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The Tunnel Effect in Chemistry Jan 01 2023 The suggestion that quantum-mechanical tunnelling might be a significant factor in some chemical reactions was first made fifty years ago by Hund, very soon after the principles of wave mechanics had been established by de Broglie, Schrodinger and Heisenberg, and similar ideas were put forward during the following thirty years by a number of authors. It was realised from the beginning that such effects would be particularly prominent in reactions involving the movement of protons or hydrogen atoms, and both theoretical and experimental work received a powerful stimulus in the discovery of deuterium in 1932. During the last twenty years theoretical predictions about the tunnel effect have been supported by an increasing body of experimental evidence, derived especially from studies of hydrogen isotope effects. The present book presents an attempt to summarize this evidence and to indicate the main lines of the basic theory. Details of mathematical manipulation are restricted mainly to Chapter 2 and the Appendices, and many readers may prefer to confine themselves to the results obtained. The main emphasis has been on the kinetics of chemical reactions involving the transfer of protons, hydrogen atoms or hydride ions, although Chapter 6 gives an account of the role of the tunnel effect in molecular spectra, and Chapter 7 makes some mention of tunnelling in solid state phenomena, biological processes and the electrolytic discharge of hydrogen. Only passing references have been made to tunnelling by electrons.

Effects of Electric Fields on Structure and Reactivity Aug 16 2021 Starting with an overview of the theory behind - and demonstrations of the effect of - electric fields on structure and reactivity, this accessible reference work aims to encourage those new to the field to consider harnessing these effects in their own work.

Effect of Chemical Structure Apr 23 2022

Solvents and Solvent Effects in Organic Chemistry Oct 30 2022 In most cases, every chemist must deal with solvent effects, whether voluntarily or otherwise. Since its publication, this has been the standard reference on all topics related to solvents and solvent effects in organic chemistry. Christian Reichardt provides reliable information on the subject, allowing chemists to understand and effectively use these phenomena. 3rd updated and enlarged edition of a classic 35% more contents excellent, proven concept includes current developments, such as ionic liquids indispensable in research and industry From the reviews of the second edition: "...This is an immensely useful book, and the source that I would turn to first when seeking virtually any information about solvent effects."

—Organometallics

Relativistic Effects in Chemistry, Theory and Techniques and Relativistic Effects in Chemistry May 13 2021 $E = mc^2$ and the Periodic Table . . . RELATIVISTIC EFFECTS IN CHEMISTRY This century's most famous equation, Einstein's special theory of relativity, transformed our comprehension of the nature of time and matter. Today, making use of the theory in a relativistic analysis of heavy molecules, that is, computing the properties and nature of electrons, is the work of chemists intent on exploring the mysteries of minute particles. The first work of its kind, *Relativistic Effects in Chemistry* details the computational and analytical methods used in studying the relativistic effects in chemical bonding as well as the spectroscopic properties of molecules containing very heavy atoms. The first of two independent volumes, Part A: *Theory and Techniques* describes the basic techniques of relativistic quantum chemistry. Its systematic five-part format begins with a detailed exposition of Einstein's special theory of relativity, the significance of relativity in chemistry, and the nature of relativistic effects, especially with molecules containing both main group atoms and transition metal atoms. Chapter 3 discusses the fundamentals of relativistic quantum mechanics starting from the Klein-Gordon equation through such advanced constructs as the Breit-Pauli and Dirac multielectron Hamiltonian. Modern computational techniques, of importance with problems involving very heavy molecules, are outlined in Chapter 4. These include the relativistic effective core potentials, ab initio CASSCF, CI, and RCI techniques. Chapter 5 describes relativistic symmetry using the double group symmetry of molecules and the classification of relativistic electronic states and is of special importance to chemists or spectroscopists interested in computing or analyzing electronic states of molecules containing very heavy atoms. An exceptional introduction to one of chemistry's foremost analytical techniques, *Relativistic Effects in Chemistry* is also evidence of the still unending reverberations of Einstein's revolutionary theory.

