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WESTON FELIPE

Stochastic and Dynamic Views of Chemical Reaction Kinetics in Solutions Courier Corporation
This book deals with a central topic at the interface of chemistry and physics—the understanding of how the transformation of matter takes place at the atomic level. Building on the laws of physics, the book focuses on the theoretical framework for predicting the outcome of chemical reactions. The style is highly systematic with attention to basic concepts and clarity of presentation. The emphasis is on concepts and insights obtained via analytical theories rather than computational and numerical aspects. Molecular reaction dynamics is about the detailed atomic-level description of chemical reactions. Based on quantum mechanics and statistical mechanics, the dynamics of uni- and bi-molecular elementary reactions are described. The book features a comprehensive presentation of transition-state theory which plays an important role in practice, and a detailed discussion of basic theories of reaction dynamics in condensed phases. Examples and end-of-chapter problems are included in order to illustrate the theory and its connection to chemical problems. The second edition includes updated descriptions of adiabatic and non-adiabatic electron-nuclear dynamics, an expanded discussion of classical two-body models of chemical reactions, including the Langevin model, additional material on quantum tunnelling and its implementation in Transition-State Theory, and a more thorough description of the Born and Onsager models for solvation.
The Microscopic Foundation of Chemical Kinetics Wiley-VCH
The Student Solutions Manual to accompany Atkins' Physical Chemistry 11th Edition provides full worked solutions to the "a" exercises, and the odd-numbered discussion questions and problems presented in the parent book. The manual is intended for students and provides helpful comments andfriendly advice to aid understanding.
An Introduction to Chemical Kinetics WCB/McGraw-Hill
This text presents a balanced presentation of the macroscopic view of empirical kinetics and the microscopic molecular viewpoint of chemical dynamics. This second edition includes the latest information, as well as new topics such as heterogeneous reactions in atmospheric chemistry, reactant product imaging, and molecular dynamics of H + H2.
Encyclopedia of Physical Organic Chemistry, 6 Volume Set PPUR presses polytechniques
"All fields of chemistry involve the principles of chemical kinetics. Important reactions take place in gases, solutions, and solids. This book provides the necessary tools for studying and understanding interactions in all of these phases. Derivations are presented in detail to make them intelligible to readers whose background in mathematics is not extensive."--BOOK JACKET.
Principles of Chemical Kinetics Elsevier
Unimolecular reactions are in principle the simplest chemical reactions, because they only involve one molecule. The basic mechanism, in which the competition between the chemical reaction step and a collisional deactivation leads to a pressure-dependent coefficient, has been understood for a long time. However, this is a rapidly developing field, and many new and important discoveries have been made in the past decade. This First Part Part of Two CCK Volumes dealing with Unimolecular Rections, deals with the Reaction Step. The first chapter is an introduction to the whole project, aiming to cover the material necessary to understand the content of the detailed chapters, as well as the history of the development of the area. Chapter 2 is a review of the modern view of the statistical theories, as embodied in the various forms of RRKM theory. Chapter 3 deals with the fully quantum mechanical view of reactive states as resonances. . Presents considerable advances in the field made during the last decade. . Treats both the statistical as well as the fully quantum mechanical view.
Invariant Manifolds for Physical and Chemical Kinetics Courier Corporation
Chemical Kinetics and Reaction Dynamics brings together the major facts and theories relating to the rates with which chemical reactions occur from both the macroscopic and microscopic point of view. This book helps the reader achieve a thorough understanding of the principles of chemical kinetics and includes: Detailed stereochemical discussions of reaction steps Classical theory based calculations of state-to-state rate constants A collection of matters on kinetics of various special reactions such as micellar catalysis, phase transfer catalysis, inhibition processes, oscillatory reactions, solid-state reactions, and polymerization reactions at a single source. The growth of the chemical industry greatly depends on the application of chemical kinetics, catalysts and catalytic processes. This volume is therefore an invaluable resource for all academics, industrial researchers and students interested in kinetics, molecular reaction dynamics, and the mechanisms of chemical reactions.
Electrolyte Solutions Elsevier
This book began as a program of self-education. While teaching under graduate physical chemistry, I became progressively more dissatisfied with my approach to chemical kinetics. The solution to my problem was to write a detailed set of lecture notes which covered more material, in greater depth, than could be presented in undergraduate physical chemistry. These notes are the foundation upon which this book is built. My background led me to view chemical kinetics as closely related to transport phenomena. While the relationship of these topics is well known, it is often ignored, except for brief discussions of irreversible thermody namics. In fact, the physics underlying such apparently dissimilar processes as reaction and energy transfer is not so very different. The intermolecular potential is to transport what the potential-energy surface is to reactivity. Instead of beginning the sections devoted to chemical kinetics with a discussion of various theories, I have chosen to treat phenomenology and mechanism first. In this way the essential unity of kinetic arguments, whether applied to gas-phase or solution-phase reaction, can be emphasized. Theories of rate constants and of chemical dynamics are treated last, so that their strengths and weaknesses may be more clearly highlighted. The book is designed for students in their senior year or first year of graduate

