1. Record Nr. UNINA9910827959203321

Autore	Henriksen Niels E
Titolo	Theories of molecular reaction dynamics : the microscopic foundation of chemical kinetics / / Niels Engholm Henriksen and Flemming Yssing Hansen
Pubbl/distr/stampa	Oxford ; ; New York, : Oxford University Press, 2008
ISBN	0-19-965275-9 1-4356-4257-0 0-19-152532-4 1-281-34141-X 9786611341411
Edizione	[1st ed.]
Descrizione fisica	1 online resource (391 p.)
Collana	Oxford graduate texts
Altri autori (Persone)	HansenFlemming Y
Disciplina	541.394
Soggetti	Molecular dynamics Chemical reaction, Conditions and laws of
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	Contents; 1 Introduction; 1.1 Nuclear dynamics: the Schrodinger equation; 1.2 Thermal equilibrium: the Boltzmann distribution; Further reading/references; Problems; PART I: GAS-PHASE DYNAMICS; 2 From microscopic to macroscopic descriptions; 2.1 Cross-sections and rate constants; 2.2 Thermal equilibrium; Further reading/references; Problems; 3 Potential energy surfaces; 3.1 The general topology of potential energy surfaces; 3.2 Molecular electronic energies, analytical results; Further reading/references; Problems; 4 Bimolecular reactions, dynamics of collisions; 4.1 Quasi-classical dynamics 4.2 Quantum dynamicsFurther reading/references; Problems; 5 Rate constants, reactive flux; 5.1 Classical dynamics; 5.2 Quantum dynamics; Further reading/references; 6 Bimolecular reactions, transition-state theory; 6.1 Standard derivation; 6.2 A dynamical correction factor; 6.3 Systematic derivation; 6.4 Quantum mechanical corrections; 6.5 Applications of transition-state theory; 6.6 Thermodynamic formulation; Further reading/references; Problems; 7 Unimolecular reactions; 7.1 True and apparent unimolecular reactions;

7.2 Dynamical theories; 7.3 Statistical theories
7.4 Collisional activation and reaction7.5 Detection and control of chemical dynamics; Further reading/references; Problems; 8 Microscopic interpretation of Arrhenius parameters; 8.1 The pre-exponential factor; 8.2 The activation energy; Problems; PART II: CONDENSED-PHASE DYNAMICS; 9 Introduction to condensed-phase dynamics; 9.1 Solvation, the Onsager model; 9.2 Diffusion and bimolecular reactions; Further reading/references; Problems; 10 Static solvent effects, transition-state theory; 10.1 An introduction to the potential of mean force
10.2 Transition-state theory and the potential of mean forceFurther reading/references; 11 Dynamic solvent effects, Kramers theory; 11.1 Brownian motion, the Langevin equation; 11.2 Kramers theory for the rate constant; 11.3 Beyond Kramers, Grote-Hynes theory and MD; Further reading/references; Problems; PART III: APPENDICES; Appendix A: Statistical mechanics; A.1 A system of non-interacting molecules; A. 2 Classical statistical mechanics; Further reading/references; Appendix B: Microscopic reversibility and detailed balance; B.1 Microscopic reversibility; B.2 Detailed balance
Further reading/referencesAppendix C: Cross-sections in various frames; C.1 Elastic and inelastic scattering of two molecules; C.2 Reactive scattering between two molecules; Appendix D: Classical mechanics, coordinate transformations; D.1 Diagonalization of the internal kinetic energy; Further reading/references; Appendix E: Small-amplitude vibrations, normal-mode coordinates; E.1 Diagonalization of the potential energy; E.2 Transformation of the kinetic energy; E.3 Transformation of phase-space volumes; Further reading/references; Appendix F: Quantum mechanics
F.1 Basic axioms of quantum mechanics

Sommario/riassunto

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. - ;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