Optical Electric And Magnetic Properties Of Molecules

#Optical Properties Molecules #Electric Properties Molecules #Magnetic Properties Molecules #Molecules #Molec

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Optical, Electric and Magnetic Properties of Molecules

This book celebrates the career and scientific accomplishments of Professor David Buckingham, who is due to retire from his Chair at Cambridge University in 1997. The adopted format comprises reprints of a number of David Buckingham's key scientific papers, each one or two of these preceded by a review of the corresponding area of David's wide-ranging research interest. Each reviewer is recognised as an expert in that field of interest and has some close association with David Buckingham, as a scientific colleague and/or a former research student. The book should serve as a distinctive reference source, both retrospective and prospective, for the field of chemical physics with which the name A.D. Buckingham is associated. The editors opted to reprint a majority of early classic Buckingham papers, balanced by some of David Buckingham's more recent publications. Reprinted papers have been placed into a general scientific context that covers prior influences on, and later impacts by, the work nominated for review.

Magnetism

Combining the contemporary knowledge from widely scattered sources, this is a much-needed and comprehensive overview of the field. In maintaining a balance between theory and experiment, the book guides both advanced students and specialists to this research area. Topical reviews written by the foremost scientists explain recent trends and advances, focusing on the correlations between electronic structure and magnetic properties. The book spans recent trends in magnetism for molecules -- as well as inorganic-based materials, with an emphasis on new phenomena being explored from both experimental and theoretical viewpoints with the aim of understanding magnetism on the atomic scale. The volume helps readers evaluate their own experimental observations and serves as a basis for the design of new magnetic materials. Topics covered include: * Metallocenium Salts of Radical Anion

Bis-(dichalcogenate) metalates * Chiral Molecule-Based Magnets * Cooperative Magnetic Behavior in Metal-Dicyanamide Complexes * Lanthanide Ions in Molecular Exchange Coupled Systems * Monte Carlo Simulation * Metallocene-Based Magnets * Magnetic Nanoporous Molecular Materials A unique reference work, indispensable for everyone concerned with the phenomena of magnetism.

Non-Linear Optical Response in Atoms, Molecules and Clusters

The aim of this brief is to present, in sufficient detail, a non-perturbative technique for calculating optical hyperpolarizabilities. The ability to efficiently compute hyperpolarizabilities, for a variety of different molecular systems, makes this brief invaluable for those engaged in the computational design of new electro-optical materials. The resulting computation is very predictable and suitable for automation, in contrast to perturbative methods that typically rely on iterative methods. The methodology which is wholly applicable to atoms, molecules, clusters (and with some modifications) to condensed matter, is described and illustrated at a level that is accessible to theoreticians and supplemented with details that should be of interest to practitioners.

Electrical, Optical, and Magnetic Properties of Organic Solid-state Materials V

This volume, the fifth in a popular series, features papers related to the development and utilization of materials with novel electrical, optical or magnetic properties. The field has experienced tremendous growth in the past years, and this volume provides a forum for materials scientists, chemists, physicists and engineers to assess the progress. In particular, light-emitting materials for displays are showing great promise for widespread commercialization. Developments in molecular engineering and self assembly, as well as in conducting polymers, are enabling better performance and greater scientific understanding of the phenomena underlying these advances. Improvements in electro-optic, photorefractive and two-photon absorbing materials are also being realized and are addressed here.

Electronic and Magnetic Properties of Chiral Molecules and Supramolecular Architectures

Time-dependent density functional response theory for electronic chiroptical properties of chiral molecules; by Jochen Autschbach, Lucia Nitsch–Velasquez, and Mark Rudolph * Chiroptical Properties of Charge-Transfer Compounds; by Yoshihisa Inoue, Tadashi Mori * G-C content independent long-range charge transfer through DNA; by Tetsuro Majima * Induced chirality in porphiryn aggregates: the role of weak and strong interactions; by Roberto Purrello * Vibrational circular dichroism spectroscopy of chiral molecules in solution; by Yunjie Xu * Magneto-electric properties of self-assembled monolayers of chiral molecules; by Zeev Vager and Ron Naaman * Theory of adsorption induced chirality and electron transfer through chiral systems; by Spiros Skourtis and David Beratan * Chiral-selective surface chemistry induced by spin-polarized secondary electrons; by Richard Rosenberg

