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Guide to the Stuart Alan Rice Papers 1947-2004



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Descriptive Summary

Identifier	ICU.SPCL.RICESA
Title	Rice, Stuart Alan. Papers
Date	1947-2004
Size	27 linear feet (54 boxes)
Repository	Special Collections Research Center University of Chicago Library 1100 East 57th Street Chicago, Illinois 60637 U.S.A.
Abstract	Stuart A. Rice (1932-) Professor of Chemistry. The collection documents Rice's research and teaching in physical and theoretical chemistry. Includes drafts, proofs and offprints of publications, research notes, and teaching materials.

Information on Use

Access

The collection is open for research.

Citation

When quoting material from this collection, the preferred citation is: Rice, Stuart Alan. Papers, [Box #, Folder #], Special Collections Research Center, University of Chicago Library

Biographical Note

Stuart Alan Rice was born in New York, New York in 1932. He received a S.B. from Brooklyn College in 1952, and was awarded his Ph.D. by Harvard University in 1955. He joined the Department of Chemistry at the University of Chicago in 1957 and has served as Director of the James Franck Institute (1961-1967), Chair of the Department of Chemistry (1971-1976) and Dean of the Division of the Physical Sciences (1981-1995). He is currently the Frank P. Hixon Distinguished Service Professor Emeritus.

Scope Note

The collection is divided into three series.

Series I: Publications includes materials associated with books and articles authored and co-authored by Rice. It is divided into four subseries. Subseries 1 contains notes, manuscripts and correspondence for The statistical mechanics of simple liquids; an introduction to the theory

of equilibrium and non-equilibrium phenomena, published by Rice and Peter Gray in 1965. Subseries 2 includes copies of articles used as sources in Rice and Meishan Zhao's Optical Control of Molecular Dynamics (2000) along with copies of associated permission requests. Subseries 3 contains files associated with Rice's work with R. Stephen Berry and John Ross on the second edition of the textbook Physical Chemistry. Subseries 4 includes offprints of articles authored and co-authored by Rice, organized chronologically and identified by short titles.

Series II: Research includes research notes, charts and calculations compiled by Stuart and his students and colleagues.

Series III: Teaching, contains lecture notes, examinations, assignments, problem solutions, for courses taught by Rice at the University of Chicago.

Related Resources

The following related resources are located in the Department of Special Collections:

<http://www.lib.uchicago.edu/e/spcl/select.html>

Subject Headings

- Rice, Stuart Alan, 1932-
- University of Chicago. Dept. of Chemistry
-
- Chemistry
-
- Chemists

INVENTORY

Series I: Publications

Subseries 1: Stuart A. Rice & Peter Gray, The statistical mechanics of simple liquids; an introduction to the theory of equilibrium and non-equilibrium phenomena, 1965

Box 1

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Rice & Gray Theory of Simple Liquids Book Chapter Notes: Chapter 1, Preface undated
Summing Up & Miscellaneous Parts undated

Box 1

Folder 2-3

Chapter 2, Equilibrium Theory, undated

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Chapter 3, Time Dependent Systems, undated

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Chapter 4, Markov Processes and Brownian Motion, undated

Box 1

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Chapter 5, The Kinetic Equations, undated

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Folder 1

Chapter 6, Applications of the Kinetic Theory of Liquids, undated

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Folder 2

Chapter 7, General Theory of Irreversibility, undated

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Folder 3-6

Corrected Chapters-Publisher's Copy, undated

Subseries 2: Stuart A. Rice & Meishan Zhao, Optical Control of Molecular Dynamics, 2000

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Articles, 1980-1995

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Permissions, 1999

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Subseries 3: R. Stephen Berry, Stuart A. Rice & John Ross Physical Chemistry, second edition, 2000

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Introduction, 2nd Edition, undated

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Chapter 12, undated

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Chapter 26, undated

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Chapters 27-29

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Folder 4

Rice Corrections, Chapters-1-31, "Solution Manual", 2000

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Articles 1978-1995

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Articles 1981-1996

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Articles 1983-1996

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Folder 6-7

Figures, undated

Box 11

Folder 1

Figures, undated

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Folder 2

Figures, GA Stimulation, undated

Subseries 4: Articles (Offprints)

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"World Aviation Statistics," Air Affairs, March, 1947

Box 11**Folder 4**

Articles, 1953-1955

- 1) Particle Scattering Factors In Polydisperse Systems
- 2) The Random Chain Model for Polyethylene by infrared Spectroscopy
- 3) The denaturation of desoxypentose nucleic acid
- 4) A Chain Model for Polyelectrolytes
- 5) A further Examination of the Molecular Weight and Size of Deoxypentose Nucleic Acid
- 6) A Note on the Kinetics of Unitary Processes.

Box 11**Folder 5**

Articles, 1956

- 1) Polyelectrolyte Gels and Ion Exchange Reactions
- 2) On The Cell Model for Solutions,
- 3) On the Bjerrum Relation and the Formation of Ion Pairs
- 4) Model for Ion Exchange Resins
- 5) Cell Model for Solutions and the Additivity of Free Energies
- 6) Electrostatic Contributions to Thermodynamic Functions of Systems Containing Polymeric Ions
- 7) On the Free Energy of Solutions
- 8) Chain Model for Polyelectrolytes. III. Equimolar Polyampholytes of Regularity Alternating Structure.

Box 11**Folder 6**

Articles, 1957

- 1) Self-consistent Monte Carlo simulations of the electron and ion distributions of inhomogeneous liquid alkali metals. II. Longitudinal and transverse density distributions in the liquid-vapor interface of binary metallic alloys
- 2) On the stability of the infinite dimensional fluid of hard hyperspheres: A statistical mechanical estimate of the density of closest packing of simple hypercubic lattices in spaces of large dimensionality
- 3) Does a Supported Monolayer Induce Structure in the Supporting Liquid: A synchrotron X-ray Study of Stearic Acid on Mercury
- 4) A self-consistent Monte Carlo Simulation of the electron and ion distributions in the liquid vapor interface of a simple metal
- 5) A generalized regular solution model of a liquid supported monolayer of long chain amphiphile molecules
- 6) Level Structure and Dynamics from Diatomics to Clusters
- 7) Coherent Pulse Sequence Control of Product Formation in Chemical Reactions
- 8) Intramolecular vibrational energy relaxation indice by van der Waals molecule fragmentation : The systems C₆H₆-nD
- 9) Lifetimes of degenerate benzene 1Bu_{2u} levels split by vibrational angular momentum
- 10) Phase space bottlenecks and statistical theories of isomerization reactions
- 11) Photon Echoes in Multilevel Systems

- 12) The Photofragmentation of Simple van der Waals Complexes
- 13) Research overview: The liquid-vapor interface of a metal as a vehicle for studying the atomic, electronic and optical properties of inhomogeneous liquid
- 14) Systematic features of the energy dependence of radiationless processes in large molecules: The substituted naphthalenes
- 15) Comment on the pair correlation function in an inhomogeneous liquid: A test of the Fischer approximation
- 16) The distribution rings of hydrogen-bonded molecules In a model of liquid water
- 17) On the use of x-ray reflectivity and fluorescence as probes of the longitudinal structure of the liquid-vapor interface

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Folder 7

Articles, 1957

- 1) The Infrared Spectrum of Cuprous Chloride Vapor
- 2) Spectra of the Alkali Halides. II. The Infrared Spectra of the Sodium and Potassium Halides, RbCl, and CsCl
- 3) Infrared Spectra of the Alkali Halides. I. Lithium Halides
- 4) Thermodynamic Properties of the Gaseous Alkali Halides
- 5) The Infrared Spectrum of Cuprous Chloride Vapor
- 6) Some Particle Scattering Factors for Rods with Inhomogeneous Mass Distributions. Application to the Molecular Configuration of Myosin
- 7) The Thermal Denaturation of Deoxyribose Nucleic Acid
- 8) A Model for Ion Binding and Exchange in Polyelectrolyte Solutions and Gels.

