

CONTENTS

IMS 2000	iii
CONTENTS	v
ORGANIZATION AND STAFF	1
COUNCIL	13
BUILDINGS AND CAMPUS	15
RESEARCH ACTIVITIES I	17

Department of Theoretical Studies

I-A Development of New Numerical Techniques in the Study of Molecular Structure	
I-A-1 Spectral Density Calculation by Using the Chebyshev Expansion	17
I-A-2 Calculation of the ZEKE Spectrum of CO	17
I-A-3 Nonadiabatic Relaxation Through a Conical Intersection	17
I-B Electron-Hydrogen Bond in Water Clusters and Their Complexes with Atomic Ions	
I-B-1 Theoretical Studies of the Water-Cluster Anions Containing the OH{e}HO Structure: Energies and Harmonic Frequencies	18
I-B-2 Electron-Hydrogen Bonds and OH Harmonic Frequency Shifts in Water Cluster Complexes with a Group 1 Metal Atom, M(H ₂ O) _n (M = Li and Na)	18
I-B-3 Theoretical Study of Photoabsorption Cross Sections of Water Cluster Anions	18
I-B-4 Theoretical Study of Photoabsorption Spectra of M(H ₂ O) _n (M = Li and Na)	19
I-C Computational Chemistry of Atomic and Molecular Processes in Atmospheric Environment	
I-C-1 Accurate Potential Energy and Transition Dipole Moment Curves for Several Electronic States of CO ⁺	19
I-C-2 Ab initio MO Study of the A, D and Third ² Π States of CO ⁺	20
I-C-3 Theoretical Studies of Einstein's A and B Coefficients of Rovibrational Transitions for Carbon Monoxide: Simulation of Temperature Distribution of CO in the Solar Atmosphere	20
I-C-4 Theoretical Study on the Hydrogen Abstraction from Saturated Hydrocarbons by OH Radical	20
I-C-5 Theoretical Study on the Reaction Mechanism for Oxidation of Isoprene	20
I-D Prediction of Protein Tertiary Structures from the First Principles	
I-D-1 Helix-Coil Transitions of Amino-Acid Homo-Oligomers in Aqueous Solution Studied by Multicanonical Simulations	21
I-D-2 Multidimensional Replica-Exchange Method for Free Energy Calculations	21
I-D-3 Replica-Exchange Multicanonical Algorithm and Multicanonical Replica-Exchange Method for Simulating Systems with Rough Energy Landscape	21
I-D-4 Multicanonical Algorithm Combined with the RISM Theory for Simulating Peptides in Aqueous Solution	21
I-D-5 A pH-dependent Variation in α-Helix Structure of the S-peptide of Ribonuclease A Studied by Monte Carlo Simulated Annealing	21
I-E Development of Simulation Algorithms for Complex Systems	
I-E-1 Replica-Exchange Monte Carlo Methods for the Isobaric-Isothermal Ensemble	22
I-E-2 Ab Initio Replica-Exchange Monte Carlo Method for Cluster Studies	22
I-F Theory of Nonadiabatic Transition	
I-F-1 Non-Adiabatic Transitions in a Two-State Exponential Potential Model	23
I-F-2 Complete Solutions of the Landau-Zener-Stueckelberg Curve Crossing Problems, and Their Generalizations and Applications	23
I-F-3 Complete Reflection in Two-State Crossing and Noncrossing Potential Systems	23
I-F-4 Nonadiabatic Transitions due to Curve Crossings: Complete Solutions of the Landau-Zener-Stueckelberg Problems and Their Applications	23
I-F-5 New Type of Nonadiabatic Dynamics: Transitions between Asymptotically Degenerate States	24
I-G Theoretical Studies of Chemical Reaction Dynamics	
I-G-1 Electronically Adiabatic Chemical Reactions Analyzed by the Semiclassical Theory of Nonadiabatic Transition	24
I-G-2 Quantum Reaction Dynamics of O(³ P) + HCl on a New Ab Initio Potential Energy Surface	24
I-G-3 Quantum-Classical Correspondence in the O(³ P) + HCl and Cl(² P) + OH Reactions for Total Angular Momentum J = 0	24

I-G-4 New Implementation of the Trajectory Surface Hopping Method with Use of the Zhu-Nakamura Theory -----	25
I-G-5 Diabatic Slow Variable Discretization Approach in Time-Independent Reactive Scattering Calculations -----	25
I-G-6 Quantum Dynamics in the DH_2^+ Reaction System -----	25
I-H New Way of Controlling Molecular Processes	
I-H-1 Laser Control of Molecular Photodissociation with Use of the Complete Reflection Phenomenon -----	25
I-H-2 New Way of Controlling Molecular Processes by Lasers -----	26
I-I New Methods to Treat Scattering Problems	
I-I-1 Analytical Treatment of Singular Equations in Dissociative Recombination -----	26
I-I-2 Stable and Efficient Evaluation of Green's Function in Scattering Problem -----	26
I-J Theoretical Study of Multi-Dimensional Tunneling	
I-J-1 Theoretical Study of Multidimensional Proton Tunneling in the Excited State of Tropolone --	26
I-K Theoretical Studies of Ultrafast Nonlinear Optical Spectroscopy of Molecules in Condensed Phases	
I-K-1 Two-Dimensional Line Shape Analysis of Photon Echo Signal -----	28
I-K-2 Cage Dynamics in the Third-Order Off-Resonant Response of Liquid Molecules: A Theoretical Realization -----	28
I-K-3 Two-Dimensional Spectroscopy for Harmonic Vibrational Modes with Nonlinear System-Bath Interactions: Gaussian-Markovian Case -----	28
I-K-4 Two-Dimensional Spectroscopy and the Harmonically Coupled Anharmonic Oscillators ----	28
I-K-5 Two-Dimensional Raman and Infrared Signals Measured from Different Phase-Matching Conditions -----	28
I-L Quantum dynamics in the condensed phases	
I-L-1 Path-Integral Approach to Rotational Relaxation Processes of a Molecule in Solvation -----	29
I-L-2 Proton Tunneling in a Dissipative Environment: Raman Response and Reaction Rate -----	29
I-M Soft Matter Physics in Biomimetic Systems	
I-M-1 On the Toughness of Biocomposites -----	29
I-M-2 Why is Nacre Strong?: Elastic Theory and Fracture Mechanics for Biocomposites with Stratified Structures -----	29
I-M-3 Mechanoelectric Effects in Ionic Gels -----	30
I-N Liquid-Liquid Phase Transition of Water and Its Potential Surface	
I-N-1 The Melting Temperature of Proton-Disordered Hexagonal Ice: A Computer Simulation of TIP4P Model of Water -----	31
I-N-2 Hydrogen Bonds between Water Molecules: Thermal Expansivity of Ice and Water -----	31
I-N-3 Potential Energy Surfaces of Supercooled Water: Intrabasin and Interbasin Structures Explored by Quenching, Normal Mode Excitation, and Basin Hopping -----	31
I-N-4 Molecular Dynamics Study of the Connectivity of Water Molecules in Supercooled States --	31
I-N-5 Ice Nanotube: What Does the Unit Cell Look Like? -----	31
I-N-6 First-Order Transition in Confined Water between High Density Liquid and Low Density Amorphous Phases -----	32
I-O Development of Techniques for Prediction of Conformations and Applications to Proteins and Organic Compounds	
I-O-1 Kinetics of a Finite One-Dimensional Spin System as a Model for Protein Folding -----	33
I-O-2 Molecular Modeling of Human Serum Transferrin for Rationalizing the Changes in Its Physicochemical Properties Induced by Iron Binding. Implication of the Mechanism of Binding to Its Receptor -----	33
I-O-3 A CoMFA Analysis with Conformational Propensity: An Attempt to Analyze the SAR of a Set of Molecules with Different Conformational Flexibility Using a 3D-QSAR Method ----	33
I-O-4 Study on Photobase Generation from α -Aminoketones: Photocrosslinking of Epoxides with Carboxylic Acids -----	34
I-P Microscopic Solvation of Alkali Atom and Aggregates in Polar Solvent Clusters	
I-P-1 Solvation Process of Na_m in Small Ammonia Clusters: Photoelectron Spectroscopy of $\text{Na}_m^-(\text{NH}_3)_n$ ($m \leq 3$) -----	35
I-P-2 Theoretical Study of $[\text{Na}(\text{H}_2\text{O})_n]^-$ ($n = 1-4$) Clusters: Geometries, Vertical Detachment Energies and IR Spectra -----	35
I-P-3 Theoretical Study of $[\text{Na}(\text{NH}_3)_n]^-$ ($n = 1-4$) -----	35
I-Q Theoretical Analyses on Nonlinear Behavior of Complex Systems	
I-Q-1 Peptide Conformations in Alcohol and Water: Analyses by the Reference Interaction Site Model Theory -----	36
I-Q-2 Binary Fluid Mixture Confined between Macroparticles: Surface-Induced Phase Transition and Long-Range Surface Forces -----	36
I-Q-3 Solvent Effects on Conformational Stability of Peptides: RISM Analyses -----	36