Electronic Effects in Organic Chemistry Aug 28 2022 The series *Topics in Current Chemistry* presents critical reviews of the present and future trends in modern chemical research. The scope of coverage is all areas of chemical science including the interfaces with related disciplines such as biology, medicine and materials science. The goal of each

thematic volume is to give the non-specialist reader, whether in academia or industry, a comprehensive insight into an area where new research is emerging which is of interest to a larger scientific audience. Each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole. The most significant developments of the last 5 to 10 years are presented using selected examples to illustrate the principles discussed. The coverage is not intended to be an exhaustive summary of the field or include large quantities of data, but should rather be conceptual, concentrating on the methodological thinking that will allow the non-specialist reader to understand the information presented. Contributions also offer an outlook on potential future developments in the field. Review articles for the individual volumes are invited by the volume editors.

Readership: research chemists at universities or in industry, graduate students

Chemistry Under Extreme and Non-Classical Conditions Mar 23 2022 The very best and latest advances compiled in a single volume—an ideal resource for graduate students and researchers . . . Here is the perfect introduction to chemistry under extreme or non-classical conditions, including use of high temperature species, high pressure, supercritical media, sonochemistry, and microwave chemistry. Written by leading experts in their respective fields, this unique text applies a unified approach to each method, including background, instrumentation, examples, information on industrial applications (where relevant), and sources for further reading. Featured topics: * Chemical Synthesis Using High Temperature Species * Effect of Pressure on Inorganic Reactions * Effect of Pressure on Organic Reactions * Organic Synthesis at High Pressure * Inorganic and Related Chemical Reactions in Supercritical Fluids * Organic Chemistry in Supercritical Fluids * Industrial and Environmental Applications of Supercritical Fluids * Ultrasound as a New Tool for Synthetic Chemists * Applications of High Intensity Ultrasound in Polymer Chemistry * Chemistry Under Extreme Conditions in Water Induced Electrohydraulic Cavitation and Pulsed-Plasma Discharges * Microwave Dielectric Heating Effects in Chemical Synthesis * Biomolecules Under Extreme Conditions

DK Eyewitness Books: Chemistry Sep 28 2022 Chemical processes have always been a part of life. They enable our bodies to function and are the basis of countless substances and processes we take for granted. This intriguing book explores the world's natural chemistry and how we understand and exploit it. From the first use of fire, people have practiced chemistry to produce food and drink, tan leather, make dyes for clothes and cosmetics, work metals, and produce glass and pottery. Today, chemicals help to purify our water, improve agriculture, and manufacture drugs, synthetic fabrics, and plastics. Our growing knowledge of the Earth's elements, the properties of atoms and DNA, and how substances interact, has resulted in many new technologies, products, and scientific advances. The most trusted nonfiction series on the market, Eyewitness Books provide an in-depth, comprehensive look at their subjects with a unique integration of words and pictures.

Principles of Chemistry Oct 25 2019

The Mössbauer Effect and its Applications in Chemistry Jun 01 2020 The Mossbauer effect is not only one of the simplest and most beautiful discoveries of nuclear physics, it is one of those discoveries which, to the highest degree, tend to produce and develop new ties between nuclear physics and the other branches of physics as well as the other natural sciences and engineering. Two of our earlier papers which form the basis of this monograph

were devoted to "propaganda" for the Mossbauer effect among chemists and "propaganda" for the chemical applications of the effect among nuclear physicists. The first paper, presented in January 1962 at the Scientific Colloquium of the Learned Council of the Theory of Chemical Structure, Kinetics, and Reactivity of the Division of Chemical Sciences of the Academy of Sciences of the USSR, gave a general description of the Mossbauer effect and the methods by which it is observed" and enumerated a number of problems in structural chemistry, chemical kinetics, and radiation chemistry that might well be studied by observing the Mossbauer spectra, in particular those of organotin compounds.

