

1. Record Nr.	UNINA9910823092403321
Autore	de Hoffmann Edmond
Titolo	Mass Spectrometry : Principles and Applications
Pubbl/distr/stampa	New York : , : John Wiley & Sons, Incorporated, , 2007 ©2013
ISBN	9780470512135 9780470033104
Edizione	[3rd ed.]
Descrizione fisica	1 online resource (503 pages)
Altri autori (Persone)	StroobantVincent De HoffmannEdmond
Disciplina	543/.0873
Soggetti	Mass spectrometry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Intro -- Mass Spectrometry -- Contents -- Preface -- Introduction -- Principles -- Diagram of a Mass Spectrometer -- History -- Ion Free Path -- 1 Ion Sources -- 1.1 Electron Ionization -- 1.2 Chemical Ionization -- 1.2.1 Proton Transfer -- 1.2.2 Adduct Formation -- 1.2.3 Charge-Transfer Chemical Ionization -- 1.2.4 Reagent Gas -- 1.2.5 Negative Ion Formation -- 1.2.6 Desorption Chemical Ionization -- 1.3 Field Ionization -- 1.4 Fast Atom Bombardment and Liquid Secondary Ion Mass Spectrometry -- 1.5 Field Desorption -- 1.6 Plasma Desorption -- 1.7 Laser Desorption -- 1.8 Matrix-Assisted Laser Desorption Ionization -- 1.8.1 Principle of MALDI -- 1.8.2 Practical Considerations -- 1.8.3 Fragmentations -- 1.8.4 Atmospheric Pressure Matrix-Assisted Laser Desorption Ionization -- 1.9 Thermospray -- 1.10 Atmospheric Pressure Ionization -- 1.11 Electrospray -- 1.11.1 Multiply Charged Ions -- 1.11.2 Electrochemistry and Electric Field as Origins of Multiply Charged Ions -- 1.11.3 Sensitivity to Concentration -- 1.11.4 Limitation of Ion Current from the Source by the Electrochemical Process -- 1.11.5 Practical Considerations -- 1.12 Atmospheric Pressure Chemical Ionization -- 1.13 Atmospheric Pressure Photoionization -- 1.14 Atmospheric Pressure Secondary Ion Mass Spectrometry -- 1.14.1 Desorption Electrospray Ionization -- 1.14.2 Direct Analysis in Real Time -- 1.15 Inorganic Ionization