Box 11

Folder 8

Articles, 1958

- 1) The Properties of Sonic Fragments of Deoxyribose Nucleic Acid
- 2) Configurations and Interactions of Macromolecules in Liquid Crystals
- 3) The Stability of the Helical DNA Molecule in Solution
- 4) Some Comments on the Theory of Denaturation
- 5) Some Further Comments on the Properties of Bolaform Electrolytes
- 6) Comments on the Paper "Potentiometric Titration, Association Phenomena, and Interaction of Neighboring Groups in Polyelectrolytes
- 7) On a Model of the Helix-Coil Transition in Macromolecules. II.
- 8) On the Theorem of Corresponding States and Its Application to Mixtures
- 9) The Statistical Mechanical Basis of the Enskog Theory of Transport in Dense Gases

Box 12

Folder 1

Articles, 1959

- 1) On a Relation between Coarse Graining and Diagonal Singularity
- 2) Effect of Pressure on Self-Diffusion in Lead
- 3) On the Dynamical Theory of Diffusion in Crystals. II. Pressure Dependence of the Self-Diffusion Constant
- 4) Polyelectrolyte
- 5) On an Approximate Theory of Transport in Dense Media

- 6) Statistical Mechanical Theory of Transport Processes. XIII. Theory of Dense Rigid Sphere Fluids
- 7) On the Dilatational Viscosity of Simple Dense Fluids.

Box 12

Folder 2

Articles, 1960

- 1) Some Aspects of the Statistical Theory of Transport
- 2) Dynamic Theory Diffusion in Crystals
- 3) The Helix-Coil Transition in Charged Macromolecules
- 4) On the Dynamical Theory of Diffusion in Crystals. III. Some Model Calculations and Relation to Continuum Theory
- 5) Dynamic Theory of Diffusion in Crystals. IV. Some Aspects of the Introduction of Irreversibility
- 6) Kinetic Theory of Moderately Dense Rigid Sphere Fluids. III. The Formulation and Solution of the Transport Equation for Binary Mixtures
- 7) On the Dynamical Theory of Diffusion in Crystals. V. Random-Walk Treatment of the Heat of Transport
- 8) Kinetic Theory of the Moderately Dense Rigid-Sphere Fluid. V. Relaxation in Momentum Sphere
- 9) Kinetic Theory of the Moderately Dense Rigid –Sphere Fluid. IV. Fluxes of Matter, Momentum, and Energy in Mixture
- 10) Principle of Corresponding States for Transport Properties
- 11) A Chain Model for Polyelectrolytes. V. A Study of the Effects of Local Charge Density
- 12) Some Further Remarks on the Coefficient of Self-Diffusion in Simple Dense Fluids
- 13) On the Dynamical Theory of Diffusion in Crystals. V. Random-Walk Treatment of the Heat of Transport.

Box 12

Folder 3

Articles, 1961

- 1) On the Kinetic theory of Dense. VIII. Some Comments on the Formal Computation of the Non-Equilibrium Distribution Function of a Fluid
- 2) An acoustic continuum model of molecular friction in simple dense fluids
- 3) On the Kinetic Theory of Dense Fluids. IX. The Fluid of Rigid Spheres with a Square-Well Attraction
- 4) On the Ionization of Polystyrene Sulfonic Acid
- 5) A Chain Model for Polyelectrolytes. VI. Some Studies of Counterion Activity and Counterion Binding in Polyethyleneimine Salts
- 6) On the Kinetic Theory of Dense Fluids. VII. The Doublet Distribution Function for Rigid Spheres with an Attractive Potential
- 7) Approximate Theory of Transport in Simple Dense Fluid Mixtures
- 8) On the Kinetic Theory of Dense Fluids. VII. The Doublet Distribution Function for Rigid Spheres with an Attractive Potential.

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Folder 4

Articles, 1962

- 1) A Conjecture Concerning the Electrical Conductance of Metal-Molten Salt Mixtures
- 2) Kinetic Theory of Ideal Ionic Melts
- 3) Exciton-Exciton Interactions and Photoconductivity in Organic Crystals
- 4) On the Kinetic Theory of Dense Fluids. XIII. The Mobility of Negative Ions in Liquid Ar, Kr, Xe. 5) Kinetic Theory of Dense Fluids. XII. Electronic Ionic Motion in Liquid He4I and Liquid He3
- 6) On the Kinetic Theory of Simple Dense Fluids. XI. Experimental and Theoretical Studies of Positive Ion Mobility in Liquid Ar, Kr, and Xe.
- 7) On the Kinetic Theory of Dense Fluids. VIII. Some Comments on the Formal Computation of the Non-Equilibrium Distribution Function of a Fluid.
- 8) An Acoustic Continuum model of Molecular Friction in Simple Dense Fluids
- 9) On the Kinetic Theory of Dense Fluids. IX. The Fluid of Rigid Spheres with a Square Well Attraction
- 10) On the Ionization of Polystyrene Sulfonic Acid
- 11) A Chain Model for Polyelectrolytes. VI. Some Studies of Counterion Activity Binding in Polyethyleneimine Salts
- 12) On the Kinetic Theory of Dense Fluids. VII. The Doublet Distribution Function for Rigid Spheres with an Attractive Potential
- 13) Approximate Theory of Transport in Simple Dense Fluid Mixtures.

Box 12

Folder 5

Articles, 1963

- 1) Theoretical and Experimental Studies of The Electronic Structure of the Xenon Fluorides
- 2) Theories and Models of Electron Binding in Solution
- 3) Theory of Electronic and Ionic Mobility in Liquid He4I and Liquid He3
- 4) Kinetic Theory of Dense Fluids. X. Measurement and Interpretation of Self-Diffusion in Liquid Ar, Kr, Xe, and CH₄
- 5) Comments on the Use of Carbon SCF Atomic Orbitals in Aromatic Molecules
- 6) Mobility of Ions in Liquid He4I and H₃ as a Function of Pressure and Temperature
- 7) Solvent Effects and a Test of the Theory of Hypochromism
- 8) Triplet Energy Transfer and Triplet-Triplet Interaction in Aromatic Crystals
- 9) On the Excess Electron and Hole Band Structures and Carrier Mobility in Naphthalene, Anthracene, and Several Polyphenyls
- 10) Triplet Excitons Band in Aromatic Crystals
- 11) On the Kinetic Theory of Dense Fluids. XIV. Experimental and Theoretical Studies of Thermal Conductivity in Liquid Ar, Kr, Xe, and CH₄
- 12) A chain Model for Polyelectrolytes. IX. The Effects of Chain Length and Charge on the Friction Constant
- 13) Speculation Concerning the Nature of Binding in Xenon Fluorine Compounds
- 14) On the Thermodynamic Properties of Solutions of Polar Polymers. A Comparison of Experiment and Theory. 15) A Chain Model for Polyelectrolytes. VIII. Further Studies of Counterion Activity in Solutions of Polyethyleneimine Hydrochloride
- 16) A Far Ultraviolet Spectroscopic Study of Xenon Tetrafluoride
- 17) The Heats of Sublimation of XeF₂ and XeF₄, and a Conjecture on Bonding in the Solids.