General Chemistry Sep 24 2019 Known for its carefully developed, thoroughly integrated approach to problem solving, this market-leading text emphasizes the conceptual understanding and visualization skills essential for first-year chemistry and science majors. The new technology program reinforces the approach of the text and provides a complete solution for teaching and learning. The Eighth Edition retains the hallmark pedagogical features of the text and builds upon the conceptual focus and art program. Students also benefit from online homework in the technology program, which features an extensive database of questions drawn from the text.

Spectroscopic Methods in Organic Chemistry Jan 27 2020 This introductory text describes the uses of the 4 spectroscopic methods, UV, IR, NMR, and mass spectra in organic chemistry. New material includes extended coverage of 2-D NMR spectra and the introduction of the powerful techniques of TOCSY, ESI and MALDI.

Nitration Nov 26 2019

High-resolution NMR Techniques in Organic Chemistry Feb 28 2020 From the initial observation of proton magnetic resonance in water and in paraffin, the discipline of nuclear magnetic resonance has seen unparalleled growth as an analytical method. Modern NMR spectroscopy is a highly developed, yet still evolving, subject which finds application in chemistry, biology, medicine, materials science and geology. In this book, emphasis is on the more recently developed methods of solution-state NMR applicable to chemical research, which are chosen for their wide applicability and robustness. These have, in many cases, already become established techniques in NMR laboratories, in both academic and industrial establishments. A considerable amount of information and guidance is given on the implementation and execution of the techniques described in this book.

Electrons, Atoms, and Molecules in Inorganic Chemistry Mar 30 2020 *Electrons, Atoms, and Molecules in Inorganic Chemistry: A Worked Examples Approach* builds from fundamental units into molecules, to provide the reader with a full understanding of inorganic chemistry concepts through worked examples and full color illustrations. The book uniquely discusses failures as well as research success stories. Worked problems include a variety of types of chemical and physical data, illustrating the interdependence of issues. This text contains a bibliography providing access to important review articles and papers of relevance, as well as summaries of leading articles and reviews at the end of each chapter so interested readers can readily consult the original literature. Suitable as a professional reference for researchers in a variety of fields, as well as course use and self-study. The book offers valuable information to fill an important gap in the field. Incorporates questions and answers to assist readers in understanding a variety of problem types. Includes detailed explanations and developed practical approaches for solving real

chemical problems Includes a range of example levels, from classic and simple for basic concepts to complex questions for more sophisticated topics Covers the full range of topics in inorganic chemistry: electrons and wave-particle duality, electrons in atoms, chemical binding, molecular symmetry, theories of bonding, valence bond theory, VSEPR theory, orbital hybridization, molecular orbital theory, crystal field theory, ligand field theory, electronic spectroscopy, vibrational and rotational spectroscopy

Isotope Effects In Chemistry and Biology Dec 20 2021 The field of isotope effects has expanded exponentially in the last decade, and researchers are finding isotopes increasingly useful in their studies. Bringing literature on the subject up to date, *Isotope Effects in Chemistry and Biology* covers current principles, methods, and a broad range of applications of isotope effects in the physical, biolo

Substituent Effects in Radical Chemistry Jul 27 2022 Proceedings of the NATO Advanced Research Workshop, Louvain-la-Neuve, Belgium, January 20-24, 1986

Caffeine Jul 15 2021 This text covers caffeine in relation to nutrition, focussing on beverages, then concentrating on chemistry, crystal structures of complexes in caffeine and biochemistry. Essays are conducted by LC-MS, capillary electrophoresis and automated flow methods. The effects of caffeine on the brain, sleep, and exercise are also considered.

Radiation Chemistry of Organic Compounds Jun 13 2021 *Radiation Effects in Materials, Volume 2: Radiation Chemistry of Organic Compounds* provides information pertinent to the fundamental aspects of radiation chemistry of organic compounds. This book reviews the published work on the radiation chemistry of organic compounds. Organized into nine chapters, this volume begins with an overview of the study of the chemical reactions produced by high-energy radiation. This text then explores the two groups of radiation sources, namely, natural and artificial, that have been equally valuable for radiation chemistry. Other chapters consider the radiation chemistry of water and aqueous systems that is important to organic radiation chemistry. This book discusses as well how radiation alters simple organic compounds, and how the response varies with the irradiation conditions and the presence of other substances. The final chapter deals with the economic aspects of the use of radiation sources in industry. This book is a valuable resource for radiation chemists.