school. A year of undergraduate physical chemistry is essential preparation. While further exposure to chemical thermodynamics, statistical thermodynamics, or molecular spectroscopy is an asset, it is not necessary.

Decoding Complexity Oxford University Press

Winner of 2018 PROSE Award for MULTIVOLUME REFERENCE/SCIENCE This encyclopedia offers a comprehensive and easy reference to physical organic chemistry (POC) methodology and techniques. It puts POC, a classical and fundamental discipline of chemistry, into the context of modern and dynamic fields like biochemical processes, materials science, and molecular electronics. Covers basic terms and theories into organic reactions and mechanisms, molecular designs and syntheses, tools and experimental techniques, and applications and future directions Includes coverage of green chemistry and polymerization reactions Reviews different strategies for molecular design and synthesis of functional molecules Discusses computational methods, software packages, and more than 34 kinds of spectroscopies and techniques for studying structures and mechanisms Explores applications in areas from biology to materials science The Encyclopedia of Physical Organic Chemistry has won the 2018 PROSE Award for MULTIVOLUME REFERENCE/SCIENCE. The PROSE Awards recognize the best books, journals and digital content produced by professional and scholarly publishers. Submissions are reviewed by a panel of 18 judges that includes editors, academics, publishers and research librarians who evaluate each work for its contribution to professional and scholarly publishing. You can find out more at: proseawards.com Also available as an online edition for your library, for more details visit Wiley Online Library

Chemical Kinetics and Process Dynamics in Aquatic Systems Royal Society of Chemistry

Recent advances in the study of structural and dynamic properties of solutions have provided a molecular picture of solute-solvent interactions. Although the study of thermodynamic as well as electronic properties of solutions have played a role in the development of research on the rate and mechanism of chemical reactions, such macroscopic and microscopic properties are insufficient for a deeper understanding of fast chemical and biological reactions. In order to fill the gap between the two extremes, it is necessary to know how molecules are arranged in solution and how they change their positions in both the short and long range. This book has been designed to meet these criteria. It is possible to develop a sound microscopic picture for reaction dynamics in solution without molecular-level knowledge of how reacting ionic or neutral species are solvated and how rapidly the molecular environment is changing with time. A variety of actual examples is given as to how and when modern molecular approaches can be used to solve specific solution problems. The following tools are discussed: x-ray and neutron diffraction, EXAFS, and XANES, molecular dynamics and Monte Carlo computer simulations, Raman, infrared, NMR, fluorescence, and photoelectron emission spectroscopic methods, conductance and viscosity measurements, high pressure techniques, and statistical mechanics methods. Static and dynamic properties of ionic solvation, molecular solvation, ion-pair formation, ligand exchange reactions, and typical organic solvents are useful for bridging the gap between classical thermodynamic studies and modern single-molecule studies in the gas phase. The book will be of interest to solution, physical, inorganic, analytical and structural chemists as well as to chemical kineticists.

Reaction Rates of Processes in Natural Waters John Wiley & Sons

By bringing together various ideas and methods for extracting the slow manifolds, the authors show that it is possible to establish a more macroscopic description in nonequilibrium systems. The book treats slowness as stability. A unifying geometrical viewpoint of the thermodynamics of slow and fast motion enables the development of reduction techniques, both analytical and numerical. Examples considered in the book range from the Boltzmann kinetic equation and hydrodynamics to the Fokker-Planck equations of polymer dynamics and models of chemical kinetics describing oxidation reactions. Special chapters are devoted to model reduction in classical statistical dynamics, natural selection, and exact solutions for slow hydrodynamic manifolds. The book will be a major reference source for both theoretical and applied model reduction. Intended primarily as a postgraduate-level text in nonequilibrium kinetics and model reduction, it will also be valuable to PhD students and researchers in applied mathematics, physics and various fields of engineering.

