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Titolo	Computational spectroscopy [[electronic resource]] : methods, experiments and applications / / edited by Jorg Grunenberg
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ISBN	3-527-64362-1 1-282-84956-5 9786612849565 3-527-63327-8 3-527-63328-6
Edizione	[4th ed.]
Descrizione fisica	1 online resource (434 p.)
Altri autori (Persone)	GrunenbergJorg
Disciplina	543.5
Soggetti	Molecular spectroscopy - Data processing Spectrum analysis - Data processing
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Computational Spectroscopy: Methods, Experiments and Applications; Contents; Preface; List of Contributors; 1 Concepts in Computational Spectrometry: the Quantum and Chemistry; 1.1 Introduction; 1.2 Quantum Laws, or the Laws of Discreteness; 1.3 Quantum Theories of a Harmonic Oscillator; 1.3.1 Matrix Mechanics; 1.3.2 Wave Mechanics; 1.3.3 Dirac.s Operators for Creation and Destruction; 1.3.4 Discussion of Quantum Theories in Relation to an Harmonic Oscillator; 1.4 Diatomic Molecule as Anharmonic Oscillator; 1.5 Quantum Mechanics and Molecular Structure; 1.6 Conclusions; References 2 Computational NMR Spectroscopy2.1 Introduction; 2.2 NMR Properties; 2.3 Chemical Shifts; 2.4 NICS and Aromaticity; 2.5 Spin-Spin Coupling Constants; 2.6 Solvent Effects; 2.7 Conclusions; 2.8 The Problem of the Error in Theoretical Calculations of Chemical Shifts and Coupling Constants; References; 3 Calculation of Magnetic Tensors and EPR Spectra for Free Radicals in Different Environments; 3.1 Introduction; 3.2 The General Model; 3.3 Spin Hamiltonian, g-Tensor, Hyperfine Coupling Constants, and Zero-Field Splitting; 3.3.1 The Spin

Hamiltonian; 3.3.2 Electronic Structure Theory
3.3.3 Additional Terms in the Hamiltonian3.3.4 Linear Response Theory; 3.3.5 Linear Response Equations for Spin Hamiltonian Parameters; 3.3.6 Computational Aspects: Functionals and Basis Sets; 3.4 Stereoelectronic, Environmental, and Dynamical Effects; 3.4.1 Structures and Magnetic Parameters; 3.4.2 Environmental Effects; 3.4.3 Short-Time Dynamical Effects; 3.5 Line Shapes; 3.6 Concluding Remarks; References; 4 Generalization of the Badger Rule Based on the Use of Adiabatic Vibrational Modes; 4.1 Introduction; 4.2 Applicability of Badger-Type Relationships in the Case of Diatomic Molecules
4.3 Dissection of a Polyatomic Molecule into a Collection of Quasi-Diatomic Molecules: Local Vibrational Modes4.3.1 Localized Vibrational Modes; 4.3.2 The Adiabatic Internal Coordinate Modes; 4.3.3 Properties of Adiabatic Internal Coordinate Modes; 4.3.4 Characterization of Normal Modes in Terms of AICoMs; 4.3.5 Advantages of AICoMs; 4.4 Local Mode Properties Obtained from Experiment; 4.4.1 Isolated Stretching Modes; 4.4.2 Local Mode Frequencies from Overtone Spectroscopy; 4.4.3 Local Mode Information via an Averaging of Frequencies: Intrinsic Frequencies; 4.4.4 Compliance Force Constants
4.5 Badger-type Relationships for Polyatomic Molecules4.6 Conclusions; References; 5 The Simulation of UV-Vis Spectroscopy with Computational Methods; 5.1 Introduction; 5.2 Quantum Mechanical Methods; 5.3 Modeling Solvent Effects; 5.4 Toward the Simulation of UV-Vis Spectra; 5.5 Some Numerical Examples; 5.6 Conclusions and Perspectives; References; 6 Nonadiabatic Calculation of Dipole Moments; 6.1 Introduction; 6.2 The Molecular Hamiltonian; 6.3 Symmetry; 6.4 The Hellmann-Feynman Theorem; 6.5 The Born-Oppenheimer Approximation; 6.6 Interaction between a Molecule and an External Field
6.7 Experimental Measurements of Dipole Moments

Sommario/riassunto

Unique in its comprehensive coverage of not only theoretical methods but also applications in computational spectroscopy, this ready reference and handbook compiles the developments made over the last few years, from single molecule studies to the simulation of clusters and the solid state, from organic molecules to complex inorganic systems and from basic research to commercial applications in the area of environment relevance. In so doing, it covers a multitude of apparatus-driven technologies, starting with the common and traditional spectroscopic methods, more recent developments (THz)

2. Record Nr. UNINA9910817401603321

Titolo	Operative techniques in breast, endocrine, and oncologic surgery / / Michael S. Sabel, MD, editor, Chief, Division of Surgical Oncology, Associate Professor of Surgery, University of Michigan Health System, Ann Arbor, Michigan, Michael W. Mulholland, MD, PhD, editor-in-chief, Professor of Surgery and Chair, Department of Surgery, University of Michigan Medical School, Ann Arbor, Michigan ; illustrations by BodyScientific International, LLC
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ISBN	1-9751-7650-2 1-4963-1908-7
Descrizione fisica	1 online resource (xvi, 447 pages) : illustrations (chiefly color)
Collana	Operative techniques in surgery
Classificazione	MED085110
Disciplina	616.99449059
Soggetti	Breast - Surgery Endocrine glands - Surgery Melanoma - Surgery Atlas
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes index.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	section I. Breast surgery -- section II. Breast reconstruction -- section III. Melanoma -- section IV. Endocrine.
Sommario/riassunto	"With an emphasis on the "hows and whys" of contemporary surgery, Operative Techniques in Breast, Endocrine, and Oncologic Surgery, Second Edition, features concise, bulleted text, full-color illustrations, and intraoperative photographs to clarify exactly what to look for and how to proceed. Drawn from the larger Operative Techniques in Surgery, Second Edition, this concise, stand-alone surgical atlas, overseen by editor-in-chief Mary T. Hawn and meticulously edited by Dr. Michael S. Sabel, focuses on the steps of each technique, rapidly directing you to the information you need to choose the right approach for each patient, perform it successfully, and achieve the best possible results. Provides comprehensive, step-by-step guidance on breast

surgery and reconstruction; cutaneous oncology; and endocrine surgery Covers open as well as laparoscopic, endoscopic, robotic, and video-assisted procedures in breast, endocrine, and oncologic surgery Features new videos, personally selected by contributing authors and editors, that accompany numerous chapters throughout the book Contains extensive updates throughout, including new coverage of the American Board of Surgery's SCORE Curricula for General Surgery and for Complex General Surgical Oncology Follows the same format for each procedure: differential diagnosis, patient history and physical findings, imaging and other diagnostic studies, surgical management, techniques, pearls and pitfalls, postoperative care, outcomes, and complications Enrich Your eBook Reading Experience Read directly on your preferred device(s), such as computer, tablet, or smartphone. Easily convert to audiobook, powering your content with natural language text-to-speech. "--