

Quantum Tunneling in Chemical Reactions

Diane Carrera
MacMillan Group Meeting
November 28, 2007

Lead References:

The Tunnel Effect in Chemistry; Bell, R. P.; Chapman and Hall: New York, 1980.

Electron Tunneling in Chemistry; Compton, R.G.; Elsevier: New York, 1989; in *Comprehensive Chemical Kinetics*, Vol. 30.

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Electron Tunneling in Chemistry R.F. Khairutdinov, K.I. Zamaraev, V.P. Zhadanov, 1989-10-17 In Volume 30 an attempt is made to consider comprehensively both theoretical and experimental data that have been obtained to date on electron tunneling reactions involving chemical compounds of various classes and to discuss the role played by these reactions in different areas of chemistry The discussion of the above problem is preceded by a review of data on tunneling phenomena in nuclear physics atomic physics solid state physics as well as on the tunneling effects in chemistry that go beyond the framework of the main subject of this monograph This review is included to acquaint the reader with the role of tunneling phenomena in physics and chemistry as a whole to show how diversified the kingdom of tunneling phenomena is and to see more distinctly the similarities and the differences between electron tunneling in chemical reactions and other tunnel phenomena

Mechanisms of Inorganic and Organometallic Reactions Volume 7 M.V. Twigg, 2013-11-11 The objective of *Mechanisms of Inorganic and Organometallic Reactions* is to provide an ongoing critical review of the literature concerned with the mechanisms of reactions of inorganic and organometallic compounds The main focus is on reactions in solution although solid state and gas phase studies are included where they provide relevant mechanistic insight Each volume covers an eighteen month literature period and this the seventh volume in the series deals with papers published during July 1988 through December 1989 Where appropriate there are references to earlier work and also to specific sections in previous volumes Coverage continues to span the whole area as comprehensively as possible in each volume and although it is impossible be absolutely complete every effort is made to include all the important for it to published work that is relevant to the elucidation of reaction mechanisms Numerical data are reported in the units used by the original authors and they are only converted to common units when making comparisons The basic format of earlier volumes is retained to facilitate tracing progress over several years in a particular topic this can now be done for more than a decade worth of research In the last volume ligand reactivity of both coordination and organometallic compounds were brought together in Chapter 12 and in response to numerous positive comments from readers this arrangement has been maintained There have been some similar suggestions about oscillating reactions and this topic may have a separate section in the next volume

Comprehensive Chemical Kinetics Nicholas Green, 2003-11-21 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 resonances Presents considerable advances in the field made during the last decade Treats both the statistical as well as the fully quantum mechanical view

Modeling of Chemical Reactions R.W. Carr,2007-09-04 Modeling of Chemical Reactions covers detailed chemical kinetics models for chemical reactions Including a comprehensive treatment of pressure dependent reactions which are frequently not incorporated into detailed chemical kinetic models and the use of modern computational quantum chemistry which has recently become an extraordinarily useful component of the reaction kinetics toolkit It is intended both for those who need to model complex chemical reaction processes but have little background in the area and those who are already have experience and would benefit from having a wide range of useful material gathered in one volume The range of subject matter is wider than that found in many previous treatments of this subject The technical level of the material is also quite wide so that non experts can gain a grasp of fundamentals and experts also can find the book useful A solid introduction to kinetics Material on computational quantum chemistry an important new area for kinetics Contains a chapter on construction of mechanisms an approach only found in this book

Modern Methods, Theory, and Data R. G. Compton,1989 **Low-temperature Combustion and Autoignition** M.J. Pilling,1997-11-27 Combustion has played a central role in the development of our civilization which it maintains today as its predominant source of energy The aim of this book is to provide an understanding of both fundamental and applied aspects of low temperature combustion chemistry and autoignition The topic is rooted in classical observational science and has grown through an increasing understanding of the linkage of the phenomenology to coupled chemical reactions to quite profound advances in the chemical kinetics of both complex and elementary reactions The driving force has been both the intrinsic interest of an old and intriguing phenomenon and the centrality of its applications to our economic prosperity The volume provides a coherent view of the subject while at the same time each chapter is self contained

New Techniques for the Study of Electrodes and Their Reactions R.G. Compton,1989-04-01 Volume 29 gives an account of new techniques for the study of electrodes and their reactions It extends and complements Volumes 26 and 27 of the series which provide an introductory treatment of modern electrochemical methodology and reactions This volume covers the various branches of spectroelectrochemistry and also some recent purely electrochemical advances In situ spectroelectrochemical techniques are covered by chapters on infrared Raman EPR ellipsometry electroreflectance and photocurrent spectroscopy Ex situ UHV experiments are treated in a separate chapter New electrochemical directions are described in chapters on hydrodynamic methods channel electrodes and microelectrodes A final chapter covers computing strategies for the on line accumulation and processing of electrochemical data

