The Jahn Teller Effect In C60 And Other Icosahedral Comple 1st Edition By Chancey C C Obrien M Cm 1997 Hardcover

Providing a general approach to understanding the properties of molecules and crystals and their origins, the Jahn-Teller effect is a fascinating phenomena in modern physics and chemistry. Its effect inspired one of the most important recent scientific discoveries--the concept of high-temperature superconductivity. This comprehensive volume presents the background of the theory and its key applications in physics and chemistry, as well as more recent achievements.

It is an introductory, reference handbook that summarizes terms and definitions, most important phenomena, regulations, experimental and theoretical tools discovered in physics, chernistry, technology and lhe application of nanostructures. We present a representative collection of fundamental terms and most important supporting definitions taken from general physics and quantum mechanics, material science and technology, mathematics and information theory, organic and inorganic chemistry, solid state physics and biology. As a result, fast progressing nanoelectronics and optoelectronics, molecular electronics and spintronics, nano- fabrication and -manufacturing, bioengineering and quantum processing of information, an area of fundamental importance for lhe information society of lhe 21st century, are covered. More than 1300 entries, from a few sentences to a page in length, are given, for beginners to professionals. Nanotechnology.

Edited by Nobel Prize-winner Ilya Prigogine and renowned authority Stuart A. Rice, the Advances in Chemical Physics series provides a forum for critical, authoritative evaluations in every area of the discipline. In a format that encourages the expression of individual points of view, experts in the field present comprehensive analyses of subjects of interest. This stand-alone, special topics volume, edited by Gert D. Billing of the University of Copenhagen and Michael Baer of the Soreq Nuclear Research Center in Yavne, Israel, reports recent advances on the role of degenerate states in chemistry. Volume 124 collects innovative papers on "Complex States of Simple Molecular Systems," "Electron Nuclear Dynamics," "Conical Intersections and the Spin-Orbit Interaction," and many more related topics. Advances in Chemical Physics remains the premier venue for presentations of new findings in its field.

Recent advances in experimental techniques now enable researchers to produce in a laboratory clusters of atoms of desired composition from any of the elements of the periodic table. This has created a new area of research into novel materials since clusters cannot be regarded either as a "large" molecule or as a fragment of the bulk. Both experimental and theoretical studies are revealing unusual properties that are not ob served in solid state environments. The structures of micro-clusters are found to be significantly distorted from the most symmetric arrangement, some even exhibiting pentagonal symmetry commonly found in icosahedric structures. The unusual stability of certain clusters, now described as "magic number species", shows striking similarities with the nuclear shell structure. The relative stabilities of clusters depend not only on the composition of the clusters but also on their charged states. The studies on spontaneous fragmentation of mUltiply charged clusters, commonly referred to as Coulomb explosion, illustrate the role of electronic bonding mechanisms on stability of clusters. The effect of foreign atoms on geometry and stability of clusters and the interaction of gas atoms with clusters are showing promise for an indepth understanding of chemisorption and catalysis. The magnetic and optical properties are dependent not only on cluster size but also on its geometry. These findings have the potential for aiding industry in the area of micro-electronics and catalysis.

Transition Metal Compounds

Dedicated to Prof. K. A. Müller on the Occasion of his 90th Birthday

Electrons in Solids

What is What in the Nanoworld

Principles of Inorganic Chemistry

Metal-Ligand Bonding

This book is based mostly on the reports presented at the XVth International lahn-Teller Symposium on Vibronic Interactions in Crystals and Molecules and NATO Advanced Research Workshop Colossal Magnetoresistance and Vibronic Interactions that took place at Boston on August 16-22 of the year 2000. This is the first time the Symposium took place in the USA where recently the giant splash of the attention to the 1 ahn-Teller effect occurred. This tremendous interest to the field all over the world is reflected not only in the numerous publications in many American and European 10urnals, but of the leading scientists from additionally in the Symposium's participation the well known Universities, National Laboratories and industrial companies, which was the largest in the history of the Symposium. The renaissance of the 1ahn-Teller physics is closely related to the three fundamental discoveries in science. The most significant among them is the discovery of high-Tc superconductivity by K. -A. Muller and G. Bednorz, for whom the "1ahn-Teller idea" was the motivation in their search. The result of this search is well known - a wide spectrum of the 1ahn-Teller ion based materials with Tc between 24K and 135K were found. The second discovery is the existence of a new polymorph of carbon - the C60. The microscopic analysis of all physical, chemical and biological properties of the buckyballs is based on 1ahn-Teller type of interactions. The third is colossal magnetoresistance.

