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Computational Molecular Spectroscopy Per Jensen, Philip R. Bunker, 2000-11-02 This book describes the use of modern computational methods in predicting high resolution molecular spectra, which allows the experimental spectroscopist to interpret and assign real spectra. * Offers a comprehensive treatment of modern computation techniques. * Provides a collection of material from different areas of theoretical chemistry and physics. * Bridges the gap between traditional quantum chemistry and experimental molecular spectroscopy.

Molecular Quantum Mechanics Peter W. Atkins, Ronald S. Friedman, 2011 This text unravels those fundamental physical principles which explain how all matter behaves. It takes us from the foundations of quantum mechanics, through quantum models of atomic, molecular, and electronic structure, and on to discussions of spectroscopy, and the electronic and magnetic properties of molecules.

Spectroscopy and Optical Diagnostics for Gases Ronald K. Hanson, R. Mitchell Spearrin, Christopher S. Goldenstein, 2015-10-26 This text provides an introduction to the science that governs the interaction of light and matter (in the gas phase). It provides readers with the basic knowledge to exploit the light-matter interaction to develop quantitative tools for gas analysis (i.e. optical diagnostics) and understand and interpret the results of spectroscopic measurements. The authors pair the basics of gas-phase spectroscopy with coverage of key optical diagnostic techniques utilized by practicing engineers and scientists to measure fundamental flow-field properties. The text is organized to cover three sub-topics of gas-phase spectroscopy: (1) spectral line positions, (2) spectral line strengths, and (3) spectral lineshapes by way of absorption, emission, and scattering interactions. The latter part of the book describes optical measurement techniques and equipment.

Key subspecialties include laser induced fluorescence, tunable laser absorption spectroscopy, and wavelength modulation spectroscopy. It is ideal for students and practitioners across a range of applied sciences including mechanical, aerospace, chemical, and materials engineering.

Introduction to Atomic Spectra Harvey Elliott White,1934

Synergetic Computers and Cognition Hermann Haken,2013-03-09 This book presents a novel approach to neural nets and thus offers a genuine alternative to the hitherto known neuro-computers. The new edition includes a section on transformation properties of the equations of the synergetic computer and on the invariance properties of the order parameter equations. Further additions are a new section on stereopsis and recent developments in the use of pulse-coupled neural nets for pattern recognition.

Introduction to Spectroscopy Donald L. Pavia,Gary M. Lampman,George S. Kriz,James R. Vyvyan,2015

Resonance Acoustic Spectroscopy Naum D. Veksler,2012-12-06 Resonance Acoustic Spectroscopy deals with the analysis of waves generated in an elastic body by a plane harmonic acoustic wave. It is the first monograph to treat new analytical and experimental methods for the investigation of the excitation, propagation and re-radiation of elastic waves in solid, thick-walled and thin-walled elastic scatterers.The material is presented systematically, comprising the formulation of the problem, method of solution, algorithm, computation and analysis. A large number of computational results are given in the form of modal resonances, form functions, dispersion curves and acoustic spectrograms. Particular attention is paid to the interpretation of the solutions.

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of us has increased immeasurably, even in recent years, but this increase has not been reflected in the level or content of courses taught at universities, many of which portray the subject as a collection of arcane recipes and poorly understood formulae of marginal importance to the mainstream of chemistry. This approach reached its nadir with the recent extraordinary furore surrounding the purported discovery of cold fusion, where two electrochemists claimed to have shown that the fusion of deuterium nuclei could be effected under ambient conditions by the electrochemically induced intercalation of deuterium atoms into palladium. Whatever the truth behind such claims, their discussion revealed a lamentable lack of knowledge of modern electrochemistry, not only among science writers for the popular press, but among many professional chemists and physicists whose acquaintance with the subject seems, for the most part, to have stopped somewhere about the time of Nernst. In a year in which Professor R.

BIOS Instant Notes in Physical Chemistry Gavin Whittaker, Andy Mount, Matthew Heal, 2000-06-15 *Instant Notes in Physical Chemistry* introduces the various aspects of physical chemistry in an order that gives the opportunity for continuous reading from front to back. The background to a range of important techniques is incorporated to reflect the wide application of the subject matter. This book provides the key to the understanding and learning of physical chemistry.

