# Symmetry And Spectroscopy Of Molecules By K Veera Reddy

As the structure and behavior of molecules and crystals depend on their different symmetries, group theory becomes an essential tool in many important areas of chemistry. It is a quite powerful theoretical tool to predict many basic as well as some characteristic properties of molecules. Whereas quantum mechanics provide solutions of some chemical problems on the basis of complicated mathematics, group theory puts forward these solutions in a very simplified and fascinating manner. Group theory has been successfully applied to many chemical problems. Students and teachers of chemical sciences have an invisible fear from this subject due to the difficulty with the mathematical jugglery. An active sixth dimension is required to understand the concept as well as to apply it to solve the problems of chemistry. This book avoids mathematical complications and presents group theory so that it is accessible to students as well as faculty and researchers. Chemical Applications of Symmetry and Group Theory discusses different applications to chemical problems with suitable examples. The book develops the concept of symmetry and group theory, representation of group, its applications to I.R. and Raman spectroscopy, U.V spectroscopy, bonding theories like molecular orbital theory, ligand field theory, hybridization, and more. Figures are included so that reader can visualize the symmetry, symmetry elements, and operations.

Winner of a 2005 CHOICE Outstanding Academic Book Award Molecular symmetry is an easily applied tool for understanding and predicting many of the properties of molecules. Traditionally, students are taught this subject using point groups derived from the equilibrium geometry of the molecule. Fundamentals of Molecular Symmetry shows how to set up symmetry groups for molecules using the more general idea of energy invariance. It is no more difficult than using molecular geometry and one obtains molecular symmetry groups. The book provides an introductory description of molecular spectroscopy and quantum mechanics as the foundation for understanding how molecular symmetry is defined and used. The approach taken gives a balanced account of using both point groups and molecular symmetry groups. Usually the point group is only useful for isolated, nonrotating molecules, executing small amplitude vibrations, with no tunneling, in isolated electronic states. However, for the chemical physicist or physical chemist who wishes to go beyond these limitations, the molecular symmetry group is almost always required.

Designed to serve as a textbook for postgraduate students of physics and chemistry, this second edition improves the clarity of treatment, extends the range of topics, and includes more worked examples with a view to providing all the material needed for a course in molecular spectroscopy—from first principles to the very useful spectral data that comprise figures, charts and tables. To improve the conceptual appreciation and to help students develop more positive and realistic impressions of spectroscopy, there are two new

chapters—one on the spectra of atoms and the other on laser spectroscopy. The chapter on the spectra of atoms is a detailed account of the basic principles involved in molecular spectroscopy. The chapter on laser spectroscopy covers some new experimental techniques for the investigation of the structure of atoms and molecules. Additional sections on interstellar molecules, inversion vibration of ammonia molecule, fibre-coupled Raman spectrometer, Raman microscope, supersonic beams and jet-cooling have also been included. Besides worked-out examples, an abundance of review questions, and end-of-chapter problems with answers are included to aid students in testing their knowledge of the material contained in each chapter. Solutions manual containing the complete worked-out solutions to chapter-end problems is available for instructors.

This book addresses the nature of the chemical bond in inorganic and coordination compounds. In particular, it explains how general symmetry rules can describe chemical bond of simple inorganic molecules. Since the complexity of studying even simple molecules requires approximate methods, this book introduces a quantum mechanical treatment taking into account the geometric peculiarities of the chemical compound. In the case of inorganic molecules, a convenient approximation comes from symmetry, which constrains both the electronic energies and the chemical bonds. The book also gives special emphasis on symmetry rules and compares the use of symmetry operators with that of Hamiltonian operators. Where possible, the reactivity of molecules is also rationalized in terms of these symmetry properties.

As practical examples, electronic spectroscopy and magnetism give experimental confirmation of the predicted electronic energy levels. Adapted from university lecture course notes, this book is the ideal companion for any inorganic chemistry course dealing with group theory.