Box 12**Folder 6**

Articles, 1964

- 1) On the Calculation of the Molecular Friction Constant
- 2) Energy Transfer Phenomena in Liquid Helium
- 3) Forbidden Electronic Transitions in XeF₂ and XeF₄
- 4) Perturbation Calculation of Mixed Pair Correlation Functions
- 5) On the Kinetic Theory of Dense Fluids. XVI. The Ideal Ionic Melt
- 6) Charge-Transfer Exciton States in Aromatic Molecular Crystals
- 7) Charge-Transfer Exciton States in Aromatic Molecular Crystals
- 8) On the Kinetic Theory of Dense Fluids. XV. Some Comments on the Rice-Allnatt Theory
- 9) On the Kinetic Theory of Dense Fluids. XVIII. The Bulk Viscosity
- 10) Guest-Host Interactions: An Examination of the Solvent-Induced Shift in a Model System
- 11) On the Excited Electronic States of Isotactic Polystyrene and Polyvinyl-naphthalene
- 12) Ion-Pair Exciton States and the Optical Spectrum of Crystalline Neon
- 13) Perturbation Theory of the Heats of Mixing of Fused Salts
- 14) On the Kinetic Theory of Dense Fluids. XVII. The Shear Viscosity.

Box 13**Folder 1**

Articles, 1965

- 1) A Brief Review of Some Aspects of the Molecular Theory of Liquids
- 2) On the Kinetic Theory of Dense Fluids. XIX. Comments on and a Rederivation of the Kinetic Equations
- 3) Deep Impurity States in Molecular Crystals: The Optical Excitation of a Substitutional Argon Atom in Crystalline Neon
- 4) Search for a Charge-Transfer State in Crystalline Anthracene
- 5) On the Singlet Exciton-States of Crystalline Anthracene
- 6) The Chemistry of Xenon
- 7) Reply to M. Blander Re: Perturbation Theory of the Heats of Mixing of Fused Salts
- 8) Exchange Effects on the Electron and Hole Mobility in Crystalline Anthracene and Naphthalene
- 9) Triplet Excitons in Crystals of Aromatic Molecules.

Box 13**Folder 2**

Articles, 1965

- 1) Chemical Predictions by MO Theory: The Rare Gas Halides
- 2) Theoretical Studies of Solvated Electrons
- 3) Productivity in Crystals of Organic Molecules
- 4) Excitons and Energy Transfer in Molecular Crystals
- 5) Electrons in Liquids
- 6) Excited Electronic States of Crystalline Benzene
- 7) Molecular Rydberg Transitions in Rare-Gas Matrices-Evidence for Interaction between Impurity States and Crystal States
- 8) Comment on the Rice Allnatt Kinetic Equations

- 9) On the Quantum-Mechanical Fokker-Planck Equation
- 10) Study of the Properties of an Excess Electron in Liquid Helium. I. The Nature of the Electron-Helium Interactions
- 11) Study of the Properties of an Excess Electron in Liquid Helium. II. A Refined Description of Configuration Changes in the Liquid
- 12) Conjecture on the Rate of Vibrational Relaxation of a Diatomic Molecule in Monatomic Lattice
- 13) On the Equation of the State of the Rigid-Sphere Fluid
- 14) A Conjecture on Conformations Leading to Energy Trapping in Helical Polymers
- 15) On the Equation of State of the Rigid-Sphere Fluid
- 16) On the Kinetic Theory of Dense Fluids. XIX. Comments on and a Rederivation of the Kinetic Equations
- 17) Experimental Study of Luminescence and Excitation Trapping in Vinyl Polymers, Paracyclophanes and Related Compounds
- 18) Low-Energy Elastic Scattering of Electrons and Positrons from Helium Atoms
- 19) Study of the Properties of an Excess Electron-in Liquid Helium. I. The Nature of the Electron-Helium Interactions
- 20) Antiresonances in Doped Molecular Solids –Experimental Evidence For Configuration Mixing of Impurity States and Conduction-Band States
- 21) Electron Mobilities in Liquid Argon
- 22) Localized Excitations in Condensed Ne, Ar, Kr, and Xe.

Box 13

Folder 3

Articles, 1966

- 1) On the Interpretation of the Factor Group Splitting in Naphthalene Crystal
- 2) Optical Properties and Electronic Structure of Metals and Alloys
- 3) The Electron-Helium Atom Pseudopotential
- 4) Reflections Spectra of Liquid Hg, In, and Bi from 2-20 eV
- 5) Conjecture on Resonant Transfer of Vibrational Energy and Radiationless Transitions in the Solid Phase: The Lifetime on Triplet Anthracene
- 6) On the Kinetic Theory of Dense Fluids
- 7) Theoretical Studies of Transannular Interactions. I. Benzene Excimer Fluorescence and the Singlet States of the Paracyclophanes
- 8) On the Intensity Distribution of Excimer Emission
- 9) Theoretical Studies of Transannular Interactions.IV. The Electronic States of the Paracyclophane Anion
- 10) Theoretical Studies of Transannular Interactions. III. The Absorption and Emission Spectra of a Multilayered Paracyclophane
- 11) Theoretical Studies of Transannular Interactions. II. The Triplet States of the Paracyclophanes
- 12) Pseudopotential Theory of Atomic and Molecular Rydberg States
- 13) Electron Drift Velocities in Liquefied Argon and Krypton at Low Electric Field Strengths
- 14) On the Calculation of Autocorrelation Functions on Dynamical Variables
- 15) Do Exciton States Exist in the Liquid Phase?
- 16) Cooperative Exciton States in Molecular Crystals.

Box 13**Folder 4**

Articles, 1967

- 1) Comments on the Theory of the Exciton States of Molecular Crystals
- 2) Triplet Excitons: Some Comments on the Properties of Triplet Excitons in Molecular Crystals
- 3) Memory Effects and the Autocorrelation Function of a Dynamical Variable
- 4) Theory of Exciton in Liquids. III. Nonresonant Broadening of Impurity Spectra in Simple Liquids
- 5) Comments on the Equation of State of the Square-Well Fluid
- 6) Conjecture Concerning an Asymptotic Modification on the Yvon-Born-Green Equation for Fluids of Rigid Spheres and Disks.

Box 14**Folder 1**

Articles, 1967

- 1) Drift Velocity and Energy of Electrons in Liquid Argon
- 2) Functional Integral Representation of Nonequilibrium Statistical Mechanics
- 3) On the Equation of State of the Rigid-Disk Fluid
- 4) Theoretical Studies of Transannular Interactions. IV. The Electronic States of the Paracyclophane Anion
- 5) A Comment on Self-Diffusion in Liquid Metals
- 6) Equation of State of a Monatomic Fluid With 6-12 Potential
- 7) Reformulation of the Representation of Transport Coefficients Using the Autocorrelation Function Formalism and the Linear-Trajectory Approximation
- 8) States of the Rydberg States of H₂
- 9) Intermediate Excitons in Molecular Crystals: A study in the Excited States of Crystalline Iodine
- 9) On the Theory of Excitons in Liquids. II A Classical Model of Polarization Waves in a Simple Liquid
- 10) Comments on the Influence of Intermediate Excitons and Exchange Forces on the Interaction in Molecular Crystals: The Crystal Structure Chlorine.

Box 14**Folder 2**

Articles, 1968

- 1) Comments on The Experimental and Theoretical Study of Transport Phenomena in Simple Liquids
- 2) Study of Exciton Dynamics in a Simple Liquid
- 3) Unified Approximation for the Velocity Autocorrelation Function and the Structure Function of a Simple Liquid
- 4) Cooperative Excitons in a Crystal with Two Molecules per Unit Cell
- 5) Optical Model Calculation on the Electronic States of Mixed Disordered Systems
- 6) Re-examination of The Theoretical Interpretations of the Spectra Crystalline Benzene and Naphtalene
- 7) Theory of Radiationless in an Isolated Molecule.

