

## Reactants And Products In Chemical Reactions Dummies

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 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 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  $H + H_2$ .

In this book we discuss both the technical and non-technical reasons science has been unable to find cures for inherited diseases such as CF, despite the exponential increase in knowledge of disease mechanisms we currently witness. New directions in scientific research and protocols are suggested that may help bring about actual cures for genetic diseases through medicinal gene therapy. A new computational approach, called the omega algorithm, is developed, implemented and applied to find compounds that could potentially correct the delta F508 mutation responsible for cystic fibrosis. Links to downloadable files, including the SMILES Chemical Reaction Database, are given in an appendix to assist the reader with their own further studies. The SMILES Chemical Reaction Database is a file containing structural information about pairs of reactants and products of two million different chemical reactions. The simplified molecular-input line-entry system (SMILES) of representing molecular structures is used to represent molecular connectivity and stereochemical relationships as strings of characters, and indeed chemical reactions. The SMILES Reaction Database is now 186.8 MB in size, and it contains two million reactant-product pairs extracted from thousands of respected journals and patents, contained in six files. The reaction data entries in each file of the database occur on consecutive lines of the file, which are delineated by newline characters. The database can be viewed using a program such as MarvinView. All computer code in the book is written in the Mathematica language and can be downloaded from links given in the book.

Collection of terms with authoritative definitions, spanning the whole range of chemistry.

Antoine Lavoisier's great accomplishments include the discovery of oxygen's role in combustion, helping to develop the metric system, writing the first extensive list of elements, helping to reform the nomenclature of chemistry, and the discovery that while matter may change shape through chemical reaction its mass remains the same. It is for these extraordinary accomplishments that he is often referred to as the "Father of Modern Chemistry." Some scholars argue that this moniker is more the result of self-promotion and that his discoveries relied heavily on the work of others, nonetheless his impact on advancing this field of science cannot be understated. "Elements of Chemistry" was first published in 1790 and is largely concerned with the chemistry of combustion. While modern students of chemistry might find the work limited in its scope, the historical impact of its publication cannot be understated. The experiments contained within helped to lay the foundation for the understanding of the role of oxygen, hydrogen, acids, and alcohols in chemical reactions and its emphasis on quantitative analysis and instrumentation helped to establish the use of chemistry as a legitimate science for understanding and defining the physical world.

Since the discovery of quantum mechanics, more than fifty years ago, the theory of chemical reactivity has taken the first steps of its development. The knowledge of the electronic structure and the properties of atoms and molecules is the basis for an understanding of their interactions in the elementary act of any chemical process. The increasing information in this field during the last decades has stimulated the elaboration of the methods for evaluating the potential energy of the reacting systems as well as the creation of new methods for calculation of reaction probabilities (or cross sections) and rate constants. An exact solution to these fundamental problems of theoretical chemistry based on quantum mechanics and statistical physics, however, is still impossible even for the simplest chemical reactions.

Therefore, different approximations have to be used in order to simplify one or the other side of the problem. At present, the basic approach in the theory of chemical reactivity consists in separating the motions of electrons and nuclei by making use of the Born-Oppenheimer adiabatic approximation to obtain electronic energy as an effective potential for nuclear motion. If the potential energy surface is known, one can calculate, in principle, the reaction probability for any given initial state of the system. The reaction rate is then obtained as an average of the reaction probabilities over all possible initial states of the reacting species. In the different stages of this calculational scheme additional approximations are usually introduced.

Written by a leader in the field, the Fundamentals of Environmental Chemistry, Second Edition puts the fundamentals of chemistry and environmental chemistry right at your students fingertips. Manahan presents the material in an understandable and interesting manner without being overly simplistic. They get basic coverage on: - Matter and the basis of its physical nature and behavior - Organic and biological chemistry - Chemistry of water, soil, and air - Industrial chemistry - Toxicological chemistry as it pertains to occupational health and human exposure to pollutants and toxicants - Energy, nuclear energy, and nuclear waste - Applications of nuclear science in areas such as tracing pesticide degradation and nuclear medicine - More than an introduction to this field, Fundamentals of Environmental Chemistry, Second Edition provides the foundation that gives your students an understanding of the chemical processes of the environment and the effects pollution on those processes.