Molecular Physics and Elements of Quantum Chemistry Hermann Haken, Hans Christoph Wolf, 2013-03-09 This textbook introduces the molecular and quantum chemistry needed to understand the physical properties of molecules and their chemical bonds. It follows the authors' earlier textbook *The Physics of Atoms and Quanta* and presents both experimental and theoretical fundamentals for students in physics and physical and theoretical chemistry. The new edition treats new developments in areas such as high-resolution two-photon spectroscopy, ultrashort pulse spectroscopy, photoelectron spectroscopy, optical investigation of single molecules in condensed phase, electroluminescence, and light-emitting diodes.

March's Advanced Organic Chemistry Michael B. Smith, Jerry March, 2007-01-29 The Sixth Edition of a classic in organic chemistry continues its tradition of excellence. Now in its sixth edition, *March's Advanced Organic Chemistry* remains the gold standard in organic chemistry. Throughout its six editions, students and chemists from around the world have relied on it as an essential resource for planning and executing synthetic reactions. The Sixth Edition brings the text completely current with the most recent organic reactions. In addition, the references have been updated to enable readers to find the latest primary and review literature with ease. New features include: More than 25,000 references to the literature to facilitate further research; Revised mechanisms, where required, that explain concepts in clear modern terms; Revisions and updates to each chapter to bring them all fully up to date with the latest reactions and discoveries; A revised Appendix B to facilitate correlating chapter sections with synthetic transformations.

Modern Spectroscopy J. Michael Hollas, 2013-04-11 The latest edition of this highly acclaimed title introduces the

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Molecular Spectroscopy Jeanne L. McHale, 2017-07-06 This textbook offers an introduction to the foundations of spectroscopic methods and provides a bridge between basic concepts and experimental applications in fields as diverse as materials science, biology, solar energy conversion, and environmental science. The author emphasizes the use of time-dependent theory to link the spectral response in the frequency domain to the behavior of molecules in the time domain, strengthened by two brand new chapters on nonlinear optical spectroscopy and time-resolved spectroscopy. Theoretical underpinnings are presented to the extent necessary for readers to understand how to apply spectroscopic tools to their own interests.

Organic Spectroscopy Lal Dhar Singh Yadav, 2013-08-30 Organic Spectroscopy presents the derivation of structural information from UV, IR, Raman, ¹H NMR, ¹³C NMR, Mass and ESR spectral data in such a way that stimulates interest of students and researchers alike. The application of spectroscopy for structure determination and analysis has seen phenomenal growth and is now an integral part of Organic Chemistry courses. This book provides: -A logical, comprehensive, lucid and accurate presentation, thus making it easy to understand even through self-study; -Theoretical aspects of spectral techniques necessary for the interpretation of spectra; -Salient features of instrumentation involved in spectroscopic methods; -Useful spectral data in the form of tables, charts and figures; -Examples of spectra to familiarize the reader; -Many varied problems to help build competence and confidence; -A separate chapter on 'spectroscopic solutions of structural problems' to emphasize the utility of spectroscopy. Organic Spectroscopy is an invaluable reference for the interpretation of various spectra. It can be used as a basic text for undergraduate and postgraduate students of spectroscopy as well as a practical resource by research chemists. The book will be of interest to chemists and analysts in academia and industry, especially those engaged in the synthesis and analysis of organic compounds including drugs, drug intermediates, agrochemicals, polymers and dyes.

Biophysics V. Pattabhi, N. Gautham, 2002-03-31 The first chapter introduces and refreshes the reader's knowledge of physics and chemistry. The next chapters cover various physico-chemical techniques used to study biomolecular structures, followed by treatments of spectroscopy, microscopy, diffraction, and computational techniques.

Hydroformylation for Organic Synthesis Maurizio Taddei, André Mann, 2014-07-08 The Role of Metals and Ligands in Organic Hydroformylation, by Luca Gonsalvi, Antonella Guerriero, Eric Monflier, Frédéric Hapiot, Maurizio Peruzzini.

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