The Jahn-Teller effect continues to be a paradigm for structural instabilities and molecular dynamical processes. This volume provides a survey of the current Jahn-Teller interactions at the interface of quantum chemistry and condensed matter physics.

Chemical physics is presently a very active field, where theoretical computation and accurate experimentation have led to a host of exciting new results. Among these are the possibility of state-to-state reactive scattering, the insights in non-adiabatic chemistry, and, from the computational perspective, the use of explicitly correlated functions in quantum chemistry. Many of these present-day developments use ideas, derivations and results that were obtained in the very early days of quantum theory, in the 1920s and 1930s. Much of this material is hard to study for readers not familiar with German. This volume presents English translations of some of the most important papers. The choice of material is made with the relevance to present-day researchers in mind. Included are seminal papers by M. Born and J.R. Oppenheimer, J. von Neurmann and E. Wigner, E.A. Hylleraas, F. London, F. Hund, H.A. Kramers, R. de L. Kronig and F. Huckel, among others.

INTRODUCING A POWERFUL APPROACH TO DEVELOPING RELIABLE QUANTUMMECHANICAL TREATMENTS OF A LARGE VARIETY OF PROCESSES IN MOLECULARSYSTEMS. The Born-Oppenheimer approximation has been fundamental tocalculation in molecular spectroscopy and molecular dynamics sincethe early days of quantum mechanics. This is despitewell-established fact that it is often not valid due to conicalintersections that give rise to strong nonadiabatic effects causedby singular nonadiabatic coupling terms (NACTs). In BeyondBorn-Oppenheimer, Michael Baer, a leading authority on molecularscattering theory and electronic nonadiabatic processes, addressesthis deficiency and introduces a rigorousapproach--diabatization--for eliminating troublesome NACTs andderiving well-converged equations to treat the interactions withinand between molecules. Concentrating on both the practical and theoretical aspects ofelectronic nonadiabatic transitions in molecules, Professor Baeruses a simple mathematical language to rigorously eliminate thesingular NACTs and enable reliable calculations of spectroscopicand dynamical cross sections. He presents models of varyingcomplexity to illustrate the validity of the theory and exploresthe significance of the study of NACTs and the relationship betweenmolecular physics and other fields in physics, particularlyelectrodynamics. The first book of its king Beyond Born-Oppenheimer: * Presents a detailed mathematical framework to treat electronicNACTs and their conical intersections * Describes the Born-Oppenheimer treatment, including the conceptsof adiabatic and diabatic frameworks * Introduces a field-theoretical approach to calculating NACTs,which offers an alternative to time-consuming ab initioprocedures * Discusses various approximations for treating a large system ofdiabatic Schrödinger equations * Presents numerous exercises with solutions to further clarify thematerial being discussed Beyond Born-Oppenheimer is required reading for physicists,physical chemists, and all researchers involved in the quantummechanical study of molecular systems.

Physics and Chemistry of Small Clusters

Electron-phonon Dynamics And Jahn-teller Effect - Proceedings Of The Xiv International Symposium

Quantum Chemistry

Time-Reversal Symmetry

Theory and Experimental Evidences

Electronic Nonadiabatic Coupling Terms and Conical Intersections

Great importance has been placed on the development of new technologies for the synthesis of nanoparticles and nanostructured materials, which are profitable for industrial production and environmentally safe. As such, in Fluorite: Structure, Chemistry and Applications, crystal structure of fluorites, point defects, specific properties, innovative methods of nanopowders synthesis and properties of ceria-based materials are discussed. Next, the dispersion and attenuation of ultrasonic bulk modes in cubic crystals is described in the framework of a phenomenological approach, whereas the contribution of the subsystem of Jahn-Teller complexes is presented through microscopic theory and Jahn-Teller effect problems.Lastly, the authors review the substitution strategies that have been attempted to introduce mixed conductivity into fluorite zirconia materials, the solubility of such transition metal dopants and the resultant electrical properties. Potential mixed conducting ternary systems are discussed.