Theory of Magnetic and Electric Susceptibilities for Optical Frequencies

Introduces an original model of the interaction between light and matter. Explains the new optical magnitudes, such as magnetic and electric susceptibilities for optical frequencies, and shows how they can obtain new correlations between the index of refraction and absorption of light, and molecular structure. The basic principle is that a substanc

Conducting and Magnetic Organometallic Molecular Materials

For several years, the two parallel worlds of Molecular Conductors in one hand and Molecular Magnetism in the other have grown side by side, the former essentially based on radical organic molecules, the latter essentially based on the high spin properties of metal complexes. Over the last few years however, organometallic derivatives have started to play an increasingly important role in both worlds, and have in many ways contributed to open several passages between these two worlds. This volume recognizes this important emerging evolution of both research areas. It is not intended to give a comprehensive view of all possible organometallic materials, and polymers for example were not considered here. Rather we present a selection of the most recent research topics where organometallic derivatives were shown to play a crucial role in the setting of conducting and/or magnetic properties in crystalline materials. First, the role of organometallic anions in tet- thiafulvalenium-based molecular conductors is highlighted by Schlueter, while Kubo and Kato describe very recent ortho-metalated chelating ligands appended to the TTF core and their conducting salts. The combination of conducting and magnetic properties and the search for p—d interactions are analyzed in two comp- mentary contributions by

Myazaki and Ouahab, while Valade focuses on the only class of metal bis(dithiolene) complexes to give rise to superconductive molecular materials, in association with organic as well as organometallic cations.

The Theory of the Electric and Magnetic Properties of Molecules

Molecular Electromagnetism aims to provide a fundamental understanding of the electromagnetic properties of molecules and molecular systems. Electric, magnetic, dielectric optical and spectroscopic properties are all discussed as are selected basic principles of spectroscopy. The book begins with a treatment of basic electromagnetism, working up to Maxwell's equations and electromagnetic radiation. A classical account of electromagnetic properties is then given. Finally the quantum- mechanical origins of electromagnetic properties are treated, building on a detailed treatment of the change of quantum state under external perturbations such as electromagnetic fields.

Molecular Electromagnetism

The MRS Symposium Proceeding series is an internationally recognised reference suitable for researchers and practitioners.

Electrical, Optical, and Magnetic Properties of Organic Solid State Materials: Volume 328

Handbook of Magnetic Materials, Volume 26, covers the expansion of magnetism over the last few decades and its applications in research, notably the magnetism of several classes of novel materials that share the presence of magnetic moments with truly ferromagnetic materials. The book is an ideal reference for scientists active in magnetism research, providing readers with novel trends and achievements in magnetism. Each article contains an extensive description given in graphical, as well as, tabular form, with much emphasis placed on the discussion of the experimental material within the framework of physics, chemistry and material science. Comprises topical review articles written by leading authorities Includes a variety of self-contained introductions to a given area in the field of magnetism without requiring recourse to the published literature Introduces given topics in the field of magnetism Describes novel trends and achievements in magnetism

Handbook of Magnetic Materials

Time-dependent density functional response theory for electronic chiroptical properties of chiral molecules; by Jochen Autschbach, Lucia Nitsch–Velasquez, and Mark Rudolph * Chiroptical Properties of Charge-Transfer Compounds; by Yoshihisa Inoue, Tadashi Mori * G-C content independent long-range charge transfer through DNA; by Tetsuro Majima * Induced chirality in porphiryn aggregates: the role of weak and strong interactions; by Roberto Purrello * Vibrational circular dichroism spectroscopy of chiral molecules in solution; by Yunjie Xu * Magneto-electric properties of self-assembled monolayers of chiral molecules; by Zeev Vager and Ron Naaman * Theory of adsorption induced chirality and electron transfer through chiral systems; by Spiros Skourtis and David Beratan * Chiral-selective surface chemistry induced by spin-polarized secondary electrons; by Richard Rosenberg

Electronic and Magnetic Properties of Chiral Molecules and Supramolecular Architectures