Solvent Effects in Chemistry Jan 21 2022 This book introduces the concepts, theory and experimental knowledge concerning solvent effects on the rate and equilibrium of chemical reactions of all kinds. It begins with basic thermodynamics and kinetics, building on this foundation to demonstrate how a more detailed understanding of these effects may be used to aid in determination of reaction mechanisms, and to aid in planning syntheses.

Consideration is given to theoretical calculations (quantum chemistry, molecular dynamics, etc.), to statistical methods (chemometrics), and to modern day concerns such as "green" chemistry, where utilization and disposal of chemical waste or by-products in an environmentally safe way is as important as achieving the desired end products by all chemists nowadays. The treatment progresses from elementary to advanced material in straightforward fashion. The more advanced topics are not developed in an overly rigorous way so that upper-level undergraduates, graduates, and newcomers to the field can grasp the concepts easily.

Steric and Stereoelectronic Effects in Organic Chemistry Feb 19 2022 In this second

edition, the author has thoroughly updated each chapter and expanded the content with addition of three new chapters. This book comments on several key aspects of stereochemical control of organic reactions in measured detail to allow the reader easily grasp these concepts. In addition, emphasis is given to key information and important aspects of steric and stereoelectronic effects and their control on conformational profile and reactivity features. This book is not only an indispensable resource for advanced undergraduate and graduate students studying the stereochemical aspects of organic reactions, but also a good reference book for all organic chemists in both industry and academia.

Magnetic Isotope Effect in Radical Reactions Jan 09 2021 In the last two decades it was demonstrated that, in addition to masses and charges, magnetic moments of nuclei are able to influence remarkably chemical reactions. This book presents the physical background (both theoretical and experimental) of the magnetic isotope effects in radical reactions in solutions. Special attention has been paid to the quantitative interpretation of the available experimental data. This book will be useful for physicists, chemists and biologists employing the isotope effect in their investigations as well as for those involved in isotope separation and isotope enrichment projects. Additionally, the magnetic isotope effect appears to be important in geochemistry and cosmochemistry. The book can be recommended for postgraduates and senior undergraduate students.

The Heavy Elements May 01 2020 This text provides a broad survey of the ten heavier elements of the p-block, which have a number of features in common as well as displaying periodic trends. Full comprehension of the chemistry of the elements is necessary before complete understanding of environmental and health effects is possible. In many texts, however, basic chemistry is avoided as too complex or uninteresting. The author's approach in this case is to use the disciplines of health and environmental science to enhance understanding of the chemistry and to provide students with an integrated approach to the influence of the elements on the world. Information is provided on concentrations, sources and speciation of the heavy elements and their effects on the health of human beings. The text is intended to stimulate students to investigate further aspects of the heavy elements, and contribute to this young but rapidly growing field.

Stereoelectronic Effects Jun 25 2022 Stereoelectronic Effects illustrates the utility of stereoelectronic concepts using structure and reactivity of organic molecules An advanced textbook that provides an up-to-date overview of the field, starting from the fundamental principles Presents a large selection of modern examples of stereoelectronic effects in organic reactivity Shows practical applications of stereoelectronic effects in asymmetric catalysis, photochemical processes, bioorganic chemistry and biochemistry, inorganic and organometallic reactivity, supramolecular chemistry and materials science