Alkali-doped fullerides have attracted strong interest since their production became possible about fifteen years ago. This book presents recent work which may solve intriguing problems arising from a variety of remarkable properties. For example, these solids are superconductors with high transition temperatures, although the similarity between the electronic and phonon energy scales should suppress superconductivity. Moreover, the Ioffe-Regel condition for electrical conductivity is strongly violated. The book shows why superconductivity is nevertheless possible, owing to a local pairing mechanism. The Ioffe-Regel condition is derived quantum-mechanically, and it is explained why the underlying assumptions are violated for fullerides and high-c cuprates, for example. The book treats electronic and transport properties, reviewing theoretical and experimental results. It focuses on superconductivity, electrical conductivity and metal-insulator transitions, emphasizing the electron-electron and electron-phonon interactions as well as the Jahn-Teller effect.

This book describes all aspects of the physics of transition metal compounds, providing a comprehensive overview of this diverse class of solids. Set within a modern conceptual framework, this is an invaluable, up-to-date resource for graduate students, researchers and industrial practitioners in solid-state physics and chemistry, materials science, and inorganic chemistry.

Uniquely describes both the crystallography and properties of perovskite related materials. Practical applications in solar cells, microelectronics and telecommunications Interdisciplinary topic drawing on materials science, chemistry, physics, and geology Contains problems and answers to enhance knowledge retention

The Jahn-Teller Effect in Molecules and Crystals

When a Boson meets a Fermion

Alkali-doped Fullerides

Vibronic Interactions: Jahn-Teller Effect in Crystals and Molecules

The Role of Degenerate States in Chemistry, Volume 124

New Aspects of the Jahn-Teller Effect in Tetrahedral Systems

The first half of the title of this book may delude the uninitiated reader. The term "'Jahn-Teller effect," taken literally, refers to a special effect inherent in particular molecular systems. Actually, this term implies a new approach to the general problem of correlations between the structure and properties of any molecular polyatomic system, including solids. Just such a new approach, or concept (in some sense, a new outlook or even a new way of thinking), which leads not to one special effect but to a series of different effects and laws, is embodied in the many (~ 4000) studies devoted to the investigation and application of the Jahn-Teller effect. The term "vibronic interactions" seems to be most appropriate to the new concept, and this explains the origin of the second half of the title. The primary objective of this book is to present a systematic develop ment of the concept of vibronic interactions and its applications, and to illustrate its possibilities and significance in modern chemistry. In the first three chapters (covering about one-third of the book) the theoretical background of the vibronic concept and Jahn-Teller effect is given. The basic ideas are illustrated fully, although a comprehensive presentation of the theory with all related mathematical deductions is beyond the scope of this book. In the last three chapters the applications of theory to spectro scopy, stereochemistry and crystal chemistry, reactivity, and catalysis, are illustrated by a series of effects and laws.

With more than 40% new and revised materials, this second edition offers researchers and students in the field a comprehensive understanding of fundamental molecular properties amidst cutting-edge applications. Including ~70 Example-Boxes and summary notes, questions, exercises, problem sets, and illustrations in each chapter, this publication is also suitable for use as a textbook for advanced undergraduate and graduate students. Novel material is introduced in description of multi-orbital chemical bonding, spectroscopic and magnetic properties, methods of electronic structure calculation, and quantum-classical modeling for organometallic and metallobiochemical systems. This is an excellent reference for chemists, researchers and teachers, and advanced undergraduate and graduate students in inorganic, coordination, and organometallic chemistry.

This book introduces vibronic coupling density and vibronic coupling constant analyses as a way to understand molecular structure and chemical reactions. After quantum study, the behavior of electrons circulating around nuclei led to the principal concept that underlies all explanations in chemistry. Many textbooks have given plausible explanations to clarify molecular structure—for example, the bond elongation of ethylene under anionization and the nonplanar structure of ammonia. Frontier molecular orbital concepts were proposed to visualize the path of chemical reactions, and conventional explanations gave students a familiarity with molecular structures in terms of the electronic state. By contrast, this book offers a more rational and more convincing path to understanding. It starts from the ab initio molecular Hamiltonian and provides systematic, rational approaches to comprehend chemical phenomena. In this way, the book leads the reader to a grasp of the quantitative evaluation of the force applied under the molecular deformation process. As well, guidelines are offered for integrating the traditional “hand-waving” approach of chemistry with more rational and general VCD and VCC alternatives along with the outlook for newly functionalized chemical systems.