Molecular magnetism is a new field of research dealing with the synthesis and study of the physical properties of molecular assemblies involving open-shell units. It is essentially interdisciplinary, joining together organic, organometallic and inorganic chemists, as well as theoreticians, physicists and materials scientists. At the core of research into molecular magnetism lie design and synthesis of new molecular assemblies exhibiting bulk properties such as long-range magnetic ordering or bistability with an hysteresis effect, which confers a memory effect on the system. In such terms, magnetism may be considered a supramolecular function. The first eight contributions to this volume present the state of the art in organic supramolecular chemistry, emphasising interlocked systems and molecular trees. The following six articles are devoted to molecular materials constructed from organic radicals and transition metal units. Molecular bistability is then focused on, followed by metal-organic and coordination magnetic materials. A new approach to nano-sized particles closes the work.

Magnetism: A Supramolecular Function

This book shows that research involving electrical, optical and magnetic properties of organic solid-state materials continues to grow both in scope and technological importance. Early studies of

charge transport in conducting polymers have evolved from the elucidation of fundamental structure/function relationships to applications such as batteries, simple electrical devices such as diodes, chemical sensors, antistatic coatings, microwave and millimeter wave-absorbing materials, and photochromic devices. A particularly exciting evolution has been the discovery and development of organic light-emitting diodes (OLEDs) which appear to be nearing commercialization in an amazingly short period of time. This application is of particular interest because both electrical and optical properties must be considered. Topics include: organic light-emitting materials and devices; photonic materials and devices; conducting and electroactive polymers and materials; molecular and supramolecular engineering; organic metals and magnetic materials and poster presentations.

Electrical, Optical and Magnetic Properties of Organic Solid-State Materials IV: Volume 488

The papers collected in this volume in honor of the late StanisBaw Kielich cover an impressive range of modern subjects in molecular science. These subjects include, among others, the nonlinear optics of molecules, new approaches to the electronic structure of large molecules, the properties of carbon nanotubes, fluorescence polarization spectroscopy, computational studies of systems of fundamental interest to collision-induced spectroscopy, the simulation of fluids, NLO materials, chemical bonding in complex molecules, the NLO properties of functionalized DNA and the magnetic properties of molecular assemblies. Written by eminent specialists, the papers should offer valuable guidance to a wide community of graduate students and researchers.

Atomic and Molecular Nonlinear Optics: Theory, Experiment and Computation

The first reference on this rapidly growing topic provides an essential up-to-date guide to current and emerging trends. A group of international experts has been carefully selected by the editors to cover all the central aspects, with a focus on molecular species while also including industrial applications. The resulting unique overview is a must-have for researchers, both in academia and industry, who are entering or already working in the field.

Lanthanides and Actinides in Molecular Magnetism

This book discusses the effect of the excitation of rotational, vibrational, and electronic degrees of freedom on the basic electrical properties of molecules and, as a consequence, on molecular optical and transport properties together with reactivity. It additionally summarizes the theory and practice of calculating state-specific electric and optical properties based on ab initio quantum chemical calculations. The book offers a clear, up-to-date review and is primarily intended for actively working researchers, graduate students, and advanced undergraduates who are interested in the electric and related properties of the electronically, rotationally, and vibrationally excited molecules.

Influence of Internal Degrees of Freedom on Electric and Related Molecular Properties

Quantum-mechanical theories -- Perturbation and variation methods -- Electric and magnetic moments -- Polarizabilities and susceptibilities -- Spin Interactions -- The effect of radiation in electric and magnetic fields -- Appendix I : Classical electrodynamics -- Appendix II : The multipole expansion.

Linear and Nonlinear Optical Properties of Molecules

Magnetic Oxides offers a cohesive up-to-date introduction to magnetism in oxides. Emphasizing the physics and chemistry of local molecular interactions essential to the magnetic design of small structures and thin films, this volume provides a detailed view of the building blocks for new magnetic oxide materials already advancing research and development of nano-scale technologies. Clearly written in a well-organized structure, readers will find a detailed description of the properties of magnetic oxides through the prism of local interactions as an alternative to collective electron concepts that are more applicable to metals and semiconductors. Researchers will find Magnetic Oxides a valuable reference.

