

Chemical Kinetics And Reaction Dynamics Solution

The book brings together, for the first time, all aspects of reactions of metallic species in the gas phase and gives an up-to-date overview of the field. Reactions covered include those of atomic, other free radical and transient neutral species, as well as ions. Experimental and theoretical work is reviewed and the efforts to establish a closer link between these approaches are discussed. The field is mainly approached from a fundamental point-of-view, but the applied problems which have helped stimulate the interest are pointed out and form the major subject of the final chapters. These emphasize the competition between purely gas-phase and gas-surface reactions. The reaction rate constant plays an essential role a wide range of processes in biology, chemistry and physics. Calculating the reaction rate constant provides considerable understanding to a reaction and this book presents the latest thinking in modern rate computational theory. The editors have more than 30 years' experience in researching the theoretical computation of chemical reaction rate constants by global dynamics and transition state theories and have brought together a global pool of expertise discussing these in a variety of contexts and across all phases. This thorough treatment of the subject provides an essential handbook to students and researchers entering the field and a comprehensive reference to established practitioners across the sciences, providing better tools to determining reaction rate constants.

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The first text to cover both molecular reaction dynamics and chemical kinetics and their respective theories in a single source. After introductory material, the monograph goes on to cover interaction potentials; relative motion and the collisional approach for chemical reaction in the gas phase; partition functions; transition state theory; unimolecular reactions; molecular reactions calculations; non-adiabatic transitions; surface kinetics; chemical reactions in solution; energetic changes in solvating a molecule; transition state theory in solution; models for diffusion; Kramers' theory of viscosity of solvent in chemical reactions; and electronic transfer reactions in solution. Also includes problems and solved exercises.

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 Reactions, 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

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resonances. . Presents considerable advances in the field made during the last decade.
. Treats both the statistical as well as the fully quantum mechanical view.
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

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computational exercises

This book gives a concise overview of the mathematical foundations of kinetics used in chemistry and systems biology. The analytical and numerical methods used to solve complex rate equations with the widely used deterministic approach will be described, with primary focus on practical aspects important in designing experimental studies and the evaluation of data. The introduction of personal computers transformed scientific attitudes in the last two decades considerably as computational power ceased to be a limiting factor. Despite this improvement, certain time-honored approximations in solving rate equations such as the pre-equilibrium or the steady-state approach are still valid and necessary as they concern the information content of measured kinetic traces. The book shows the role of these approximations in modern kinetics and will also describe some common misconceptions in this field.

This series of volumes aims to publish authoritative review articles on a wide range of exciting and contemporary topics in gas and condensed phase kinetics. Research in Chemical Kinetics complements the acclaimed series Comprehensive Chemical Kinetics, and is edited by the same team of professionals. The reviews contained in this volume are concise, topical accounts of specific research written by acknowledged experts. The authors summarize their latest work and place it in a general context. Particular strengths of the volume are the quality of the contributions and their topicality, and the rapid publication realized.

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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.

"Kinetics and Dynamics" on molecular modeling of dynamic processes opens with an introductory overview before discussing approaches to reactivity of small systems in the

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gas phase. Then it examines studies of systems of increasing complexity up to the dynamics of DNA. This title has interdisciplinary character presenting wherever possible an interplay between the theory and the experiment. It provides basic information as well as the details of theory and examples of its application to experimentalists and theoreticians interested in modeling of dynamic processes in chemical and biochemical systems. All contributing authors are renowned experts in their fields and topics covered in this volume represent the forefront of today's science.

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.

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

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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.

Chemical Kinetics and Reaction Dynamics Courier Corporation

Molecular reaction dynamics is the study of chemical and physical transformations of matter at the molecular level. The understanding of how chemical reactions occur and how to control them is fundamental to chemists and interdisciplinary areas such as materials and nanoscience, rational drug design, environmental and astrochemistry. This book provides a thorough foundation to this area. The first half is introductory, detailing experimental techniques for initiating and probing reaction dynamics and the essential insights that have been gained. The second part explores key areas including photoselective chemistry, stereochemistry, chemical reactions in real time and chemical reaction dynamics in solutions and interfaces. Typical of the new challenges are molecular machines, enzyme action and molecular control. With problem sets included, this book is suitable for advanced undergraduate and graduate students, as well as being supplementary to chemical kinetics, physical chemistry, biophysics and materials

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science courses, and as a primer for practising scientists.