Optical Spectra of Transparent Rare Earth Compounds investigates the optical spectra of transparent rare earth (RE) compounds such as europium chalcogenides. Emphasis is placed on the underlying physics in selected examples, and theoretical results are usually presented without proof in a form that allows their application to the interpretation of experimental data. This book is comprised of 11 chapters and begins with an overview of the spectra of RE ions in ionic crystals, paying particular attention to the sharpness of many lines in the absorption and emission spectra. How these very narrow lines arise, what interactions determine their energy, and how they can be used to investigate particular properties of the solid state are explained in detail. Subsequent chapters explore the energy structure of RE free ions in solids; trivalent RE ions in a static crystal field and in a phonon field; magnetic interactions and hyperfine interactions; and Jahn-Teller systems. The absorption spectra of europium chalcogenides are also considered, along with REs in glasses and RE lasers. This monograph is written primarily for solid state physicists and those who need an overall view of the basic features of rare earth spectra in transparent solids, such as new workers.

Vibronic Coupling Density

Hybrid Organic-Inorganic Perovskites

Fundamentals and Implications for Physics and Chemistry

Atomic and Molecular Photoabsorption

Theory and Applications

Classic Scientific Papers

Earlier books have discussed the theory of Jahn-Teller interactions in lower symmetry structures (e.g. cubic, tetrahedral, tetragonal, and trigonal); this is the first that focuses on the new icosahedral systems, whose most famous example is Buckminster-fullerene, C[subscript]60.

This is a standard work on defects in solids, an important subject in materials science.

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 Schr ö dinger 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 Schr ö dinger equation, namely, (1) by using a diatomic molecule in the rovibronic Schr ö dinger 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 symposium was a dedication to John L Hall, who was recently awarded the Nobel Prize in Physics, (report below). The symposium was a celebration of his striking career in physics and his impressive record of achievements. Papers included in this volume offer brief and personal glimpses of some of his achievements, the research he inspired, and the great friendships he has built.Nobel Prize Report:John L Hall, a Scientist Emeritus of the National Institute of Standards and Technology and a Fellow of JILA (joint institute of NIST and University of Colorado) has been awarded the 2005 Nobel Prize in Physics.Hall shared the Nobel with Theodor W H ä nsch of the Max Planck Institute for Quantum Optics and a professor of physics at Ludwig Maximilians University in Munich, Germany, and Roy J Glauber, a professor of physics at Harvard University.Hall and H ä nsch were awarded half the Nobel Prize for their contributions to the development of laser-based precision spectroscopy, including the optical frequency comb technique. An optical frequency comb is generated by a laser specially designed to produce a series of extremely short — a few billionths of a second — equally spaced pulses of light.

Understanding Molecular Deformation

A Textbook of Inorganic Chemistry – Volume 1

Perovskites

A Guide to Spirituality Without Religion

High-Tc Copper Oxide Superconductors and Related Novel Materials

Seven Time-Reversal Operators for Spin Containing Systems

This book by Kaplan and Vekhter brings together the molecular world of the chemist with the condensed matter world of the physicist. Prior to the collapse of the Soviet Union, chemists in the West devoted lit to relationships between molecular electronic structure and tle attention solid-state vibronic phenomena. Treating quantum mechanical problems wherein the adiabatic Born-Oppenheimer approximation fails was done by "brute force. " With bigger and better computers available in the West, molecular orbital calculations were done on observed and conceived static structures with little concern for any cooperativity of vibrational behavior that might connect these states. While it had long been understood in the West that situations do occur in which different static structures are found for molecules that have identical or nearly identical electronic structures, little attention had been paid to understanding the vibrational states that could connect such structures. It was easier to calculate the electronic structure observed with several possible distortions than to focus on ways to couple electronic and vibrational behavior. In the former Soviet Union, computational power was not as acces sible as in the West. Much greater attention, therefore, was devoted to conserving computational time by considering fundamental ways to han dle the vibrational connectivity between degenerate or nearly degenerate electronic states.