The Theory of the Electric and Magnetic Properties of Molecules

Investigating the relationship between the magnetic properties and structure of molecules, molecular magnetochemistry, is an area of growing interest to scientists in a variety of fields, including physical, organic and inorganic chemistry, molecular physics, and biophysics. For the first time, systematic results on magnetic properties of molecules such as mean magnetic susceptibility, their anisotropies

and principal magnetic axes are presented. Molecular Magnetochemistry is a comprehensive and up-to-date view on experimental methods not covered in previous volumes, including the Zeeman effect in vapor phase and magnetic birefringence of diamagnetic systems (Cotton-Mouton Effect). The relationship between magnetic and related electrical phenomena is also described, summing up experimental data on magnetic and electrical anisotropies and components of molecular quadrupole moments.

Magnetic Oxides

acids. The achievements of molecular biology testify to the success of material science in a realm which, until recently, appeared totally enig matic and mysterious. Further scientific developments should bring to mankind vast developments both in theoretical knowledge and in practical applications, namely, in agriculture, medicine, and technology. The purpose of this book is to explain molecular biophysics to all who might wish to learn about it, to biologists, to physicists, to chemists. This book contains descriptive sections, as well as sections devoted to rigorous mathematical treatment of a number of problems, some of which have been studied by the author and his collaborators. These sections may be omitted during a first reading. Each chapter has a selected bibliography. This book is far from an exhaustive treatise on molecular biophysics. It deals principally with questions related to the structures and functions of proteins and nucleic acids. M. V. Vol'kenshtein Leningrad, September, 1964 3 Molecular Biophysics 9 Thermodynamics and Biology......

Molecular Magnetochemistry

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 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 lnorganic, 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.

Molecules and Life

Papers written during the last 40 years by Claude Cohen-Tannoudji and his collaborators on various physical effects which can be observed on atoms interacting with electromagnetic fields.

Dielectric and Related Molecular Processes

This textbook can be used to teach electromagnetism to a wide range of undergraduate science majors in physics, electrical engineering or materials science. By making lesser demands on mathematical knowledge than typical texts, and by emphasizing electromagnetic properties of materials and their applications, this text is particularly appropriate for students of materials science. Many competing books focus on the study of propagation waves either in the microwave or optical domain, whereas

Basic Electromagnetism and Materials covers the entire electromagnetic domain and the physical response of materials to these waves.

Atoms in Electromagnetic Fields

Ranging from the physics of elementary particles to the structure of viruses, the subject matter of this book stresses the importance of optical activity and chirality in modern science and will be of interest to a wide range of scientists. Using classical and quantum methods with a strong emphasis on symmetry principles, the volume develops the theory of varied optical activity and related phenomena from the perspective of molecular scattering of polarized light. First Edition Hb (1983): 0-521-24602-4

Basic Electromagnetism and Materials

Existing texts on liquid theory are limited to simple liquids of spherical molecules, but nearly all liquids of practical interest have molecules that are non-spherical, resulting in more diverse phenomena. This text is the first to provide the molecular theory for such liquids, and describes applications to a wide range of physical properties.

Theory and Applications of Molecular Paramagnetism

This volume brings together selected contributed papers presented at the International Conference of Computational Methods in Science and Engineering (ICCMSE 2006), held in Chania, Greece, October 2006. The conference aims to bring together computational scientists from several disciplines in order to share methods and ideas. The ICCMSE is unique in its kind. It regroups original contributions from all fields of the traditional Sciences, Mathematics, Physics, Chemistry, Biology, Medicine and all branches of Engineering. It would be perhaps more appropriate to define the ICCMSE as a conference on computational science and its applications to science and engineering. Topics of general interest are: Computational Mathematics, Theoretical Physics and Theoretical Chemistry. Computational Engineering and Mechanics, Computational Biology and Medicine, Computational Geosciences and Meteorology, Computational Economics and Finance, Scientific Computation, High Performance Computing, Parallel and Distributed Computing, Visualization, Problem Solving Environments, Numerical Algorithms, Modelling and Simulation of Complex System, Web-based Simulation and Computing, Grid-based Simulation and Computing, Fuzzy Logic, Hybrid Computational Methods, Data Mining, Information Retrieval and Virtual Reality, Reliable Computing, Image Processing, Computational Science and Education etc. More than 800 extended abstracts have been submitted for consideration for presentation in ICCMSE 2005. From these 500 have been selected after international peer review by at least two independent reviewers.

