass spectral measurements derived from different platforms, which may complicate analyses, comparison, and interpretation of results.

Interpretation of Mass Spectra, say the authors, "aims at correlating ion dissociation mechanisms on a much broader scale, with emphasis on basic attributes such as ionization energies, proton affinities, and bond dissociation energies". They stress that

the most important part of learning how to interpret unknown mass spectra is to practise doing it. "Prof. McLafferty's text has become a classic for classroom or self study concerned with interpreting mass spectra in order to discern molecular structures or identities of compounds." International Journal of Mass Spectrometry

With usage of mass spectrometry continually expanding, an increasing number of scientists, technicians, students, and physicians are coming into contact with this valuable technique. Mass spectrometry has many uses, both qualitative and quantitative, from analyzing simple gases to environmental contaminants, pharmaceuticals, and complex biopolymers. The extraordinary versatility can make mass spectrometers daunting to novices. Consequently, new users would benefit greatly from an understanding of the basic concepts as well as the processes that occur in these instruments. Mass Spectrometry for the Novice provides exactly that, with detailed, straightforward descriptions and clear illustrations of principles of operations and techniques. The book begins with an overview that includes essential definitions and then provides information on the components of and the strategies used in the most common instruments. The authors discuss the methodologies available, classes of compounds analyzed, and the types of data that can be generated. A group of representative applications from published articles is summarized, demonstrating the diversity of mass spectrometry. The authors also condense the essentials of the topic into one invaluable chapter that provides a set of concise take-home messages on all aspects of mass spectrometry. The final section provides a collection of resources including books, reviews, and useful websites. Using simple language, new color figures, clever cartoons, and assuming no prior knowledge, this book provides a readily understandable entrée to mass spectrometry. A CD-ROM with selected figures and cartoons is included.

This book offers a balanced mixture of practice-oriented information and theoretical background as well as numerous references, clear illustrations, and useful data tables. Problems and solutions are accessible via a special website. This new edition has been completely revised and extended; it now includes three new chapters on tandem mass spectrometry, interfaces for sampling at atmospheric pressure, and inorganic mass spectrometry.

Protein study experiments generate thousands of mass spectra, generating an overload of data that necessitates the development of sophisticated data analysis methods. Our work aims at developing the following methods that allow for extraction of biochemically relevant information from mass spectra.

Provides comprehensive coverage of the interpretation of LC–MS–MS mass spectra of 1300 drugs and pesticides Provides a general discussion on the fragmentation of even-electron ions (protonated and deprotonated molecules) in both positive-ion and negative-ion modes This is the reference book for the interpretation of MS–MS mass spectra of small organic molecules Covers related therapeutic classes of compounds such as drugs for cardiovascular diseases, psychotropic compounds, drugs of abuse and designer drugs, antimicrobials,

among many others Covers general fragmentation rule as well as specific fragmentation pathways for many chemical functional groups Gives an introduction to MS technology, mass spectral terminology, information contained in mass spectra, and to the identification strategies used for different types of unknowns

Completely revised and updated, this text provides an easy-to-read guide to the concept of mass spectrometry and demonstrates its potential and limitations. Written by internationally recognised experts and utilising "real life" examples of analyses and applications, the book presents real cases of qualitative and quantitative applications of mass spectrometry. Unlike other mass spectrometry texts, this comprehensive reference provides systematic descriptions of the various types of mass analysers and ionisation, along with corresponding strategies for interpretation of data. The book concludes with a comprehensive 3000 references. This multi-disciplined text covers the fundamentals as well as recent advance in this topic, providing need-to-know information for researchers in many disciplines including pharmaceutical, environmental and biomedical analysis who are utilizing mass spectrometry

With contributions from noted experts from Europe and North America, Mass Spectrometry Instrumentation, Interpretation, and Applications serves as a forum to introduce students to the whole world of mass spectrometry and to the many different perspectives that each scientific field brings to its use. The book emphasizes the use of this important analytical technique in many different fields, including applications for organic and inorganic chemistry, forensic science, biotechnology, and many other areas. After describing the history of mass spectrometry, the book moves on to discuss instrumentation, theory, and basic applications.

DART-MS is a relatively new, but very fast evolving technology. Due to its versatility, it addresses fields of crucial importance to people and community, e.g. food or agricultural, forensic, industrial, environmental, medicinal and clinical analysis.

The chapter includes an introduction to the main ionisation techniques in mass spectrometry and the way the resulting fragments can be analysed. First, the fundamental notions of mass spectrometry are explained, so that the reader can easily cover this chapter (graphs, main pick, molecular ion, illogical pick, nitrogen rule, et cetera). Isotopic percentage and nominal mass calculation are also explained along with fragmentation mechanism. A paragraph emphasises the ionisation energy issues, the basics of ionisation voltage, the developing potential and the energy balance. A frame time of the main theoretical milestones in both theory and experimental mass spectrometry is highlighted here. In the second part of the chapter, the molecular fragmentation for alkanes, iso-alkanes, cycloalkanes, halogen, alcohols, phenols, ethers, carbonyl compounds, carboxylic acids and functional derivatives, nitrogen compounds (amines, nitro compounds), sulphur compounds, heterocycles and biomolecules (amino acids, steroids, triglycerides) is explained. Fragmentation schemes are followed by the simplified spectra, which help the understanding of such complex phenomena. At the end of the chapter, acquisition of mass spectrum is discussed. The chapter presented here is an introduction to mass spectrometry, which, we think, helps the understanding of the mechanism of fragmentation corroborating

