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Nota di contenuto	VIBRATIONAL OPTICAL ACTIVITY: Principles and Applications; Contents; Preface; 1 Overview of Vibrational Optical Activity; 1.1 Introduction to Vibrational Optical Activity; 1.1.1 Field of Vibrational Optical Activity; 1.1.2 Definition of Vibrational Circular Dichroism; 1.1.3 Definition of Vibrational Raman Optical Activity; 1.1.4 Unique Attributes of Vibrational Optical Activity; 1.1.4.1 VOA is the Richest Structural Probe of Molecular Chirality; 1.1.4.2 VOA is the Most Structurally Sensitive Form of Vibrational Spectroscopy 1.1.4.3 VOA Can be Used to Determine Unambiguously the Absolute Configuration of a Chiral Molecule1.1.4.4 VOA Spectra Can be Used to Determine the Solution-State Conformer Populations; 1.1.4.5 VOA Can be Used to Determine the ee of Multiple Chiral Species of Changing Absolute and Relative Concentration; 1.2 Origin and Discovery of Vibrational Optical Activity; 1.2.1 Early Attempts to Measure VOA; 1.2.2 Theoretical Predictions of VCD; 1.2.3 Theoretical Predictions of ROA; 1.2.4 Discovery and Confirmation of ROA; 1.2.5 Discovery and Confirmation of VCD; 1.3 VCD Instrumentation Development 1.3.1 First VCD Measurements - Dispersive, Hydrogen-Stretching Region1.3.2 Near-IR VCD Measurements; 1.3.3 Mid-IR VCD

Measurements; 1.3.4 Fourier Transform VCD Instrumentation; 1.3.5 Commercially Available VCD Instrumentation; 1.4 ROA Instrumentation Development; 1.4.1 First ROA Measurements - Single Channel ICP-ROA; 1.4.2 Multi-Channel ROA Measurements; 1.4.3 Backscattering ROA Measurements; 1.4.4 SCP-ROA Measurements; 1.4.5 DCP-ROA Measurements; 1.4.6 Commercially Available ROA Instruments; 1.5 Development of VCD Theory and Calculations; 1.5.1 Models of VCD Spectra
1.5.1.1 Coupled Oscillator Model1.5.1.2 Fixed Partial Charge Model; 1.5.1.3 Localized Molecular Orbital Model; 1.5.1.4 Charge Flow Model; 1.5.1.5 Ring Current Model; 1.5.2 Vibronic Coupling Theory of VCD; 1.5.3 Magnetic Field Perturbation Formulation of VCD; 1.5.4 Nuclear Velocity Perturbation Formulation of VCD; 1.5.5 Ab Initio Calculations of VCD Spectra; 1.5.6 Commercially Available Software for VCD Calculations; 1.6 Development of ROA Theory and Calculations; 1.6.1 Original Theory of ROA; 1.6.2 Models of ROA Spectra; 1.6.3 General Unrestricted Theory of Circular Polarization ROA
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1.8.1 Frequency Ranges and Structural Sensitivities

Sommario/riassunto

This unique book stands as the only comprehensive introduction to vibrational optical activity (VOA) and is the first single book that serves as a complete reference for this relatively new, but increasingly important area of molecular spectroscopy. Key features:A single-source reference on this topic that introduces, describes the background and foundation of this area of spectroscopy.Serves as a guide on how to use it to carry out applications with relevant problem solving.Depth and breadth of the subject is presented in a logical, complete and progressive fashion. A