Box 14**Folder 3**

Articles, 1968 II

- 1) Elementary Description of the Equation of State of a Simple Fluid
- 2) Theory of Excitons in Liquids. IV A Simplified Treatment of the Shift and Damping of Polarization Waves
- 3) Intramolecular Formation of p-Methylbenzyl Radical from p-Xylene
- 4) Properties of Simple Liquids
- 5) Studies of the Electronic States of Simple Liquids
- 6) Use of Model Potentials in the Study of Molecular Rydberg States
- 7) Conjecture Concerning Asymptotic Modifications on the Yvon-Born-Green Equation for Fluids of Rigid Spheres and Disks
- 8) New Approximation for the Calculation of Neutron Scattering from a Simple Liquid
- 9) Theoretical Study of the Low Energy Photoionization of Large Molecules: Benzene
- 10) Secular Behavior and Friedman's Multiple-Time-Scale Theory of Irreversible Processes
- 11) Use of Pseudopotentials in Atomic-Structure Calculations
- 12) Cooperative Excitons in a Crystal with Two Molecules per Unit Cell, 1968

Box 14

Folder 4

Articles, 1969

- 1) On the Use of Pseudopotentials in the Quantum Theory of Atoms and Molecules
- 2) Radiationless Transitions in Photochemistry
- 3) Coupling-Parameter Expansion in the Kirkwood Integral Equation for Dense Fluids
- 4) Reflections in a Pool of Mercury: An Experimental and Theoretical Study of the Interaction between Electromagnetic Radiation and a Liquid Metal
- 5) Reflection Spectrum of Liquid Mercury from 4500 to 10 000 Å
- 6) Theory of Electron Transport in Disordered Systems: The Nearly Free-Electron and Nearly Bound-Electron Limits
- 7) Analysis of The Most Probable Path Description of Irreversible Processes
- 8) Some Formal Results in a Theory of Molecular Rearrangements: Photoisomerism, 1969

Box 15

Folder 1

Articles, 1970

- 1) Relaxation Phenomena in Excited Molecules
- 2) An analytic approach to the Theory of Phase Transitions
- 3) Electronic States of Simple Dielectric Liquids
- 4) Energy Trapping in Solid He, Ne, Ar, Kr, and Xe by Molecule Formation-A Theoretical Interpretation
- 5) Some Comments on the Theory of Phase Transitions
- 6) Boltzmann Statistics and Radiationless Decay in Large Molecules: optical Selection Studies
- 7) Stochastic Theory of Vibrational Relaxation and Dissociation
- 8) Elementary Model of the Broadening of Localized Transitions in a simple liquid
- 9) Perturbation Treatment of the Equation of State of Simple Mixtures
- 10) Study of the Reflection Spectrum of Crystalline Anthracene: Evidence for the Existence of Defects

- 11) Conjecture the Width of the Lowest-Singlet-Singlet Transition in Crystalline Anthracene
- 12) Generalization of Hydrodynamics to Include Single Particle Modes and Fluctuations
- 13) Analytic Approach to the Theory of Phase Transitions
- 14) Internal Rotation and the Breakdown of the Adiabatic Approximation: Many-Phonon Radiationless Transitions
- 15) Frenkel Excitons in Vibrating Molecular Crystal.

Box 15

Folder 2

Articles, 1971

- 1) Correlation of Pi-Electron Density with Vibrational Frequencies of Linear Polyenes
- 2) Radiationless Processes in Aromatic Molecules Studied in Shpolskii Matrices
- 3) The Stability Nonpolynomial Kinetics
- 4) Study of Impurity-Host Coupling in Shpolskii Matrices
- 5) Study of Concentration Fluctuations in Model Systems
- 6) Relaxation Phenomena in Excited Molecules
- 7) Interference Effects in the Rydberg Spectra of Naphthalene and Benzene
- 8) Comments on the Theory of Electron Mobility in Simple Fluids
- 9) Absorption Band Profile of the Origin Region of the b-polarized 4000 Å Anthracene Crystal Transition
- 10) Study of the Lifetimes of Individual Vibronic States of the Isolated Benzene Molecule
- 11) Some Comments on the Theory of Photochemical Reactions.

Box 15

Folder 3

Articles, 1972

- 1) Antiresonances in the Rydberg Spectrum of Naphthalene a New Analysis
- 2) Reflectivities of Hg-In Liquid Alloys from 0.31 to 9 eV
- 3) A Theoretical Interpretation of the Electronic Properties of Metal Molten Salt Mixtures
- 4) Competition between Photon Emission and Photodissociation in electronically excited chloro-and bromoacetylene
- 5) Comments in the Rydberg Spectrum Pyrazine
- 6) A Re-examination on the Theory of Phase Transitions in Crystalline Heavy Methane
- 7) Decay of Fluorescence from Single Vibronic States of SO₂
- 8) A new model of liquid water
- 9) Random Matrix Theory and the Master Equation for Finite Systems
- 10) Some Theoretical Results for the Photochemical Decomposition of Large Molecules
- 11) On the calculation of the density of localized states in a dense fluid
- 12) Lifetimes in Quantum Yields of Individual Vibronic States of C₆D₄ and C₆H₅F
- 13) Preparation of Amorphous Solid Water.

Box 15

Folder 4

Articles, 1973

- 1) Spectroscopic properties of polyenes. I. The lowest energy allowed single-singlet transition for cis- and trans-1,3,5-hexatriene
- 2) Comment on "Decay Fluorescence From Single Vibronic Levels of SO₂
- 3) Surface Plasmons at the Surface of Liquid Mercury
- 4) Spectroscopic properties of polyenes. II. The vacuum ultraviolet spectra of cis and trans-1,3,5-hexatriene
- 5) The Electronic Spectra of Hg-In Alloys
- 6) Primary Photochemical and Photophysical Processes in Chloro and Bromo-Acetylene
- 7) Substitution Reactions of Fluorine Atoms with Unsaturated Hydrocarbons
- 8) Comment on the applicability of Urbach's Rule to Molecular Crystals
- 9) Crossed molecular beams study reaction $F + C_2H_2Cl_2 \rightarrow Cl + \{C_2H_2ClF\}$
- 10) Phase transitions and end effects in models of biopolymers
- 11) ITFITS model for vibration-translation energy partitioning in atom-polyatomic molecule collisions
- 12) Unimolecular decomposition of long-lived complexes of fluorine and substituted mono-olefins, cyclic olefins, and dienes
- 13) Unimolecular decomposition of the long-lived complex formed in the reaction $F + C_4H_8$
- 14) Reactions of F atoms and aromatic and heterocyclic molecules: Energy distribution in the reaction complex
- 15) Laboratory angular dependence and the recoil-energy spectrum of the products of the reaction $F + C_6D_6 \rightarrow D + C_6D_5F$
- 16) Quantum ergodicity and vibrational relaxation in isolated molecules
- 17) Quantum ergodicity and vibrational relaxation in isolated molecules
- 18) Influence of large amplitude vibrational motion on the rate of intersystem crossing: A study of single vibronic level fluorescence from aniline N, N-d₂, aniline-d₅, and aniline-d₇
- 19) Intramolecular energy transfer in cis-trans isomerization: A study of fluorescence from single vibronic levels of styrene, trans- α -styrene-d₁, styrene-d₈, and ethynylbenzene
- 20) Nonradiative processes in p-C₆H₄F₂ and m-C₆H₄F₂, 21) Fluorescence lifetimes of individual vibronic levels of partially deuterated benzenes: A further test of the theory of radiationless processes
- 22) Intramolecular vibrational energy transfer: A study of representations.