I-Q-4	Effects of a Trace Amount of Hydrophobic Molecules on Phase Transition for Water Confined between Hydrophobic Surfaces: Theoretical Results for Simple Models	---36
I-Q-5	Methodology for Predicting Approximate Shape and Size Distribution of Micelles	-----37
I-R	Electronic Structure of a Molecule in Solution	
I-R-1	Ab initio Study of Water: Liquid Structure, Electronic and Thermodynamic Properties over a Wide Range of Temperature and Density	-----38
I-R-2	Solvent Effects on a Diels-Alder Reaction in Supercritical Water: RISM-SCF Study	-----39
I-R-3	A Theoretical Study on a Diels-Alder Reaction in Ambient and Supercritical Water: Viewing Solvent Effects through Frontier Orbitals	-----39
I-R-4	Self-Consistent Field, <i>Ab initio</i> Molecular Orbital and Three-Dimensional Reference Interaction Site Model Study for Solvation Effect on Carbon Monoxide in Aqueous Solution	---39
I-R-5	Which Carbon Oxide is More Soluble? Ab initio Study on Carbon Monoxide and Dioxide in Aqueous Solution	-----39
I-R-6	NMR Chemical Shifts in Solution: A RISM-SCF Approach	-----39
I-R-7	ElectronL Self-Trapping in Two Dimensional Fluid	-----40
I-S	Solvation Thermodynamics of Protein and Related Molecules	
I-S-1	Salt Effect on Stability and Solvation Structure of Peptide: An Integral Equation Study	-----40
I-S-2	Theoretical Study for Partial Molar Volume of Amino Acids in Aqueous Solution: Implication of Ideal Fluctuation Volume	-----40
I-T	Collective Density Fluctuations in Polar Liquids and Their Response to Ion Dynamics	
I-T-1	Relaxation of Average Energy and Rearrangement of Solvent Shells in Various Polar Solvents in Connection with Solvation Dynamics: Studied by RISM Theory	--41
I-T-2	Importance of Acoustic Solvent Mode and Solute-Solvent Radial Distribution Functions in Solvation Dynamics: Studied by RISM Theory	-----41
I-U	Liquid-Solid Interface	
I-U-1	Potentials of Mean Force of Simple Ions in Ambient Aqueous Solution. I. Three-Dimensional Reference Interaction Site Model Approach	-----42
I-U-2	Potentials of Mean Force of Simple Ions in Ambient Aqueous Solution. II. Solvation Structure from the Three-Dimensional Reference Interaction Site Model Approach, and Comparison with Simulations	-----43
I-U-3	Hydration Free Energy of Hydrophobic Solutes Studied by a Reference Interaction Site Model with a Repulsive Bridge Correction and a Thermodynamic Perturbation Method	-----43
I-U-4	Liquid Structure at Metal Oxide-Water Interface: Accuracy of a Three-Dimensional RISM Methodology	-----43
I-U-5	Self-Consistent, Kohn-Sham DFT and Three-Dimensional RISM Description of a Metal-Molecular Liquid Interface	-----43
I-V	Dimensional Crossovers and Excitation Spectra in Quasi-One-Dimensional Organic Conductors	
I-V-1	Quantum Phase Transitions and Collapse of the Mott Gap in the $d = 1 + \epsilon$ Dimensional Hubbard Model with $2k_F$ Umklapp Scattering	-----45
I-V-2	One- and Two-Band Hubbard Models in $d = 1 + \epsilon$ Dimensions: Dimensionality Effects on the Charge and Spin Gap Phases	-----45
I-V-3	Interplay of Randomness, Electron Correlation, and Dimensionality Effects in Quasi-One-Dimensional Conductors	-----45
I-V-4	Charge Gap and Dimensional Crossovers in Quasi-One-Dimensional Organic Conductors	--45
I-V-5	Dimensionality Effects on the Charge Gap in the Dimerized Hubbard Model at Quarter Filling: the Density-Matrix and Perturbative Renormalization-Group Approaches	-----46
I-V-6	Intra- and Inter-Chain Dynamic Response Functions in Quasi-One-Dimensional Conductors	46
I-W	Optical Excitations in Charge-Lattice-Ordered Phases of One-Dimensional Materials	
I-W-1	Charge Ordering and Lattice Modulation in Quasi-One-Dimensional Halogen-Bridged Binuclear Metal Complexes	-----46
I-W-2	Charge Ordering and Lattice Modulation in MMX Chains	-----46
I-W-3	Charge Ordering and Optical Conductivity of MMX Chains	-----46
I-W-4	Charge Excitations in an Alternate Charge Polarization Phase of a One-Dimensional Two-Band Extended Peierls-Hubbard Model for MMX Chains	-----47
I-W-5	Highly Doped Nondegenerate Conjugated Polymers—A Theory Using the DMRG Method	-----47
I-X	Magnetic and Optical Properties of Two-Dimensional Metal-Complex and Organic Conductors	
I-X-1	Collective Excitations around Charge Ordered States and Coexistent States with Different Orders	-----47
I-X-2	Anisotropic Collective Excitations around Various Charge Ordering States	-----48
I-X-3	Stability and Cation Dependence of Magnetic Orders in $(Et_nMe_{4-n}Z)[Pd(dmit)_2]_2$	-----48
I-Y	Multi-Phase Stability and Nonlinear Dynamics near Phase Boundary	
I-Y-1	Influence of Short-Range Interference on Ionization Threshold Law	-----49
I-Y-2	Potential Analysis for Neutral-Ionic Phase Transition	-----49