Molecular Light Scattering and Optical Activity

Molecular magnets show many properties not met in conventional metallic magnetic materials, id est low density, transparency to electromagnetic radiation, sensitivity to external stimuli such as light, pressure, temperature, chemical modification or magnetic/electric fields, and others. They can serve as "functional" materials in sensors of different types or be applied in high-density magnetic storage or nanoscale devices. Research into molecule-based materials became more intense at the end of the 20th century and is now an important branch of modern science. The articles in this Special Issue, written by physicists and chemists, reflect the current work on molecular magnets being carried out in several research centers. Theoretical papers in the issue concern the influence of spin anisotropy in the low dimensional lattice of the resulting type of magnet, as well as thermodynamics and magnetic excitations in spin trimers. The impact of external pressure on structural and magnetic properties and its underlying mechanisms is described using the example of Prussian blue analogue data. The other functionality discussed is the magnetocaloric effect, investigated in coordination polymers and high spin clusters. In this issue, new molecular magnets are presented: (i) ferromagnetic high-spin [Mn6] single-molecule magnets, (ii) solvatomagnetic compounds changing their structure and magnetism dependent on water content, and (iii) a family of purely organic magnetic materials. Finally, an advanced calorimetric study of anisotropy in magnetic molecular superconductors is reviewed.

Theory of Molecular Fluids

This thesis demonstrates the novel magnetic functionalities in cyanido-bridged metal assemblies, and as such appeals to readers in the field of materials science. The utilization of octacyanidometalates

as building blocks enables the observation of (i) photo-induced magnetization due to a light-induced spin-crossover in an iron octacyanidoniobate-based assembly, (ii) photo-induced magnetization with a two-step spin-crossover behavior in an iron octacyanidoniobate-based material, and (iii) the coexistence of super-ionic conductivity and metamagnetism in a manganese-octacyanoniobate system. These multi-functionalities are achieved by incorporating a spin-crossover moiety or a hydrogen-bonding network into a cyanido-bridged network structure with a strong magnetic interaction. In particular, in light-induced spin-crossover magnets, a magnetically non-ordered state can be altered to a magnetically ordered state by photo-irradiation, which is one of the attractive mechanisms for novel optical switching devices.

Recent Progress in Computational Sciences and Engineering (2 vols)

Molecular systems are assemblies of molecules designed to possess special qualities and desired functionality. Such systems are important because they provide materials with novel properties, and they will be particularly useful for minimizing electronic devices. Molecular systems often form organized molecular crystals, polymers, or thin films that are significantly more complex than current materials. To provide a sound basis for understanding these levels of complexity, this book provides an analysis of the fundamentals of electronic structures, dynamic processes in condensed phases, and the unique properties of organic molecular solids and the environmental effects on these properties. Also covered are the latest methods in physical chemistry that are particularly useful for deriving and controlling the functionality of molecular systems. A second volume subtitled From Molecular Systems to Molecular Devices is also being published.

Some Optical Properties of Molecules

Presented here is a discussion of the measurement and interpretation of diamagnetism and optics of molecular crystals.

Molecular Magnets

This book is an in-depth review of experiment and theory on electric-dipole polarizabilities. It is broad in scope, encompassing atomic, molecular, and cluster polarizabilities. Both static and dynamic polarizabilities are treated (in the absence of absorption) and a full tensor picture of the polarizability is used. Traditional experimental techniques for measuring electric polarizabilities are described in detail. Recently developed experimental methods, including light forces, position-sensitive time-of-flight deflection, and atom interferometry, are also extensively discussed. Theoretical techniques for calculating polarizabilities are reviewed, including a discussion on the use of Gaussian basis sets. Many important comparisons between theory and experiment are summarized in an extensive set of tables of polarizabilities of important atoms, molecules, and clusters. Applications of polarizabilities to many areas of chemistry and physics are described, including optics, chemical structure, interactions of gases and particles with surfaces, and the interaction of molecules with light. The emphasis is on a lucid presentation of the ideas and results with up-to-date discussions on important applications such as optical tweezers and nanostructure fabrication. This book provides an excellent overview of the importance of polarizabilities in understanding the physical, electronic, and optical properties of particles in a regime that goes from free atoms to condensed-phase clusters.