Symmetry and group theory provide us with a formal method for the description of the geometry of objects by describing the patterns in their structure. In chemistry it is a powerful method that underlies many apparently disparate phenomena. Symmetry allows us to accurately describe the types of bonding that can occur between atoms or groups of atoms in molecules. It also governs the transitions that may occur between energy levels in molecular systems, which in turn allows us to predict the absorption properties of molecules and hence their spectra. Molecular Symmetry lays out the formal language used in the area using illustrative examples of particular molecules throughout. It then applies the ideas of symmetry to describe molecular structure, bonding in molecules and consider the implications in spectroscopy.Topics covered include: Symmetry elements Symmetry operations and products of operations Point groups used with molecules Point group representations, matrices and basis sets Reducible and irreducible representations Applications in vibrational spectroscopy Symmetry in chemical bonding Molecular Symmetry is designed to introduce the subject by combining symmetry with spectroscopy in a clear and accessible manner. Each chapter ends with a summary of learning points, a selection of self-test questions, and

suggestions for further reading. A set of appendices includes templates for paper models which will help students understand symmetry groups. Molecular Symmetry is a must-have introduction to this fundamental topic for students of chemistry, and will also find a place on the bookshelves of postgraduates and researchers looking for a broad and modern introduction to the subject

This handbook on group theory is geared toward chemists and experimental physicists who use spectroscopy and require knowledge of the electronic structures of the materials they investigate. Accessible to undergraduate students, it takes an elementary approach to many of the key concepts. Rather than the deductive method common to books on mathematics and theoretical physics, the present volume introduces fundamental concepts with simple examples, relating them to specific chemical and physical problems. The text is centered on detailed analysis of examples. Since neither chemists nor spectroscopists require theorem proofs, very few appear here. Instead, the focus remains on the principal conclusions, their meaning, and their use. In keeping with the text's practical bias, the main results of group theory are presented in all sections as procedures, making possible their systematic and step-by-step-application. Each chapter contains problems that develop practical skill and provide a valuable supplement to the text.

The fourth edition of Modern Spectroscopy introduces the reader to a wide range of spectroscopies and includes both the background theory and applications to

structure determination and chemical analysis. It covers rotational, vibrational, electronic, photoelectron and Auger spectroscopy, as well as EXAFS, and the theory of lasers and laser spectroscopy. New material includes laser detection and ranging (LIDAR), cavity ring-down spectroscopy, femtosecond lasers, femtosecond spectroscopy and very high resolution fluorescence of large molecules. In addition, the clarity of figures has been greatly improved and Professor Ben van der Veken at the University of Antwerp has run some new infrared spectra especially for this new edition. A revised and updated edition of a successful, clearly written textbook Modern Spectroscopy, Fourth Edition: includes the latest developments in modern laser techniques. contains a discussion of molecular symmetry. provides numerous worked examples, calculations and questions at the end of chapters. improved clarity of many of the figures Written by an author with many years' teaching and research experience, Modern Spectroscopy, Fourth Edition will prove invaluable for students of chemistry, physics, and chemical physics studying atomic and molecular spectroscopy, lasers and laser spectroscopy, and molecular symmetry.

Prof. McClain has, quite simply, produced a new kind of tutorial book. It is written using the logic engine Mathematica, which permits concrete exploration and development of every concept involved in Symmetry Theory. It is aimed at students of chemistry and molecular physics who need to know mathematical group theory and its applications, either for their own research or for understanding the language and concepts of their field. The book begins with the most elementary symmetry concepts, then presents mathematical

group theory, and finally the projection operators that flow from the Great Orthogonality are automated and applied to chemical and spectroscopic problems.