I-Y-3 Localized Vibrational Modes of Excitations in Electroluminescent Polymers	49
I-Y-4 Photoinduced Polarization Inversion in a Polymeric Molecule.....	49

RESEARCH ACTIVITIES II -----51

Department of Molecular Structure

II-A Laser Cooling and Trapping of Metastable Helium Atoms	
II-A-1 Magneto-Optical Trap of Metastable Helium-3 Atoms	51
II-B Spectroscopic Studies on Atoms and Ions in Liquid Helium	
II-B-1 Theoretical Studies on the Spectra of Yb ⁺ Ions in Liquid Helium	51
II-B-2 Measurements of Fine Structure Changing Cross Sections of Ca ⁺ and Sr ⁺ in Collisions with He Atoms	51
II-C Endohedral Metallofullerenes: New Fullerene Molecules with Novel Properties	
II-C-1 La@C ₈₂ Anion. An Usually Stable Metallofullerene	53
II-C-2 Transient Spectroscopic Properties of Endohedral Metallofullerenes, La@C ₈₂ and La ₂ @C ₈₀	53
II-C-3 Vibrational Spectroscopy of Endohedral Dimetallofullerene, La ₂ @C ₈₀	53
II-D Structure and Function of Respiratory Terminal Oxidases	
II-D-1 Probing Molecular Structure of Dioxygen Reduction Site of Bacterial Quinol Oxidases through Ligand Binding to the Redox Metal Centers	54
II-D-2 Active Site Structure of SoxB-Type Cytochrome <i>bo</i> ₃ Oxidase from Thermophilic Bacillus -54	
II-E Structure and Function of Transmembrane Electron Transfer System in Neuroendocrine Secretory Vesicles	
II-E-1 Reduction of Heme Iron Suppresses the Carboxylation of Two Histidyl and One Tyrosyl Residues Indispensable for the Transmembrane Electron Transfer Reaction of Cytochrome <i>b</i> ₅₆₁	55
II-E-2 Planarian Cytochrome <i>b</i> ₅₆₁ : A Transmembrane Electron Transfer Protein Unique to Neuroendocrine Secretory Vesicles	55
II-F Structure and Function of Steroidogenic Cytochrome P450 System	
II-F-1 Direct Heme-Steroid Interaction in Cytochrome P450c21 Studied by FTIR Spectroscopy ---55	
II-F-2 Adrenodoxin-Cytochrome P450scc Interaction as Revealed by EPR Spectroscopy: Comparison with Putidaredoxin-Cytochrome P450cam System	56
II-G Biomolecular Science	
II-G-1 Resonance Raman Investigation of Fe–N–O Structure of Nitrosylheme in Myoglobin and Its Mutants	57
II-G-2 Novel Iron Porphyrin-Alkanethiolate Complex with Intramolecular NH···S Hydrogen Bond: Synthesis, Spectroscopy, and Reactivity	57
II-G-3 Mechanism of the Anionic Cyclopolymerization of Bis(dimethylvinylsilyl)methane	58
II-G-4 Synthesis and Characterization of Novel Alkylperoxo Mononuclear Iron(III) Complexes with a Tripod: Pyridylamine Ligand: A Model for Peroxo Intermediates in Reactions Catalyzed by Non-Heme Iron Enzymes	58
II-G-5 Interactions of Phosphatidylinositol 3-Kinase Src Homology 3 Domain with Its Ligand Peptide Studied by Absorption, Circular Dichroism, and UV Resonance Raman Spectroscopies	58
II-G-6 Resonance Raman Studies of Oxo Intermediates in the Reaction of Pulsed Cytochrome <i>bo</i> with Hydrogen Peroxide	59
II-G-7 A New Measurement System for UV Resonance Raman Spectra of Large Proteins and Its Application to Cytochrome <i>c</i> Oxidase	59
II-G-8 An Approach to the O ₂ Activating Mononuclear Non-heme Fe Enzymes: Structural Characterization of Fe(II)-Acetato Complex and Formation of Alkylperoxoiron(III) Species with the Highly Hindered Hydrotris(3-tert-butyl-5-isopropyl-1-pyrazolyl)borate	59
II-G-9 Structures of Reaction Intermediates of Bovine Cytochrome <i>c</i> Oxidase Probed by Time-Resolved Vibrational Spectroscopy	59
II-G-10 Heme Structure of Hemoglobin M Iwate [α87(F8)His → Tyr]: A UV and Visible Resonance Raman Study	60
II-G-11 Model Complexes for the Active Form of Galactose Oxidase. Physicochemical Properties of Cu(II)- and Zn(II)-Phenoxy Radical Complexes	60
II-G-12 Characterization of Imidazolate-Bridged Cu(II)-Zn(II) Heterodinuclear and Cu(II)-Cu(II) Homodinuclear Hydroperoxo Complexes as Reaction Intermediate Models of Cu, Zn-SOD	60
II-H Fast Dynamics of Photoproducts in Solution Phases	
II-H-1 Saturation Raman Spectroscopy as a tool for Studying the Excited States of Complex Organic Molecules: Application to Nickel Octaethylporphyrin	61
II-H-2 Construction of Novel Nanosecond Temperature Jump Apparatuses Applicable to Raman Measurements and Direct Observation of Transient Temperature	61

II-H-3 Identification of Histidine 77 as the Axial Heme Ligand of Carbonmonoxy CooA by Picosecond Time-Resolved Resonance Raman Spectroscopy	61
II-H-4 A Role of Solvent in Vibrational Energy Relaxation of Metalloporphyrins	62
II-I Molecular and Electronic Structures of Metallofullerenes and the Fullerene Radical Anions	
II-I-1 2D-HYSCORE Measurements of ^{13}C -La@C ₈₂	63
II-I-2 ESR Measurements of La@C _n	63
II-J State Correlated Raman Spectroscopy	
II-J-1 Investigations of Orientational Order for an Antiferroelectric Liquid Crystal by Polarized Raman Scattering Measurements	64
II-J-2 Polarized Raman Scattering Study for Frustoelectric Liquid Crystals	64