Oxoacidity: Reactions of Oxo-compounds in Ionic Solvents Victor L. Cherginets,2005-02-15 The generally accepted definitions of acids and bases together with the generalized definition for the solvent system introduced by the author for the description of both molecular and ionic solvents are discussed The

oxobasicity index introduced as a measure of relative oxoacidic properties of ionic melts pIL and methods of its determination are presented Moreover the oxoacidity scales of ionic melts based on alkali metal halides at different temperatures are constructed The sequential addition method SAM proposed by the author to investigate the effect of oxide particle size on oxide solubilities is presented This book is meant for specialists developing theoretical and applied aspects of molten salt chemistry acid base theories and solubility phenomena It will also be useful for those chemists who wish to extend their knowledge of physical and solution chemistry First book devoted to oxoacids and oxobases Aimed at specialists developing theoretical and applied aspects of molten salt chemistry acid base theories and solubility phenomena The perfect handbook for beginners looking for preliminary knowledge about methods of investigation Mechanism and Kinetics of Addition Polymerizations M. Kucera, 1991-11-26 This volume presents an up to date survey of knowledge concerning addition type polymerizations It contains nine chapters each of which covers a particular basic term Whenever necessary the phenomena are discussed from the viewpoint of both stationary and non stationary state of radical ionic i e anionic and cationic and coordination polymerization Special attention has been paid to the propagation process It provides not only a general overview but also information on important special cases theoretical conditions of propagation influence of external factors controlled propagation copolymerization mechanism of various propagation types etc The book is arranged according to the basic steps in chain reactions which is a novel approach in a monograph on this topic It facilitates the identification of common features of various polymerization types which may appear quite different This useful comprehensive text should prove invaluable to all those involved in the field of macromolecular chemistry It will also be of interest to all chemists who beside the profound study of their own field are looking for interdisciplinary liaison points **Kinetics of Multistep Reactions** Friedrich G. Helfferich, 2004-09-15 This book addresses primarily the engineer in industrial process development the research chemist in academia and industry and the graduate student intending to become a reaction engineer In industry competitive pressures put a premium on scale up by large factors to cut development time To be safe such development should be based on fundamental kinetics that reflect the elementary steps of which the reaction consists The book forges fundamental kinetics into a practical tool by presenting new effective methods for elucidation of mechanisms and reduction of complexity without unacceptable sacrifice in accuracy fewer equations lesser computational load fewer coefficients fewer experiment to determine them For network elucidation new rules relating network configurations to observable kinetic behaviour allow incorrect networks to be ruled out by whole classes instead of one by one For modelling general equations and algorithms are given from which equations for specific networks can be recovered by simple substitutions The procedures are illustrated with examples of industrial reactions including among others paraffin oxidation ethoxylation hydroformylation hydrocyanation shape selective catalysis ethane pyrolysis styrene polymerization and ethene oligomerization Many of the rate equations have not been published before The expanded edition of the 2001 title Kinetics of

Homogeneous Multistep Reactions includes new chapters on heterogeneous catalysis and periodic and chaotic reactions new sections on adsorption statistical methods and lumping and other new detail Contains new chapters on heterogeneous catalysis oscillations and chaos Includes new sections on statistical methods lumping adsorption and software and databases Provides a better understanding of complex reaction mechanisms

Kinetics of Homogeneous Multistep Reactions

Friedrich G. Helfferich, 2001-01-25 This book addresses primarily the chemist and engineer in industrial research and process development where competitive pressures put a premium on scale up by large factors to cut development time To be safe such scale up should be based on fundamental kinetics that is mathematics that reflect the elementary steps of which the reactions consist The book forges fundamental kinetics into a practical tool by presenting new effective methods for elucidation of mechanisms and reduction of mathematical complexity without unacceptable sacrifice in accuracy

Kinetic Models of Catalytic Reactions G.S. Yablonskii, V.I. Bykov, V.I. Elokhin, A.N. Gorban, 1991-04-17 This book has been written by a group of mathematicians and chemists whose common interest is in the complex dynamics of catalytic reactions Based on developments in mathematical chemistry a general theory is described that allows the investigation of the relationships between the kinetic characteristics of complex reactions and their detailed reaction mechanism Furthermore a comprehensive analysis is made of some typical mechanism of catalytic reactions in particular for the oxidation of carbon monoxide on platinum metals In fact the book presents three kinetics a detailed oriented to the elucidation of a detailed reaction mechanism according to its kinetic laws b applied with the aim of obtaining kinetic relationships for the further design of chemical reactors and c mathematical kinetics whose purpose is the analysis of mathematical models for heterogeneous catalytic reactions taking place under steady or unsteady state conditions

Applications of Kinetic Modelling G. Hancock, R.G. Compton, 1999-05-07 Volume 37 is concerned with the use and role of modelling in chemical kinetics and seeks to show the interplay of theory or simulation with experiment in a diversity of physico chemical areas in which kinetics measurements provide significant physical insight Areas of application covered within the volume include electro and interfacial chemistry physiology biochemistry solid state chemistry and chemical engineering A leading contributor to this general area has been Professor W John Albery FRS to whom the contributors and editors dedicate this book

