

# Molecular Spectroscopy 02

Nearly all information about the Universe comes from the study of light as it reaches us. However, understanding the information contained in this light requires both telescopes capable of resolving it into its component colours and a detailed knowledge of the quantum mechanical behaviour of atoms and molecules. This book, which is based on a third-year undergraduate course taught by the author at University College London, presents the basic atomic and molecular physics necessary to understand and interpret astronomical spectra. It explains how and what kind of information

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can be extracted from these spectra. Contemporary astronomical spectra are used extensively to study the underlying atomic physics and illustrate the results.

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 accessible the energy levels and selection rules that govern microwave spectroscopy without

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recourse to detailed rotational eigenstates. Also covers triatomic molecules, aromatic hydrocarbons, lasers, multiphoton spectroscopies, and diagrammatic perturbation techniques.

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

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spectroscopy. Theoretical underpinnings are presented to the extent necessary for readers to understand how to apply spectroscopic tools to their own interests.

Molecular Spectroscopy, Second Edition

MOLECULAR STRUCTURE AND SPECTROSCOPY

Advances in Molecular Spectroscopy

An Introduction to Modern Molecular Spectroscopy. Second Edition

The first edition, by P.R. Bunker, published in 1979, remains the sole textbook that explains the use of the molecular symmetry

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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,

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symmetry groups, character tables and the Hamiltonian have been introduced. A description of the symmetry in the three-dimensional rotation group  $K(\text{spatial})$ , 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

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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. Since the publication in 1950 of Vol. I, Spectra of Diatomic Molecules of Molecular Spectra and

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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



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observation of new electronic 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

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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.

Gas phase molecular spectroscopy is a powerful

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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

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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

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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

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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

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latest practical applications in areas such as metrology, probing of gas media, and climate prediction

Collisional Effects on Molecular Spectra  
Biomedical Index to PHS-supported Research

Technical Publications  
Announcements with Indexes  
Elements Of Molecular Spectroscopy, 2nd Edition  
2nd Hungarian Conference :

Papers

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

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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



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standards, fundamental constants, atomic masses, and conversion factors of interest to spectroscopists. Spectroscopists, chemists, and researchers will find this work invaluable.

Laboratory-based pressure-broadening data has long provided information that is both of practical importance for technological applications and of fundamental interest for understanding molecular interactions and dynamics. During this project period the temperature dependence of the collision-broadened line widths of H<sub>2</sub>O and HDO were studied between 100 deg K and 600 deg K. Selected transitions were between 250 GHz and 500 GHz and the broadening gases were O<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>, and He. Low temperature

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measurements were made in a collisionally cooled cell to circumvent the limitations imposed by the low vapor pressure of the sample gas at temperatures far below their freezing points. The experimentally determined values were compared with earlier experimental and theoretical works. Introduction to Infrared and Raman Spectroscopy focuses on the theoretical and experimental aspects of infrared and Raman spectroscopy, with emphasis on detailed group frequency correlations and their vibrational origin. Topics covered include vibrational and rotational spectra, molecular symmetry, methyl and methylene groups, triple bonds and cumulated double bonds, and olefin groups. Aromatic and

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heteroaromatic rings are also considered, along with carbonyl compounds and molecular vibrations. This book is comprised of 14 chapters and begins with a discussion on the use of Raman and infrared spectroscopy to study the vibrational and rotational frequencies of molecules, paying particular attention to photon energy and degrees of freedom of molecular motion. The quantum mechanical harmonic oscillator and the anharmonic oscillator are described. The next chapter focuses on the experimental techniques and instrumentation needed to measure infrared absorption spectra and Raman spectra. Symmetry is then discussed from the standpoint of the spectroscopist. The following

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chapters explore the vibrational origin of group frequencies, with an emphasis on mechanical effects; spectra-structure correlations; and the spectra of compounds such as ethers, alcohols, and phenols. The final chapter demonstrates how the frequencies and forms of a nonlinear molecule's normal modes of vibration may be calculated mathematically. This monograph will be a useful resource for spectroscopists and physical scientists.