Carbonyl Compounds Discover how carbonyl compounds bridge reactants, catalysts, and specific products Carbonyl-containing molecules represent some of the most versatile functionalities in organic chemistry, with applications in a wide variety of areas. In Carbonyl Compounds: Reactants, Catalysts and Products, accomplished chemists and authors Feng Shi, Hongli Wang, and Xingchao Dai deliver a comprehensive treatment of these multi-functional compounds. You'll discover how to build carbonyl molecules with traditional and non-traditional methods, how to transform carbonyl-containing molecules into fine chemicals, and how to use carbonyl-containing molecules as catalytic materials for the synthesis of fine chemicals. The book is a comprehensive and systematic treatment of carbonyl compounds as reactants, catalysts, and products. From the use of carbon monoxide in the hydroformylation of alkenes and alkynes to the reactions via carbonyl and hydroxyl groups recycling, you'll find everything you need to know about these versatile compounds. Readers will also benefit from the inclusion of: A thorough introduction to carbonyl molecules as reactants, including treatments of carbon monoxide, carbon dioxide, HCHO, HCOOH, and CO surrogates An exploration of carbonyl compounds as catalysts, including acid catalyzed reactions with  $-CO_2H$  and reactions via carbonyl and hydroxyl groups recycling A practical discussion of the synthetic applications of carbonyl compounds, including the synthesis of functional molecules and the synthesis of functional materials A concise treatment of future perspectives and potential research trends for carbonyl molecules Perfect for organic, catalytic, pharmaceutical, and physical chemists, Carbonyl Compounds will also earn a place in the libraries of chemical engineers and materials scientists seeking a one-stop reference for up-to-date information about the building, transformation, and

applications of carbonyl-containing molecules.

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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CK-12 Foundation's Chemistry - Second Edition FlexBook covers the following chapters: Introduction to Chemistry - scientific method, history. Measurement in Chemistry - measurements, formulas. Matter and Energy - matter, energy. The Atomic Theory - atom models, atomic structure, sub-atomic particles. The Bohr Model of the Atom electromagnetic radiation, atomic spectra. The Quantum Mechanical Model of the Atom energy/standing waves, Heisenberg, Schrodinger. The Electron Configuration of Atoms Aufbau principle, electron configurations. Electron Configuration and the Periodic Table- electron configuration, position on periodic table. Chemical Periodicity atomic size, ionization energy, electron affinity. Ionic Bonds and Formulas ionization, ionic bonding, ionic compounds. Covalent Bonds and Formulas nomenclature, electronic/molecular geometries, octet rule, polar molecules. The Mole Concept formula stoichiometry. Chemical Reactions balancing equations, reaction types. Stoichiometry limiting reactant equations, yields, heat of reaction. The Behavior of Gases molecular structure/properties, combined gas law/universal gas law. Condensed Phases: Solids and Liquids intermolecular forces of attraction, phase change, phase diagrams. Solutions and Their Behavior concentration, solubility, colligative properties, dissociation, ions in solution. Chemical Kinetics reaction rates, factors that affect rates. Chemical Equilibrium forward/reverse reaction rates, equilibrium constant, Le Chatelier's principle, solubility product constant. Acids-Bases strong/weak acids and bases, hydrolysis of salts, pH Neutralization dissociation of water, acid-base indicators, acid-base titration, buffers. Thermochemistry bond breaking/formation, heat of reaction/formation, Hess' law, entropy, Gibb's free energy. Electrochemistry oxidation-reduction, electrochemical cells. Nuclear Chemistry radioactivity, nuclear equations, nuclear energy. Organic Chemistry straight chain/aromatic hydrocarbons, functional groups. Chemistry Glossary

The Chemical Reactions Student Learning Guide includes self-directed readings, easy-to-follow illustrated explanations, guiding questions, inquiry-based activities, a lab investigation, key vocabulary review and assessment review questions, along with a post-test. It covers the following standards-aligned concepts: Changes of Matter; Chemical Reactions; Formulas & Equations; Balancing Equations; Types of Chemical Reactions (1); Types of Chemical Reactions (2); Energy in Chemical Reactions; Evidence of Chemical Reactions; and Chemical Reaction Rates & Catalysts. Aligned to Next Generation Science Standards (NGSS) and other state standards.