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.

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.

This book is a progressive presentation of kinetics of the chemical reactions. It provides

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complete coverage of the domain of chemical kinetics, which is necessary for the various future users in the fields of Chemistry, Physical Chemistry, Materials Science, Chemical Engineering, Macromolecular Chemistry and Combustion. It will help them to understand the most sophisticated knowledge of their future job area. Over 15 chapters, this book presents the fundamentals of chemical kinetics, its relations with reaction mechanisms and kinetic properties. Two chapters are then devoted to experimental results and how to calculate the kinetic laws in both homogeneous and heterogeneous systems. The following two chapters describe the main approximation modes to calculate these laws. Three chapters are devoted to elementary steps with the various classes, the principles used to write them and their modeling using the theory of the activated complex in gas and condensed phases. Three chapters are devoted to the particular areas of chemical reactions, chain reactions, catalysis and the stoichiometric heterogeneous reactions. Finally the non-steady-state processes of combustion and explosion are treated in the final chapter.

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. Molecular reaction dynamics is about the detailed atomic-level description of chemical reactions. Based on quantum mechanics and statistical mechanics or, as an approximation, classical mechanics, the dynamics of uni- and bi-molecular elementary reactions are described. The book features a detailed presentation of transition-state theory which plays an important role in practice, and a comprehensive discussion of basic theories of

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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 book is a short primer on chemical reaction rates based on a six-lecture first-year undergraduate course taught by the author at the University of Oxford. The book explores the various factors that determine how fast or slowly a chemical reaction proceeds and describes a variety of experimental methods for measuring reaction rates. The link between the reaction rate and the sequence of steps that makes up the reaction mechanism is also investigated.

Chemical reaction rates is a core topic in all undergraduate chemistry courses.

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

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detailed theoretical calculations * Of special interest to Industrial Chemistry and Biochemistry Chemical Kinetics and Process Dynamics in Aquatic Systems is devoted to chemical reactions and biogeochemical processes in aquatic systems. The book provides a thorough analysis of the principles, mathematics, and analytical tools used in chemical, microbial, and reactor kinetics. It also presents a comprehensive, up-to-date description of the kinetics of important chemical processes in aquatic environments. Aquatic photochemistry and correlation methods (e.g., LFERs and QSARs) to predict process rates are covered. Numerous examples are included, and each chapter has a detailed bibliography and problems sets. The book will be an excellent text/reference for professionals and students in such fields as aquatic chemistry, limnology, aqueous geochemistry, microbial ecology, marine science, environmental and water resources engineering, and geochemistry.

The book on Advanced Chemical Kinetics gives insight into different aspects of chemical reactions both at the bulk and nanoscale level and covers topics from basic to high class. This book has been divided into three sections: (i) "Kinetics Modeling and Mechanism," (ii) "Kinetics of Nanomaterials," and (iii) "Kinetics Techniques." The first section consists of six chapters with a variety of topics like activation energy and complexity of chemical reactions; the measurement of reaction routes; mathematical modeling analysis and simulation of enzyme kinetics; mechanisms of homogeneous charge compression ignition combustion for the fuels; photophysical processes and photochemical changes; the mechanism of hydroxyl radical, hydrate electron, and hydrogen atom; and acceptorless alcohol dehydrogenation. The understanding of the kinetics of nanomaterials, to bridge the knowledge gap, is presented in the second section. The third section highlights an overview of experimental techniques used

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to study the mechanism of reactions.