RESEARCH ACTIVITIES III -----65

Department of Electronic Structure

III-A Photochemical Synthesis of Exotic Atomic-Molecular Binary Clusters in Solution:	
π Radical -Transition Metal Alternatively Stacking (π-d)_n Clusters	
III-A-1 π Radical-Transition Metal Alternatively Stacking (π -d) _n - π Clusters: (I) V ₆ (C ₅ H ₅) ₇ , a Pentagonal Ring ((C ₅ H ₅)V) with a Rolling Axis Vanadocene (C ₅ H ₅)V(C ₅ H ₅)? ---	65
III-A-2 Development of a New Mass Spectrometer Allowing the Injection of Solution Directly into Vacuum and the Desolvation through the Collision of Liquid Jet with Solvent Gas Flow Rebounded from a Rotating Titanium Drum for Solute Deposition	66
III-B States of Neutral and Ionic Molecular Associates in Solutions	
III-B-1 Monomeric and Cluster States of Acetic Acid Molecules in Solutions: A Raman Spectroscopic Study	66
III-B-2 Comparison of the Theoretical Models for Calculating Acetic Acid Clusters in Aqueous Solution	67
III-C Ultrafast Dynamics and Structural Changes of Excited Cation Radicals in Solution	
III-C-1 First Observation of the Formation Process of a Solvated Aromatic Cation Radical in Polar Solvents: A Two-Photon Pumped Femtosecond Time-Resolved Absorption Study	68
III-C-2 Vibrational Relaxation Process of Solvated Aromatic Cation Radicals in Polar Solvents: A Two-Photon Pumped Picosecond Time-Resolved Raman Study	69
III-D Spectroscopic and Dynamical Studies on Charge Delocalization and Charge Transfer in Aromatic Molecular Cluster Ions	
III-D-1 Photodissociation Spectroscopy of Benzene Cluster Ions in Ultraviolet and Infrared Regions. Static and Dynamic Behavior of Positive Charge in Cluster Ions	70
III-D-2 Charge Transfer Complex of Benzene Cation Vertically Coordinated with Acetic Acid	71
III-D-3 Vibrational and Electronic Spectra of (Benzene-Benzyl Alcohol) ⁺ ; Predominance of Charge Resonance Interaction over Hydrogen-Bonding Interaction	71
III-D-4 Electronic and Vibrational Spectra of Aniline-Benzene Hetero-Dimer and Aniline Homo-Dimer Ions	71
III-E Structures and Reactivities of Metal Clusters	
III-E-1 Construction of Apparatus for Mass Analysis of Metal Clusters	73
III-F Spectroscopy and Dynamics of Vibrationally Excited Molecules and Clusters	
III-F-1 IR dip Spectra of Photochemical Reaction Products in a Phenol/Ammonia Cluster —Examination of Intracuster Hydrogen Transfer	74
III-F-2 Structural Characterization of the Acridine-(H ₂ O) _n (n = 1–3) Clusters by Fluorescence Dip Infrared Spectroscopy	74
III-F-3 Internal Methyl Group Rotation in o-Cresol Studied by Pulsed Field Ionization-ZEKE Photoelectron Spectroscopy	74
III-F-4 Pulsed Field Ionization-ZEKE Spectroscopy of Cresoles and Their Aqueous Complex: Internal Rotation of Methyl Group and Intermolecular Vibrations	75
III-F-5 Butterfly Vibration of the Tetrafluorobenzene Cation Studied by Pulsed Field Ionization-ZEKE Photoelectron Spectroscopy	75
III-G Time-Resolved Photoelectron Imaging on Ultrafast Chemical Dynamics	
III-G-1 Femtosecond Time-Resolved Photoelectron Imaging on Ultrafast Dephasing in Pyrazine --	76
III-H Crossed Beam Studies on Bimolecular Reaction Dynamics	
III-H-1 State-Resolved Differential Cross Section Measurements for the Inelastic Scattering of NO + Ar	76
III-I Non-Adiabatic Molecular Photodissociation Dynamics Studied by Polarization Spectroscopy	
III-I-1 Atomic Orbital Orientation in Photodissociation of OCS	77
III-J Photochemistry on Well-Defined Surfaces	
III-J-1 Excitation Mechanisms and Photochemistry of Adsorbates with Spherical Symmetry	78
III-J-2 Photo-induced Oxygen Elimination Reaction at an Ag(110)-p(2×1)-O Surface	78

III-K Structure and Properties of Polyoxometalates with a Magnetic, Electronic, or Biological Significance

III-K-1 Luminescence and Energy Transfer Phenomena in Tb ³⁺ /Eu ³⁺ -Mixed Polyoxometallolanthanoates K ₁₅ H ₃ [Tb _{1.4} Eu _{1.6} (H ₂ O) ₃ (SbW ₉ O ₃₃)(W ₅ O ₁₈) ₃].25.5H ₂ O and Na ₇ H ₁₉ [Tb _{4.3} Eu _{1.7} O ₂ (OH) ₆ (H ₂ O) ₆ Al ₂ (Nb ₆ O ₁₉) ₅].47H ₂ O	79
III-K-2 Mixed-Valence Ammonium Trivanadate with a Tunnel Structure Prepared by Pyrolysis of Polyoxovanadate	79
III-K-3 Photoassisted Dehalogenation of Organo-Chlorine Compounds by Paratungstate A in Aqueous Solutions	79
III-K-4 A Novel-Type Mixed-ligand Polyoxotungstolanthanoate, [Ln(W ₅ O ₁₈)(BW ₁₁ O ₃₉)] ¹²⁻ (Ln = Ce ³⁺ and Eu ³⁺)	79
III-K-5 Photoreduction Processes of α-Dodecamolybdophosphate, α-[PMo ₁₂ O ₄₀] ³⁻ : ³¹ P-NMR, Electrical Conductivity, and Crystallographic Studies	80
III-K-6 Na ₁₀ (glycine) ₂ [H ₂ W ₁₂ O ₄₂].28H ₂ O	80
III-K-7 Crystal and Electronic Structure and Magnetic Susceptibility of the Photochemically Prepared Layered Vanadyl Phosphate, Na(VO) ₂ (PO ₄) ₂ .4H ₂ O	80

