

CONTENTS

OPENING REMARKS	xxxi
<i>J. Solvay</i>	
FEMTOCHEMISTRY: FROM ISOLATED MOLECULES TO CLUSTERS	
FEMTOCHEMISTRY: CHEMICAL REACTION DYNAMICS AND THEIR CONTROL	3
<i>A. H. Zewail</i>	
<i>Discussion on the Report by A. H. Zewail</i>	
COHERENT CONTROL WITH FEMTOSECOND LASER PULSES	47
<i>T. Baumert, J. Helbing, and G. Gerber</i>	
<i>Discussion on the Report by G. Gerber</i>	
GENERAL DISCUSSION ON FEMTOCHEMISTRY: FROM ISOLATED MOLECULES TO CLUSTERS	83
FEMTOCHEMISTRY: FROM CLUSTERS TO SOLUTIONS	
SIZE-DEPENDENT ULTRAFAST RELAXATION PHENOMENA IN METAL CLUSTERS	101
<i>R. S. Berry, V. Bonačić-Koutecký, J. Gaus, Th. Leisner, H. Ruppe, S. Rutz, E. Schreiber, St. Vajda, S. Wolf, L. Wöste, J. Manz, B. Reischl-Lenz, and R. de Vivie-Riedle</i>	
<i>Discussion on the Report by L. Wöste</i>	
FEMTOSECOND CHEMICAL DYNAMICS IN CONDENSED PHASES	141
<i>G. R. Fleming, T. Joo, and M. Cho</i>	
<i>Discussion on the Report by G. R. Fleming</i>	
FEMTOSECOND LASER CONTROL OF ELECTRON BEAMS FOR ULTRAFAST DIFFRACTION	185
<i>V. S. Letokhov</i>	
<i>Discussion on the Communication by V. S. Letokhov</i>	
	xxv

GENERAL DISCUSSION ON FEMTOCHEMISTRY: FROM CLUSTERS TO SOLUTIONS	193
LASER CONTROL OF CHEMICAL REACTIONS	
PERSPECTIVES ON THE CONTROL OF QUANTUM MANY-BODY DYNAMICS: APPLICATION TO CHEMICAL REACTIONS	213
<i>S. A. Rice</i> <i>Discussion on the Report by S. A. Rice</i>	
EXPERIMENTAL OBSERVATION OF LASER CONTROL: ELECTRONIC BRANCHING IN THE PHOTODISSOCIATION OF Na ₂	285
<i>A. Shnitman, I. Sofer, I. Golub, A. Yogev, M. Shapiro, Z. Chen, and P. Brumer</i> <i>Discussion on the Communication by M. Shapiro</i>	
COHERENT CONTROL OF BIMOLECULAR SCATTERING	295
<i>P. Brumer and M. Shapiro</i>	
LASER HEATING, COOLING, AND TRANSPARENCY OF INTERNAL DEGREES OF FREEDOM OF MOLECULES	301
<i>D. J. Tannor, R. Kosloff, and A. Bartana</i> <i>Discussion on the Communication by D. J. Tannor</i>	
RAMIFICATIONS OF FEEDBACK FOR CONTROL OF QUANTUM DYNAMICS	315
<i>H. Rabitz</i> <i>Discussion on the Communication by H. Rabitz</i>	
THEORY OF LASER CONTROL OF VIBRATIONAL TRANSITIONS AND CHEMICAL REACTIONS BY ULTRASHORT INFRARED LASER PULSES	327
<i>M. V. Korolkov, J. Manz, and G. K. Paramonov</i> <i>Discussion on the Communication by J. Manz</i>	
TIME-FREQUENCY AND COORDINATE-MOMENTUM WIGNER WAVEPACKETS IN NONLINEAR SPECTROSCOPY	345
<i>S. Mukamel, C. Ciordas-Ciurdariu, and V. Khidekel</i>	
GENERAL DISCUSSION ON LASER CONTROL OF CHEMICAL REACTIONS	373