The aim of this research is to gain insight into hydrogen combustion as a prototype of complex chemistry via classical molecular dynamics (CMD) simulations given the presently available reactive force field, ReaxFF. We focus on developing computational and theoretical methods to analyze CMD simulations of hydrogen combustion and glean the details of chemistry to identify major sequential elementary reactions connecting reactants to products. In Chapter 1 we explain the problem exists in understanding complex chemistry followed by a brief overview of currently popular methods used to study complex chemical processes with an emphasis on hydrogen combustion. Then, we propose our approach that is based on CMD simulations to tackle the problem and elaborate on the goals of the study. In Chapter 2 we introduce an algorithm that identifies every elementary molecular event such as reactions and formation/dissociation of hydrogen-bond complexes in CMD simulations of hydrogen combustion. After validating the ReaxFF force field for the equation of state and interaction energy, we then present ReaxFF-based results of CMD simulations for the early chemistry of hydrogen combustion. The CMD simulations predict two major pathways for production of initial radicals; a termolecular elementary reaction  $2\text{O}_2 + \text{H}_2 \rightarrow 2\text{HO}_2$  and the widely-accepted bimolecular reaction  $\text{O}_2 + \text{H}_2 \rightarrow \text{H} + \text{HO}_2$ . Later in Chapter 2, we present and discuss the effects of density on the early chemistry of hydrogen combustion; which show that at elevated density and low temperature the termolecular reaction dominates the chemistry. We describe a method based on collision gas theory that can be used with CMD simulations to explain the observed trends. In Chapter 3, we provide results for Nudged Elastic Band method (NEB) to characterize potential energy profiles for the bi- and ter-molecular reactions predicted by ReaxFF. Then, we use state-of-the-art electronic structure calculations to examine accuracy of the ReaxFF predictions for the energies and stationary points of the reactions. Later in Chapter 3 we discuss the effect of temperature on the occurrence probability of the ter- and bi-molecular reactions based on the electronic structure predictions of the energy barriers. Lastly, we identify the steric requirements predicted by ReaxFF for each reaction based on the CMD simulations. In Chapter 4, we present a method based on Tolman's interpretation of activation energy that can be applied to thermal and non-thermal chemical reactions in molecular dynamics simulations of bulk gases. We use Boyd's assumption of local equilibrium thermodynamics to generalize Tolman's concept for application to individual reaction clusters, which include all chemical species that participate in an isolated reaction, for which we define the reaction cluster local energy (RCLE). The RCLE is shown to be conserved during the course of a reaction. We identify the transition configuration (TC), which is the point where the local energy of the reactants crosses that of the products. The TC is a unique point that separates reactants and products and can be used as an estimation of the transition state in accordance with Marcus theory for proton transfer reactions. We demonstrate application of the method by computing activation energies of the several reactions in molecular dynamics simulations.

Bishop's text shows students how to break the material of preparatory chemistry down and master it. The system of objectives tells the students exactly what they must learn in each chapter and where to find it.

Chemistry in Quantitative Language, second edition is an invaluable guide to solving chemical equations and calculations. It provides readers with intuitive and systematic strategies to carry out the many kinds of calculations they will meet in general chemistry.

Advances in Enzymology and Related Areas of Molecular Biology is a seminal series in the field of biochemistry, offering researchers access to authoritative reviews of the latest discoveries in all areas of enzymology and molecular biology.

These landmark volumes date back to 1941, providing an unrivaled view of the historical development of enzymology. The series offers researchers the latest understanding of enzymes, their mechanisms, reactions and evolution, roles in complex biological process, and their application in both the laboratory and industry. Each volume in the series features contributions by leading pioneers and investigators in the field from around the world. All articles are carefully edited to ensure thoroughness, quality, and readability. With its wide range of topics and long historical pedigree, *Advances in Enzymology and Related Areas of Molecular Biology* can be used not only by students and researchers in molecular biology, biochemistry, and enzymology, but also by any scientist interested in the discovery of an enzyme, its properties, and its applications.