spectral data and molecular structures.
Clearly structured, easy to read and optimal to understand, this extensive compendium fills the gap between textbooks devoted to either spectra interpretation or basic physical principles. The original Chinese editions have already sold over 18,500 copies, and the material is taken from the latest literature from around the world, plus technical information provided by the manufacturers of spectroscopic instruments. Alongside basic methods, Professor Ning presents up-to-date developments in NMR, MS, IR and Raman spectroscopy, such as pulsed-field gradient technique, LC-NMR, and DOSY. He stresses the application of spectroscopic methods, interpreting them in great detail and depth since most of the selected spectra may be applied to practical work, as well as summarizing the rules for their interpretation. He also incorporates his original ideas, including a comparison of the common points in different spectroscopic techniques. This monograph features a unique structure, a typical example being the discussion of 2D NMR starting from pulse sequence units, which construct various pulse sequences for related 2D NMR. A complete chapter deals with the determination of configurations and conformations of organic compounds and even biological molecules from the viewpoint of spectroscopic methodologies, while one whole section is dedicated to the interpretation of mass spectra produced by soft ionization techniques. The principles of mass analyzers, especially the ion trap, are discussed in great depth, together with a concise summary of the MS fragmentation and rearrangement of common compounds, allowing readers to easily predict related mass spectrometric reactions. All the three kinds of library retrieval of mass spectra are presented in detail, together with recent developments in molecular vibration spectroscopy. The whole is rounded off with several appendices, including a subject index for rapid reference. With a foreword by the Nobel prizewinner, Richard R. Ernst.
This book is a logical, step-by-step guide to identification of organic compounds by mass spectrometry. The book is organized into chapters covering the major types of organic compounds, including alcohols, acids and esters, aldehydes and ketones, ethers, hydrocarbons, halogenated compounds, amines and amides, and sulfur-containing compounds. In each chapter, the mechanisms of the major fragmentation pathways are discussed, with reference to several simple sample compounds. By teaching the user to recognize typical fragmentations, the book removes the need to search databases, often limited, of electronic spectra. Key features of the book include: * 200 representative spectra of common organic compounds * Functional group approach to mass spectra interpretation * Appendix of 'unknown' spectra with step-by-step guide to identification This book is a must for anyone who needs to identify organic molecules by mass spectrometry but does not need to know the detailed workings of a mass spectrometer.
Analysis of Neuropeptides by Liquid Chromatography and Mass Spectrometry
Trace Analysis by Mass Spectrometry deals with trace analysis of solids and liquids by mass spectrometric techniques. Topics include the physics and techniques of electrical discharge ion sources, transmission of ions through double focusing mass spectrometers, and detection and measurement of ions by ion-sensitive plates. The ion sources used are principally electrical discharge type sources. This book is comprised of 14 chapters. The first several chapters focus on the basic physics of electrical discharge ion sources, double focusing mass spectrometry, and the measurement of

arrays of mass resolved ion beams by electrical detection methods and with ion sensitive emulsions. The discussion then shifts to the problem of obtaining the chemical composition of the recorded mass resolved ion sample and relating this composition to that of the original sample. The chapters that follow describe specific techniques for analyzing special samples such as insulators, powders, microsamples, biological materials, reactive and low melting point substances, radioactive materials, and gases in solids. The remaining chapters include the use of laser ion sources in the analysis of solids and the analysis of surfaces particularly with sputter ion sources. This book will be of interest to students and practitioners of physics and chemistry.

Interpretation of Mass Spectra of Organic Compounds outlines the basic instrumentation, sample handling techniques, and procedures used in the interpretation of mass spectra of organic compounds. The fundamental concepts of ionization, fragmentation, and rearrangement of ions as found in mass spectra are covered in some detail, along with the rectangular array and interpretation maps. Computerization of mass spectral data is also discussed. This book consists of nine chapters and begins with a historical overview of mass spectrometry and a discussion on some important developments in the field, along with a summary of interpretation objectives and methods. The following chapters focus on instruments, ion sources, and detectors; recording of the mass spectrum and the instrumental and sample variables affecting the mass spectrum; sample introduction systems; and fragmentation reactions. Correlations as applied to interpretations are also considered, with emphasis on applications of the branching rule as well as beta-bond and alpha-bond cleavages. Example interpretations, calculations, data-processing procedures, and computer programs are included. This monograph is intended for organic chemists, biochemists, mass spectroscopists, technicians, managers, and others concerned with the whys and wherefores of mass spectrometry.

Instructional units designed to serve the continuing education needs of chemists and chemical engineers. Includes an introduction and brief overview of principles of basic mass spectrometry, introduciton to electron-impact spectra and interpretation, alternative ionization methods, additional mass spectrometric techniques (instrumental and chemical), interpretation of selected spectra. Guide includes illustrations,problems, bibliography, and glossary.