Hybrid organic-inorganic perovskites (HOIPs) have attracted substantial interest due to their chemical variability, structural diversity and favorable physical properties the past decade. This materials class encompasses other important families such as formates, azides, dicyanamides, cyanides and dicyanometallates. The book summarizes the chemical variability and structural diversity of all known hybrid organic-inorganic perovskites subclasses including halides, azides, formates, dicyanamides, cyanides and dicyanometallates. It also presents a comprehensive account of their intriguing physical properties, including photovoltaic, optoelectronic, dielectric,

magnetic, ferroelectric, ferroelastic and multiferroic properties. Moreover, the current challenges and future opportunities in this exciting field are also been discussed. This timely book shows the readers a complete landscape of hybrid organic-inorganic pervoskites and associated multifuctionalities.
To appreciate the chemistry and physical properties of complexes of the transition series, an understanding of metal-ligand interactions applied to complexes of the d-block is needed. Metal Ligand Bonding aims to provide this through an accessible, detailed, non-mathematical approach. Initial chapters detail the crystal-field model, using it to describe the use of magnetic measurements to distinguish complexes with different electronic configurations and geometries. Subsequent chapters look at the molecular orbital theory of transition metal complexes using a pictorial approach. Bonding in octahedral complexes is explored and electronic spectra and magnetic properties are given extensive coverage. The material addressed in this book forms the foundation of undergraduate lecture courses on d-block chemistry and facilitates learning through various key features, including: full colour diagrams; in-text questions with answers; revision exercises and clearly defined learning outcomes to encourage a reflective approach to study; an associated website; and experimental data and observations from everyday life. A basic knowledge of atomic and molecular orbitals as applied to main group elements is assumed.
The concepts of the Jahn-Teller effect and vibronic coupling are being applied to more and more systems in both chemistry and physics. Aspects of structural chemistry such as the distortion of the nuclear framework to a lower-symmetry conformation have received an increasing attention, as well as the dynamics on the coupled potential energy surfaces. The Jahn-Teller intersections are now recognized as prototype cases of conical intersections where the nuclear motion is known to be inherently nonadiabatic in nature and interchanges freely between the different potential energy surfaces. In the condensed phase especially, the significance of the Jahn-Teller effect has been increasingly appreciated, following the discovery of superconductivity in the fullerides and of very large ("colossal") magnetoresistance in the manganite perovskites. Indeed, these materials are particularly challenging since the Jahn-Teller interaction competes with electronic correlation effects. Vibronic Interactions and the Jahn-Teller Effect: Theory and Applications provides an in-depth discussion of the Jahn-Teller effect and vibronic interactions as reflected by the contributions presented at the XX International Conference on the Jahn-Teller effect, Fribourg, Switzerland, 2010. The following topics have been treated in a clear and concise way: • Complex topologies of Jahn-Teller effect and conical intersections • Multi-state vibronic interactions on strongly coupled potential energy surfaces • Interplay of vibronic and spin-orbit coupling • Strain in Jahn-Teller systems and cooperative Jahn-Teller effect • Orbital ordering and its relation to ferromagnetism, ferroelectricity and molecular magnets • The Jahn-Teller effect in icosahedral systems • The Jahn-Teller effect and high temperature superconductivity This book is of interest to a wide audience including academic and industrial theoretical and experimental physicists, chemists, spectroscopists, and crystallographers.
Dr. Gregory Boyd ' s Myth of a Christian Nation
The Jahn Teller Effect in C_1hn_346_1tn6_1tn0
Structure-Property Relationships
Narrow-band Solids with Unusual Properties
The Jahn-Teller Effect
High-order Expansions of the Electrostatic Hamiltonian and Relativistic Jahn-Teller Couplings
This book provides a comprehensive discussion of the Jahn-Teller Effect (JTE), focusing on the boson-fermion interaction. While current research is concerned with measuring and calculating ever more sophisticated and complex manifestations of the JT effect, the present volume takes away the epicycles of the theory and focuses on the symmetry dilemma at its core. When fermions and bosons meet, they get entangled and form a new dynamic reality. According to the rules of Molecular Symmetry, this reality is limited to a small set of patterns, with degeneracy cardinalities: 2, 3, 4, 5, and 6. The novelty of the book is that it adopts a unique mathematical technique, known as the Bargmann-Fock representation, and treats all degeneracies in detail. So far, this method was only applied to the simplest doublet case therefore its extension to the entire range of cases offers a new unified perspective. This volume will help the reader acquire a clear understanding of the JT effect, discover its universal mechanism and it will be a great tool for researchers and graduates working on this topic.