RESEARCH ACTIVITIES IV -----81

Department of Molecular Assemblies

IV-A Spectroscopic Study of Organic Conductors

IV-A-1 Charge Disproportionation of θ-(BEDT-TTF) ₂ RbZn(SCN) ₄ Studied by Raman Spectroscopy	81
IV-A-2 Isotope Shift and Charge Susceptibility of C=C Related Normal Modes of BEDT-TTF Molecule	81
IV-A-3 Raman-Active C=C Stretching Vibrations of κ-(BEDT-TTF) ₂ Cu[N(CN) ₂]Br	81
IV-A-4 An Influence of the Cooling Rate to the Raman and IR Spectra of Partially Deuterated κ-(BEDT-TTF) ₂ Cu[N(CN) ₂]Br	82
IV-A-5 Spectroscopic Evidence for the Charge Disproportionation in a Two-Dimensional Organic Conductor, θ-(BDT-TTP) ₂ Cu(NCS) ₂	82
IV-A-6 ESR Properties of a Quasi-Two-Dimensional Organic Conductor, θ-(BDT-TTP) ₂ Cu(NCS) ₂	83
IV-A-7 Infrared Spectroscopic Study of the Band Structure of (EO-TTP) ₂ AsF ₆	83
IV-A-8 Optical Properties and Metal-Insulator Transitions in Organic Metals (BEDT-ATD) ₂ X(solvent) (X = PF ₆ , AsF ₆ , BF ₄ ; solvent = THF, DHF, DO)	83

IV-B Solid State Properties of Organic Conductors with p-d Interaction

IV-B-1 Magnetic Exchange Interactions in Quasi-One-Dimensional Organic Alloy of Co _{0.01} Ni _{0.99} Pc(AsF ₆) _{0.5}	84
IV-B-2 Pressure Dependence of Resistivity in Quasi-One-Dimensional Conductor CoPc(AsF ₆) _{0.5}	84
IV-B-3 Antiferromagnetic Phase Transition of DMTSA-FeCl ₄	85

IV-C Microscopic Investigation of Molecular-Based Conductors

IV-C-1 Low-Temperature Electronic States in (EDT-TTF) ₂ AuBr ₂	86
IV-C-2 Low Temperature Electronic States of β'-type Pd(dmit) ₂ Compounds	86
IV-C-3 Magnetic Investigation of Organic Conductors Based on TTP Derivatives	87
IV-C-4 Possible Charge Disproportionation and New Type Charge Localization in θ-(BEDT-TTF) ₂ CsZn(SCN) ₄	87

IV-D Development of Magnetic Organic Superconductors

IV-D-1 BETS as a Source of Molecular Magnetic Superconductors (BETS = Bis(ethylenedithio)tetraselenafulvalene)	88
IV-D-2 Superconductivity, Antiferromagnetism and Phase Diagram of a Series of Organic Conductors, λ-(BETS) ₂ Fe _x Ga _{1-x} Br _y Cl _{4-y}	88
IV-D-3 Fermi Surface and Phase Transition in Magnetic Field Parallel to the Conducting Plane in λ-(BETS) ₂ FeCl ₄	89
IV-D-4 Anisotropy of Magnetic Susceptibilities of λ-(BETS) ₂ FeBr _x Cl _{4-x}	89
IV-D-5 A Novel Antiferromagnetic Organic Superconductor κ-(BETS) ₂ FeBr ₄ [where BETS = Bis(ethylenedithio)tetraselenafulvalene]	90
IV-D-6 The x-Dependence of Electrical Properties and Antiferromagnetic Ordering between Fe ³⁺ Ions in κ-BETS ₂ FeCl _x Br _{4-x} System	90
IV-D-7 Successive Antiferromagnetic and Superconducting Transition in an Organic Metal, κ-(BETS) ₂ FeCl ₄	90

IV-E Structural and Electrical Properties of Molecular Crystals at Low Temperature and/or High Pressure

IV-E-1 Origin of Ferromagnetic Exchange Interactions in a Fullerene-Organic Compound	91
--	----

IV-E-2	Low temperature X-ray Crystal Structure Determination of α -(BEDT-TTF) $_2$ I $_3$ —Stripe-Like Charge Distribution at Low Temperature -----	92
IV-E-3	Crystal and Band Structure Examinations of High-Pressure Molecular Superconductor [(C $_2$ H $_5$) $_2$ (CH $_3$) $_2$ N][Pd(dmit) $_2$] $_2$ at 10 kbar -----	92
IV-E-4	Superconducting Transition of (TMTTF) $_2$ PF $_6$ above 50 kbar [TMTTF = Tetramethyltetrafulvalene] -----	92
IV-E-5	Electrical Resistivity Measurements of Organic Single Crystals by Diamond Anvil Cell up to 15 GPa -----	93
IV-F	Development of New Functional Molecular Materials	
IV-F-1	A Three-Dimensional Synthetic Metallic Crystal Composed of Single Component Molecules -----	93
IV-F-2	Development of Single-Component Molecular Metals Based on Transition Metal Complexes with Extended-TTF Dithiolate Ligands -----	94
IV-F-3	Synthesis and Properties of a New Organic Donor Containing a TEMPO Radical -----	94
IV-F-4	Synthesis, Structures and Properties of an New TSeF Derivative Containing Pyrazino-Ring and Its Cation Radical Salts -----	95
IV-G	Electrical Properties of Organic Semiconductors in Ultrahigh Vacuum	
IV-G-1	Quasi-Intrinsic Semiconducting State of Titanyl-phthalocyanine Films Obtained under Ultrahigh Vacuum Conditions -----	96
IV-H	Preparation and Characterization of Highly Oriented Organic Films	
IV-H-1	Substrate-Induced Order and Multilayer Epitaxial Growth of Substituted Phthalocyanine Thin Films -----	96
IV-H-2	Ordered Growth of Substituted Phthalocyanine Thin Films: Hexadecafluorophthalocyaninatozinc on Alkali Halide (100) and Microstructured Si Surfaces --	97
IV-H-3	Energy Transfer in Highly Oriented Permethyloctadecasilane and -Octadecasilane Films --	97
IV-I	Properties of Gas Adsorption on Single-Walled Carbon Nanotube Aggregates	
IV-I-1	Properties of Micropores in Single-Walled Carbon Nanotubes Studied by N $_2$ Gas Adsorption Isotherm Measurements -----	98
IV-I-2	Direct Evidence of Xenon Gas Adsorption Inside of Single-Walled Carbon Nanotubes Studied by ^{129}Xe -NMR -----	98
IV-J	Electronic Properties of Pristine and Doped Single-walled Carbon Nanotubes aggregates	
IV-J-1	Electronic States of Single-Walled Carbon Nanotube Aggregates Studied by Low Temperature ^{13}C -NMR -----	99
IV-J-2	Electronic States of Alkali-Metal Doped Single-Walled Carbon Nanotube Aggregates ----	99
IV-J-3	Electronic States of Br $_2$ Doped Single-Walled Carbon Nanotube Aggregates -----	100
IV-K	Structural and Electronic Properties of Fullerene-based Compounds	
IV-K-1	Study on the Physical Properties of Na $_4$ C $_{60}$ -----	101
IV-L	Development of Pulsed Field Gradient NMR Spectroscopy	
IV-L-1	Direct Measurement of Self-Diffusion Coefficients in Solids: Plastic Crystalline Hexamethylethane -----	102
IV-M	Phase Transition Mechanism of Reentrant Liquid Crystal	
IV-M-1	Neutron Small-Angle Scattering of Reentrant Liquid Crystal CBOBP -----	102
IV-N	Systematic Study of Organic Conductors	
IV-N-1	Structural Genealogy of BEDT-TTF-Based Organic Conductors III. Twisted Molecules: δ and α' Phases -----	104
IV-N-2	Raman and Optical Investigations on Charge Localization in the One-Dimensional Organic Conductors (TTM-TTP)(I $_3$) $_{5/3}$ and (TSM-TTP)(I $_3$) $_{5/3}$ -----	104
IV-N-3	Raman Investigation of the One-Dimensional Organic Conductor with a Half-Filled Band, (TTM-TTP)I $_3$ -----	105
IV-N-4	ESR Investigation of Organic Conductors (DTM-TTP)(TCNQ)(TCE) and (TMET-TTP)(TCNQ) -----	105
IV-N-5	Structural and Magnetic Properties of Cu[C(CN) $_3$] $_2$ and Mn[C(CN) $_3$] $_2$ -----	105
IV-O	Photoelectron Spectroscopy of Organic Solids in Vacuum Ultraviolet Region	
IV-O-1	Angle-Resolved Photoemission Measurements of ω -(<i>n</i> -pyrrolyl)alkanethiol Self-Assembled Monolayers Using <i>in-situ</i> Sample Preparation Apparatus -----	107
IV-O-2	Photoemission Spectra of LiNiO $_2$ Catalyst for Oxidative Coupling of Methane -----	107
IV-O-3	Intramolecular Energy-Band Dispersion in Oriented Thin Films of <i>n</i> -CF $_3$ (CF $_2$) $_{22}$ CF $_3$ Observed by Angle-Resolved Photoemission with Synchrotron Radiation -----	107