Box 15

Folder 5

Articles, 1974

- 1) 2,3-Naphthi-2,5-bicyclo[2.2.0]hexadiene
- 2) Comments on the Ultraviolet Spectrum and Photophysical Properties of Trimethylenecyclopropane
- 3) A Model Calculation of the Intramolecular Vibration Spectrum of Liquid Water
- 4) Can the Optical Excitations of Surface Plasmons be Used to Study (Liquid) Metal Surfaces?
- 5) A Quantum ergodic theory approach to unimolecular fragmentation
- 6) Amorphous Solid Water: An X-ray Diffraction Study
- 7) Comment on the application of the absorption sum rule to the optical properties of liquid metals

- 8) On the use of Raman scattering to probe exciton-phonon coupling in molecular crystals
- 9) A Raman spectral study of amorphous solid water*
- 10) Surface plasmons in liquid mercury: Propagation in a nonuniform transition layer
- 11) Random coupling model for molecular dissociation
- 12) Quantum ergodicity and vibrational relaxation in isolated molecules. II. \hbar -independent effects and relaxation to the asymptotic limit.

Box 16

Folder 1

Articles, 1975

- 1) Some Comments on the Dynamics of Primary Photochemical Processes
- 2) Stabilization of a Mode-Locked Nd: Glass Laser by Intracavity Second-Harmonic Generation
- 3) Topics in Current Chemistry
- 4) Extended Generalized Langevin Equations: Calculation of the Velocity Autocorrelation Function of a Simple Fluid
- 5) The stimulated Raman spectrum of water and its relationship to liquid structure
- 6) Comment: Reinterpretation of hexatriene spectrum and comparison with theory
- 7) Theory of photochemical isomerization in polyenes
- 8) Diffraction pattern and structure of amorphous solid water at 10 and 77 K*
- 9) A reply to "Comment on stimulated Raman scattering from water"
- 10) Angular Momentum Conservation in Photochemical Fragmentation a Simple Model
- 11) Amorphous Solid Water: A Neutron Diffraction Study.

Box 16

Folder 2

Articles, 1976

- 1) Surface Plasmons at an Inhomogeneous Liquid Metal/Dielectric Interface: Evidence for a Second Branch Dispersion Curve
- 2) An optical model of dipolar exciton band structure
- 3) Response to the comment by Conwell on dispersion of surface plasmons in inhomogeneous media
- 4) A simulation of the Conformation of All-Trans-Retinal by Trans-Retinal by Transfer of local conformations
- 5) Tunable Infrared Ultrashort Pulses From a Mode-Locked Parametric Oscillator
- 6) On Vibrational Relaxation in Liquids
- 7) Nonlinear resonance and stochasticity in intramolecular energy exchange
- 8) An experimental and theoretical study of the dispersion of the shift surface exciton on anthracene crystals
- 9) Surface Plasmon dispersion in liquid mercury
- 10) Surface polaritons on molecular crystals: An experimental study of anthracene.

Box 16

Folder 3

Articles, 1978

- 1) An interpretation of the OH stretching Region of the vibrational Spectrum of Ice I

- 2) The 2500-4000 cm^{-1} Raman and Infrared Spectra of Low Density Amorphous Solid Water and Polycrystalline Ice I
- 3) Large amplitude vibrational motion in a one dimensional chain: Coherent state representation
- 4) On Vibrational Population Relaxation in Solution
- 5) On the existence of a nonmonotonic nuclear density profile at the jellium-vacuum interface
- 6) Response to a second comment by Conwell on dispersion of surface plasmons in inhomogeneous media
- 7) Internal Energy Transfer in Isolated Molecules: Ergodic and Nonergodic Behavior
- 8) A conjectured interpretation of the OH stretching spectrum of low density amorphous solid water
- 9) A theoretical study of the OH stretching region of the vibrational spectrum of ice Ih
- 10) The OH stretching region infrared spectra of low density amorphous solid water and polycrystalline ice Ih
- 11) Raman spectroscopic studies of the OH stretching region of low density amorphous solid water and of polycrystalline ice Ih
- 12) Determination of the density profile in the liquid-vapor interface near the triple pointa)
- 13) On the existence of a nonmonotone surface ion density in liquid metals: Perturbative introduction of discrete ions into jellium
- 14) Spectroscopic properties of polyenes. III. 1,3,5,7-Octatetraene.

Box 16

Folder 4

Articles, 1978

- 1) On the Relationship Between Low-Density Amorphous Solid Water and Ice Ih
- 2) Angular momentum constraints in radiationless processes: The symmetric top molecule
- 3) The intramolecular potential of water molecules engaged in hydrogen bonding from analysis of the overtone spectrum of ice I
- 4) On the role of Fermi resonance in the spectrum of water in its condensed phases
- 5) Low energy collisional relaxation of I_2^* in He: Evidence for resonance enhanced vibrational deactivation
- 6) Azeroth order random network model of liquid water
- 7) Collision induced intramolecular vibrational energy transfer in 1B2 aniline (includes supplemental material)
- 8) Single vibronic Fluorescence from aniline
- 9) Vibrational Relaxation in Liquid Diethylamine
- 9) Dynamics of Radiationless Processes Studied in Pulsed Supersonic Free Jets: Some Naphthalene Lifetimes
- 10) A numerical study of large amplitude motion on a chain of coupled nonlinear oscillators
- 11) On the Continuity of State between Amorphous Solid and Liquid Water
- 12) On the influence of nonrandom sequential coupling on radiationless relaxation processes.

Box 16

Folder 5

Articles, 1979

- 1) Quantum Effects in Intramolecular Energy Transfer: The Role of Observations
- 2) Closing Remarks
- 3) Comments on a semigroup formalism for the description of phase and population relaxation processes
- 3) The mean spherical approximation and effective pair potentials in liquids
- 4) The entropy of liquid water from the random network model
- 5) The enthalpy and heat capacity of liquid water and the ice polymorphs from a random network model
- 6) The water-water pair potential near the hydrogen bonded equilibrium configuration
- 7) The influence of rotational motion on intersystem crossing in isolated molecules.

Box 16

Folder 6

Articles, 1980

- 1) On rotational Effects in Radiationless Processes in Polyatomic Molecules
- 2) Quasiperiodic and Stochastic Intramolecular Dynamics: the Nature of Intramolecular Energy Transfer
- 3) Measurement of the Group Refractive Indices of Several Liquids
- 4) A random network model calculation of the free energy of liquid water
- 5) Very Low energy cross sections for collision-induced rotational relaxation of I₂ seeded in a supersonic free jet
- 6) Collision induce relaxation of an electronically excited molecule: Evidence for low energy resonance enhanced vibrational deactivation
- 7) A test of the random network model of water using molecular dynamics simulation Data
- 8) The Influence of quantization on the onset chaos in Hamiltonian systems: The Kolmogorov entropy interpretation, 9) Simulation Studies of the Scattering of a Solitary Wave by a Mass impurity in a chain nonlinear oscillators
- 10) Mode dependent enhanced vibrational relaxation in low energy He-1B₂ aniline collisions
- 11) Comment on the rotational state dependence of indirect photodissociation of a polyatomic molecule.

Box 16

Folder 7

Articles, 1980

- 1) A test of the random network model of water using molecular dynamics simulation data
- 2) Dynamical correlations and chaos in classical Hamiltonian systems
- 3) An accurate integral equation for the pair and triplet distribution functions of a simple liquid
- 4) A study of the rotational state dependence of predissociation of a polyatomic molecule: The case of ClO₂
- 5) A correlation diagram model for interpreting propensity rules in collision induced vibrational relaxation

- 6) Intramolecular vibrational energy transfer in 1B2 aniline induced by collisions with H₂O and CH₃F
- 7) Collision induced intramolecular vibrational energy transfer in 1B_{3u} pyrazine
- 8) Single level fluorescence form 1B_{3u} pyrazine: The role of Fermi resonance and Duschinski rotation.