Multifunctional Molecular Magnets Based on Octacyanidometalates

This book, Introduction to Optics I: Interaction of Light with Matter, is the first book in a series of four covering the introduction to optics and optical components. The author's targeted goal for this series is to provide clarity for the reader by addressing common difficulties encountered while trying to understand various optics concepts. This first book is organized and written in a way that is easy to follow, and is meant to be an excellent first book on optics, eventually leading the way for further study. Those with technical backgrounds as well as undergraduate students studying optics for the first time can benefit from this book series. The current book includes three chapters on light and its characteristics (Chapter 1), on matter from the standpoint of optics (Chapter 2), and on the interaction of light with matter (Chapter 3). Among the characteristics of light, the ones characterizing its speed, color, and strength are covered. The polarization of light will be covered in the next book of the series, where we discuss optical components. Chapter 2 discusses various atomic and molecular transitions activated by light (optical transitions). Different kinds of natural bulk material media are described: crystalline and amorphous, atomic and molecular, conductive and insulating. Chapter 3 on the interaction of light

with matter describes naturally occurring phenomena such as absorption, dispersion, and nonlinear optical interactions. The discussion is provided for the natural bulk optical materials only. The interfaces between various materials will be covered in the next book on optical components. The following three books of the series are planned as follows. In the second book, we will focus on passive optical components such as lenses, mirrors, guided-wave, and polarization optical devices. In the third book, we will discuss laser sources and optical amplifiers. Finally, the fourth book in the series will cover optoelectronic devices, such as semiconductor light sources and detectors.

From Molecules to Molecular Systems

This book explains the theory and methods by which gas molecules can be polarized by light, a subject of considerable importance for what it tells us about the electronic structure of molecules and properties of chemical reactions. Starting with a brief review of molecular angular momentum, the text goes on to consider resonant absorption, fluorescence, photodissociation and photoionization, as well as collisions and static fields. A variety of macroscopic effects are considered, among them angular distribution and the polarization of emitted light, ground state depopulation, laser-induced dichroism, the effect of collisions and external magnetic and electric field effects. Most examples in the book are for diatomic molecules, but symmetric-top polyatomic molecules are also included. The book concludes with a short appendix of essential formulae, tables for vector calculus, spherical functions, Wigner rotation matrices, Clebsch-Gordan coefficients, and methods for expansion over irreducible tensors.

Magnetism and Optics of Molecular Crystals

This brief investigates the diradical character, which is one of the ground-state chemical indices for "bond weakness" or "electron correlation" and which allows researchers to explore the origins of the electron-correlation-driven physico-chemical phenomena concerned with electronic, optical and magnetic properties as well as to control them in the broad fields of physics and chemistry. It then provides the theoretical fundamentals of ground and excited electronic structures of symmetric and asymmetric open-shell molecular systems by using model molecular systems. Moreover, it presents the theoretical design guidelines for a new class of open-shell singlet molecular systems for nonlinear optics (NLO) and singlet fission.

Electric-dipole Polarizabilities of Atoms, Molecules, and Clusters

With the central importance of electric polarizability and hyperpolarizability for a wide spectrum of activities, this book charts the trends in the accurate theoretical determination of these properties in specialized fields. The contributions include reviews and original papers that extend from methodology to applications in specific areas of primary importance such as cluster science and organic synthesis of molecules with specific properties./a

Introduction to Optics I

Molecular and Colloidal Electro-Optics presents cohesive coverage from internationally recognized experts on new approaches and developments in both theoretical and experimental areas of electro-optic science. It comprises a well-integrated yet multi-disciplinary treatment of fundamental principles, strategies, and applications of electro-op

Optical Polarization of Molecules

Excitation Energies and Properties of Open-Shell Singlet Molecules