The first edition, by P.R. Bunker, published in 1979, remains the sole textbook that explains the use of the molecular symmetry group in understanding high resolution molecular spectra. Since 1979 there has been considerable progress in the field and a second edition is required; the original author has been joined in its writing by Per Jensen. The Material of the first edition has been reorganized and much has been added. The molecular symmetry group is now introduced early on, and the explanation of how to determine nuclear spin statistical weights has been consolidated in one chapter, after groups, symmetry groups, character tables and the Hamiltonian have been introduced. A description of the symmetry in the three-dimensional rotation group K(spatial), irreducible spherical tensor operators, and vector coupling coefficients is now included. The chapters on energy levels and selection rules contain a great deal of material that was not in the first edition (much of it was undiscovered in 1979), concerning the Jahn-Teller effect, the Renner effect, Multichannel Quantum Defect Theory, the use of variational methods for calculating rotational-vibration energy levels, and the contact transformed rotation-vibration Hamiltonian. A new chapter is devoted entirely to weakly bound cluster molecules (often called Van der Waals molecules). A selection of experimental spectra is included in order to illustrate particular theoretical points.

Vibrational Spectroscopy Provides In A Very Readable Fashion A Comprehensive Account Of The Fundamental Principles Of Infrared And Raman Spectroscopy For Structural Applications To Inorganic, Organic And Coordination Compounds. Theoretical Analyses Of The Spectra By Normal Coordinate Treatment, Factor Group

Analysis And Molecular Mechanics Are Delineated.The Book Features: * Coverage From First Principles To Recent Advances * Relatively Self-Contained Chapters * Experimental Aspects * Step By Step Treatment Of Molecular Symmetry And Group Theory * Recent Developments Such As Non-Linear Raman Effects * Comprehensive Treatment Of Rotation Spectroscopy * Band Intensities * Spectra Of Crystals * End-Of-Chapter Exercises.Suitable For Students And Researchers Interested In The Field Of Vibrational Spectroscopy. No Prior Knowledge Of Concepts Specific To Vibrational Spectroscopy Is Necessary. Mathematical Background Such As Matrices And Vectors Are Provided.

This unified treatment introduces upper-level undergraduates and graduate students to the concepts and methods of modern molecular spectroscopy and their applications to quantum electronics, lasers, and related optical phenomena. Starting with a review of the prerequisite quantum mechanical background, the text examines atomic spectra and diatomic molecules, including the rotation and vibration of diatomic molecules and their electronic spectra. A discussion of rudimentary group theory advances to considerations of the rotational spectra of polyatomic molecules and their vibrational and electronic spectra; molecular beams, masers, and lasers; and a variety of forms of spectroscopy, including optical resonance spectroscopy, coherent transient spectroscopy, multiple-photon spectroscopy, and spectroscopy beyond molecular constants. The text concludes with a series of useful appendixes.

The mathematical fundamentals of molecular symmetry and group theory are comprehensibly described in this book. Applications are given in context of electronic and vibrational spectroscopy as well as chemical reactions following orbital symmetry rules. Exercises and examples compile and deepen the content in a lucid manner.

Encompassing a wide range of techniques, spectroscopy is used to analyze chemicals, biological and pharmaceutical compounds, food and beverages, and high-tech materials. Covering the whole range of spectroscopic techniques, this book provides a thorough overview of underlying principles, techniques and applications. Dr. Hollas is a well-known author and authority in the field, and this book is an expanded version of his well-received lower-level book, Modern Spectroscopy, now in its third edition (0-471-96523-5). "The first edition of High Resolution Spectroscopy (the big book version of Modern Spectroscopy) was undoubtedly the best textbook on spectroscopy written at an undergraduate / beginning graduate level, and the second edition is an improvement... ...The coverage is broad, deep and even. The first chapters give a concise and clear introduction to spectroscopy, covering much that is accessible elsewhere only in more complicated discussions... ...The production values of High Resolution Spectroscopy are high, diagrams are well reproduced and the whole text is lavishly illustrated with many spectra and diagrams of apparatus.... ... it contains a great deal of material and is beautifully written; every library should contain a copy; every student of spectroscopy (no-matter what age!) should have a copy on their shelves." Extracts from a Review in Spectroscopy Europe, 11/3 (1999) The latest edition of this highly acclaimed title introduces the reader to a wide range of spectroscopies, and includes both the background theory and applications to structure determination and chemical analysis. It covers rotational, vibrational, electronic, photoelectron and Auger spectroscopy, as well as EXAFs and the theory of lasers and laser spectroscopy. A revised and updated edition of a successful, clearly written book Includes the latest developments in modern laser techniques, such as cavity ring-down spectroscopy and femtosecond lasers Provides numerous