Box 17

Folder 1-2

Articles, 1981

- 1) A Pseudoatom Theory for the Structure of the Liquid-metal-Vapour Interface
- 2) Rotational Analysis of Bands at the Long-Wavelength End of the A₂A₂-X₂B₁ Electronic Transition of ClO₂
- 3) Collision-Induced Intramolecular Energy Transfer in Electronically Excited Polyatomic Molecules
- 4) Structural test for intermolecular force models of crystalline HCl
- 5) An improved analysis of the OH stretching region of the vibrational spectrum of ice I_h
- 6) Is Dynamical Chaos the Same Phenomenon in Classical and Quantum Mechanical Hamiltonian Systems
- 7) The Ewald-Oseen theorem in the x-ray frequency region: A microscopic analysis
- 8) Improved method for calculating the dispersion of surface excitations on homogeneous media
- 9) Structure in the Density Profile at the Liquid-Metal-Vapor Interface
- 10) Mode-to-mode energy transfer in 1B₂ aniline induced by very low energy collisions with He.

Box 17

Folder 3

Articles, 1982

- 1) Cooperative vibrational excitation in molecular solids
- 2) The structure of the liquid-vapour interface of sodium-caesium alloys
- 3) Comparison of vibrational relaxation of 1Au Glyoxal Induced by very-low-energy collisions and by photodissociation of Van der Waals complexes
- 4) Triplet correlation functions in the Lennard-Jones fluid: Tests against molecular dynamics simulations
- 5) Experimental and theoretical studies of the density profile in the liquid-vapour interface of Cs
- 6) Further comments concerning large amplitude motion in an anharmonic chain with nearest neighbor interactions
- 7) Very low energy collision induced vibrational relaxation of 1Au glyoxal
- 8) The OH stretching spectrum of liquid water: A random network model interpretation
- 9) An improved analysis of the OH stretching spectrum of amorphous solid water
- 10) A theoretical analysis of very low energy collision induced vibrational relaxation in the system He-I₂ (3×10^{-4} eV)
- 11) Atom molecule collisions at very low energies: A correlation function approach
- 12) A study of the liquid-vapor interface of mercury: Computer simulation results

- 13) Theoretical and experimental characterization of supersonic expansions from split sources
- 14) Theoretical and Experimental Characterization of Supersonic Expansions from Slit Sources
- 15) Some properties of large amplitude motion in an anharmonic chain with nearest neighbor interactions
- 16) A pseudoatom theory for the liquid-vapor interface of simple metals: Computer simulation studies of sodium and cesium
- 17) Test of effective pair potentials for water: Predicted ice structures, 18) Amorphous solid water and Its Relationship to Liquid Water: A random Network Model for Water.

Box 17

Folder 4

Articles, 1983

- 1) SVL fluorescence spectroscopy and collision-induced intramolecular vibrational energy transfer in 1B1 difluorodiazirine
- 2) A theoretical Analysis of the Stretching Spectra of Ice Ih, Liquid Water, and Amorphous Solid Water
- 3) Classical Trajectory Studies of energy transfer in Ar-difluorodiazirine collisions
- 4) A study of the freezing transition in the Leonard-Jones system
- 5) An X-ray reflectance study of the liquid-vapor of Cs
- 6) Theoretical analysis of the achievement of random close packing of hard spheres and a conjecture on spinodal decomposition
- 7) Contribution to the theory of freezing.

Box 17

Folder 5

Articles, 1984

- 1) Comment on the structures of the liquid-vapor interfaces of Na and Na-Cs alloys
- 2) Calculations of the lattice mode spectra of proton ordered ices: A test of the accuracy of water-water potentials
- 3) Crystallization of the classical one-component plasma
- 4) Shot-noise-limited detection scheme for two-beam laser spectroscopy
- 5) 1B2u \leftrightarrow 1A1g spectroscopy of jet-cooled benzene: Single vibronic level fluorescence studies
- 6) Freezing of the two classical two-dimensional, one component plasma
- 7) Relaxation dynamics of photexcited benzene-rare gas van der Waals complexes
- 8) Vibrational state dependence of radiationless processes in 1B2u benzene
- 9) Comment on vibrational energy redistribution in the isolated dimethyltetrazine dimer
- 10) Relaxation of large molecules following ultrafast excitation
- 11) Model based calculations of the lattice mode spectra of ice Ih and amorphous solid water
- 12) Potential Barrier, Penetration Of
- 13) Very Low Energy Collision Induced Vibrational: An overview
- 14) Intramolecular Dephasing
- 15) Joseph Edward Mayer (1904-1983)

- 16) A comment on dynamical chaos in classical and quantum mechanical Hamiltonian systems
- 17) A generalization of the Ewald-Oseen extinction theorem: Relation to surface polariton modes
- 18) Very-Low-Energy Collision-Induce Rotational Relaxation: A theoretical Analysis
- 19) A Test of an effective pair potential for liquid water
- 20) Theory of the electrical conductivity in the liquid-vapor interface of a simple metal
- 21) X-ray total external reflectance-diffraction as a probe of the structure of the liquid-vapor interface.

Box 17

Folder 6

Articles, 1985

- 1) X-ray reflection from liquids
- 2) Structure of the liquid-vapor interface of water
- 3) A conjecture concerning transformation of a supercooled hard sphere to a metastable disordered solid
- 4) Comment on the lattice mode spectra of ST-2 potential model of proton ordered ices
- 5) Wave Packet evolution in isolated pyrazine molecules: Coherence triumphs over chaos
- 6) Rotational state dependence of pyrazine fluorescence: Initial decays for the vibrationless 1B_{3u} state
- 7) The elastic constants of condensed matter: A direct-correlation function approach
- 8) Picosecond CARS as a probe of ground electronic state intramolecular vibrational redistribution
- 9) Control of selectivity of Chemical reaction via control of wave packet evolution
- 10) A scattering resonance description of very low energy collision induced vibrational relaxation
- 11) A Comment on the consistency of truncated nonlinear integral equation based theories of freezing.

Box 18

Folder 1

Articles, 1986

- 1) Fractal Behavior in classical collisional energy transfer
- 2) Science Must Grow
- 3) The Infrared spectra of pentagonal, hexagonal and heptagonal Rings of water Molecules: A model Study
- 2) Coherent pulse sequence induced control of selectivity of reactions: Exact quantum mechanical calculations
- 3) Bottlenecks to Unimolecular Reactions and an Alternative from Classical RRKM Theory
- 4) Selectivity of Elementary Molecular Processes Associated with Energy Transfer and Chemical Reaction
- 5) Distribution of atoms at the surface of liquid mercury
- 6) Fluorescence Lifetimes of Mode 61 in Deuterobenzenes: Fine Structure in the Decay Lifetime Spectrum
- 7) Coherent Pulse Sequence Induced Control of Selectivity of Reactions

- 8) An experimental study of the in-plane distribution in the liquid-vapor interface of mercury
- 9) A self-consistent Monte Carlo simulation of the electron and ion distributions in the liquid-vapor interface of a simple metal
- 10) The classical mechanics of vibrational predissociation: A model based study of phase space structure and its influence on fragmentation rates
- 11) The vibrational spectrum of the water dimer: Some model based predictions.

