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An insightful analysis of confined chemical systems for theoretical and experimental scientists Chemical Reactivity in Confined Systems: Theory and Applications presents a theoretical basis for the molecular phenomena observed in confined spaces. The book highlights state-of-the-art theoretical and computational approaches, with a focus on obtaining physically relevant clarification of the subject to enable the reader to build an appreciation of underlying chemical principles. The book includes real-world examples of confined systems that highlight how the reactivity of atoms and molecules change upon encapsulation. Chapters include discussions on recent developments related to several host-guest systems, including cucurbit[n]uril, ExBox+4, clathrate hydrates, octa acid cavitand, metal organic frameworks (MOFs), covalent organic frameworks (COFs), zeolites, fullerenes, and carbon nanotubes. Readers will learn how to carry out new calculations to understand the physicochemical behavior of confined quantum systems. Topics covered include: A thorough introduction to global reactivity descriptors, including electronegativity, hardness, and electrophilicity An exploration of the Fukui function, as well as dual descriptors, higher order derivatives, and reactivity through information theory A practical discussion of spin dependent reactivity and temperature dependent reactivity Concise treatments of population analysis, reaction force, electron localization functions, and the solvent effect on reactivity Perfect for academic researchers and graduate students in theoretical and computational chemistry and confined chemical systems, Chemical Reactivity in Confined Systems: Theory and Applications will also earn a place in the libraries of professionals working in the areas of catalysis, supramolecular chemistry, and porous materials.

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

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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

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

Chemistry and chemical engineering have changed significantly in the last decade. They have broadened their scope into biology, nanotechnology, materials science, computation, and advanced methods of process systems engineering and control so much that the programs in most chemistry and chemical engineering departments now barely resemble the classical notion of chemistry. Beyond the Molecular Frontier brings together research, discovery, and invention across the entire spectrum of the chemical sciences from fundamental, molecular-level chemistry to large-scale chemical processing technology. This reflects the way the field has evolved, the synergy at universities between research and education in chemistry and chemical engineering, and the way chemists and chemical engineers work together in industry. The astonishing developments in science and engineering during the 20th century have made it possible to dream of new goals that might previously have been considered unthinkable. This book identifies the key opportunities and challenges for the chemical sciences, from basic research to societal needs and from terrorism defense to environmental protection, and it looks at the ways in which chemists and chemical engineers can work together to contribute to an improved future.

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