worked examples, calculations and questions at the end of chapters

Coverage of Physical Chemistry. Each volume includes a large number of illustrative numericals and typical problems to highlight the principles involved. IUPAC recommendations and SI units have been adopted throughout. The present book describes Wave Mechanics, Energy Quantization and Atomic Structure, Theories of Covalent Bond, Electrical and Magnetic Properties of Molecules, Molecular Spectroscopy, Molecular Symmetry and its Applications. Salient Features: • Comprehensive coverage of wave mechanics, energy quantization and atomic structure, theories of covalent bond, electrical and magnetic properties of molecules, molecular spectroscopy, molecular symmetry and its applications • Emphasis given to applications and principles • Explanation of equations in the form of solved problems and numericals • IUPAC recommendations and SI units have been adopted throughout • Rich and illustrious pedagogy

Key Features:Concepts built from strong and ground origins. Brief presentation on atomic, hybrid and molecular orbital concepts. Molecular structure and symmetry presented in pedagogical manner. Illustrations with a variety of molecular examples. Self-study exercises for thorough understanding. crossword puzzles provide test of learning. Appendices at the end provide an essential

supplement.About the Book:This book is designed with an exclusive coverage of symmetry & structure of molecules. Also, the teachers would find a classroom-friendly narration of all the topics presented in the book.An exclusive excursion-like treatment is given for the concepts of structure, symmetry and orbitals (atomic, hybrid and molecular) with a semi-pedagogical coverage. The primary focus of the book is on 'root-learning' than on 'rote- learning', paving the way for strong foundations. Secondly, the treatment given in the book helps in learning the correct concept by both the teacher and the taught. The method of presentation chosen for the book is the one that is well tested in the classroom for few decades. The book attempts a systematic approach in mastering the subject layer by layer and a smooth transition is maintained throughout from chapter to chapter for a successful take off.

The group theory is a powerful tool that is used to determine symmetry of molecules. It is a key component in the present-day Physical Sciences, Chemical Sciences, Mathematics, Statistics and Computer Sciences. Groups - "set of all the permutation of the roots of an algebraic expression that exhibit the characteristics that the combination of any two of these permutations belongs to the set." Group theory has a huge number of applications in the real world. Group theory is not only confined to

determination of molecular symmetry but also symmetry of molecular orbitals, atoms, rotation and vibration of bonds, and is thus very useful in spectroscopy. The symmetry of molecules / molecular orbital provides information regarding the positions of orbitals in various energy levels and the molecular transitions in them.

The book reviews the results of vibration-rotational spectroscopy of molecules obtained recently by combining modern computational methods of quantum chemistry with the new techniques of high-resolution rotational and vibration-rotational spectroscopy. It shows for example that the tunneling vibration-rotational spectroscopy of the van der Waals complexes provides a new look at intermolecular forces while the high precision and sensitivity of the submillimeter-wave and Fourier transform microwave spectroscopy make it possible to study complex rotational spectra of molecules in excited vibrational states. New results of high level ab initio quantum chemical computations of vibrational and rotational energy levels and dipole moment functions of unusual molecules will be discussed together with the recent discovery of clustering of energy levels in asymmetric tops. Group theoretical analysis of floppy molecules, especially the tunneling effects in nonrigid molecules, will also be discussed. Contents:High-Resolution Spectroscopy of Transient Molecules and