Box 18

Folder 2

Articles, 1987

- 1) On the structure of the liquid metal-polar adsorbate interface: Monte Carlo simulations
- 2) Mode-Specific Intramolecular Vibrational Relaxation in S1 Tetrazine-Argon: A Perturbation Theory Analysis
- 3) A molecular dynamics study of the structure of a model Langmuir monolayer of amphiphile molecules
- 4) Direct measurements of vibrational predissociation of p-difluorobenzene-argon
- 5) Hyperthermal Scattering of Atoms from Disordered Surfaces
- 6) Is a Liquid Supported Amphiphile Monolayer Aptly Described as a Two-Dimensional System?
- 7) The Atomic Structure of the Liquid-Vapor Interface of a Metal: An Example of the Influence of Strong Density Dependence of the Interatomic Potential
- 8) How Robust are Bottlenecks to Unimolecular Fragmentation? 9) Ensemble dephasing in vibrationally excited jet-cooled tetrazine and its complexes with Ar, Kr, and Xe
- 10) Intramolecular vibrational relaxation in S0 state of s-tetrazine-X (X=Ar,Kr,Xe)
- 11) X-Ray diffraction study of a Langmuir monolayer of C₂₁H₄₃OH 12) A lattice model of a supported monolayer of amphiphile molecules: Monte Carlo simulations
- 13) Studies of the Atomic Distributions in the Liquid-Vapor Interfaces of Simple Metals and Alloys*.

Box 18

Folder 3

Articles, 1989

- 1) A Study of the Influence of an amphiphile monolayer on the structure of the supporting liquid
- 2) Solitonlike Structure in the Parametric Distortions of Bounded-System Energy Spectra
- 3) Hamiltonian Mapping Models of Molecular Fragmentation
- 4) Light scattering with incident evanescent waves: A method for studying the properties of adsorbed polymers
- 5) Kinetics of a structural phase transition in Langmuir monolayers studied using x-ray diffraction
- 6) Semiclassical quantization of the scattering from a classically chaotic repeller
- 7) Scattering from a classically chaotic repeller
- 8) Exact quantization of the scattering from classically chaotic repeller.

Box 18

Folder 4

Articles, 1990

- 1) Langmuir Monolayers: Structures and Phase Transitions
- 2) Van der Waals Molecules as a Vehicle for the Study of Unimolecular Reactions
- 3) An Interpretation of the multiple fluid-fluid transitions in liquid supported amphiphile monolayers
- 4) On using shaped light pulses to control the selectivity of product formation in a chemical reaction: An application to a multiple level system
- 5) Unimolecular Reactions Revisited
- 6) Influence of vibrational frequency mismatch on phase-space bottlenecks to intramolecular energy redistribution and molecular fragmentation
- 7) Uniaxial compression induced collective tilting and distorted hexagonal structure in Langmuir monolayers
- 8) An interpretation of the bifurcation orientational relaxation processes in a supercooled liquid
- 9) The influence of the structure of the surface of a liquid on the properties of a supported monolayer
- 10) Parametric motion of energy levels: Curvature distribution
- 11) Light scattering with evanescent waves: Intermolecular interference and the structure factor for an ideal flexible chain at an interacting interface.

Box 18

Folder 5

Articles, 1991

- 1) From Discrete to Continuous Quantum Spectra: Parametric Sensitivity and Statistical Properties
- 2) Active Control of Selectivity of Product Formation in a Chemical Reaction: What's new? 3) A Generalized method of Stimulated Emission Pumping
- 4) Molecular dynamics studies of the liquid-vapor interface of water
- 5) Their Most Productive Years: Young Physics Faculty in 1990
- 6) Long-Chain Amphiphile Monolayers on an Anisotropic Substrate: A Computer Simulation Study
- 7) The Use of Pulse Shaping To Control the Photodissociation of a Diatomic Molecule: Preventing the Best from Being the Enemy of the Good
- 8) Comment concerning the optimum control of transformations in an unbounded quantum system
- 9) Fluorescence-detected wave packet interferometry: Time resolved molecular spectroscopy with sequences of femtosecond phase-locked pulses.

Box 18

Folder 6

Articles, 1992

- 1) Signatures of Chaos in Quantum Dynamics and the Controllability of Evolution in a Quantum System
- 2) An approximate classical unimolecular reaction rate theory
- 3) Comment on the tilting transition in Langmuir monolayers
- 4) Grazing incidence x-ray diffraction study of the transverse structure function of the liquid-vapor interface of Ga

- 5) Molecular-dynamics studies of the structure and properties of monolayers of perfluorinated amphiphiles
- 6) Unimolecular fragmentation rate theory revisited: An improved classical theory
- 7) Structural in a monolayer of fluorinated amphiphile molecules
- 8) A molecular dynamics study of the packing structures in monolayers of partially fluorinated amphiphiles
- 9) Spectroscopy with Nonimaging Optics: Application to the Infrared Spectroscopy of Langmuir Monolayers
- 10) Comment on the classical theory of the rate of isomerization
- 11) Comment on the rate of vibrational predissociation of some $RgCl_2$ and $RgCl$ molecules
- 12) Field-theoretical model inspired by adiabatic-ansatz eigenvalue problems
- 13) Comment on the rate of isomerization in molecules with a symmetric triple well potential.

Box 19

Folder 1

Articles, 1993

- 1) Intermediate ordering in a liquid supported monolayer: A molecular dynamics study
- 2) A molecular dynamics study of the structure of a long chain amphiphile monolayer adsorbed on ice Ih
- 3) Intermediate ordering in a liquid supported monolayer: A molecular dynamics study
- 4) Infrared external reflection spectroscopic studies of phase transitions in Langmuir monolayers of stearyl alcohol
- 5) Molecular parking in water supported monolayers of $F(CF_2)_{11}COOH$ and $F(CF_2)_{10}CH_2COOH$.

Box 19

Folder 2

Articles, 1993

- 1) Infrared external reflection spectroscopic studies of phase transitions in Langmuir monolayers of stearyl alcohol
- 2) Intermediate ordering in a liquid supported monolayer: A molecular dynamics study
- 2) In-Plane Structure of the Liquid-Vapor Interface of an Alloy: A grazing Incidence X-ray Diffraction Study of Bismuth:Gallium
- 3) Infrared external reflection spectroscopic studies of phase transitions in Langmuir monolayers of heneicosanol. 4) Infrared external reflection spectroscopy of adsorbates on dielectric substrates: Determining adsorbate orientation in Langmuir monolayers
- 5) Evanescent wave light scattering study of a diblock copolymer adsorbed at the air/water interface
- 6) Comment on the rate of isomerization of 3-phospholene
- 7) Comment on molecular dynamics simulations of monolayers of fluorinated amphiphiles
- 8) Hydrogen negative ion: Semiclassical quantization and weak-field effect
- 9) Differences in the Structures of Relaxed and Unrelaxed Langmuir Monolayers of Heneicosanol: Dependence of Collective Molecular Tilt on Chain Conformation
- 10) Population in a multilevel System: A model Study

- 11) In-Plane Structure of the Liquid-Vapor Interface of an Alloy: A Grazing Incidence X-ray Diffraction Study of Bismuth: Gallium
- 12) Comment on the Influence of Molecular Flexibility on Molecular packing in Langmuir Monolayers
- 13) Reaction Path Analysis of the Rate of Unimolecular isomerization
- 14) Static and Dynamic evanescent wave light scattering studies of diblock copolymers adsorbed at the air/water interface
- 15) Intermediate ordering in a liquid supported monolayer: A molecular dynamics study.

Box 19

Folder 3

Articles, 1994

- 1) Self-consistent Monte Carlo simulation of the electron ion distributions in the liquid-vapor interface of magnesium
- 2) Resonance State Approach to Quantum Transition State Theory
- 3) Formation of an ordered Langmuir monolayer by a non-polar chain molecule
- 4) Laser Techniques for State-Selected and State-to-State Chemistry II
- 5) Nonadiabatic transitions and gauge structure
- 6) In-plane X-Ray diffraction from monolayers of perfluorinated fatty acids: evidence for azimuthal ordering in the condensed phase
- 7) Remarks concerning the theory of the tilting transition in expanded Langmuir monolayers
- 8) Laser Techniques for State-Selected and State-to-State Chemistry II
- 9) Optimal control theory approach to enhancement of HgAr photodissociation
- 10) On the classical theory of the rate of isomerization of HCN.