Organophosphates Chemistry, Fate, and Effects Oct 18 2021 This volume pulls together a wealth of up-to-date information on the toxicology of this diverse and ubiquitous class of insecticides. Leading experts review the reactivity of organophosphorus compounds with cholinesterase, as well as their metabolism and biological effects on humans and other nontarget organisms. The book not only covers the anticholinesterase actions of organophosphates, but also other, presumably independent, effects, such as teratogenicity, delayed neuropathy, immunotoxicity, and behavioral toxicity. Offers crucial overviews of

chemical and biochemical reactivity and biological responsiveness of mainly nontarget organisms Reviews new developments in assessment of metabolism and disposition of organophosphorus compounds Examines organophosphorus compound-induced toxicity mediated by mechanisms other than inhibition of acetylcholinesterase Covers new research on differences in toxicity induced by the variety of organophosphorus Analyzes current controversies on the relevance of certain biochemical parameters in actual organophosphate toxicity in vivo

Chemistry Nov 30 2022 Explores the world of chemical reactions and shows the role that chemistry plays in our world.

Carbocation Chemistry Dec 08 2020

Tunnelling in Molecules Oct 06 2020 Quantum tunnelling is one of the strangest phenomena in chemistry, where we see the wave nature of atoms acting in “impossible” ways. By letting molecules pass through the kinetic barrier instead of over it, this effect can lead to chemical reactions even close to the absolute zero, to atypical spectroscopic observations, to bizarre selectivity, or to colossal isotopic effects. Quantum mechanical tunnelling observations might be infrequent in chemistry, but it permeates through all its disciplines producing remarkable chemical outcomes. For that reason, the 21st century has seen a great increase in theoretical and experimental findings involving molecular tunnelling effects, as well as in novel techniques that permit their accurate predictions and analysis. Including experimental, computational and theoretical chapters, from the physical and organic to the biochemistry fields, from the applied to the academic arenas, this new book provides a broad and conceptual perspective on tunnelling reactions and how to study them. Quantum Tunnelling in Molecules is the obligatory stop for both the specialist and those new to this world.

Orbitals in Chemistry Nov 18 2021 This text presents a unified and up-to-date discussion of the role of atomic and molecular orbitals in chemistry, from the quantum mechanical foundations to the recent developments and applications. The discussion is mainly qualitative, largely based on symmetry arguments. It is felt that a sound mastering of the concepts and qualitative interpretations is needed, especially when students are becoming more and more familiar with numerical calculations based on atomic and molecular orbitals. The text is mathematically less demanding than most traditional quantum chemistry books but still retains clarity and rigour. The physical insight is maximized and abundant illustrations are used. The relationships between the more formal quantum mechanical formalisms and the traditional chemical descriptions of chemical bonding are critically established. This book is of primary interest to undergraduate chemistry students and others taking courses of which chemistry is a significant part.

Stereoelectronic Effects in Organic Chemistry Jul 03 2020

Radiochemistry and Nuclear Chemistry Aug 23 2019 Origin of Nuclear Science; Nuclei, Isotopes and Isotope Separation; Nuclear Mass and Stability; Unstable Nuclei and Radioactive Decay; Radionuclides in Nature; Absorption of Nuclear Radiation; Radiation Effects on Matter; Detection and Measurement Techniques; Uses of Radioactive Tracers; Cosmic Radiation and Elementary Particles; Nuclear Structure; Energetics of Nuclear Reactions; Particle Accelerators; Mechanics and Models of Nuclear Reactions; Production of Radionuclides; The Transuranium Elements; Thermonuclear Reactions: the Beginning

and the Future; Radiation Biology and Radiation Protection; Principles of Nuclear Power; Nuclear Power Reactors; Nuclear Fuel Cycle; Behavior of Radionuclides in the Environment; Appendices; Solvent Extraction Separations; Answers to Exercises; Isotope Chart; Periodic Table of the Elements; Quantities and Units; Fundamental Constants; Energy Conversion Factors; Element and Nuclide Index; Subject Index.