Sources -- 1.15.1 Thermal Ionization Source -- 1.15.2 Spark Source -- 1.15.3 Glow Discharge Source -- 1.15.4 Inductively Coupled Plasma Source -- 1.15.5 Practical Considerations -- 1.16 Gas-Phase Ion-Molecule Reactions -- 1.17 Formation and Fragmentation of Ions: Basic Rules -- 1.17.1 Electron Ionization and Photoionization Under Vacuum -- 1.17.2 Ionization at Low Pressure or at Atmospheric Pressure -- 1.17.3 Proton Transfer -- 1.17.4 Adduct Formation. 1.17.5 Formation of Aggregates or Clusters -- 1.17.6 Reactions at the Interface between Source and Analyser -- 2 Mass Analysers -- 2.1 Quadrupole Analysers -- 2.1.1 Description -- 2.1.2 Equations of Motion -- 2.1.3 Ion Guide and Collision Cell -- 2.1.4 Spectrometers with Several Quadrupoles in Tandem -- 2.2 Ion Trap Analysers -- 2.2.1 The 3D Ion Trap -- 2.2.2 The 2D Ion Trap -- 2.3 The Electrostatic Trap or 'Orbitrap' -- 2.4 Time-of-Flight Analysers -- 2.4.1 Linear Time-of-Flight Mass Spectrometer -- 2.4.2 Delayed Pulsed Extraction -- 2.4.3 Reflectrons -- 2.4.4 Tandem Mass Spectrometry with Time-of-Flight Analyser -- 2.4.5 Orthogonal Acceleration Time-of-Flight Instruments -- 2.5 Magnetic and Electromagnetic Analysers -- 2.5.1 Action of the Magnetic Field -- 2.5.2 Electrostatic Field -- 2.5.3 Dispersion and Resolution -- 2.5.4 Practical Considerations -- 2.5.5 Tandem Mass Spectrometry in Electromagnetic Analysers -- 2.6 Ion Cyclotron Resonance and Fourier Transform Mass Spectrometry -- 2.6.1 General Principle -- 2.6.2 Ion Cyclotron Resonance -- 2.6.3 Fourier Transform Mass Spectrometry -- 2.6.4 MSⁿ in ICR/FTMS Instruments -- 2.7 Hybrid Instruments -- 2.7.1 Electromagnetic Analysers Coupled to Quadrupoles or Ion Trap -- 2.7.2 Ion Trap Analyser Combined with Time-of-Flight or Ion Cyclotron Resonance -- 2.7.3 Hybrids Including Time-of-Flight with Orthogonal Acceleration -- 3 Detectors and Computers -- 3.1 Detectors -- 3.1.1 Photographic Plate -- 3.1.2 Faraday Cup -- 3.1.3 Electron Multipliers -- 3.1.4 Electro-Optical Ion Detectors -- 3.2 Computers -- 3.2.1 Functions -- 3.2.2 Instrumentation -- 3.2.3 Data Acquisition -- 3.2.4 Data Conversion -- 3.2.5 Data Reduction -- 3.2.6 Library Search -- 4 Tandem Mass Spectrometry -- 4.1 Tandem Mass Spectrometry in Space or in Time -- 4.2 Tandem Mass Spectrometry Scan Modes. 4.3 Collision-Activated Decomposition or Collision-Induced Dissociation -- 4.3.1 Collision Energy Conversion to Internal Energy -- 4.3.2 High-Energy Collision (keV) -- 4.3.3 Low-Energy Collision (between 1 and 100 eV) -- 4.4 Other Methods of Ion Activation -- 4.5 Reactions Studied in MS/MS -- 4.6 Tandem Mass Spectrometry Applications -- 4.6.1 Structure Elucidation -- 4.6.2 Selective Detection of Target Compound Class -- 4.6.3 Ion-Molecule Reaction -- 4.6.4 The Kinetic Method -- 5 Mass Spectrometry/Chromatography Coupling -- 5.1 Elution Chromatography Coupling Techniques -- 5.1.1 Gas Chromatography/mass Spectrometry -- 5.1.2 Liquid Chromatography/mass Spectrometry -- 5.1.3 Capillary Electrophoresis/mass Spectrometry -- 5.2 Chromatography Data Acquisition Modes -- 5.3 Data Recording and Treatment -- 5.3.1 Data Recording -- 5.3.2 Instrument Control and Treatment of Results -- 6 Analytical Information -- 6.1 Mass Spectrometry Spectral Collections -- 6.2 High Resolution -- 6.2.1 Information at Different Resolving Powers -- 6.2.2 Determination of the Elemental Composition -- 6.3 Isotopic Abundances -- 6.4 Low-Mass Fragments and Lost Neutrals -- 6.5 Number of Rings or Unsaturation -- 6.6 Mass and Electron Parities, Closed-Shell Ions and Open-Shell Ions -- 6.6.1 Electron Parity -- 6.6.2 Mass Parity -- 6.6.3 Relationship between Mass and Electron Parity -- 6.7 Quantitative Data -- 6.7.1 Specificity -- 6.7.2 Sensitivity and Detection Limit -- 6.7.3 External Standard Method -- 6.7.4 Sources of