As a continuation of classical condensed matter physics texts, this graduate textbook introduces advanced topics of correlated electron systems, mesoscopic transport,quantum computing, optical excitations and topological insulators. The book is focusing on an intuitive understanding of the basic concepts of these rather complex subjects.
Aimed at senior undergraduates and first-year graduate students, this book offers a principles-based approach to inorganic chemistry that, unlike other texts, uses chemical applications of group theory and molecular orbital theory throughout as an underlying framework. This highly physical approach allows students to derive the greatest benefit of topics such as molecular orbital acid-base theory, band theory of solids, and inorganic photochemistry, to name a few. Takes a principles-based, group and molecular orbital theory approach to inorganic chemistry The first inorganic chemistry textbook to provide a thorough treatment of group theory, a topic usually relegated to only one or two chapters of texts, giving it only a cursory overview Covers atomic and molecular term symbols, symmetry coordinates in vibrational spectroscopy using the projection operator method, polyatomic MO theory, band theory, and Tanabe-Sugano diagrams Includes a heavy dose of group theory in the primary inorganic textbook, most of the pedagogical benefits of integration and reinforcement of this material in the treatment of other topics, such as frontier MO acid--base theory, band theory of solids, inorganic photochemistry, the Jahn-Teller effect, and Wade's rules are fully realized Very physical in nature compare to other textbooks in the field, taking the time to go through mathematical derivations and to compare and contrast different theories of bonding in order to allow for a more rigorous treatment of their application to molecular structure, bonding, and spectroscopy Informal and engaging writing style; worked examples throughout the text; unanswered problems in every chapter; contains a generous use of informative, colorful illustrations
This book introduces new developments in the field of Time-Reversal Symmetry presenting, for the first time, the Wigner time-reversal operator in the form of a product of two- or three time-reversal operators of lower symmetry. The action of these operators leads to the sign change of only one or two angular momentum components, not of all of them. It demonstrates that there are six modes of time-reversal symmetry breaking that do not lead to the complete disappearance of the symmetry but to its lowering. The full restoration of the time-reversal symmetry in the six cases mentioned is possible by introducing six types of metaparticles. The book also confirms the presence of six additional time-reversal operators using a group-theoretical method. The problem is only where to seek these metaparticles. The book discusses time-reversal symmetry in classical mechanics, classical and relativistic electrodynamics, quantum mechanics and theory of quantized fields, including dynamical reversibility and statistical irreversibility of the time, Wigner ' s and Herring ' s criteria, Kramers theorem, selection rules due to time-reversal symmetry, Onsager ' s relations, Poincar é recurrence theorem, and CPT theorem. It particularly focuses attention on time-reversal symmetry violation. It is proposed a new method of testing the time-reversal symmetry, which is confirmed experimentally by EPR spectroscopy data. It shows that the traditional black-white point groups of magnetic symmetry are not applicable to magnetic systems with Kramers degeneration of energy levels and that magnetic groups of four-color symmetry are adequate for them. Further, it addresses the predicted structural distortions in Kramers three-homonuclear magnetic clusters due to time-reversal symmetry that have been identified experimentally. Lastly, it proposes a method of synthesis of two-nuclear coordination compounds with predictable magnetic properties, based on the application of the time-reversal transformation that was confirmed experimentally.
Molecular Symmetry and Spectroscopy
Manifestations of the Jahn-Teller effect in the optical spectra of transition metal impurities in crystals
Waking Up
Beyond Born-Oppenheimer
Fluorite
The Jahn-Teller Effect and Vibronic Interactions in Modern Chemistry