RESEARCH ACTIVITIES V -----109

Department of Applied Molecular Science

V-A Molecular Mechanisms of Oxygen Activation by Heme Enzymes

- V-A-1 Investigations of the Myoglobin Cavity Mutant H93G with Unnatural Imidazole Proximal Ligands as a Modular Peroxide O-O Bond Cleavage Model System -----109
- V-A-2 Formation and Catalytic Roles of Compound I in the Hydrogen Peroxide-Dependent Oxidations by His64 Myoglobin Mutants -----109
- V-A-3 Proximal Ligand Control of Heme Iron Coordination Structure and Reactivity with Hydrogen Peroxide: Investigations of the Myoglobin Cavity Mutant H93G with Unnatural Oxygen Donor Proximal Ligands -----110
- V-A-4 Mechanisms of Sulfoxidation Catalyzed by High-Valent Intermediates of Heme Enzymes: Electron Transfer vs. Oxygen Transfer Mechanism -----110

V-B Model Studies of Non-Heme Proteins

- V-B-1 A Bis(μ -oxo)dicopper(III) Complex with Aromatic Nitrogen Donors: Structural Characterization and Reversible Conversion between Copper(I) and Bis(μ -oxo)dicopper(III) Species -----111
- V-B-2 Characterization of Imidazolate-Bridged Cu(II)-Zn(II) Heterodinuclear and Cu(II)-Cu(II) Homodinuclear Hydroperoxo Complexes as Reaction Intermediate Models of Cu, Zn-SOD ---111
- V-B-3 Synthesis and X-ray Crystal Structure of a Novel Mn(II)-Semiquinone Complex [Mn^{II}(TPA)(DTBSQ)]BPh₄, and Its Dioxygenase-like Activity: Relevance to Manganese(II)-Dependent Catechol Dioxygenases -----111
- V-B-4 Infrared Spectroscopic Features of the Cyclic Hydrogen-Bonded *cis*(Hydroxo)-Fe^{III}-(Carboxylato) Unit of Lipoygenase Active Site Models -----112

V-C Aqueous Organometallic Chemistry

- V-C-1 pH-Selective Hydrogenation with an Organometallic Aqua Complex as a Catalyst Precursor in Very Acidic Media -----112

V-D Magnetic Structure of Oligo-Nitroxide-Transition Metal Complexes

- V-D-1 Influence of the Thermal Excitations of the Ferrimagnetic ($-1/2, 5/2, -1/2$) Linear Trimer on the Paramagnetic Behavior of the Layered Metal-Radical Complex {Mn(hfac)₂}₃(R_X)₂ $\cdot n$ -C₇H₁₆ -----113
- V-D-2 Synthesis and Magnetic Properties of Bis(hexafluoroacetylacetonate) Copper(II) Complex with 5-Bromo-1,3-Phenylenebis(*N*-*tert*-butylaminoxyl) as a Bridging Ligand -----113
- V-D-3 Magnetic Behaviour of the Ferrimagnetic ($-1/2, 5/2, -1/2$) Linear Trimer in Complexes of Mn(hfac)₂ with Bis- and Trisnitroxide Radicals -----113
- V-D-4 Exchange Coupling Parameters and Energy Levels for Cyclic Metal-Radical Complexes of Bis(hexafluoroacetylacetonato) manganese(II) with 5-*tert*-butyl-1,3-phenylenebis(*N*-*tert*-butylaminoxyl) and (4-*N*-*tert*-butyl-*N*-oxyamino)pyridine -----114
- V-D-5 Synthesis and Magnetic Properties of a New Complex Made up of Mn(hfac)₂ and a Radical with a Triplet Ground State -----114
- V-D-6 Two-Dimensional Complexes of the General Formula [Mn(hfac)₂]₃(R)₂ with Variable Metal-Radical Exchange Interactions -----115

V-E Synthesis of Chiral Molecule-Based Magnets

- V-E-1 Synthesis and Characterization of a Chiral Molecule-Based Metamagnet Made by a Chiral Triplet Organic Radical and Transition Metal Ion -----116
- V-E-2 Synthesis, Structure and Magnetic Properties of a Chiral One-Dimensional Molecule-Based Magnet -----116

V-F Synthesis and Characterization of Quantum-Spin Systems

- V-F-1 Construction of a Quantum-Spin System of $S = 1/2$ Antiferromagnetic Chain with the Next-Nearest-Neighbor Interactions -----117
- V-F-2 Magnetic Properties of Low Dimensional Quantum Spin Systems Made of Stable Organic Biradicals PNNNO, F₂PNNNO and PIMNO -----118
- V-F-3 Singlet Ground States in an Organic $S = 1/2$ Spin Ladder and a Novel Double Spin Chain of Ferromagnetic Dimers Formed by an Organic Tetraradical -----118
- V-F-4 Observation of Magnetization Plateau of 1/4 in a Novel Double Spin Chain of Ferromagnetic Dimers Formed by an Organic Tetraradical -----119

V-G Pressure Effects on Molecular Magnetism

- V-G-1 Pressure Effect on Mn Complexes of Bisaminoxyl Radicals -----119
- V-G-2 Pressure Effect on Cu(hfac)₂ Complex with 5-Bromo-1,3-phenylenebis(*N*-*tert*-butylaminoxyl)—Suppression of the Structural Change under Pressure -----120