Unimolecular Kinetics, Part 1. The Reaction Step Elsevier

The transition state is the critical configuration of a reaction system situated at the highest point of the most favorable reaction path on the potential-energy surface, its characteristics governing the dynamic behavior of reacting systems decisively. This text presents an accurate survey of current theoretical investigations of chemical reactions, with a focus on the nature of the transition state. Its scope ranges from general basic theories associated with the transition states, to their computer-assisted applications, through to a number of reactions in a state-of-the-art fashion. It covers various types of gas-phase elementary reactions, as well as some specific types of chemical processes taking place in the liquid phase. Also investigated is the recently developing transition state spectroscopy. This text will not only serve as a contemporary reference book on the concept of the transition state, but will also assist the readers in gaining valuable key principles regarding the essence of chemical kinetics and dynamics.

Chemical Kinetics and Reaction Mechanisms Gulf Professional Publishing

Materials Kinetics: Transport and Rate Phenomena provides readers with a clear understanding of how physical-chemical principles are applied to fundamental kinetic processes. The book integrates advanced concepts with foundational knowledge and cutting-edge computational approaches, demonstrating how diffusion, morphological evolution, viscosity, relaxation and other kinetic phenomena can be applied to practical materials design problems across all classes of materials. The book starts with an overview of thermodynamics, discussing equilibrium, entropy, and irreversible processes. Subsequent chapters focus on analytical and numerical solutions of the diffusion equation, covering Fick’s laws, multicomponent diffusion, numerical solutions, atomic models, and diffusion in crystals, polymers, glasses, and polycrystalline materials. Dislocation and interfacial motion, kinetics of phase separation, viscosity, and advanced nucleation theories are examined next, followed by detailed analyses of glass transition and relaxation behavior. The book concludes with a series of chapters covering molecular dynamics, energy landscapes, broken ergodicity, chemical reaction kinetics, thermal and electrical conductivities, Monte Carlo simulation techniques, and master equations. Covers the full breadth of materials kinetics, including organic and inorganic materials, solids and liquids, theory and experiments, macroscopic and microscopic interpretations, and analytical and computational approaches Demonstrates how diffusion, viscosity microstructural evolution, relaxation, and other kinetic phenomena can be leveraged in the practical design of new materials Provides a seamless connection between thermodynamics and kinetics Includes practical exercises that reinforce key concepts at the end of each chapter