Its Applications to Molecular Dynamics (E Hirota & Y Endo)Vibration-Rotation Spectra of Reactive Molecules: Interplay of Ab Initio Calculations and High-Resolution Experimental Studies (H Bürger & W Thiel)Rotational Spectra of Symmetric Top Molecules: Correlation-Free Reduced Forms of Hamiltonians, Advances in Measuring Techniques, and Determination of Molecular Parameters from Experimental Data (K Sarka et al.)Hot Bands in Infrared Spectra of Symmetric Top and Some Other Molecules. A Useful Tool to Reach Hidden Information (G Graner & H Bürger)The Formation of Four-Fold Rovibrational Energy Clusters in H2S, H2Se, and H2Te (P Jensen et al.)Phase Angles in the Matrix Elements of Molecular Spectroscopy (C di Lauro & F Lattanzi)High-Resolution Infrared Spectroscopy and One-Dimensional Large Amplitude Motion in Asymmetric Tops: HNO3 and H2O2 (J-M Flaud & A Perrin)Extended Molecular Symmetry Groups: Symmetry Analysis of Molecules Consisting of Two Coaxial Rotors (P Soldán)Quantum-Mechanical Studies of Radiative Association Reactions: Formation of HeH+, NeH+ and ArH+ (W P Kraemer et al.) Readership: Chemists, astrophysicists, laser physicists and other general physicists. keywords:Transient and Reactive Molecules;Reduced Hamiltonians;Hot Bands;Rovibrational Energy Clusters;Phase Angles in Matrix Elements;Large Amplitude

Vibrations;Molecular Symmetry Groups;Radiation Association Reactions

The Students Of Chemistry Have Access A Variety Of Excellent Books Dealing With The Applications Of The Techniques Of Group Theory For Solving Chemical Problems. Most Of The Books Are Too Advance For Beginners. It Is Hoped That This Book Will Help Them For Having A Firm Grip Of The Subject Matter. The Book Contains Not Only The Symmetry Of The Molecules But Also That Of Crystals. The Idea Of Space Group Is Introduced Along With The Idea Of The Point Group For Crystals Is Often Neglected In Introductory Textbooks. Simple Mnemonic Device Is Also Introduced For Understanding The Molecular Orbital Energy Levels For Certain Cyclic And Acyclic Systems. Hopefully, I Believe That After Grasping The Ideas Presented Here, The Learners Will Be In Better Position To Appriciate The Ideas Presented In The More Advance And Comprehensive Textbooks Listed In The Bibilography Which Is By No Means Exhaustive. Content Highlights : - Preface # Symmetry # Symmetry And Mathematical Tools # Reducible And Irreducible Representation # Symmetry And Vibronic Spectroscopy # Symmetry And Bond Theory # Symmetry And Molecular Orbital Energies # Symmetry And Crystallographic Groups # Bibiliography # Appendix # Index

Symmetry and group theory provide us with a

rigorous method for the description of the geometry of objects by describing the patterns in their structure. In chemistry it is a powerful concept that underlies many apparently disparate phenomena. Symmetry allows us to accurately describe the types of bonding that can occur between atoms or groups of atoms in molecules. It also governs the transitions that may occur between energy levels in molecular systems, leading to a predictive understanding of the absorption properties of molecules and hence their spectra. Molecular Symmetry lays out the formal language used in the area, with illustrative examples of particular molecules throughout. It then applies the ideas of symmetry and group theory to describe molecular structure, bonding in molecules and to consider the implications in spectroscopy. Topics covered include: Symmetry elements Symmetry operations and products of operations Point groups used with molecules Point group representations, matrices and basis sets Reducible and irreducible representations Applications in vibrational spectroscopy Molecular orbital theory of chemical bonding Molecular Symmetry is designed to introduce the subject by combining symmetry with spectroscopy and bonding in a clear and accessible manner. Each chapter ends with a summary of learning points, a selection of self-test questions, and suggestions for further reading. A set of appendices includes templates for paper models

which will help students understand symmetry operations and cover key aspects of the material in depth. Molecular Symmetry is a must-have introduction to this fundamental topic for students of chemistry, and will also find a place on the bookshelves of postgraduates and researchers looking for a broad and modern introduction to the subject.

