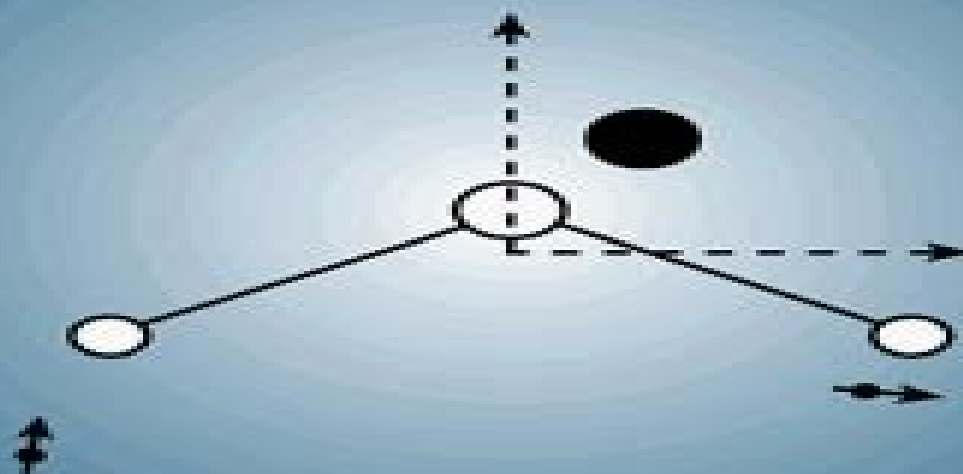


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MOLECULAR SYMMETRY AND SPECTROSCOPY

SECOND EDITION



**Philip R. Bunker
and Per Jensen**

Molecular Symmetry And Spectroscopy

Robert Glaser



Molecular Symmetry And Spectroscopy:

Molecular Symmetry and Spectroscopy Philip R. Bunker, Per Jensen, 2006 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

Symmetry and Spectroscopy Daniel C. Harris, Michael D. Bertolucci, 1989-01-01 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

Fundamentals of Molecular Symmetry P.R. Bunker, 2018-10-03 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

Symmetry and Spectroscopy of Molecules K. Veera Reddy, 2007

Molecular Symmetry David J. Willock, 2009-03-16 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 considers 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.

Molecular Symmetry and Group Theory R. C. Maurya, J.M. Mir, 2019-09-02. The mathematical fundamentals of molecular symmetry and group theory are comprehensively 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. **Molecular Symmetry and Group Theory** Robert L. Carter, 1997-12-16. A

thorough introduction to molecular symmetry and group theory as applied to chemical problems. Readers will discover by example the power of symmetry arguments in understanding otherwise intimidating theoretical problems in chemistry. This book demonstrates the centrality of symmetry and group theory to a complete understanding of the theory of structure and bonding. **Molecular Symmetry and Group Theory** Alan Vincent, 2013-06-05. This substantially revised and expanded

new edition of the bestselling textbook addresses the difficulties that can arise with the mathematics that underpins the study of symmetry and acknowledges that group theory can be a complex concept for students to grasp. Written in a clear, concise manner, the author introduces a series of programmes that help students learn at their own pace and enable them to understand the subject fully. Readers are taken through a series of carefully constructed exercises designed to simplify the mathematics and give them a full understanding of how this relates to the chemistry. This second edition contains a new chapter on the projection operator method. This is used to calculate the form of the normal modes of vibration of a molecule and the normalised wave functions of hybrid orbitals or molecular orbitals. The features of this book include: A concise, gentle introduction to symmetry and group theory. Takes a programmed learning approach. New material on projection operators and the calculation of normal modes of vibration and normalised wave functions of orbitals. This book is suitable for all students of chemistry taking a first course in symmetry and group theory. Symmetry, Spectroscopy, and Crystallography

Robert Glaser, 2015-09-28 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

Spectra of Atoms and Molecules Peter F. Bernath, 2020-04-20 This fourth edition of Peter Bernath's successful Spectra of Atoms and Molecules is designed to provide advanced undergraduate 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 as needed to understand spectroscopy detailed worked examples and a large number of excellent problems at the end of each chapter 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 as well Bernath's treatment clears the confusing topic of line strengths as needed for quantitative applications Responding to student requests the fourth addition features detailed and worked examples in each chapter This book has also been updated to include the 2018 CODATA revision of physical constants and a large number of corrections and clarifications New chapters on atmospheric and astronomical spectroscopy have been added Spectra of Atoms and Molecules demystifies spectroscopy by showing readers the intermediate steps in a derivation as well as the final result

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