The Spectra and Structures of Simple Free Radicals

Fundamentals of Molecular Spectroscopy

Laser Spectroscopy

An Introduction to Molecular Spectroscopy

Revised and Enlarged Edition

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*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*

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*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.*

*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*

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*molecular spectroscopy, including information on near and midrange 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.*

*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*

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*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*



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*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.*

*Air Force Scientific Research  
Bibliography: 1950-56  
Molecular Spectroscopy  
Introduction to Infrared and*

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*Raman Spectroscopy Abstracts - Symposium on Molecular Spectroscopy Advances, Applications, and Practical Advice on Modern Spectroscopic Analysis*  
***Infrared and Raman Spectroscopy, Principles and Spectral Interpretation, Second Edition provides a solid introduction to vibrational spectroscopy with an emphasis on developing critical interpretation skills. This book fully integrates the use of both IR and Raman***

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*spectroscopy as spectral interpretation tools, enabling the user to utilize the strength of both techniques while also recognizing their weaknesses. This second edition more than doubles the amount of interpreted IR and Raman spectra standards and spectral unknowns. The chapter on characteristic group frequencies is expanded to include increased discussions of sulphur and phosphorus organics, aromatic and*

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*heteroaromatics as well as inorganic compounds. New topics include a discussion of crystal lattice vibrations (low frequency/THz), confocal Raman microscopy, spatial resolution in IR and Raman microscopy, as well as criteria for selecting Raman excitation wavelengths. These additions accommodate the growing use of vibrational spectroscopy for process analytical monitoring, nanomaterial investigations, and*

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***structural and identity determinations to an increasing user base in both industry and academia. Integrates discussion of IR and Raman spectra Pairs generalized IR and Raman spectra of functional groups with tables and text Includes over 150 fully interpreted, high quality IR and Raman reference spectra Contains fifty-four unknown IR and Raman spectra, with a corresponding answer key The Book Has 15 Chapters***

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***In All. The First Two Chapters Are Related To Atomic Structure And Atomic Spectra. The Next Chapter Is Devoted To Nature Of Chemical Bonds As Looked Upon Through Quantum Mechanics, Followed By All Types Of Spectroscopy. Every Aspect Is Explained With Some Typical Spectra. The Underlying Theory So Developed Will Help Students To Carry Out Spectral Analysis. Only Simple Quantum Mechanics Relevant To Simple Molecular Structure Has***

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***Been Given. Attempt Has Been Made To Relate The Characteristic Chemical Behavior Of These Molecules With Its Mo And Thus To Molecular Spectra. One Will Not Find Such Relationship In Any Book, But This Will Make Chemistry, As Such, Still More Interesting. Application Of Infrared And Ultra-Violet Spectroscopy, Nmr And Mass Spectra In Structure Determination Of Organic Molecules Are Very Elegantly Presented. In The***

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***Fourteenth Chapter, Lasers And Their Applications To Various Types Of Second, Third, And Fourth Order Scattering Spectroscopy Have Been Developed. The Book Has Minimum But Essential Mathematics With Very Easy Format In Its Text. Such An Approach Will Give A Clear Understanding Of The Subject And Provides Knowledge To Excel At Any Level University Examination, Competitive Examination, And Before Interview Boards.***



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*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*

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*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),*

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*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,*

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*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,*

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*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

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*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*

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***methods, concepts, models, and computational schemes described in this book.***

***June 16-20, 1997***

***Techniques and Applications***

***Modern Research***

***Government-wide Index to Federal Research & Development Reports***

***IV. Constants of Diatomic Molecules***

This work describes experimental techniques using laser spectroscopy and presents specific practical applications for this technology in many fields, including physics, engineering, chemistry, medicine

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and bioscience. The general spectroscopic features of molecules are delineated; transition metal and rare earth complexes are examined; and transition selection rules are explained.

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



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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

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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.

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

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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

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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.

Molecular Spectra and Molecular Structure  
Infrared and Raman Spectroscopy  
Molecular Spectroscopy Workbench  
Fundamentals of Molecular Spectroscopy.  
Scientific and Technical Aerospace

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### Reports

*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. Reflecting the growing volume of published work in this field, researchers will find this book an invaluable source of information on current methods and applications. Designed to serve as a textbook for postgraduate students of physics and chemistry, this second edition improves the*

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*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*

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*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*

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*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.*

*Flash Index*

*Molecules and Radiation*

*Astronomical Spectroscopy*

*Proceedings of the IVth*

*International Meeting on*

*Molecular Spectroscopy*

*Principles and Spectral*

*Interpretation*

Molecular Spectroscopy  
CRC Press

Advances in Molecular Spectroscopy, Volume 1 covers



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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.

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Part III considers the general theories on molecular spectroscopy. This topic is followed by surveys on electron energy, orbital valency, 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. It is still the only available text that presents from a consistent theoretical perspective an introduction both to classical atomic and molecular spectroscopy and to the spectroscopic advances made possible by modern optics,

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particularly laserbased methods.

Grants and Awards for the

Fiscal Year Ended ...

PROCEEDINGS- 2ND

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Molecular Spectroscopy

Research Awards Index