Volume 4 is the fourth of the 7-volume series on Physical Chemistry written by Dr. K L Kapoor. This book is useful for 4th and 5th semester students of B.Sc Chemistry (Hons and Gen). Updated sixth edition on Quantum Chemistry and Molecular Spectroscopy is divided into 5 chapters and focuses on atomic structure, chemical bonding, electrical and magnetic properties, molecular spectroscopy and its applications. IUPAC recommendations along with SI units have been incorporated in this book. The revised edition includes probability of finding harmonic oscillator in classical forbidden region; commutator of xn and pm; E-type and P-type of delayed fluorescence; and Jablonski diagram to display electronic transitions in a molecule. Salient Features: • Strictly in accordance with latest IUPAC recommendations and SI units being adopted throughout the text • Comprehensive coverage of wave mechanics, energy quantization and atomic structure, theories of covalent bond, electrical and magnetic properties of molecules, molecular

spectroscopy, molecular symmetry and its applications • Perfect blend of both theoretical and application-based concepts • Extensive chapter-end numericals including Revisionary Problems, Try Yourself Problems and Numerical Problems

Informal, effective undergraduate-level text introduces vibrational and electronic spectroscopy, presenting applications of group theory to the interpretation of UV, visible, and infrared spectra without assuming a high level of background knowledge. 200 problems with solutions. Numerous illustrations. "A uniform and consistent treatment of the subject matter." — Journal of Chemical Education.

Written in a clear and understandable manner, this book provides a comprehensive, yet non-mathematical, treatment of the topic, covering the basic principles of symmetry and the important spectroscopic techniques used to probe molecular structure. The chapters are extensively illustrated and deal with such topics as symmetry elements, operations and descriptors, symmetry guidelines, high-fidelity pseudosymmetry, crystallographic symmetry, molecular gears, and experimental techniques, including X-ray crystallography and NMR spectroscopy. As an additional feature, 3D animations of most of the structures and molecules covered are available online at wiley.com. As a result, chemists learn how to understand and predict molecular structures and reactivity. Authored by a renowned expert with numerous publications and an excellent track record in research and teaching, this is a useful source for graduate students and researchers working in the field of organic synthesis, physical chemistry, biochemistry, and crystallography, while equally serving as supplementary reading for courses on stereochemistry, organic synthesis, or crystallography.

An introduction to one of the fundamental tools in chemicalresearch—spectroscopy and photophysics in condensed-phase andextended systems A great deal of modern research in chemistry and materialsscience involves the interaction of radiation with condensed-phasesystems such as molecules in liquids and solids as well asmolecules in more complex media, molecular aggregates, metals,semiconductors, and composites. Condensed-Phase MolecularSpectroscopy and Photophysics was developed to fill the needfor a textbook that introduces the basics of traditional molecularspectroscopy with a strong emphasis on condensed-phase systems. Italso examines optical processes in extended systems such as metals,semiconductors, and conducting polymers, and addresses the uniqueoptical properties of nanoscale systems. Condensed-Phase Molecular Spectroscopy and Photophysicsbegins with an introduction to quantum mechanics that sets a solidfoundation for understanding the text's subsequent topics,including: Electromagnetic radiation and radiation-matterinteractions Molecular vibrations and infrared spectroscopy Electronic spectroscopy Photophysical processes and light scattering Nonlinear and pump-probe spectroscopies Electron transfer processes Each chapter contains problems ranging from simple to complex,enabling readers to gradually build their skills andproblem-solving abilities. Written for upper-level undergraduateand graduate courses in physical and materials chemistry, this textis uniquely designed to equip readers to solve a broad array ofcurrent problems and challenges in chemistry.

This third edition of Peter Bernath's successful Spectra of Atoms and Molecules is designed to provide advanced undergraduates and graduate students a working knowledge of the vast field of spectroscopy. Also of interest to chemists, physicists, astronomers, atmospheric scientists, and

engineers, this volume emphasizes the fundamental principles of spectroscopy with the primary goal of teaching the interpretation of spectra. Features include a presentation of group theory needed to understand spectroscopy, detailed worked examples and a large number of excellent problems at the end of each chapter. Prof. Bernath provides a large number of diagrams and spectra which have been specifically recorded for this book. Molecular symmetry, matrix representation of groups, quantum mechanics, and group theory are among the topics covered; atomic, rotational, vibrational, electronic and Raman spectra are analyzed. Bernath's clear treatment of the confusing topic of line strengths as needed for quantitative applications is featured. This much-needed new edition has been updated to include the 2010 CODATA revision of physical constants, and a large number of corrections and clarifications. Responding to student requests, the main new feature is the addition of detailed worked examples in each chapter. Spectra of Atoms and Molecules, 3e will help demystify spectroscopy by showing readers the necessary steps in a derivation, as well as the final result.