Box 19

Folder 4

Articles, 1995

- 1) Thermal Expansion Coefficient of a Water-Supported Perfluoron-n-eicosane Monolayer
- 2) Experimental evidence for the divergence of a transport coefficient in a quasi-two-dimensional fluid
- 3) Backbone ordering in amphiphile monolayers.

Box 19

Folder 5

Articles, 1996

- 1) Chromophore Rich Nanodomains in Bulk and Ultra Thin Film Polymer Blends
- 2) Phase transitions in a confined quasi-two-dimensional colloid suspension
- 3) Dynamics of Quasi Two Dimensional Colloidal Systems
- 4) In-plane structure of the liquid-vapor interfaces of dilute bismuth: gallium alloys: X-ray-scattering studies
- 5) The influence of high-frequency modes on ultrashort pulse absorption initiated processes
- 6) Observations of First-Order Liquid-to-Hexatic and Hexatic-to-Solid Transitions in a Confined Colloid Suspension
- 7) Dynamics of Quasi Two-Dimensional Colloidal Systems

- 8) Comment on Quantum Transition State Theory
- 9) Structure of the liquid-vapor interfaces of metals and binary alloys
- 10) Molecular dynamics studies of Langmuir monolayers of F(CF₂)₂₀F, 24) Molecular dynamics studies of Langmuir monolayers of F(CF₂)₁₁COOH
- 11) Surface segregation and layering in the liquid-vapor interface of a dilute bismuth: gallium alloy
- 12) Self-diffusion in dilute quasi-two-dimensional hard sphere suspensions: Evanescent wave light scattering and video microscopy studies
- 13) Structure and equation of state of a long chain amphiphile monolayer adsorbed on ice Ih: A molecular dynamics study
- 14) Structural studies of semifluorinated hydrocarbon monolayers at the air/water interface
- 15) A generalized approach to the control of the evolution of a molecular system
- 16) Infrared spectroscopic studies of structure and phase transitions in a Langmuir monolayer of H(CH₂)₂₃COOH, 31) New approaches to a Classical Theory of Unimolecular Reaction Rate.

Box 19

Folder 6

Articles, 1997

- 1) Active Control of the Dynamics of Atoms and Molecules
- 2) Perspectives on the control of quantum many-body dynamics application to chemical reactions
- 3) A synchrotron x-ray liquid surface spectrometer
- 4) Structure of liquid Ga and the liquid-vapor interface of Ga
- 5) Re-examination of Chirped Pulse Control of Wave Packet Motion in NaI
- 6) The influence of high-frequency modes on two spectroscopy
- 7) Structure of the liquid-vapor interface of a Sn:Galloy.

Box 19

Folder 7

Articles, 1998

- 1) Quantum Monte Carlo simulations of the structure in the liquid-vapor interface of BiGa binary alloys
- 2) Intramolecular energy transfer in the isomerization cyclobutanone
- 3) Semiclassical quantum unimolecular reaction rate theory revisited
- 4) Self-consistent quantum Monte Carlo Simulations of the structure of the liquid-vapor interface of eutectic indium-gallium alloy
- 5) Selective photochemistry via adiabatic passage for degenerate final states
- 6) Theoretical studies of the Structures of the Liquid-Vapor Interfaces of Metals and Binary Alloys
- 7) Phase Transitions in a quasi-two-dimensional system
- 8) Unusual structure in a quasi-two-dimensional binary colloid fluid
- 9) Comparison of the structures of the liquid-vapor interfaces of Al, Ga, and Tl
- 10) Structure of the liquid-vapor interface of a metal from a simple model potential: Corresponding States of the Alkali metals
- 11) Equivalence of the Kobra-Rice photoselective adiabatic passage and the Brumer-Shapiro strong field methods for control of product formation in a reaction 12)

Computer simulation study of the structure of the liquid-vapor interface of mercury, at 20, 100, and 200C

- 13) Coherent population transfer via a resonant intermediate state: The breakdown of adiabatic passage
- 14) Coherent population transfer via a resonant intermediate state: The breakdown of adiabatic passage.

Box 20

Folder 1

Articles, 1999

- 1) John Gamble Kirkwood
- 2) Protein folding at the air-water interface studied with x-ray reflectivity
- 3) A sufficient condition for the angle parameter of the complex dilatation Transformation
- 4) Urease and Hexadecylamine-Urease Films at the Air-Water Interface: An X-Ray Reflection and Grazing Incidence X-Ray Diffraction Study,
- 5) The Structure of the liquid-vapor interface of a gallium-tin binary alloy
- 6) Computational Chemistry in the Undergraduate Chemistry Curriculum: Development of a Comprehensive Course Formula
- 7) Two—Dimensional freezing in the liquid-vapor interface of a dilute Pb:Ga alloy, A sufficient condition for the angle parameter of the complex dilatation transformation
- 8) Experimental observations of non-Gaussian behavior and stringlike cooperative dynamics in concentrated quasi-two-dimensional colloidal liquids
- 9) Controlling quantum wavepacket motion in reduced-dimensional spaces: reaction path analysis in optimal control of HCN isomerization
- 10) Quantum Monte Carlo Simulation Studies of the Structures of the Liquid-Vapor Interfaces of Sn and Pb
- 11) A sufficient condition for the angle parameter complex dilatation transformation
- 12) Computer Simulation study of the structure of the liquid-vapor interface of mercury at 20, 100 and 200°C.

Box 20

Folder 2

Articles, 2000

- 1) Optical control reactions
- 2) Active Control of Molecular Dynamics: Coherence versus Chaos
- 3) Structure of the liquid-vapor interface of a dilute alloy of Pb in Ga
- 4) A test of the dependence of an optimal control field on the number of molecular degrees of freedom : HCN isomerization
- 5) Test of the universal local pseudopotential for the description of an inhomogeneous metal
- 6) Diffusion of an isolated colloidal sphere confined between flat plates
- 7) Direct measurements of constrained Brownian motion of an isolated sphere between two walls
- 8) Melting transition in a quasi-two-dimensional colloid suspension: Influence of the colloid-colloid interaction
- 9) Nature of the transition from two- to three-dimensional ordering in a confined colloidal suspension

- 10) Hexagonal to square lattice conversion in bilayer systems.

Box 20

Folder 3

Articles, 2001

- 1) Sequential STIRAP-based control of the HCN->CNH isomerization. 2) Sensitivity of the Extended STIRAP Method of Selective Population Transfer to Coupling to Background States
- 3) Interfering for the good of a chemical reaction
- 4) Density distribution in the liquid-vapor interface of a dilute alloy of Pb in Ga
- 5) Melting of a quasi-two-dimensional metallic system
- 6) Dynamical heterogeneity in a dense quasi-two-dimensional colloidal liquid.

Box 20

Folder 4

Articles, 2002

- 1) Population Transfer to a Predissociating Target State Using Pulsed Coherent Excitation: Sensitivity to Coupling to Background States
- 2) Variations on the Theme of Stimulated Raman Adiabatic, Passage: Control of Chemical Reactions
- 3) Equilibrium structure and effective pair in a quasi-one-dimensional colloid liquid
- 4) Optical control of molecular dynamics in a liquid
- 5) Active control of product selection in a chemical reaction: a view of the current scene
- 5) Structure of the liquid-vapor interface of a dilute ternary alloy: Pb and Sn in Ga
- 6) Controllability of population transfer to degenerate states: Analytical and numerical results for a four-level system.

Box 20

Folder 5

Articles, 2003

- 1) Phase diagram of a quasi-two-dimensional colloid assembly
- 2) High-Precision Molecular Wave-Packet Interferometry With HgAr Dimers
- 3) Structure of the liquid-vapor interface of a dilute ternary alloy: Pb and In in Ga
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