V-H Desorption Induced by Electronic Transitions at the Surface of Van der Waals Condensates

- V-H-1 Absolute Measurement of Total Photo Desorption Yield of Solid Ne in Vacuum Ultraviolet Range -----121

V-H-2 Desorption of Excimers from the Surface of Solid Ne by Low Energy Electron or Photon Impact -----	121
V-I Bioinorganic Studies on Structures and Functions of Non-Heme Metalloenzymes Using Model Complexes	
V-I-1 A Novel Diiron Complex as a Functional Model for Hemerythrin -----	122
V-I-2 Reactivity of Hydroperoxide Bound to a Mononuclear Non-Heme Iron Site -----	122
V-J Synthesis and Physical Properties of Novel Molecular Metals	
V-J-1 Preparation, Structures and Physical Properties of Selenium Analogues of DTEDT as Promising Donors for Organic Metals -----	123
V-J-2 Preparation and Properties of Gold Complexes with TTF Dithiolato Ligands -----	123
V-J-3 New TTP Donors Containing Chalcogenopyran-4-ylidene: Preparation, Structures, and Electrical Properties -----	124
V-J-4 Structures and Properties of CHEO-TTP Salts -----	124
V-J-5 Structures and Physical Properties of (CHTM-TTP) ₂ TCNQ -----	124
V-K Fast Bimolecular Reaction Kinetics in Solution	
V-K-1 Ultrafast Bimolecular Reaction Kinetics between S ₁ <i>trans</i> -Stilbene and Carbon Tetrachloride Studied by Sub-Picosecond Time-Resolved Visible Absorption Spectroscopy -----	126
V-L Development of Model Core Potentials and Post Hartree-Fock Calculations to Atoms and Molecules	
V-L-1 A Theoretical Study on the Ionization of CO ₂ and CS ₂ with Analysis of the Vibrational Structure of the Photoelectron Spectra -----	127
V-L-2 A Theoretical Study on the Ionization of OCS with Analysis of the Vibrational Structure of the Photoelectron Spectrum -----	127
V-L-3 Configuration Interaction Study of Differential Correlation Energies in Ca ⁺ , Ca and Ca ⁻ --	127
V-L-4 Spin-Orbit Configuration Interaction Calculations of Low-Lying Electronic States of NaCl Using Model Core Potential -----	127
V-M Theoretical Study of the Electronic Structures of Weakly Bound Molecules	
V-M-1 Ab initio Molecular Orbital Study of Fe(CO) _n (n = 1, 2, and 3) -----	128
V-M-2 Ab initio CASSCF and MRSDCI Calculations of the (C ₆ H ₆) ³⁺ Radical -----	128
V-M-3 Molecular Orbital Study on OH Stretching Frequency of Phenol Dimer and its Cation ----	128
V-N Theory for Quantum Liquids and Molecular Dynamics Study Using Potentials by <i>ab initio</i> Molecular Orbital Calculations	
V-N-1 An Integral Equation Theory for Quantum Liquids: Finite-Temperature Kohn-Sham Density-Functional Formulation -----	129
V-N-2 Structure Change of Supercritical Mercury -----	129
V-O Determination of Structures of Neutral Clusters	
V-O-1 Focusing of DCl and HCl Dimers by an Electrostatic Hexapole Field —The Role of the Tunneling Motion -----	130
V-O-2 Tunneling Motion in (HCl) ₂ Hydrogen-Bonded Dimer Probed by Electrostatic Hexapole and Doppler-Selected TOF Measurement for the Internal Energy Distribution of [ClHCl] -----	130
V-P Reaction Dynamics in the Gas Phase and on Surface	
V-P-1 Evidence for Steric Effect in Methyl Chloride Ionization by Metastable Argon Atoms ----	131
V-P-2 Direct Observation of Steric Effect in Penning Ionization Reaction of Ar* + CHCl ₃ → CHCl ₂ ⁺ + Cl + e ⁻ + Ar -----	131
V-P-3 Hydrogen Adsorption and Reaction on the Ir{100}-(1×5) Surface -----	131
V-P-4 Hot Atom Mechanism in Hydrogen Exchange Reaction on the Ir{100} Surface -----	131
V-Q Millimeter-Wave Spectroscopy Combined with Pulsed-Jet Expansion Technique for the Detection of the Novel Unstable Species and the van der Waals Mode Transitions of Molecular Clusters	
V-Q-1 Millimeter-Wave Spectroscopy of the van der Waals Bending Band of He–HCN -----	132
V-Q-2 Millimeter Wave Spectroscopy of the HCN–H ₂ Cluster -----	133
V-Q-3 Millimeter Wave Spectra of the H ₂ –H ₂ O van der Waals Complex -----	133
V-Q-4 Millimeter Wave Spectroscopy of the van der Waals Bending Band of OCO-DF Generated in a Supersonic Jet Expansion -----	134
V-R Ion-Molecule Reactions in the Troposphere	
V-R-1 Measurements of Mobility and Mass Spectra of Tropospheric Ions -----	135
V-R-2 Experimental Study of Ion-Induced Nucleation in the Troposphere -----	135
V-S Monte Carlo Simulation of Molecular Clusters	
V-S-1 Boson Localization on the Superfluid-Insulator Transition by Quantum Loop Algorithm --	136
V-S-2 Monte Carlo Simulation of the Formation of Chemical Gel and Clusters -----	136
V-S-3 Linear-shaped Motion of DNA in Concentrated Polymer Solutions Under a Steady Field --	136
V-T Development of Shaped Pulse Solid-State NMR Spectroscopy	
V-T-1 Shaped Pulse Solid-State NMR Experiment -----	137

**V-U Development of ^{13}C High-Resolution NMR Spectroscopy
for Nematic and Cholesteric Liquid Crystals**

- V-U-1 Direct Determination of ^{13}C Chemical Shift Anisotropies of Liquid Crystals
by Combining OMAS NMR and Rotor-Synchronous Pulses with Hankel Transformation -----138

RESEARCH ACTIVITIES VI -----139

Department of Vacuum UV Photoscience

VI-A Electronic Structure and Decay Mechanism of Inner-Shell Excited Molecules

- VI-A-1 Exchange Interaction in the $1s\text{-}\sigma^*$ Resonance of the Triplet Ground State of S_2
in Comparison with O_2 -----139
- VI-A-2 Polarization Dependence of O^+/O_2^+ Fragmentations at the Terminal $\text{O}1s\text{-to-}\sigma^*$ Excitation
of Ozone: A Memory Effect of Core-Hole Localization During the Auger Decay -----139
- VI-A-3 Molecular Field and Spin-Orbit Splittings in the $2p$ Ionization of Second-Row Elements:
A Breit-Pauli Approximation Applied to OCS , SO_2 , and PF_3 -----140