Recent advances in infrared molecular spectroscopy have resulted in sophisticated theoretical and laboratory methods that are difficult to grasp without a solid understanding of the basic principles and underlying theory of vibration-rotation absorption spectroscopy. Rotational Structure in Molecular Infrared Spectra fills the gap between these recent, complex topics and the most elementary methods in the field of rotational structure in the infrared spectra of gaseous molecules. There is an increasing need for people with the skills and knowledge to interpret vibration-rotation spectra in many scientific disciplines, including applications in atmospheric and planetary research. Consequently, the basic principles of vibration-rotation absorption spectroscopy are

addressed for contemporary applications. In addition to covering operational quantum mechanical methods, spherical tensor algebra, and group theoretical methods applied to molecular symmetry, attention is also given to phase conventions and their effects on the values of matrix elements. Designed for researchers and PhD students involved in the interpretation of vibration-rotation spectra, the book intentionally separates basic theoretical arguments (in the appendices), allowing readers who are mainly concerned with applications to skip the principles while at the same time providing a sound theoretical basis for readers who are looking for more foundational information. Reviews basic theory and contemporary methods of vibration rotation absorption spectroscopy, including operational quantum mechanical methods, spherical tensor algebra, and group theoretical methods applied to molecular symmetry Covers sophisticated mathematical topics in simple, easy-to-read language Discusses methods and applications separately from basic theoretical arguments for quick reference

This book presents a range of fundamentally new approaches to solving problems involving traditional molecular models. Fundamental molecular symmetry is shown to open new avenues for describing molecular dynamics beyond standard perturbation techniques. Traditional concepts used to describe molecular dynamics are based on a few fundamental assumptions, the ball-and-stick picture of molecular structure and the respective perturbative treatment of different kinds of couplings between otherwise separate motions. The book points out the conceptual limits of these models and, by focusing on the most essential idea of theoretical physics, namely symmetry, shows how to overcome those limits by introducing fundamentally new concepts. The book begins with an introduction to molecular symmetry in general, followed by a discussion of nuclear spin

symmetry. Here, a new correlation between identical particle exchange and spin angular momentum symmetry of nuclei is exhibited. The central part of the book is the discussion of extremely floppy molecules, which are not describable in the framework of traditional theories. The book introduces a fundamentally new approach to describing the molecular dynamics of these molecules - the super-rotor model, which is based on a five-dimensional symmetry that has never been observed in molecules before. By applying the super-rotor theory to the prototype of floppy molecules, protonated methane, this model can consistently predict the symmetry and energy of low-energy states, which were characterized experimentally only a few years ago. The theoretical predictions agree with the experimental results, which makes the prospect of further developing the super-rotor theory and applying it to other molecules a promising one. In the final section, the book also covers the topic of ultrafast rotations, where usual quantum calculations reach their natural limits. A semi-classical method for determining rotational energies, developed in the early 1990s, is shown to be attachable to quantum calculations of the vibrational states. This new combined method is suitable for efficiently calculating ro-vibrational energies, even for molecular states with large angular momentum.

