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4A3 - SANAA DEVAN

BASIC Molecular Spectroscopy discusses the utilization of the Beginner's All-purpose Symbolic Instruction Code (BASIC) programming language in molecular spectroscopy. The book is comprised of five chapters that provide an introduction to molecular spectroscopy through programs written in BASIC. The coverage of the text includes rotational spectra, vibrational spectra, and Raman and electronic spectra. The book will be of great use to students who are currently taking a course in molecular spectroscopy.
Since the publication in 1950 of Vol. I, Spectra of Diatomic Molecules of Molecular Spectra and Molecular Structure, much progress has been made in the field. While there have been some important refinements in the theory of diatomic molecular spectra, most of the advances have been in the further exploration of individual spectra. Not only has the number of molecules about which some spectroscopic data are available been increased by a factor of 2 to 3, but also the spectroscopic information about the molecules known in 1950 has been vastly extended. This is due to the observation of new elec tronic states (about three times as many as known before), the enormous improvements in the accuracy of the constants of the states known in 1950, and the determination of higher order constants. In view of the increasing use of spectroscopic information on diatomic molecules in other fields of physics, in chemistry, and in astrophysics, it appeared desirable to prepare an up-to-date version of the table of molecular constants in the appendix of Vol. I. This updating proved to be far more time-consuming than originally anticipated, and it is only now, 10 years that we are able to present such a table, which, instead after its initiation, of the original 80 pages (plus 30 pages of bibliography), now fills a volume of 700 pages. In the interest of economy, and unlike the original version, the new table has been

produced by photo-offset from the final manuscript.
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.

This book is written for graduate students just beginning research, for theorists curious about what experimentalists actually can and do measure, and for experimentalists bewildered by theory. It is a guide for potential users of spectroscopic data, and uses language and concepts that bridge the frequency-and time-domain spectroscopic communities. Key topics, concepts, and techniques include: the assignment of simple spectra, basic experimental techniques, definition of Born-Oppenheimer and angular momentum basis sets and the associated spectroscopic energy level patterns (Hund's cases), construction of effective Hamiltonian matrices to represent both spectra and dynamics, terms neglected in the Born-Oppenheimer approximation (situations intermediate between Hund's cases, spectroscopic perturbations), nonlinear least squares fitting, calculation and interpretation of coupling terms, semi-classical (WKB) approximation, transition intensities and interference effects, direct photofragmentation (dissociation and ionization) and indirect photofragmentation (predissociation and autoionization) processes, visualization of intramolecular dynamics, quantum beats and wavepackets, treatment of decaying quasi-eigenstates using a complex Heff model, and concluding with some examples of polyatomic molecule dynamics. Students will discover that there is a fascinating world of cause-and-effect localized dynamics concealed beyond the reduction of spectra to archival molecular constants and the exact ab initio computation of molecular properties. Professional spectroscopists, kinetics, ab initio theorists will appreciate the practical, simplified--model, and rigorous theoretical approaches discussed in this book. Key Features: • A fundamental reference for all spectra of small, gas-phase molecules. • It is the most up-to-date and comprehensive book on the electronic spectroscopy and dynamics of diatomic molecules. • The authors pioneered the development of many of the experimental methods, concepts, models, and computational schemes described in this book. A fundamental reference for all spectra of small, gas-phase molecules. It is the most up-to-date and comprehensive book on the electronic spectroscopy and dynamics of diatomic molecules. The authors pioneered the development of many of the experimental methods, concepts, models, and computational schemes described in this book.
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Advances in Molecular Spectroscopy, Volume 1 covers the proceedings of the Fourth Meeting of Molecular Spectroscopy, held in Bologna, Italy on September 7-12, 1959. This book is organized into three parts encompassing 69 chapters. The first part presents first some experimental and correlations studies on molecular structure, followed by discussions on the application of molecular spectroscopic techniques for molecular structure determination. Part II reviews experimental determination of Raman intensities, vibrations of aromatic rings, and IR spectra and electronic structure of various organic compounds. Part III considers the general theories on molecular spectroscopy. This topic is followed by surveys on electron energy, orbital va-

lency, relations among potential energy of diatomic molecules, and determination of rotation structure. This book will be of value to molecular spectroscopists and analytical and organic chemists.