INTRAMOLECULAR DYNAMICS**SOLVENT DYNAMICS AND RRKM THEORY OF CLUSTERS** 391*R. A. Marcus**Discussion on the Report by R. A. Marcus***HIGH-RESOLUTION SPECTROSCOPY AND INTRAMOLECULAR DYNAMICS** 409*H. J. Neusser and R. Neuhauser**Discussion on the Report by H. J. Neusser***GENERAL DISCUSSION ON INTRAMOLECULAR DYNAMICS** 449**REGULAR AND IRREGULAR FEATURES IN UNIMOLECULAR SPECTRA AND DYNAMICS****INTRAMOLECULAR DYNAMICS IN THE FREQUENCY DOMAIN** 463*R. W. Field, J. P. O'Brien, M. P. Jacobson, S. A. B. Solina,
W. F. Polik, and H. Ishikawa***EMERGENCE OF CLASSICAL PERIODIC ORBITS AND CHAOS IN INTRAMOLECULAR AND DISSOCIATION DYNAMICS** 491*P. Gaspard and I. Burghardt***GENERAL DISCUSSION ON REGULAR AND IRREGULAR FEATURES IN UNIMOLECULAR SPECTRA AND DYNAMICS** 583**MOLECULAR RYDBERG STATES AND ZEKE SPECTROSCOPY****ZEKE SPECTROSCOPY** 607*E. W. Schlag**Discussion on the Report by E. W. Schlag***SEPARATION OF TIME SCALES IN THE DYNAMICS OF HIGH MOLECULAR RYDBERG STATES** 625*R. D. Levine***GENERAL DISCUSSION ON MOLECULAR RYDBERG STATES AND ZEKE SPECTROSCOPY: PART I** 647

FROM RYDBERG STATE DYNAMICS TO ION–MOLECULE REACTIONS USING ZEKE SPECTROSCOPY	667
<i>T. P. Softley, S. R. Mackenzie, F. Merkt, and D. Rolland</i> <i>Discussion on the Report by T. P. Softley</i>	
QUANTUM DEFECT THEORY OF THE DYNAMICS OF MOLECULAR RYDBERG STATES	701
<i>Ch. Jungen</i> <i>Discussion on the Report by Ch. Jungen</i>	
SUBPICOSECOND STUDY OF BUBBLE FORMATION UPON RYDBERG STATE EXCITATION IN CONDENSED RARE GASES	711
<i>M.-T. Portella-Oberli, C. Jeannin, and M. Chergui</i> <i>Discussion on the Communication by M. Chergui</i>	
GENERAL DISCUSSION ON MOLECULAR RYDBERG STATES AND ZEKE SPECTROSCOPY: PART II	719
TRANSITION-STATE SPECTROSCOPY AND PHOTODISSOCIATION	
PHOTODISSOCIATION SPECTROSCOPY AND DYNAMICS OF THE VINOXY (CH ₂ CHO) RADICAL	729
<i>D. L. Osborn, H. Choi, and D. M. Neumark</i> <i>Discussion on the Report by D. M. Neumark</i>	
RESONANCES IN UNIMOLECULAR DISSOCIATION: FROM MODE-SPECIFIC TO STATISTICAL BEHAVIOR	745
<i>R. Schinke, H.-M. Keller, H. Flöthmann, M. Stumpf,</i> <i>C. Beck, D. H. Mordaunt, and A. J. Dobbyn</i> <i>Discussion on the Report by R. Schinke</i>	
PHOTODISSOCIATING SMALL POLYATOMIC MOLECULES IN THE VUV REGION: RESONANCES IN THE $^1\Sigma^+ - ^1\Sigma^+$ BAND OF OCS	789
<i>K. Yamanouchi, K. Ohde, and A. Hishikawa</i> <i>Discussion on the Communication by K. Yamanouchi</i>	
PHASE AND AMPLITUDE IMAGING OF EVOLVING WAVEPACKETS BY SPECTROSCOPIC MEANS	799
<i>M. Shapiro</i> <i>Discussion on the Communication by M. Shapiro</i>	

GENERAL DISCUSSION ON TRANSITION-STATE SPECTROSCOPY AND PHOTODISSOCIATION	809
REACTION RATE THEORIES	
RECENT ADVANCES IN STATISTICAL ADIABATIC CHANNEL CALCULATIONS OF STATE-SPECIFIC DISSOCIATION DYNAMICS	819
<i>J. Troe</i>	
<i>Discussion on the Report by J. Troe</i>	
QUANTUM AND SEMICLASSICAL THEORIES OF CHEMICAL REACTION RATES	853
<i>W. H. Miller</i>	
<i>Discussion on the Report by W. H. Miller</i>	
FEMTOSPECTROCHEMISTRY: NOVEL POSSIBILITIES WITH THREE-DIMENSIONAL (SPACE–TIME) RESOLUTION	873
<i>V. S. Letokhov</i>	
<i>Discussion on the Communication by V. S. Letokhov</i>	
ACADEMIC SESSION AT THE CASTLE OF LAEKEN: PRESENTATION TO KING ALBERT II	889
MODERN PHOTOCHEMISTRY	889
<i>S. A. Rice</i>	
FEMTOCHEMISTRY	892
<i>A. H. Zewail</i>	
CONCLUDING REMARKS	893
<i>S. A. Rice and V. S. Letokhov</i>	
AUTHOR INDEX	899
SUBJECT INDEX	927