In his best-selling book, The Myth of a Christian Nation, Dr. Gregory Boyd, a widely-respected theologian and pastor, argues that the church was established to serve the world with a Christ-like love that is diametrically opposed to the pursuit of political power. Christians are called to manifest a " kingdom of the cross " that impacts culture through self-sacrificial love, not the Romans 13 " kingdom of the sword " that impacts culture through coercive force. Dr. Boyd ' s radical separatism leaves committed Christians with no choice other than to abandon the civic realm. His is a call to effect change through spiritual disciplines, such as prayer, not by taking up the reins of government to exercise " power over " others. For Boyd, there is no room for Christians to serve in government or any of its arms, including the military or police. At last—there is now a reply, refutation and rebuttal to Dr. Boyd ' s treatise and conclusions, which result from misunderstandings of fundamental biblical principles and the selective treatment of Scripture. In this volume, John Teller sets forth a systematic reply to each of Dr. Boyd ' s arguments against Christians ' participation in civil government, the military and other civil institutions. This reply and rebuttal to Dr. Boyd ' s treatise shows that far from being called to eschew the " power over " kingdom of the sword, Christians are called to be God ' s co-laborers in redeeming the kingdom of sword, just as they are called to transform every other aspect of the fallen creation.
For the millions of Americans who want spirituality without religion, Sam Harris ' s latest New York Times bestseller is a guide to meditation as a rational practice informed by neuroscience and psychology. From Sam Harris, neuroscientist and author of numerous New York Times bestselling books, Waking Up is for the twenty percent of Americans who follow no religion but who suspect that important truths can be found in the experiences of such figures as Jesus, the Buddha, Lao Tzu, Rumi, and the other saints and sages of history. Throughout this book, Harris argues that there is more to understanding reality than science and secular culture generally allow, and that how we pay attention to the present moment largely determines the quality of our lives. Waking Up is part memoir and part exploration of the scientific underpinnings of spirituality. No other book marries contemplative wisdom and modern science in this way, and no author other than Sam Harris—a scientist, philosopher, and famous skeptic—could write it.
Atomic and Molecular Photoabsorption: Partial Cross Sections is a companion work to Joseph Berkowitz's earlier work, Atomic and Molecular Photoabsorption: Absolute Total Cross Sections, published with Academic Press in 2002. In this work Joseph Berkowitz selected the "best" absolute partial cross sections for the same species as included in the companion work. A contrast, however, is that photoabsorption measurements, being of order I/Io, do not require the most intense light sources, whereas acquiring data on the products of light interactions with gaseous matter (ions, electrons, various coincidence measurements) has benefited significantly with the arrival of second- and third-generation synchrotrons. The newer devices have also extended the energy range of the light sources to include the K-shells of the species discussed here. The newer light sources encouraged experimentalists to develop improved instrumentation. Thus, the determination of partial cross sections continues to be an active field, with more recent results in some cases superseding earlier ones. Where the accuracy of the absolute partial cross sections is deemed sufficient (less than five percent), numerical tables are included in this new work. In other cases, the available data are presented graphically. Includes data on atoms, diatomic molecules, triatomic molecules, and polyatomic molecules Written by world-leading pioneer in the field of photoionization mass spectrometry Very clear presentation of the useful, quantitative information in both tables and graphs
Because of the high symmetry involved, the Jahn-Teller effect is the natural starting point for considering electron-phonon (or vibronic) interactions in icosahedral molecules. This work is the first comprehensive theoretical analysis of the Jahn-Teller interaction in C60 and other icosahedral complexes. The importance of this research derives in part from the increasing, widespread interest in C60 and other molecular clusters and their application in science and industry. The electrical and spectroscopic properties of fullerene and fulleride compounds depend intimately on the coupling between the electronic and vibrational modes of these systems, and this book addresses the fundamental theoretical questions. In particular, a chapter is devoted to the connection between the theory and experimental observations, such as ESR (electron spin resonance) effects and molecular spectra. Earlier books have discussed the theory of Jahn-Teller interactions in lower symmetry structures (cubic, tetrahedral, tetragonal, trigonal,...); this is the first that focuses on the new icosahedral systems, whose most famous example is Buckminsterfullerene, C60. The book's authors have over fifty years of combined research experience into the theoretical aspects of the Jahn-Teller effect.