This text teaches the principles underlying modern chemical kinetics in a clear, direct fashion, using several examples to enhance basic understanding. Solutions to selected problems. 2001 edition. /div

Covering chemical kinetics from the working chemist's point of view, this book aims to prepare chemists to devise experiments to test different hypothesis. A number of examples from research literature have been included.

Principles of Chemical Kinetics is devoted to the principles and applications of chemical kinetics. The phenomenology and commonly used theories of chemical kinetics are presented in a critical manner, with particular emphasis on collision dynamics. How and what mechanistic information can be obtained from various experimental approaches is stressed throughout this book. Comprised of nine chapters, this text opens with an overview of reaction rates and their empirical analysis, along with theories of chemical kinetics. The following chapters consider reactions and unimolecular decompositions in the gas phase; chemical reactions in molecular beams; and energy transfer and partitioning in chemical reactions. Kinetics in liquid solutions and fast reactions in liquids are also described. The final chapter looks at the kinetics of enzymes, with particular reference to steady state and transient state kinetics, the pH and temperature dependence of kinetic parameters, and the mechanism underlying enzymatic action. This monograph is intended for students with a general college background in chemistry, physics, and mathematics, and with a typical undergraduate course in physical chemistry.

This text presents a balanced presentation of the macroscopic view of empirical kinetics and

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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 $H + H_2$.

A comprehensive, in-depth presentation of theoretical underpinnings and mathematical techniques This is the first book of its kind to combine all the theories of molecular reaction dynamics and chemical kinetics in a single source. It provides a sophisticated treatment of the material that functions both as a professional reference and a high-level text for PhD and postdoctoral researchers. *Advanced Molecular Dynamics and Chemical Kinetics* offers exceptional, in-depth coverage and includes a complete discussion of the theoretical as well as mathematical presentation of techniques. It features relevant exercises as well as comprehensive coverage of: * Second Quantization * Semiclassical Theory * Quantum Theory of Reaction Rates * Feynman Path Integrals * Wavepacket Propagation and Grid Methods * Photodissociation * Molecular Properties of Solvated Molecules * Quantum Model for Electron Transfer * Electron Transfer Coupling Elements * Proton Transfer Reactions in Solution This is the ideal reference for seasoned professionals in molecular reaction dynamics as well as for younger researchers who may want to enter the field or simply wish to learn more about it. Also available: *Introduction to Molecular Dynamics and Chemical Kinetics* Gert D. Billing and Kurt V. Mikkelsen

A practical approach to chemical reaction kinetics—from basic concepts to laboratory methods—featuring numerous real-world examples and case studies This book focuses on fundamental aspects of reaction kinetics with an emphasis on mathematical methods for analyzing experimental data and interpreting results. It describes basic concepts of reaction

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kinetics, parameters for measuring the progress of chemical reactions, variables that affect reaction rates, and ideal reactor performance. Mathematical methods for determining reaction kinetic parameters are described in detail with the help of real-world examples and fully-worked step-by-step solutions. Both analytical and numerical solutions are exemplified. The book begins with an introduction to the basic concepts of stoichiometry, thermodynamics, and chemical kinetics. This is followed by chapters featuring in-depth discussions of reaction kinetics; methods for studying irreversible reactions with one, two and three components; reversible reactions; and complex reactions. In the concluding chapters the author addresses reaction mechanisms, enzymatic reactions, data reconciliation, parameters, and examples of industrial reaction kinetics. Throughout the book industrial case studies are presented with step-by-step solutions, and further problems are provided at the end of each chapter. Takes a practical approach to chemical reaction kinetics basic concepts and methods Features numerous illustrative case studies based on the author's extensive experience in the industry Provides essential information for chemical and process engineers, catalysis researchers, and professionals involved in developing kinetic models Functions as a student textbook on the basic principles of chemical kinetics for homogeneous catalysis Describes mathematical methods to determine reaction kinetic parameters with the help of industrial case studies, examples, and step-by-step solutions Chemical Reaction Kinetics is a valuable working resource for academic researchers, scientists, engineers, and catalyst manufacturers interested in kinetic modeling, parameter estimation, catalyst evaluation, process development, reactor modeling, and process simulation. It is also an ideal textbook for undergraduate and graduate-level courses in chemical kinetics, homogeneous catalysis, chemical reaction

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engineering, and petrochemical engineering, biotechnology.