Error -- 6.7.5 Internal Standard Method -- 6.7.6 Isotopic Dilution Method -- 7 Fragmentation Reactions -- 7.1 Electron Ionization and Fragmentation Rates -- 7.2 Quasi-Equilibrium and RRKM Theory -- 7.3 Ionization and Appearance Energies -- 7.4 Fragmentation Reactions of Positive Ions -- 7.4.1 Fragmentation of Odd-Electron Cations or Radical Cations. 7.4.2 Fragmentation of Cations with an Even Number of Electrons (EE) -- 7.4.3 Fragmentations Obeying the Parity Rule -- 7.4.4 Fragmentations not Obeying the Parity Rule -- 7.5 Fragmentation Reactions of Negative Ions -- 7.5.1 Fragmentation Mechanisms of Even Electron Anions (EE -) -- 7.5.2 Fragmentation Mechanisms of Radical Anions -- 7.6 Charge Remote Fragmentation -- 7.7 Spectrum Interpretation -- 7.7.1 Typical Ions -- 7.7.2 Presence of the Molecular Ion -- 7.7.3 Typical Neutrals -- 7.7.4 A Few Examples of the Interpretation of Mass Spectra -- 8 Analysis of Biomolecules -- 8.1 Biomolecules and Mass Spectrometry -- 8.2 Proteins and Peptides -- 8.2.1 ESI and MALDI -- 8.2.2 Structure and Sequence Determination Using Fragmentation -- 8.2.3 Applications -- 8.3 Oligonucleotides -- 8.3.1 Mass Spectra of Oligonucleotides -- 8.3.2 Applications of Mass Spectrometry to Oligonucleotides -- 8.3.3 Fragmentation of Oligonucleotides -- 8.3.4 Characterization of Modified Oligonucleotides -- 8.4 Oligosaccharides -- 8.4.1 Mass Spectra of Oligosaccharides -- 8.4.2 Fragmentation of Oligosaccharides -- 8.4.3 Degradation of Oligosaccharides Coupled with Mass Spectrometry -- 8.5 Lipids -- 8.5.1 Fatty Acids -- 8.5.2 Acylglycerols -- 8.5.3 Bile Acids -- 8.6 Metabolomics -- 8.6.1 Mass Spectrometry in Metabolomics -- 8.6.2 Applications -- 9 Exercises -- Questions -- Answers -- Appendices -- 1 Nomenclature -- 1.1 Units -- 1.2 Definitions -- 1.3 Analysers -- 1.4 Detection -- 1.5 Ionization -- 1.6 Ion Types -- 1.7 Ion-Molecule Reaction -- 1.8 Fragmentation -- 2 Acronyms and Abbreviations -- 3 Fundamental Physical Constants -- 4A Table of Isotopes in Ascending Mass Order -- 4B Table of Isotopes in Alphabetical Order -- 5 Isotopic Abundances (in %) for Various Elemental Compositions CHON -- 6 Gas-Phase Ion Thermochemical Data of Molecules. 7 Gas-Phase Ion Thermochemical Data of Radicals -- 8 Literature on Mass Spectrometry -- 9 Mass Spectrometry on Internet -- Index.

Sommario/riassunto

The latest edition of a highly successful textbook, *Mass Spectrometry, Third Edition* provides students with a complete overview of the principles, theories and key applications of modern mass spectrometry. All instrumental aspects of mass spectrometry are clearly and concisely described: sources, analysers and detectors. Tandem mass spectrometry is introduced early on and then developed in more detail in a later chapter. Emphasis is placed throughout the text on optimal utilisation conditions. Various fragmentation patterns are described together with analytical information that derives from the mass spectra. This new edition has been thoroughly revised and updated and has been redesigned to give the book a more contemporary look. As with previous editions it contains numerous examples, references and a series of exercises of increasing difficulty to encourage student understanding. Updates include: Increased coverage of MALDI and ESI, more detailed description of time of flight spectrometers, new material on isotope ratio mass spectrometry, and an expanded range of applications. *Mass Spectrometry, Third Edition* is an invaluable resource for all undergraduate and postgraduate students using this technique in departments of chemistry, biochemistry, medicine, pharmacology, agriculture, material science and food science. It is also of interest for researchers looking for an overview of the latest

techniques and developments.