The Theory of the Jahn-Teller Effect
Electronic Structure of Defects in Insulators and Semiconductors
Structure, Chemistry, and Applications
The Jahn-Teller Effect:A Bibliographic Review
Electronic Structure and Properties of Transition Metal Compounds
Cooperative Phenomena in Jahn—Teller Crystals
An advanced-level textbook of inorganic chemistry for the graduate (B.Sc) and postgraduate (M.Sc) students of Indian and foreign universities. This book is a part of four volume series, entitled "A Textbook of Inorganic Chemistry – Volume I, II, III, IV". CONTENTS: Chapter 1. Stereochemistry and Bonding in Main Group Compounds: VSEPR theory, dπ -pπ bonds, Bent rule and energetic of hybridization. Chapter 2. Metal-Ligand Equilibria in Solution: Stepwise and overall formation constants and their interactions, Trends in stepwise constants, Factors affecting stability of metal complexes with reference to the nature of metal ion and ligand, Chelate effect and its thermodynamic origin, Determination of binary formation constants by pH-metry and spectrophotometry. Chapter 3. Reaction Mechanism of Transition Metal Complexes – I: Inert and labile complexes, Mechanisms for ligand replacement reactions, Formation of complexes from aquo ions, Ligand displacement reactions in octahedral complexes- acid hydrolysis, Base hydrolysis, Racemization of tris chelate complexes, Electrophilic attack on ligands. Chapter 4. Reaction Mechanism of Transition Metal Complexes – II: Mechanism of ligand displacement reactions in square planar complexes, The trans effect, Theories of trans effect, Mechanism of electron transfer reactions – types; Outer sphere electron transfer mechanism and inner sphere electron transfer mechanism, Electron exchange. Chapter 5. Isopoly and Heteropoly Acids and Salts: Isopoly and Heteropoly acids and salts of Mo and W: structures of isopoly and heteropoly anions. Chapter 6. Crystal Structures: Structures of some binary and ternary compounds such as fluorite, antifluorite, rutile, antirutile, crystobalite, layer lattices- CdI2, BiI3; ReO3, Mn2O3, corundum, pervoskite, Ilmenite and Calcite. Chapter 7. Metal-Ligand Bonding: Limitation of crystal field theory, Molecular orbital theory, octahedral, tetrahedral or square planar complexes, π-bonding and molecular orbital theory. Chapter 8. Electronic Spectra of Transition Metal Complexes: Spectroscopic ground states, Correlation and spin-orbit coupling in free ions for Ist series of transition metals, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d1 – d9 states), Calculation of Dq, B and β parameters, Effect of distortion on the d-orbital energy levels, Structural evidence from electronic spectrum, John-Tellar effect, Spectrochemical and nephalauxetic series, Charge transfer spectra, Electronic spectra of molecular addition compounds. Chapter 9. Magantic Properties of Transition Metal Complexes: Elementary theory of magneto - chemistry, Guoy ' s method for determination of magnetic susceptibility, Calculation of magnetic moments, Magnetic properties of free ions, Orbital contribution, effect of ligand-field, Application of magneto-chemistry in structure determination, Magnetic exchange coupling and spin state cross over. Chapter 10. Metal Clusters: Structure and bonding in higher boranes, Wade ' s rules, Carboranes, Metal Carbonyl Clusters - Low Nuclearity Carbonyl Clusters, Total Electron Count (TEC). Chapter 11. Metal-π Complexes: Metal carbonyls, structure and bonding, Vibrational spectra of metal carbonyls for bonding and structure elucidation, Important reactions of metal carbonyls; Preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; Tertiary phosphine as ligand.
Authored by many of the world's leading experts on high-Tc superconductivity, this volume presents a panorama of ongoing research in the field, as well as insights into related multifunctional materials. The contributions cover many different and complementary aspects of the physics and materials challenges, with an emphasis on superconducting materials that have emerged since the discovery of the cuprate superconductors, for example pnictides, MgB2, H2S and other hydrides. Special attention is also paid to interface superconductivity. In addition to superconductors, the volume also addresses materials related to polar and multifunctional ground states, another class of materials that owes its discovery to Prof. M ü ller's ground-breaking research on SrTiO3.
Absolute Partial Cross Sections
Introduction to the Theory
The Jahn-Teller Effect in C60 and Other Icosahedral Complexes
Optical Spectra of Transparent Rare Earth Compounds
A Handbook on Nanoscience and Nanotechnology
Theory of Defects in Solids