Exothermic reactions used for the production of chemicals present a hazard if they proceed without control. Runaway reactions can result in a blow-off of the reactor top and an emission of reactants and products, possibly followed by a gas explosion. Undesired exothermic reactions initiated during production, purification or storage by excessive temperatures or other causes have similar destructive effects, even if the origin is different. Although the hazards connected with exothermic reactions have been known since the inception of the chemical industry, a systematic knowledge of the possible effects has only been developed in the last 25 years. A number of incidents in the chemical industry, which have been investigated by groups of experts from various companies, have promoted the understanding of these hazards. The author has investigated incidents in plants and tested experimental methods for more than 20 years. In particular he was interested in collecting and comparing safety-relevant data of products. At the end of his industrial career he now believes that it is important to pass on information about this field of activity to younger colleagues who are interested in the safety of chemical plants. The purpose of this book is to provide a basis for understanding the hazards arising from exothermic reactions. Knowledge of the relevant properties is necessary for a safe processing of products and mixtures. The test methods which have been used and developed together with the increasing understanding of the hazards of reactions are particularly important. A critical survey of extensive experimental techniques is provided.

Introductory chemistry students need to develop problem-solving skills, and they also must see why these skills are important to them and to their world. *Introductory Chemistry, Fourth Edition* extends chemistry from the laboratory to the student's world, motivating students to learn chemistry by demonstrating how it is manifested in their daily lives.

Throughout, the *Fourth Edition* presents a new student-friendly, step-by-step problem-solving approach that adds four steps to each worked example (Sort, Strategize, Solve, and Check). Tro's acclaimed pedagogical features include Solution Maps, Two-Column Examples, Three-Column Problem-Solving Procedures, and Conceptual Checkpoints. This proven text continues to foster student success beyond the classroom with MasteringChemistry®, the most advanced online tutorial and assessment program available. This package contains: Tro, *Introductory Chemistry with MasteringChemistry® Long*, *Introductory Chemistry Math Review Toolkit*

This graduate textbook, written by experienced lecturers, features the study and computation of efficient reactive processes. The text begins with the problem of determining the chemical reaction properties by first decomposing complex processes into their elementary components. Next, the problem of two colliding mass points is investigated and relationships between initial conditions and collision outcomes are discussed. The failure of classical approaches to match experimental information is discussed and a quantum formulation of the calculation of the properties of two colliding bodies is provided. The authors go on to describe how the formalism is extended to structured collision partners by discussing the methods used to compute the electronic structure of polyelectronic reactants and products and the formalism of atom diatom reactions. Additionally, the relationships between the features of the potential energy surface and the outcomes of the reactive dynamics, are discussed. Methods for computing quantum, classical, and semi-classical reactive probabilities based on the already discussed concepts and tools are also featured and the resulting main typical reactive behaviors are analyzed. Finally, the possibility of composing the computational tools and technologies needed to tackle more complex simulations as well as the various competences and distributed computing infrastructure needed for developing synergistic approaches to innovation are presented.

In recent years, a significant amount of progress has been made using green chemistry in the synthesis of synthetically useful compounds and molecules by replacing hazardous chemicals with greener alternatives. However, there is still room for improvement, especially in the pharmaceutical sector where new drugs are being formulated. This book examines green approaches to overcoming hazardous organic transformations. Summarizing recent developments, the book features a detailed description of some of the high impact active pharmaceutical ingredients that have been developed considering green chemistry approaches. It explores the design, engineering and process development and the calculations to account for waste. The book includes strategies to further advance green approaches in the development of generic pharmaceutical industries and features novel, innovative approaches that promote waste-free organic synthesis. This book is of interest to industrialists working in pharmaceuticals and researchers working in green chemistry.

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 to study the mechanism of reactions.

The calculation of cross sections and rate constants for chemical reactions in the gas phase has long been a major problem in theoretical chemistry. The need for reliable and applicable theories in this field is evident when one considers the significant recent advances that have been made in developing experimental techniques, such as lasers and molecular beams, to probe the microscopic details of chemical reactions. For example, it is now becoming possible to measure cross sections for chemical reactions state selected in the vibrational rotational states of both reactants and products. Furthermore, in areas such as atmospheric, combustion and interstellar chemistry, there is an urgent need for reliable reaction rate constant data over a range of temperatures, and this information is often difficult to obtain in experiments. The classical trajectory method can be applied routinely to simple reactions, but this approach neglects important quantum mechanical effects such as tunnelling and resonances. For all these reasons, the quantum theory of reactive scattering is an area that has received considerable attention recently. This book describes the proceedings of a NATO Advanced Research Workshop held at CECAM, Orsay, France in June, 1985. The Workshop concentrated on a critical examination and discussion of the recent developments in the theory of chemical reaction dynamics, with particular emphasis on quantum theories. Several papers focus on exact theories for reactions.