FEMTOCHEMISTRY: CHEMICAL REACTION DYNAMICS AND THEIR CONTROL

A. H. ZEWAIL

*Arthur Amos Noyes Laboratory of Chemical Physics
California Institute of Technology
Pasadena, California*

CONTENTS

- I. Introductory Remarks
- II. Concept of Coherence and the Evolution to Femtochemistry
 - A. Coherence and Dephasing
 - B. Coherence Control by Phase-Coherent Pulses
 - C. Coherence in the States of Isolated Molecules: IVR
 - D. Coherence in Orientation: Molecular Structures
 - E. Coherence in Reactions: Wavepackets and Nuclear Motions
 - F. Coherence in Solvation: Clusters and Dense Fluids
 - G. Coherence Control of Wavepackets: Reactive and Nonreactive Systems
 - H. Coherence in Electron Diffraction: Complex Molecular Structures
- III. Prototype Systems: Uni- and Bimolecular Reactions
 - A. Resonances in Unimolecular Reactions
 - B. Barrier Reactions: Saddle-Point Transition State
 - C. Bimolecular Reactions: Ground-State Dynamics
 - D. Complex Organic Reactions
 - E. Electron Transfer Reactions
 - F. Tautomerization Reactions of DNA Models
- IV. Scope of Reactions Studied
- V. Concluding Remarks
- Bibliography
- References

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard,

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.

ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

COHERENT CONTROL WITH FEMTOSECOND LASER PULSES

T. BAUMERT, J. HELBING, and G. GERBER*

*Physikalisches Institut
Universität Würzburg
Würzburg, Germany*

CONTENTS

- I. Introduction
- II. Experiment
- III. Pump–Probe Schemes
- IV. Phase-Sensitive Pump–Probe Experiments
- V. Coherent Control with Phase-Modulated Femtosecond Laser Pulses
- VI. Influence of Laser Pulse Duration
- VII. Coherent Control with Intense Laser Pulses
- VIII. Conclusion
- References

SIZE-DEPENDENT ULTRAFAST RELAXATION PHENOMENA IN METAL CLUSTERS

R. S. BERRY

*Department of Chemistry and the James Franck Institute
The University of Chicago
Chicago, Illinois*

V. BONAČIĆ-KOUTECKÝ and J. GAUS

*Walter Nernst-Institut
Humboldt-Universität zu Berlin
Berlin, Germany*

Th. LEISNER, J. MANZ, B. REISCHL-LENZ,
H. RUPPE, S. RUTZ, E. SCHREIBER, S. VAJDA,
R. de VIVIE-RIEDLE, S. WOLF, and L. WÖSTE*

*Institut für Experimentalphysik and
Institut für Physikalische und Theoretische Chemie
Freie Universität Berlin
Berlin, Germany*

CONTENTS

- I. Introduction
- II. Dimers
- III. Triatomics
 - A. NeNePo Experiments with Triatomics
 - B. Pump-Probe Experiments of Bound Excited Trimer States
 - C. Time-Resolved Spectroscopy of Bound-Free Trimer Transitions

*Report presented by L. Wöste

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.
ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

IV. Larger Clusters

A. Bound-Free Transitions into Excited States

B. NeNePo Experiments

References

FEMTOSECOND CHEMICAL DYNAMICS IN CONDENSED PHASES

G. R. FLEMING* and T. JOO†

*Department of Chemistry and James Franck Institute
University of Chicago
Chicago, Illinois*

M. CHO‡

*Department of Chemistry
Massachusetts Institute of Technology
Cambridge, Massachusetts*

CONTENTS

- I. Introduction
- II. Vibrational Dynamics
 - A. Multilevel Redfield Theory
 - B. Experimental Studies
- III. System–Bath Interactions
 - A. Line Shape Function
 - B. Echo Spectroscopies
- IV. Discussion
- References