A Life Scientist's Guide to Physical Chemistry Wiley-Interscience
Selecting the best type of reactor for any particular chemical reaction, taking into consideration safety, hazard analysis, scale-up, and many other factors is essential to any industrial problem. An understanding of chemical reaction kinetics and the design of chemical reactors is key to the success of the of the chemist and the chemical engineer in such an endeavor. This valuable reference volume conveys a basic understanding of chemical reactor design methodologies, incorporating control, hazard analysis, and other topics not covered in similar texts. In addition to covering fluid mixing, the treatment of wastewater, and chemical reactor modeling, the author includes sections on safety in chemical reaction and scale-up, two topics that are often neglected or overlooked. As a real-world introduction to the modeling of chemical kinetics and reactor design, the author includes a case study on ammonia synthesis that is integrated throughout the text. The text also features an accompanying CD, which contains computer programs developed to solve modeling problems using numerical methods. Students, chemists, technologists, and chemical engineers will all benefit from this comprehensive volume. Shows readers how to select the best reactor design, hazard analysis, and safety in design methodology Features computer programs developed to solve modeling problems using numerical methods
Theories of Molecular Reaction Dynamics McGraw-Hill Science, Engineering & Mathematics
This second, extended and updated edition presents the current state of kinetics of chemical reactions, combining basic knowledge with results recently obtained at the frontier of science. Special attention is paid to the problem of the chemical reaction complexity with theoretical and methodological concepts illustrated throughout by numerous examples taken from heterogeneous catalysis combustion and enzyme processes. Of great interest to graduate students in both chemistry and chemical engineering.
Chemical Kinetics Oxford University Press on Demand
Chemical Kinetics The Study of Reaction Rates in Solution Kenneth A. Connors This chemical kinetics book blends physical theory, phenomenology and empiricism to provide a guide to the experimental practice and interpretation of reaction kinetics in solution. It is suitable for courses in chemical kinetics at the graduate and advanced undergraduate levels. This book will appeal to students in physical organic chemistry, physical inorganic chemistry, biophysical chemistry, biochemistry, pharmaceutical chemistry and water chemistry all fields concerned with the rates of chemical reactions in the solution phase.
Tutorials in Molecular Reaction Dynamics Springer Science & Business Media
Introduction to Chemical Kinetics is a compilation of lecture notes of the author about principles, concepts, and theories in chemical kinetics. The book tackles the nature of chemical kinetics, reaction rates and order, and thermodynamic consistency of rate laws. The effects of temperature on kinetics, prediction of reaction rates, gas-phase reactions, and controlled reactions are also discussed. The text also explains the reactions catalyzed by enzymes; reactions in solids and heterogenous systems; oxidation of metals; catalysis of reactions by solids; and methods for different reaction rates. The monograph is recommended as a textbook for undergraduate students in chemistry who are currently taking up kinetics, as it is an easily understood and concise book that can also be used as reference.
Introduction to Molecular Dynamics and Chemical Kinetics Wiley-VCH Verlag GmbH
Chemical Kinetics bridges the gap between beginner and specialist with a path that leads the reader from the phenomenological approach to the rates of chemical reactions to the state-of-the-art calculation of the rate constants of the most prevalent reactions: atom transfers, catalysis, proton transfers, substitution reactions, energy transfers and electron transfers. For the beginner provides the basics: the simplest concepts, the fundamental experiments, and the underlying theories. For the specialist shows where sophisticated experimental and theoretical methods combine to offer a panorama of time-dependent molecular phenomena connected by a new rational. Chemical Kinetics goes far beyond the qualitative description: with the guidance of theory, the path becomes a reaction path that can actually be inspected and calculated. But Chemical Kinetics is more about structure and reactivity than numbers and calculations. A great emphasis in the clarity of the concepts is achieved by illustrating all the theories and mechanisms with recent examples, some of them described with sufficient detail and simplicity to be used in general chemistry and lab courses. * Looking at atoms and molecules, and how molecular structures change with time. * Providing practical examples and detailed theoretical calculations * Of special interest to Industrial Chemistry and Biochemistry
The Study of Reaction Rates in Solution Springer Science & Business Media
Reaction Rate Theory and Rare Events bridges the historical gap between these subjects because the increasingly multidisciplinary nature of scientific research often requires an understanding of both reaction rate theory and the theory of other rare events. The book discusses collision theory, transition state theory, RRKM theory, catalysis, diffusion limited kinetics, mean first passage times, Kramers theory, Grote-Hynes theory, transition path theory, non-adiabatic reactions, electron transfer, and topics from reaction network analysis. It is an essential reference for students, professors and scientists who use reaction rate theory or the theory of rare events. In addition, the book discusses transition state search algorithms, tunneling corrections, transmission coefficients, microkinetic models, kinetic Monte Carlo, transition path sampling, and importance sampling methods. The unified treatment in this book explains why chemical reactions and other rare events, while having many common theoretical foundations, often require very different computational modeling strategies. Offers an integrated approach to all simulation theories and reaction network analysis, a unique approach not found elsewhere Gives algorithms in pseudocode for using molecular simulation and computational chemistry methods in studies of rare events Uses graphics and explicit examples to explain concepts Includes problem sets developed and tested in a course range from pen-and-paper theoretical problems, to computational exercises
From Classical Macroscopic Descriptions to Modern Microscopic Details Elsevier
Methods in Reaction Dynamics is a collection of lectures given at the 1999 Mariapfarr Workshop in Theoretical Chemistry. Arranged as a series of detailed reviews, it provides an overview of quantum mechanical techniques used to describe and simulate the dynamics and kinetics of elementary chemical reactions. The volume provides in-depth discussions of selected topics in Theoretical Chemistry, such as quantum methods in theoretical and computational reaction dynamics and kinetics; time-dependent, time-independent and mixed quantum-classical techniques. Some of the topics have not been reviewed before in detail.
Second Revised Edition Cambridge University Press
Chemical Kinetics and Reaction DynamicsCourier Corporation