Written by an author internationally renowned in the field of molecular spectroscopy, this book provides an up-to-date account of the new experimental and theoretical methods on the high resolution infrared spectroscopy of small molecules. The approach uses a visual approach to spectral analysis, containing large numbers of energy level diagrams and spectra specra to show the progress in identification and line assignment. Covering new and important techniques on laser and Fourier Transform, it also contains both theoretical and experimental chapters. Divided into 3 parts, features covered in the first part include: * Calculations of the vibration-rotation energy levels of rigid and non-rigid molecules * Calculations of the intensities of vibration-rotation transitions * Introduction to linear and non-linear molecular spectroscopy * Use of interferometric and laser spectrometers for measuring infrared spectra The second part presents a detailed treatment of the analysis of the high resolution vibration-rotation spectra of linear, quasilinear, symmetric rotor and asymmetric rotor molecules. In the final part of the book the following topics of current interest are examined in depth: * Electric and magnetic resonance spectroscopy * Spectroscopy of transient species, free radicals and ions, and Van der Waals clusters * Atmospheric and astrophysical spectroscopy, including the spectroscopy of the atmosphere of the Earth and nearby planets, cool stars and molecules in the interstellar medium This comprehensive book is an essential reference for researchers who want to be at the cutting edge in the field of spectroscopy and physical chemistry, atmospheric science and infrared astonomy.

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.

Specialist Periodical Reports provide systematic and detailed review coverage of progress in the major areas of chemical re-

search. Written by experts in their specialist fields the series creates a unique service for the active research chemist, supplying regular critical in-depth accounts of progress in particular areas of chemistry. For over 80 years the Royal Society of Chemistry and its predecessor, the Chemical Society, have been publishing reports charting developments in chemistry, which originally took the form of Annual Reports. However, by 1967 the whole spectrum of chemistry could no longer be contained within one volume and the series Specialist Periodical Reports was born. The Annual Reports themselves still existed but were divided into two, and subsequently three, volumes covering Inorganic, Organic and Physical Chemistry. For more general coverage of the highlights in chemistry they remain a 'must'. Since that time the SPR series has altered according to the fluctuating degree of activity in various fields of chemistry. Some titles have remained unchanged, while others have altered their emphasis along with their titles; some have been combined under a new name whereas others have had to be discontinued. The current list of Specialist Periodical Reports can be seen on the inside flap of this volume.

Molecular Spectroscopy: Modern Research explores the advances in several phases of research in molecular spectroscopy. This eight-chapter book commemorates the 25th anniversary of the annual Columbus Symposium on Molecular Structure and Spectroscopy, held in September, 1970. This book highlights the spectroscopic studies of molecular species in the gas phase and in matrices. Representative articles are also included that cover the applications of molecular studies in a wide variety of areas such as biophysics, astrophysical problems, and energy transfer processes. Other chapters describe the progress achieved in the technology of high resolution spectroscopy and the techniques and terminology of Lamb-dip spectroscopy. A comprehensive bibliography is included for most of the subjects discussed and this text concludes with tables of standard data listing secondary wavelength standards, fundamental constants, atomic masses, and conversion factors of interest to spectroscopists. Spectroscopists, chemists, and researchers will find this work invaluable.

An introduction to one of the fundamental tools in chemical research—spectroscopy and photophysics in condensed-phase and extended systems A great deal of modern research in chemistry and materials science involves the interaction of radiation with condensed-phase systems such as molecules in liquids and solids as well as molecules in more complex media, molecular aggregates, metals, semiconductors, and composites. Condensed-Phase Molecular Spectroscopy and Photophysics was developed to fill the need for a textbook that introduces the basics of traditional molecular spectroscopy with a strong emphasis on condensed-phase systems. It also examines optical processes in extended systems such as metals, semiconductors, and conducting polymers, and addresses the unique optical properties of nanoscale systems. Condensed-Phase Molecular Spectroscopy and Photophysics begins with an introduction to quantum mechanics that sets a solid foundation for understanding the text's subsequent topics, including: Electromagnetic radiation and radiation-matter

interactions 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 and problem-solving abilities. Written for upper-level undergraduate and graduate courses in physical and materials chemistry, this text is uniquely designed to equip readers to solve a broad array of current problems and challenges in chemistry.

Applications of Numerical Methods in Molecular Spectroscopy provides a mathematical background, theoretical perspective, and review of spectral data processing methods. The book discusses methods of complex spectral profile separation into bands, factor analysis methods, methods of quantitative analysis in molecular spectroscopy and reflectance spectroscopy, and new data processing methods. Mathematical methods in special areas of molecular spectroscopy, such as color science, electron spin resonance, and nuclear magnetic resonance spectroscopies are also covered. The book will benefit researchers and postgraduate students in fields of chemistry, physics, and biology.

Written by a Nobel Laureate, this introduction to molecular spectroscopy covers rotational, vibrational, and electronic energy levels of diatomic molecules and ions; linear, nonlinear polyatomic radicals and ions; more. 1971 edition.

This book compiles and updates the best articles to date from the eleven-year history of Spectroscopy magazine's successful "Molecular Spectroscopy Workbench" column. From the fundamentals of important techniques to novel time- and money-saving ideas, it draws from a broad spectrum of recent developments in the field of molecular spectroscopy, including information on near and mid-range infrared techniques, optical rotation/circular dichroism, UV/Vis and fluorescence, mass spectrometry, acousto-optic tunable filters (AOTFs), fiber optics, and miscellaneous techniques and new hardware.