PERSPECTIVES ON THE CONTROL OF QUANTUM MANY-BODY DYNAMICS: APPLICATION TO CHEMICAL REACTIONS

S. A. RICE

*Department of Chemistry and The James Franck Institute
The University of Chicago
Chicago, Illinois*

CONTENTS

- I. Introduction
- II. General Considerations
- III. The Brumer–Shapiro Method
- IV. The Tannor–Rice–Kosloff–Rabitz Method
- V. Generic Conditions for Control of Quantum Dynamics
- VI. How Much Control of Quantum Many-Body Dynamics Is Attainable?
- VII. Reduced Space Analyses of the Control of Quantum Dynamics
 - A. Reduced Representation in State Space
 - B. Reduced Representation in Coordinate Space
 - C. Reduction by Factorization: Time-Dependent Hartree Approximation
- VIII. The Control of Dynamics-Inverse Scattering Duality
- IX. Conclusions
- References

LASER HEATING, COOLING, AND TRANSPARENCY OF INTERNAL DEGREES OF FREEDOM OF MOLECULES

D. J. TANNOR*

*Department of Chemical Physics
Weizmann Institute of Science
Rehovot Israel*

R. KOSLOFF AND A. BARTANA

*Department of Physical Chemistry and the
Fritz Haber Research Center
The Hebrew University
Jerusalem Israel*

CONTENTS

- I. Introduction
 - II. Instantaneous Dipole Moment: Generalized Einstein B Coefficient
 - III. Vibrational Heating Using Nondestructive Optical Cycling
 - IV. Nonevaporative Cooling
- References

RAMIFICATIONS OF FEEDBACK FOR CONTROL OF QUANTUM DYNAMICS

H. RABITZ

*Department of Chemistry
Princeton University
Princeton, New Jersey*

CONTENTS

- I. Introduction
- II. The Ubiquitous Role of Feedback
 - A. Feedback in the Design of Molecular Controls
 - B. Feedback in the Laboratory Control of Molecular Dynamics
 - C. Feedback in the Inversion of Molecular Dynamics
- III. Conclusion
- References

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.
ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

THEORY OF LASER CONTROL OF VIBRATIONAL TRANSITIONS AND CHEMICAL REACTIONS BY ULTRASHORT INFRARED LASER PULSES

M. V. KOROLKOV, J. MANZ,* and G. K. PARAMONOV

*Freie Universität Berlin
Institut für Physikalische und Theoretische Chemie
Berlin, Germany*

CONTENTS

- I. Introduction
- II. Models and Techniques
- III. Applications
 - A. Individual Vibrational-State-to-Vibrational-State Transitions
 - B. Series of Vibrational Transitions
 - C. Vibrational Transitions in Competition with Dissipative Processes
 - D. Above-Threshold Dissociation
 - E. Isomerization
- IV. Conclusions
- References

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.

ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

TIME-FREQUENCY AND COORDINATE-MOMENTUM WIGNER WAVEPACKETS IN NONLINEAR SPECTROSCOPY

S. MUKAMEL, C. CIORDAS-CIURDARIU, AND V. KHIDEKEL

*Department of Chemistry
University of Rochester
Rochester, New York*

CONTENTS

- I. Introduction
- II. Correlation Function Expression for Spontaneous Light Emission
- III. Wigner Wavepackets in Phase Space: The Doorway—Window Picture
- IV. Nuclear Wavepackets in Pump–Probe Spectroscopy
- V. Extension to Heterodyne-Detected Four-Wave Mixing
 - Appendix A: Time- and Frequency-Gated Autocorrelation Signals
 - Appendix B: The Signal and the Optical Polarization
 - Appendix C: Four-Point Correlation Function Expression for Fluorescence Spectra
 - Appendix D: Phase-Space Doorway–Window Wavepackets for Fluorescence
 - Appendix E: Doorway–Window Phase-Space Wavepackets for Pump–Probe Signals
- References

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.
ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

SOLVENT DYNAMICS AND RRKM THEORY OF CLUSTERS

R. A. MARCUS

*Noyes Laboratory of Chemical Physics
California Institute of Technology
Pasadena, California*

CONTENTS

- I. Introduction
- II. Microcanonical Solvent Dynamics Modified RRKM Theory
 - A. One-Coordinate Type Treatment
 - B. Vibrational Assistance Treatment
- III. Discussion
- References

