1. Record Nr. UNINA9910828592303321

Titolo	Rate constant estimation for thermal reactions : methods and applications / / edited by Herbert DaCosta, Maohong Fan
Pubbl/distr/stampa	Hoboken, N.J., : Wiley, c2012
ISBN	9786613401250 9781283401258 1283401258 9781118166116 1118166116 9781118166093 1118166094
Edizione	[1st ed.]
Descrizione fisica	1 online resource (360 p.)
Classificazione	SCI007000
Altri autori (Persone)	DaCostaHerbert FanMaohong
Disciplina	541/.36
Soggetti	Chemical kinetics - Effect of temperature on - Mathematics Numerical calculations Thermochemistry - Mathematics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Rate Constant Calculation for Thermal Reactions: Methods and Applications; CONTENTS; PREFACE; CONTRIBUTORS; PART I: METHODS; 1. Overview of Thermochemistry and Its Application to Reaction Kinetics; 1.1. History of Thermochemistry; 1.2. Thermochemical Properties; 1.3. Consequences of Thermodynamic Laws to Chemical Kinetics; 1.4. How to Get Thermochemical Values?; 1.4.1. Measurement of Thermochemical Values; 1.4.2. Calculation of Thermochemical Values; 1.4.2.1. Quantum Chemical Calculations of Molecular Properties; 1.4.2.2. Calculation of Thermodynamic Functions from Molecular Properties 1.5. Accuracy of Thermochemical Values1.5.1. Standard Enthalpies of Formation; 1.5.2. Active Thermochemical Tables; 1.6. Representation of Thermochemical Data for Use in Engineering Applications; 1.6.1. Representation in Tables; 1.6.2. Representation with Group Additivity

Values; 1.6.3. Representation as Polynomials; 1.6.3.1. How to Change f H298K Without Recalculating NASA Polynomials; 1.7. Thermochemical Databases; 1.8. Conclusion; References; 2. Calculation of Kinetic Data Using Computational Methods; 2.1. Introduction; 2.2. Stationary Points and Potential Energy Hypersurfaces
2.3. Calculation of Reaction and Activation Energies: Levels of Theory and Solvent Effects2.3.1. Hartree-Fock and Post-Hartree-Fock Methods; 2.3.2. Methods Based on Density Functional Theory; 2.3.3. Computational Treatment of Solvent Effects; 2.4. Estimate of Relative Free Energies: Standard States; 2.5. Theoretical Approximate Kinetic Constants and Treatment of Data; 2.6. Selected Examples; 2.6.1. Relative Reactivities of Phosphines in Aza-Wittig Reactions; 2.6.2. Origins of the Stereocontrol in the Staudinger Reaction Between Ketenes and Imines to Form -Lactams
2.6.3. Origins of the Stereocontrol in the Reaction Between Imines and Homophthalic Anhydride2.7. Conclusions and Outlook; References; 3. Quantum Instanton Evaluation of the Kinetic Isotope Effects and of the Temperature Dependence of the Rate Constant; 3.1. Introduction; 3.2. Arrhenius Equation, Transition State Theory, and the Wigner Tunneling Correction; 3.3. Quantum Instanton Approximation for the Rate Constant; 3.4. Kinetic Isotope Effects; 3.4.1. Transition State Theory Framework for KIE
3.6.6. Statistical Errors and Efficiency

Sommario/riassunto

Providing an overview of the latest computational approaches to estimate rate constants for thermal reactions, this book addresses the theories behind various first-principle and approximation methods that have emerged in the last twenty years with validation examples. It presents in-depth applications of those theories to a wide range of basic and applied research areas. When doing modeling and simulation of chemical reactions (as in many other cases), one often has to compromise between higher-accuracy/higher-precision approaches (which are usually time-consuming) and approximate/lower-preci