Gas phase molecular spectroscopy is a powerful tool for obtaining information on the geometry and internal structure of isolated molecules and their interactions with others. It enables the understanding and description, through measurements and modeling, of the influence of pressure on light absorption, emission, and scattering by gas molecules, which must be taken into account for the correct analysis and prediction of the resulting spectra. Collisional Effects on Molecular Spectra: Laboratory Experiments and Models, Consequences for Applications, Second Edition provides an updated review of current experimental techniques, theoretical knowledge, and practical applications. After an introduction to collisional effects on molecular spectra, the book moves on by taking a threefold approach: it highlights key models, reviews available data, and discusses the consequences for applications. These include areas such as heat transfer, remote sensing, optical sounding, metrology, probing of gas media, and climate predictions. This second edition also contains, with respect to the first one, significant amounts of new information, including 23 figures, 8 tables, and around 700 references. Drawing on

the extensive experience of its expert authors, Collisional Effects on Molecular Spectra: Laboratory Experiments and Models, Consequences for Applications, Second Edition, is a valuable guide for all those involved with sourcing, researching, interpreting, or applying gas phase molecular spectroscopy techniques across a range of fields Provides updated information on the latest advances in the field, including isolated line shapes, line-broadening and -shifting, line-mixing, the far wings and associated continua, and collision-induced absorption Reviews recently developed experimental techniques of high accuracy and sensitivity Highlights the latest practical applications in areas such as metrology, probing of gas media, and climate prediction

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.

Molecular Symmetry and Spectroscopy deals with the use of group theory in quantum mechanics in relation to problems in molecular spectroscopy. It discusses the use of the molecular symmetry group, whose elements consist of permutations of identical nuclei with or without inversion. After reviewing the permutation groups, inversion operation, point groups, and representation of groups, the book describes the use of representations for labeling molecular energy. The text explains an approximate time independent Schrödinger equation for a molecule, as well as the effect of a nuclear permutation or the inversion of E* on such equation. The book also examines the expression for the complete molecular Hamiltonian and the several groups of operations commuting with the Hamiltonian. The energy levels of the Hamiltonian can then be symmetrically labeled by the investigator using the irreducible representations of these groups. The text explains the two techniques to change coordinates in a Schrödinger equation, namely, (1) by using a diatomic molecule in the rovibronic Schrödinger equation, and (2) by a rigid nonlinear polyatomic molecule. The book also explains that using true symmetry, basis symmetry, near symmetry, and near quantum numbers, the investigator can label molecular energy levels. The text can benefit students of molecular spectroscopy, academicians, and investigators of molecular chemistry or quantum mechanics.

This 1972 monograph is devoted to the analysis and interpretation of the infrared and Raman spectra of solid compounds, frequently used for their identification and characterization. It was thought unsatisfactory to analyse

such spectra by the theory applicable to gas-phase samples, though this was frequently done. Furthermore, the results obtained by far infrared and laser Raman spectrometers, which detect the movement of atoms and/or molecules as a whole, had no gas-phase analogy. A separate approach to solid state vibrational spectra was therefore proposed within this volume. Dr Sherwood describes the solid state physics of vibrational spectroscopy and extends it to the more complex structures of low symmetry. He assumes an understanding of the infrared and Raman spectra of gases.

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.

The authors discuss and analyse various spectroscopic effects in relation to the interaction mechanisms of molecules with laser fields. The contents are organized according to the aspects of molecular spectra that reflect intra- and intermolecular interactions and the influence of the molecular environment. After a brief summary of molecular energy levels and spectra, the discussion centers on molecular spectroscopy, with balanced treatments of the coarse and fine structures of molecular two-photon spectra, Doppler-free spectra via nonlinear uncoupling interactions of lasers with molecules, the spectral effects of nonlinear coupling interactions of lasers with molecules, and methods of selective simplification and identification of molecular spectra. The theory is given throughout in terms of the density matrix equations. Concepts are illustrated by examples based on simple molecules.

A concise introduction to the spectroscopy of atoms and molecules. Treatment emphasizes an intuitive understanding of topics and the development of problem-solving techniques. Provides background material on time-dependent perturbation theory and second quantization, and incorporates many illustrative spectra from the literature. Examines electronic band spectra and polyatomic rotations, which makes ac-

cessible the energy levels and selection rules that govern microwave spectroscopy without recourse to detailed rotational eigenstates. Also covers triatomic molecules, aromatic hydrocarbons, lasers, multiphoton spectroscopies, and diagrammatic perturbation techniques.