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.
ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

HIGH-RESOLUTION SPECTROSCOPY AND INTRAMOLECULAR DYNAMICS

H. J. NEUSSER* and R. NEUHAUSER

*Institut für Physikalische und Theoretische Chemie
Technische Universität München
Garching, Germany*

CONTENTS

- I. Introduction
- II. Intramolecular Dynamics in Electronically Excited S_1 State of Benzene
 - A. Mechanism of Intramolecular Dynamics in Polyatomic Molecular System
 - B. Intramolecular Dynamics in Benzene
 - 1. States at Low Excess Energy
 - 2. Dynamic Behavior of States at Intermediate Vibrational Excess Energy
 - C. Influence of Van der Waals Bonded Noble-Gas Atoms on Intramolecular Dynamics
- III. Laser-Driven Population Dynamics and Coherent Ion Dip Spectroscopy
 - A. Introduction
 - B. Incoherent Population Dynamics
 - C. Coherent Population Dynamics
 - D. Coherent Population Dynamics for Special Pulse Sequences
 - E. Coherent Ion Dip Pulse Sequence
 - F. Experimental Results
 - 1. Experimental Setup
 - 2. Experimental Procedure of Coherent Ion Dip Spectroscopy
 - 3. Spectra
- IV. Intramolecular Dynamics of High Rydberg States in Polyatomic Molecules
 - A. General Remarks
 - B. Experimental
 - C. Experimental Results
- V. Conclusion

**Report presented by H. J. Neusser*

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.

ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

INTRAMOLECULAR DYNAMICS IN THE FREQUENCY DOMAIN

R. W. FIELD*, J. P. O'BRIEN, M. P. JACOBSON,
S. A. B. SOLINA, W. F. POLIK[†], AND H. ISHIKAWA[‡]

*Department of Chemistry
Massachusetts Institute of Technology
Cambridge, Massachusetts*

CONTENTS

- I. Introduction
 - II. Dispersed Fluorescence Spectrum of Acetylene
 - III. From Spectrum to Potential to Dynamics
 - IV. A Change in Resonance Structure
 - V. Summary
- References

EMERGENCE OF CLASSICAL PERIODIC ORBITS AND CHAOS IN INTRAMOLECULAR AND DISSOCIATION DYNAMICS

P. GASPARD* and I. BURGHARDT†

*Service de Chimie Physique and Center for
Nonlinear Phenomena and Complex Systems
Université Libre de Bruxelles
Brussels, Belgium*

CONTENTS

- I. Introduction
- II. Semiclassical Quantization around Equilibrium Points and Periodic Orbits
 - A. Time Evolution in Quantum Mechanics and Trace Formulas
 - B. Quantization around Isolated Equilibrium Points
 - C. Gutzwiller Trace Formula for Isolated Periodic Orbits
 - D. Zeta Function and Interferences between Isolated Periodic Orbits
 - E. Periodic-Orbit Expression for Eigenfunction Averages
 - F. Berry–Tabor Trace Formula and Nonisolated Periodic Orbits
 - G. Bifurcating Periodic Orbits
 - H. Semiclassical Scattering: Scattering Orbits versus Trapped Orbits
 - I. Emergence of Rate and Relaxation Behaviors: Quasiclassical Regime
- III. Bounded Systems
 - A. Energy Spectrum and Its Different Scales
 - 1. Average Level Density
 - 2. Periodic-Orbit Structures
 - 3. Energy Scale below Mean Spacing
 - B. Statistics of Level Curvature and Other Parametric Properties

**Report presented by P. Gaspard*

*†Present address: Institut für Physikalische und Theoretische Chemie der Universität Bonn,
Bonn, Germany*

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.
ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