Both molecular spectroscopy and computational chemistry have witnessed rapid significant progresses in recent years. On the one hand, it is nowadays possible to compute, to quite a reasonable degree of accuracy, almost all fundamental spectroscopic properties for small molecular systems. The theoretical approach is now properly considered to be of fundamental importance in attaining a high degree of understanding of spectroscopic information. Moreover, it may be also a great help in designing and planning experiments. On the other hand, new and very powerful experimental

techniques have been developed. This book combines an advanced teaching standpoint with an emphasis on the interplay between theoretical and experimental molecular spectroscopy. It covers a wide range of topics (such as molecular dynamics and reactivity, conformational analysis, hydrogen bonding and solvent effects, spectroscopy of excited states, complex spectra interpretation and simulation, software development and biochemical applications of molecular spectroscopy) and considers a large variety of molecular spectroscopic techniques, either from an experimental or from a theoretical perspective. (short text) This book combines an advanced teaching standpoint with an emphasis on the interplay between theoretical and experimental molecular spectroscopy. It covers a wide range of topics (such as molecular dynamics and reactivity, conformational analysis, hydrogen bonding and solvent effects, spectroscopy of excited states, complex spectra interpretation and simulation, software development and biochemical applications of molecular spectroscopy) and considers a large variety of molecular spectroscopic techniques either from an experimental or from a theoretical perspective.

"Authoritative and clearly written."—Applied Optics The direct observation of short-lived free radicals and the consequent study of their structure and reactions have led to important developments in almost every branch of chemistry as well as in other areas. This volume by a Nobel laureate offers an excellent introduction to the essentials of molecular spectroscopy. The introductory chapter discusses experimental methods and illustrates the observed spectra of various molecules and free radicals.

Subsequent chapters explore rotational, vibrational, and electronic energy levels of diatomic molecules and ions; radiative transitions; linear and nonlinear polyatomic radicals and ions; continuous and diffuse spectra; predissociation and pre-ionization; and recombination. The well-illustrated text features more than 100 figures and spectra. A distilled version of the author's monumental three-volume study, Molecular Spectra and Molecular Structure, it constitutes a superb resource for anyone wishing a concise but complete treatment of the fundamentals of molecular spectroscopy.

This Comprehensive Text Clearly Explains Quantum Theory, Wave Mechanics, Structure Of Atoms And Molecules And Spectroscopy.The Book Is In Three Parts, Namely, Wave Mechanics; Structure Of Atoms And Molecules; And Spectroscopy And Resonance Techniques.In A Simple And Systematic Manner, The Book Explains The Quantum Mechanical Approach To Structure, Along With The Basic Principles And Application Of Spectroscopic Methods For Molecular Structure Determination.The Book Also Incorporates The Electric And Magnetic Properties Of Matter, The Symmetry, Group Theory And Its Applications.Each Chapter Includes Many Solved Examples And Problems For A Better Understanding Of The Subject.With Its Exhaustive Coverage And Systematic Approach, This Is An Invaluable Text For B.Sc. (Hons.) And M.Sc.

Chemistry Students.

This volume contains a selection of scientific papers related to the structure and dynamics of non-rigid molecules. This frontline topic was born a few decades ago, when Longuet-Higgins proposed his famous theory of Molecular Symmetry Groups (Mol. Phys. 6, (1962) 457). Unfortunately, since this early paper, very few publications have been devoted to the study of non-rigid molecules. Let us mention some books which dedicate some chapters to them: Induced Representations in Crystals and Molecules, by S. L. Altmann, Academic Publishers, 1977; Molecular Symmetry and Spectroscopy, by P. R. Bunker, Academic Publishers, 1979; and finally Large Amplitude Motion in Molecules, Vols. I and II, by several authors, Springer Verlag, 1979. More recently an International Symposium on Non-Rigid Molecules was held in Paris, France, from 1-7 July 1982, the proceedings of which were published in the volume entitled Symmetries and Properties of Non-Rigid Molecules. A Comprehensive Survey, edited by J. Maruani et al., Elsevier, 1983. Finally, we should mention the very specialized work The Permutational Approach to Dynamic Stereochemistry, by J. Brocas et al., McGraw-Hill, 1983. The purpose of this book is to fill in this information on the structure and dynamics of non-rigid systems. To this aim, we have gathered a collection of recent papers written by the most

qualified specialists in the world, covering a large field from van der Waals molecules to inorganic complexes and organic polyrotor molecules, as well as considering statistical and dynamic aspects.