Modern Aspects of Diffusion-Controlled Reactions E. Kotomin, V. Kuzovkov, 1996-10-24 This monograph deals with the effects of reactant spatial correlations arising in the course of basic bimolecular reactions describing defect recombination energy transfer and exciton annihilation in condensed matter These effects lead to the kinetics considered abnormal from the standard chemical kinetics point of view Numerous bimolecular reaction regimes and conditions are analysed in detail Special attention is paid to the development and numerous applications of a novel many point density MPD formalism which is based on Kirkwood's superposition approximation used for decoupling three particle correlation functions The book demonstrates that incorporation of the reaction induced spatial correlations of similar reactants e.g. vacancy

vacancy leads to the development of an essentially non Poisson spectrum of reactant density fluctuations This can completely change the kinetics at longer times since it no longer obeys the law of mass action The language of the correlation lengths and critical exponents similar to physics of critical phenomena is used instead A relation between MPD theory and synergistics is discussed The validity of the theorem giving a critical complexity for the two step reactions exhibiting self organization phenomena is questioned Theoretical results are illustrated by numerous experimental data **Catastrophe**

Theory A. Okninski,1992-06-12 This book aims to provide a straightforward introduction to chemical applications of the catastrophe theory It is primarily intended for chemists interested in placing chemical reactions in the broader context of non linear science but it has a practical relevance for scientists in general Catastrophe theory deals with those non linear phenomena in which a continuous change in the control parameters results in a discontinuous alteration of a characteristic quantity of the system The author discusses the origins of catastrophe theory giving examples of occurrences in the areas of physics chemistry and biology Elementary theory and non chemical applications are also described The chemical kinetics and methods of analysis of chemical kinetic equations arising from elementary and generalized catastrophe theories are reviewed Finally the theory is applied to analyse and classify phenomena associated with the stability loss that may occur in chemical reactions The book contains over 100 figures and an extensive subject index **Chemical Synergies** Nuno A.G.

Bandeira,Bartosz Tylkowski,2018-05-07 This book gives an overview of recent integrated and inter disciplinary approaches between chemical experiment and theory in a variety of fields from polymer science to materials chemistry and ranging from the design of tailored properties to catalysis and reactivity building on the well established success of Density Functional Theory as the foremost quantum chemical method to provide qualitative and quantitative interpretation of results from the chemical laboratory The combination of several characterization techniques with an understanding at the molecular level of chemical and physical phenomena are the main focal point of the subject matter Mechanisms of Inorganic and Organometallic Reactions ,1983 **Advances in Chemical Physics, Volume 75** Ilya Prigogine,Stuart A. Rice,2009-09-08

The Advances in Chemical Physics series provides the chemical physics and physical chemistry fields with a forum for critical authoritative evaluations of advances in every area of the discipline Filled with cutting edge research reported in a cohesive manner not found elsewhere in the literature each volume of the Advances in Chemical Physics series serves as the perfect supplement to any advanced graduate class devoted to the study of chemical physics *Mechanisms of Inorganic and*

Organometallic Reactions M. V. Twigg,1983 *Photokinetics* H. Mauser,G. Gauglitz,1998-09-02 Many books cover the determination of rate constants under different experimental conditions and different chemical composition of the reaction mixture in their formal treatment of thermal kinetics However most textbooks are limited to simple mechanisms In contrast analogous treatment of photochemical reactions is limited to the publication of special reactions and investigations Therefore this book is aimed at providing an overall description of formal photokinetics covering a wider scope than the usual books on

kinetics This volume attempts to provide a concise treatment of both thermo and photochemical reactions by means of generalised differential equations their set up in matrix notation and their solution by a formalism using numerical integration At a first glance this approach might be surprising However apart from the argument that the didactics of thermal reactions are easier to handle than those of kinetics the book provides additional reasons in support of this approach Therefore the formalism derived allows the evaluation of photochemical reactions which are superimposed thermal reactions taking into account that the amount of light absorbed varies during the reaction Because of this any approximation either by using total absorbance or negligible absorbance will cause considerable errors even for simple reactions The approach chosen to transform the axis of the radiation time into a new variable that includes the photokinetic factor proves that formal kinetics can be applied to thermal and photochemical reactions as well and even allows the handling of solutions that cannot be homogenised or solid samples in which the concentration varies locally By using this approach to introduce partial photochemical quantum yields even complex mechanisms can be determined quantitatively A large number of examples for different mechanisms and an introduction to many spectroscopic and chromatographic methods suitable for photokinetic analyses are provided to enable the reader to carry out a step by step evaluation of his own measurements To reduce the number of formula in some chapters an appendix has been included which contains a detailed description of the calculus of some essential examples For the convenience of the reader the following has been included A large number of examples describing the use of formula A detailed description of the procedure for applying photokinetics to complex consecutive photoreactions An Internet address where the reader can find a tutorial for this procedure <http://www.barolo.ipc.uni-tuebingen.de/tele/photokin> A simple macro to help in programming his own evaluation procedure

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