- C. Time Domain
 - 1. Beyond Heisenberg Time
 - 2. Emergent Classical Orbits and Vibrograms
- D. Diatomic Molecules
 - 1. Morse-Type Model for $I_2(\tilde{X}^1\Sigma)$
 - 2. Experimental Vibrogram of NaI by Zewail and Co-workers
- E. Triatomic Molecules
 - 1. $CS_2(\tilde{X}^1\Sigma_g^+)$
 - 2. $NO_2(\tilde{X}^2A_1-A^2B_2)$
- F. Tetra-atomic Molecules
 - 1. $^{12}C_2HD(\tilde{X}^1\Sigma^+)$
 - 2. $^{12}C_2H_2(\tilde{X}^1\Sigma^+)$
- G. Synthesis
- IV. Open Systems
 - A. Energy and Time Domains
 - B. Unimolecular Dissociation Rates: RRKM Theory and Distribution of Resonances
 - C. Dissociation on Potentials with a Saddle: Classical Properties
 - 1. Classical Dynamics: The Repeller
 - 2. Bifurcation Scenario Associated with Transition to Chaos
 - 3. Fully Chaotic Regime: Smale Horseshoes
 - D. Dissociation on Potentials with a Saddle: Semiclassical Quantization
 - 1. Quantization in Periodic Regime
 - 2. Quantization in Transition Regime
 - 3. Periodic-Orbit Quantization in Fully Chaotic Regime
 - E. Ultrashort-Lived Resonances in Triatomic Molecules
 - 1. HgI_2
 - 2. CO_2
 - 3. H_3
 - 4. O_3
 - 5. H_2O
 - 6. Comparison of Lifetimes
- V. Conclusions
- References

ZEKE SPECTROSCOPY

E. W. SCHLAG

*Institut für Physikalische und Theoretische Chemie
Technische Universität München
Garching, Germany*

CONTENTS

- I. Introduction
 - II. ZEKE Spectroscopy
 - III. Conclusion
- References

SEPARATION OF TIME SCALES IN THE DYNAMICS OF HIGH MOLECULAR RYDBERG STATES

R. D. LEVINE

*The Fritz Haber Research Center for Molecular Dynamics
The Hebrew University
Jerusalem, Israel*

*and
Department of Chemistry and Biochemistry
University of California Los Angeles
Los Angeles, California*

CONTENTS

- I. Background
- II. Preliminaries
- III. Dynamics
 - A. Effective Hamiltonian
 - B. Trapping Versus Dilution
- IV. Concluding Remarks
- References

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.

ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

FROM RYDBERG STATE DYNAMICS TO ION–MOLECULE REACTIONS USING ZEKE SPECTROSCOPY

T. P. SOFTLEY,* S. R. MACKENZIE, F. MERKT, and D. ROLLAND

*Physical and Theoretical Chemistry Laboratory
Oxford, United Kingdom*

CONTENTS

- I. Introduction
- II. State-Selected Ion–Molecule Reactions
 - A. Principles of State Selection
 - B. Experimental
- III. Examples of Preparation of State-Selected Ions
 - A. Hydrogen, H_2^+
 - B. Carbon monoxide, CO^+
 - C. Nitrogen, N_2^+
 - D. Nitric oxide, NO^+
- IV. Studies of Ion–Molecule Reactions
 - A. $H_2^+ + H_2 \rightarrow H_3^+ + H$
 - B. Collision Energy Resolution
 - C. Transmission Effects
 - D. Rydberg State Perturbation by Collision
- V. Rydberg State Lifetimes
- VI. Experimental Measurements of Rydberg Lifetimes
- VII. MQDT Calculations of Spectra of Autoionizing Rydberg States
 - A. Method Employed in the Calculations
 - B. Calculations for Argon
 - C. Calculations for Nitrogen
- VIII. Conclusions
- References

**Report presented by T. P. Softley*

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.

ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

QUANTUM DEFECT THEORY OF THE DYNAMICS OF MOLECULAR RYDBERG STATES

CH. JUNGEN

*Laboratoire Aimé Cotton du CNRS
Université de Paris-Sud
Orsay, France*

CONTENTS

- I. Introduction
- II. Frame Transformations and Bound States
- III. High Orbital Angular Momentum States
- IV. States in the Electronic Continuum
- V. Determination of Quantum Defects from Experiment
- VI. Conclusion
- References

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.
ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

PHOTODISSOCIATION SPECTROSCOPY AND DYNAMICS OF THE VINOXY (CH_2CHO) RADICAL

D. L. OSBORN, H. CHOI, and D. M. NEUMARK*

*Department of Chemistry
University of California
Berkeley, California
and
Chemical Sciences Division
Lawrence Berkeley Laboratory
Berkeley, California*

CONTENTS

I.	Introduction
II.	Experimental
III.	Results
IV.	Discussion
	A. $\text{CH}_3 + \text{CO}$ Channel
	B. $\text{D} + \text{CD}_2\text{CO}$ Channel
V.	Conclusions
	References