This book covers the basic concepts found in introductory high-school and college chemistry courses.

IUPAC Compendium of Chemical Terminology The Gold Book

Separation processes— or processes that use physical, chemical, or electrical forces to isolate or concentrate selected constituents of a mixture—are essential to the chemical, petroleum refining, and materials processing industries. In this volume, an expert panel reviews the separation process needs of seven industries and identifies technologies that hold promise for meeting these needs, as well as key technologies that could enable separations. In addition, the book recommends criteria for the selection of separations research projects for the Department of Energy's Office of Industrial Technology.

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.

General Chemistry for Engineers explores the key areas of chemistry needed for engineers. This book develops material from the basics to more advanced areas in a systematic fashion. As the material is presented, case studies relevant to engineering are included that demonstrate the strong link between chemistry and the various areas of engineering. Serves as a unique chemistry reference source for professional engineers Provides the chemistry principles required by various engineering disciplines Begins with an 'atoms first' approach, building from the simple to the more complex chemical concepts Includes engineering case studies connecting chemical principles to solving actual engineering problems Links chemistry to contemporary issues related to the interface between chemistry and engineering practices "Explores the simplicity of basic chemical reactions and then builds to the more complex, giving readers a history of the years and the minds that contributed to the research that led to chemistry as we know it today."--

Gearing up for the AP Chemistry exam? AP Chemistry For Dummies is packed with all the resources and help you need to do your very best. This AP Chemistry study guide gives you winning test-taking tips, multiple-choice strategies, and topic guidelines, as well as great advice on optimizing your study time and hitting the top of your game on test day. This user-friendly guide helps you prepare without perspiration by developing a pre-test plan, organizing your study time, and getting the most out of your AP course. You'll get help understanding atomic structure and bonding, grasping atomic geometry, understanding how colliding particles produce states, and much more. Two full-length practice exams help you build your confidence, get comfortable with test formats, identify your strengths and weaknesses, and focus your studies. Discover how to Create and follow a pretest plan Understand everything you must know about the exam Develop a multiple-choice strategy Figure out displacement, combustion, and acid-base reactions Get familiar with stoichiometry Describe patterns and predict properties Get a handle on organic chemistry nomenclature Know your way around laboratory concepts, tasks, equipment, and safety Analyze laboratory data Use practice exams to maximize your score AP Chemistry For Dummies gives you the support, confidence, and test-taking know-how you need to demonstrate your ability when it matters most.

The book "Chemical Reactions in Inorganic Chemistry" describes an overview of chemical reagents used in inorganic chemical reactions for the synthesis of different compounds including coordination, transition metal, organometallic, cluster, bioinorganic, and solid-state compounds. This book will be helpful for the graduate students, teachers, and researchers, and chemistry professionals who are interested to fortify and expand their knowledge about sol-gel preparation and application, porphyrin and phthalocyanine, carbon nanotube nanohybrids, triple bond between arsenic and group 13 elements, and N-heterocyclic carbene and its heavier analogues. It comprises a total of five chapters from multiple contributors around the world including China, India, and Taiwan.

A very challenging subject IB chemistry requires tremendous effort to understand fully and attain a high grade. 'IB Chemistry Revision Guide' simplifies the content and provides clear explanations for the material.

Chemical Kinetics and Mechanism considers the role of rate of reaction. It begins by introducing chemical kinetics and the analysis of reaction mechanism, from basic well-established concepts to leading edge research. Organic reaction mechanisms are then discussed, encompassing curly arrows, nucleophilic substitution and E1 and E2 elimination reactions. The book concludes with a Case Study on Zeolites, which examines their structure and internal dimensions in relation to their behaviour as molecular sieves and catalysts. The accompanying CD-ROM contains the "Kinetics Toolkit", a graph-plotting application designed for manipulation and analysis of kinetic data, which is built into many of the examples, questions and exercises in the text. There are also interactive activities illustrating reaction mechanisms. The Molecular World series provides an integrated introduction to all branches of chemistry for both students wishing to specialise and those wishing to gain a broad understanding of chemistry and its relevance to the everyday world and to other areas of science. The books, with their Case Studies and accompanying multi-media interactive CD-ROMs, will also provide valuable resource material for teachers and lecturers. (The CD-ROMs are designed for use on a PC running Windows 95, 98, ME or 2000.)

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