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

This book is focused on mathematical modelling of chemical kinetics. The authors present the classification of basic models of chemical kinetics, thermokinetics and macrokinetics, as well as their application for the most important chemical transformations, such as combustion and catalysis. Readers will find a detailed description and analysis of different mathematical instruments which can be applied for simulation of reaction dynamics.

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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.

Motivating students to engage with physical chemistry through biological examples, this textbook demonstrates how the tools of physical chemistry can be used to illuminate biological questions. It clearly explains key principles and their relevance to life science students, using only the most straightforward and relevant mathematical tools. More than 350 exercises are spread throughout the chapters, covering a wide range of biological applications and explaining issues that students often find challenging. These, along with problems at the end of

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each chapter and end-of-term review questions, encourage active and continuous study. Over 130 worked examples, many deriving directly from life sciences, help students connect principles and theories to their own laboratory studies. Connections between experimental measurements and key theoretical quantities are frequently highlighted and reinforced. Answers to the exercises are included in the book. Fully worked solutions and answers to the review problems, password-protected for instructors, are available at www.cambridge.org/rousseau.

Over the last decade, increased attention to reaction dynamics, combined with the intensive application of computers in chemical studies, mathematical modeling of chemical processes, and mechanistic studies has brought graph theory to the forefront of research. It offers an advanced and powerful formalism for the description of chemical reactions and their intrinsic reaction mechanisms. *Chemical Reaction Networks: A Graph-Theoretical Approach* elegantly reviews and expands upon graph theory as applied to mechanistic theory, chemical kinetics, and catalysis. The authors explore various graph-theoretical approaches to canonical representation, numbering, and coding of elementary steps and chemical reaction mechanisms, the analysis of their topological structure, the complexity estimation, and classification of reaction mechanisms. They discuss topologically distinctive features of multiroute catalytic and noncatalytic and chain reactions involving metal complexes. With its careful balance of clear language and mathematical rigor, the presentation of the authors' significant original work, and emphasis on practical applications and examples, *Chemical Reaction Networks: A Graph Theoretical Approach* is both an outstanding reference and valuable tool for chemical research.

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Chemical Kinetics and Reaction Dynamics is a modern textbook for advanced courses. Houston emphasizes the essential principles of kinetics and dynamics through relevant examples and current research, providing students with a clear, basic understanding. Many processes of the chemical industry are based upon heterogeneous catalysis. Two important items of these processes are the development of the catalyst itself and the design and optimization of the reactor. Both aspects would benefit from rigorous and accurate kinetic modeling, based upon information on the working catalyst gained from classical steady state experimentation, but also from studies using surface science techniques, from quantum chemical calculations providing more insight into possible reaction pathways and from transient experimentation dealing with reactions and reactors. This information is seldom combined into a kinetic model and into a quantitative description of the process. Generally the catalytic aspects are dealt with by chemists and by physicists, while the chemical engineers are called upon for mechanical aspects of the reactor design and its control. The symposium "Dynamics of Surfaces and Reaction Kinetics in Heterogeneous Catalysis" aims at illustrating a more global and concerted approach through a number of prestigious keynote lectures and severely screened oral and poster presentations.

Kinetics and Dynamics of Elementary Gas Reactions surveys the state of modern knowledge on elementary gas reactions to understand natural phenomena in terms of molecular behavior. Part 1 of this book describes the theoretical and conceptual background of elementary gas-phase reactions, emphasizing the assumptions and limitations of each theoretical approach, as well as its strengths. In Part 2, selected experimental results are considered to demonstrate the scope of present day techniques and illustrate the application of the theoretical ideas

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introduced in Part 1. This publication is intended primarily for working kineticists and chemists, but is also beneficial to graduate students.

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