RESONANCES IN UNIMOLECULAR DISSOCIATION: FROM MODE-SPECIFIC TO STATISTICAL BEHAVIOR

R. SCHINKE,* H.-M. KELLER, H. FLÖTHMANN,
M. STUMPF, C. BECK, D. H. MORDAUNT, and A. J. DOBBYN

*Max-Planck-Institut für Strömungsforschung
Göttingen, Germany*

CONTENTS

- I. Introduction
- II. Potential-Energy Surfaces
- III. Quantum Mechanical Calculations
- IV. HCO: A Textbook Example of Regular Dynamics
- V. DCO: A Spectroscopic Challenge
- VI. HNO: A Mixed Regular-Irregular System
- VII. HO₂: Classical Chaos Reflected in Dissociation Rates and Product-State Distributions
- VIII. Resume and Outlook
- References

**Report presented by R. Schinke*

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.
ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

PHOTODISSOCIATING SMALL POLYATOMIC MOLECULES IN THE VUV REGION: RESONANCES IN THE ${}^1\Sigma^+ - {}^1\Sigma^+$ BAND OF OCS

K. YAMANOUCHI,* K. OHDE, and A. HISHIKAWA

*Department of Pure and Applied Sciences
College of Arts and Sciences
The University of Tokyo
Tokyo, Japan*

CONTENTS

- I. Spectra of Dissociating Molecules
 - II. Absorption Spectrum of OCS in the VUV Region
 - III. PHOFEX Spectrum of the ${}^1\Sigma^+ - {}^1\Sigma^+$ Band of OCS
 - IV. Fano Profile in the VUV-PHOFEX Spectrum of OCS
 - V. Concluding Remarks
- References

Advances in Chemical Physics, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale, XXth Solvay Conference on Chemistry, Edited by Pierre Gaspard, Irene Burghardt, I. Prigogine, and Stuart A. Rice.
ISBN 0-471-18048-3 © 1997 John Wiley & Sons, Inc.

PHASE AND AMPLITUDE IMAGING OF EVOLVING WAVEPACKETS BY SPECTROSCOPIC MEANS

MOSHE SHAPIRO

*Department of Chemical Physics
The Weizmann Institute
Rehovot 76100,
Israel*

CONTENTS

I.	Introduction
II.	Theory of Wavefunction Imaging
III.	Imaging of a Highly Rotating Na ₂ Molecule
	Acknowledgments
	References

RECENT ADVANCES IN STATISTICAL ADIABATIC CHANNEL CALCULATIONS OF STATE-SPECIFIC DISSOCIATION DYNAMICS

J. TROE

*Institut für Physikalische Chemie
Universität Göttingen
Göttingen, Germany*

CONTENTS

- I. Introduction
- II. Adiabatic Channel Potential Curves
- III. Thermal Capture Rate Constants
- IV. Specific Rate Constants for Dissociation
- V. Comparison of Statistical Adiabatic Channel and Variational Transition-State Treatments
 - A. Comparison of SACM and VTST for Isotropic Charge-Locked Permanent Dipole Systems
 - B. Comparison of SACM and VTST for Anisotropic Charge-Permanent Dipole Systems
 - C. Comparison of SACM and VTST for General Potentials
- VI. Recent SACM Applications to More Complex Reaction Systems
- References

QUANTUM AND SEMICLASSICAL THEORIES OF CHEMICAL REACTION RATES

W. H. MILLER

*Department of Chemistry, University of California, and
Chemical Sciences Division, Lawrence Berkeley National Laboratory
Berkeley, California*

CONTENTS

- I. Introduction
 - II. Quantum Theory
 - III. Semiclassical Approximation for the CRP
 - IV. Concluding Remarks
- References

FEMTOSPECTROCHEMISTRY: NOVEL POSSIBILITIES WITH THREE-DIMENSIONAL (SPACE–TIME) RESOLUTION

V. S. LETOKHOV

*Institute of Spectroscopy
Russian Academy of Sciences,
Troitzk, Moscow Region 142092, Russia*

CONTENTS

- I. Introduction
 - II. Principal Idea
 - III. Femtosecond MPI of Chromophores
 - IV. Laser Resonance Photoelectron Spectromicroscopy
 - V. Toward Femtosecond Laser Photoion Microscopy
 - VI. Conclusion
- References