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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	UNDERSTANDING MASS SPECTRA Second Edition; CONTENTS; Preface to the Second Edition; Acknowledgments; Abbreviations and Notations Used in This Book; 1 Instrumentation; 1.1. Introduction; 1.1.1. Overview; 1.1.2. Sample Introduction; 1.2. Ionization Source; 1.2.1. Electron Ionization Source; 1.2.2. Chemical Ionization; 1.2.3. Other Ionization Methods; 1.2.3.1. Electrospray Ionization; 1.2.3.2. Desorption Ionization; 1.3. m/z Analysis; 1.3.1. Time-of-Flight (TOF); 1.3.2. Magnetic Sector; 1.3.3. Transmission Quadrupole; 1.3.3.1. Selected Ion Monitoring (SIM); 1.3.4. Quadrupole Ion Trap (QIT) 1.3.5. Other Types of Mass Analysis1.3.5.1. Mass Spectrometry/Mass Spectrometry(MS/MS); 1.3.5.2. Accurate m/z Analysis; 1.3.6. Spectral Skewing; 1.4. Ion Detection; 1.4.1. Electron Multiplier; 1.4.2. Photomultiplier Detector; 1.5. Data System; 1.5.1. Instrument Tuning and Calibration; 1.5.2. The Mass Spectrum; 1.5.2.1. Production of the Mass Spectrum; 1.5.2.2. Terminology: Ions vs. Peaks; 1.5.3. Library

Searches; 1.5.4. Using the Data System to Analyze GC/MS Data; 1.6. Criteria for Good-Quality Spectra; Additional Problems; Mass Spectrometric Resources on the Internet

References and Suggested Reading

2 Elemental Composition from Peak Intensities; 2.1. Natural Isotopic Abundances; 2.1.1. Atomic and Molecular Mass; 2.1.2. Calculated Exact Masses and Mass Defects; 2.2. Determining Elemental Composition from Isotope Peak Intensities; 2.2.1. One or More Atoms of a Single Element; 2.2.1.1. Chlorine and Bromine; 2.2.1.2. Ion Designation and Nomenclature; 2.2.1.3. Probability Considerations with Multiple Numbers of Atoms; 2.2.1.4. Isotope Peak Intensity Ratios for Carbon-Containing Ions-The X + 1 Peak; 2.2.1.5. A, A + 1, and A + 2 Elements

2.2.1.6 Isotope Peak Intensity Ratios for Carbon-Containing Ions-The X + 2 Peak

2.2.1.7. Overlapping Peak Clusters-Contributions from  $(^{13}\text{C})$  Only; 2.2.1.8. Silicon; 2.2.2. Complex Isotope Clusters; 2.2.2.1. Sulfur Dioxide; 2.2.2.2. Diazepam; 2.3. Obtaining Elemental Compositions from Isotope Peak Intensities; Examples; Additional Problems; References;

3 Ionization, Fragmentation, and Electron Accounting; 3.1. A Brief Review of Orbitals and Bonding; 3.2. Even- and Odd-Electron Species; 3.3. Site of Initial Ionization; 3.4. Types of Fragmentation; 3.5. The Nitrogen Rule

3.6. Energy Considerations in Fragmentation Processes

3.6.1. Fragmentation Rates; 3.6.2. Metastable Ions; 3.6.3. Energy Diagrams; 3.6.4. Stevenson's Rule; Additional Examples; Problems; References;

4 Neutral Losses and Ion Series; 4.1. Neutral Losses; 4.1.1. Losses from the Molecular Ion; 4.1.2. Loss of Small Molecules from Aromatic Ions; 4.2. Low-Mass Ion Series; 4.2.1. n-Alkane Spectra; 4.2.2. Effect of Chain Branching on the Spectra of Aliphatic Hydrocarbons; 4.2.3. Ion Series for Nonaromatic Compounds; 4.2.4. Aromatic Ion Series; 4.2.5. Use of Ion Series: Mass Chromatograms

Additional Problems

## Sommario/riassunto

Understanding Mass Spectra: A Basic Approach, Second Edition combines coverage of the principles underlying mass spectral analysis with clear guidelines on how to apply them in a laboratory setting. Completely revised from the first edition, an updated and unified approach to mass spectral interpretation emphasizes the application of basic principles from undergraduate organic, analytical, and physical chemistry courses. A detailed overview of theory and instrumentation, this useful guide contains step-by-step descriptions of interpretative strategies and convenient lists and tables detail