Nuclear chemistry and effects of irradiation Feb 07 2021

Calcium Dec 28 2019 Calcium's importance in health and disease is clear when listing its multiple roles in the body, which include building strong bones and teeth, vascular calcification, muscle function, hormonal regulation and maintaining a normal heartbeat. This book will examine these roles and will also cover areas such as chemical analysis, sources of calcium based on geography, influence of Vitamin D, hypercalcemia and the effects of dietary calcium. This edited volume will pool knowledge across scientific disciplines in a way that increases its applicability to a wide range of audiences and fills the gap identified in providing comprehensive synopses of food substances. Chemists, analytical scientists, forensic scientists, food scientists, as well as course lecturers and university librarians, will all benefit from this title.

Fluorine Sep 04 2020 Fluorine is best known for its role in the prevention of cavities and in improving oral and bone health however equally there are millions of people around the world suffering from dental fluorosis due to chronic exposure to high levels of fluoride in drinking water. This volume, written by leading researchers in this area, examines the positives and negatives of fluorine and its effects on humans for example fluoride-induced oxidative stress in the liver, effects of fluoride on insulin and preventing fluoride toxicity. Extremely useful for underpinning cross-disciplinary fluorine research, this book provides a fascinating insight for those with an interest in the health and nutritional sciences.

Organic Chemistry, Part 1 of 3 Apr 11 2021 This textbook is where you, the student, have an introduction to organic chemistry. Regular time spent in learning these concepts will make your work here both easier and more fun.

Environmental Inorganic Chemistry for Engineers Mar 11 2021 Environmental Inorganic Chemistry for Engineers explains the principles of inorganic contaminant behavior, also applying these principles to explore available remediation technologies, and providing the design, operation, and advantages or disadvantages of the various remediation technologies. Written for environmental engineers and researchers, this reference provides the tools and methods that are imperative to protect and improve the environment. The book's three-part treatment starts with a clear and rigorous exposition of metals, including topics such as preparations, structures and bonding, reactions and properties, and complex formation and sequestering. This coverage is followed by a self-contained section concerning complex formation, sequestering, and organometallics, including hydrides and carbonyls. Part Two, Non-Metals, provides an overview of chemical periodicity and the fundamentals of their structure and properties. Clearly explains the principles of inorganic contaminant behavior in order to explore available remediation technologies Provides the design, operation, and advantages or disadvantages of the various remediation technologies Presents a clear exposition of metals, including topics such as preparations, structures, and bonding, reaction and properties, and complex formation and sequestering

The Jahn-Teller Effect Aug 04 2020 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.

The Jahn-Teller Effect and Vibronic Interactions in Modern Chemistry Sep 16 2021 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 development 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 spectroscopy, stereochemistry and crystal chemistry, reactivity, and catalysis, are illustrated by a series of effects and laws.

Effect-Directed Analysis of Complex Environmental Contamination May 25 2022

Today more than 5 million chemicals are known and roughly 100,000 of them are frequently used, with both numbers rising. Many of these chemicals are ultimately released into the environment and may cause adverse effects to ecosystems and human health. Effect-directed analysis (EDA) is a promising tool for identifying predominant toxicants in complex, mostly environmental mixtures combining effect testing, fractionation and chemical analysis. In the present book leading experts in the field provide an overview of relevant approaches and tools used in EDA. This includes diagnostic biological tools, separation techniques and advanced analytical and computer tools for toxicant identification and structure elucidation. Examples of the successful application of EDA are discussed such as the identification of mutagens in airborne particles and sediments, of endocrine disruptors in aquatic ecosystems and of major toxicants in pulp and paper mill effluents. This book is a valuable, comprehensive and interdisciplinary source of information for environmental scientists and environmental agencies dealing with the analysis, monitoring and assessment of environmental contamination.

Stereoelectronic Effects Nov 06 2020 Stereoelectronic effects control the way molecules are put together and account for the "rules of engagement" which operate when molecules meet and react. Understanding these effects is the key to understanding molecular behavior, since the same basic three-dimensional interactions are responsible for both structure and reactivity. This concise and very accessible volume provides a comprehensive, intentionally non-mathematical coverage of stereochemistry, along with an in-depth discussion of the main classes of organic reactions, promoting a logical and simple way of thinking about chemistry.