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Radiation; 1.4 Electromagnetic Spectrum; 1.5 Interaction of Radiation with Matter; 1.6 Magnetic Spectroscopies; 1.7 Pulse Techniques in NMR Spectroscopy; 1.8 Line Widths; 1.9 Selection Rules; 1.10 Summary of Spectroscopic Techniques; References; Chapter 2: Computational Spectroscopy Tools for Molecular Structure Analysis; 2.1 Introduction; 2.2 Potential Energy Surface and Molecular Structure 2.3 Computational Aspects for Spectroscopic Techniques 2.4 Application and Case Studies; Acknowledgments; References; Chapter 3: Absolute Configuration and Conformational Analysis of Chiral Compounds via Experimental and Theoretical Prediction of Chiroptical Properties: ORD, ECD, and VCD; 3.1 Introduction; 3.2 Chirality; 3.3 What is a Chiroptical Method?; 3.4 Quantum Mechanical (Ab Initio) Methods for Predicting Chiroptical Properties; 3.5 Electronic Circular Dichroism (ECD); 3.6 Vibrational Circular Dichroism (VCD); 3.7 Optical Rotatory Dispersion (ORD) 3.8 When More than One Method is Needed 3.9 Concluding Remarks; References; Chapter 4: Mass Spectrometry Strategies in the Assignment of Molecular Structure: Breaking Chemical Bonds before Bringing the Pieces of the Puzzle Together; 4.1 Introduction; 4.2 Instrumentation and Technology; 4.3 Breaking Chemical Bonds - Fragmentation Reactions; 4.4 Confirmation of Identity; 4.5 Putting the Puzzle Together - Structure Elucidation of Unknowns; 4.6 Conclusions and Perspectives; Abbreviations; References; Chapter 5: Basic Principles of IR/Raman: Applications in Small Molecules Structural Elucidation 5.1 Introduction 5.2 Characteristic Vibrational Modes: Diatomics and Chemical Bonds; 5.3 Fundamental Vibrational Modes and Molecular Structure; 5.4 Selection Rules and Finding the Number of Normal Modes in Each Symmetry Species; 5.5 The Vibrational Assignment of Raman and Infrared Spectra; 5.6 Conclusions; References; Chapter 6: Solid-State NMR Applications in the Structural Elucidation of Small Molecules; 6.1 Introduction; 6.2 Line-Narrowing and Sensitivity Enhancement Methods in ssNMR Spectroscopy; 6.3 Probing Dynamics in Solids; 6.4 Application of ssNMR Spectroscopy to Small Molecules 6.5 NMR of Molecules on Surfaces (DNP) 6.6 NMR Crystallography; Acronyms; References; Chapter 7: Simplified NMR Procedures for the Assignment of the Absolute Configuration; 7.1 Introduction; 7.2 Single Derivatization Methods for Mono- and Polyfunctional Compounds; 7.3 Resin-Bound Chiral Derivatizing Agents (Mix and Shake Method); 7.4 Non-resin in Tube Assignment (BPG and BINOL Borates); 7.5 Tandem HPLC-NMR: Simultaneous Enantioresolution and Configurational Assignment; 7.6 Assignment Based on the Chemical Shifts from the Auxiliaries; 7.7 Scope and Conclusions; References Chapter 8: Structural Elucidation of Small Organic Molecules Assisted by NMR in Aligned Media

Sommario/riassunto

Intended for advanced readers, this is a review of all relevant techniques for structure analysis in one handy volume. As such, it provides the latest knowledge on spectroscopic and related techniques for chemical structure analysis, such as NMR, optical spectroscopy, mass spectrometry and X-ray crystallography, including the scope and limitation of each method. As a result, readers not only become acquainted with the techniques, but also the advantages of the synergy between them. This enables them to choose the correct analytical method for each problem, saving both time and resources. Speci