**VI-B Soft X-ray Photoelectron-Photoabsorption Spectroscopy and Electronic Structure
of Transition Metal Compounds**

- VI-B-1 Ni $2p$ Photoabsorption and Resonant Photoelectron Spectroscopy of High-Spin Ni Complex,
 $\text{Ni}(\text{N,N}'\text{-dimethylethylenediamine})_2\text{Cl}_2$ -----140
- VI-B-2 Mg and Al K-edge XAFS Measurements with a KTP Crystal Monochromator -----141

**VI-C Observation of Vibrational Coherence (Wavepacket Motion) in Solution-Phase Molecules
Using Ultrashort Pulses**

- VI-C-1 Observation of Vibrational Coherence of S_1 *trans*-Stilbene in Solution
by 40-fs-Resolved Absorption Spectroscopy -----142
- VI-C-2 Generation of Two Independently-Tunable Pulses
for Extremely-Fast Pump-Probe Absorption Spectroscopy -----142
- VI-C-3 Measurement of Impulsive Stimulated Raman Scattering Using Ultra-Short Pulses
Generated by a Krypton Gas-Filled Hollow Fiber -----143
- VI-C-4 Construction of an Apparatus for Optical Heterodyne Detected Impulsive Stimulated Raman
Scattering Measurement Using a Phase Mask -----144

VI-D Studies of Primary Photochemical/physical Processes

Using Femtosecond Electronic Spectroscopy

- VI-D-1 Ultrafast Excited-State Proton Transfer Dynamics of 1,8-dihydroxyanthraquinone (chrysozin)
Studied by Femtosecond Time-Resolved Fluorescence Spectroscopy -----145
- VI-D-2 Femtosecond Dynamics of Photoexcited *trans*-Azobenzene
Observed by Time-Resolved Fluorescence Up-Conversion Spectroscopy -----145
- VI-D-3 S_2 Emission of a Series of Zinc(II) Porphyrins
Studied by Femtosecond Fluorescence Spectroscopy -----146
- VI-D-4 Construction of Femtosecond IR-IR Pump-Probe Spectrometer -----146

VI-E Studies of Photochemical Reactions Using Picosecond Time-Resolved Vibrational Spectroscopy

- VI-E-1 Observation of Picosecond Time-Resolved Raman Spectra of *p*-Nitroaniline -----147
- VI-E-2 Femtosecond and Picosecond Time-Resolved Spectra of 5-Dibenzosuberone -----148
- VI-E-3 Resonance Hyper-Raman Scattering of *all-trans* Retinal from a Diluted Solution:
Excitation Profile and Energy Levels of the Low-Lying Excited Singlet States -----148

VI-F Synchrotron Radiation Stimulated Surface Reaction and Application to Nanoscience

- VI-F-1 SR-Stimulated Etching and OMVPE Growth
for Semiconductor Nanostructure Fabrication -----150
- VI-F-2 Aligned Island Formation Using Step-Band Networks on $\text{Si}(111)$ -----150
- VI-F-3 Scanning Tunneling Microscopy Study of Surface Morphology of $\text{Si}(111)$
after Synchrotron Radiation Stimulated Desorption of SiO_2 -----151
- VI-F-4 Assignments of Bending and Stretching Vibrational Spectra
and Mechanisms of Thermal Decomposition of SiH_2 on $\text{Si}(100)$ Surfaces -----151
- VI-F-5 Control of Surface Composition on $\text{Ge}/\text{Si}(001)$ by Atomic Hydrogen Irradiation -----151
- VI-F-6 Reconstruction of BL4A Beam Line
and Infrared Reflection Absorption Spectroscopy System -----151

VI-G Photoionization Dynamics Studied by Electron Spectroscopy

Combined with a Continuous Synchrotron Radiation Source

- VI-G-1 Superexcitation and Subsequent Decay of Triatomic Molecules
Studied by Two-Dimensional Photoelectron Spectroscopy -----153
- VI-G-2 Photoelectron Spectroscopy of Atomic and Molecular Radicals
Prepared by RF Atom Source -----153

VI-H Development of a Laser-Synchrotron Radiation Combination Technique to Study Photoionization of Polarized Atoms	
VI-H-1 Laser Photoionization of Polarized Ar Atoms Produced by Excitation with Synchrotron Radiation -----	154
VI-H-2 Development of a New Angle-Resolved Energy Analyzer for Photoelectron Spectroscopy of Polarized Atoms -----	154
VI-I Vacuum UV Spectroscopy Making Use of a Combination of Synchrotron Radiation and a Mode-Locked or Pulsed UV Laser	
VI-I-1 Rotational State Distribution of N_2^+ Produced from N_2 or N_2O Observed by a Laser-Synchrotron Radiation Combination Technique -----	155
VI-J Monochromator Newly Developed on the Beam Line BL2B2 in UVSOR	
VI-J-1 Performance of the Dragon-Type Monochromator at UVSOR -----	156
VI-J-2 Anisotropy of the Fragment Ions from Small Molecules Excited with Synchrotron Radiation -----	156
VI-K Thin Film Preparation with Chemical Vapor Deposition Using Vacuum Ultraviolet Radiation	
VI-K-1 Silica Film Preparation by Chemical Vapor Deposition Using Vacuum Ultraviolet Excimer Lamps -----	157
VI-K-2 Silica Film Preparation by Chemical Vapor Deposition Using Vacuum Ultraviolet Excimer Lamps -----	157
VI-L Ultraviolet, Visible and Infrared Spectroscopy of Solids	
VI-L-1 Performance of IR-VUV Normal Incidence Monochromator Beamline at UVSOR -----	158
VI-L-2 Pseudogap Formation in the Intermetallic Compounds $(Fe_{1-x}V_x)_3Al$ -----	158
VI-M Dynamics and Relaxation of Atoms and Molecules Following Core-Level Excitation	
VI-M-1 Site-Specific Phenomena in Si:2p Core-Level Photoionization of $X_3Si(CH_2)_nSi(CH_3)_3$ ($X = F$ or Cl , $n = 0-2$) Condensed on a Si(111) Surface -----	159
VI-M-2 Site-Specific Fragmentation Following C:1s Core-Level Photoionization of 1,1,1-Trifluoroethane Condensed on a Au Surface and of a 2,2,2-Trifluoroethanol Monolayer Chemisorbed on a Si(100) Surface -----	159
VI-M-3 Ion Desorption Induced by Core-Electron Transitions Studied with Electron-Ion Coincidence Spectroscopy -----	159
VI-M-4 Electron-Ion Coincidence Study for the $TiO_2(110)$ Surface -----	160
VI-M-5 Development of Electron-Ion Coincidence Spectroscopy for Study of Vapor-Phase Dynamics -----	160
VI-M-6 High-Resolution Angle-Resolved Ion-Yield Measurements of H_2O and D_2O in the Region of O 1s to Rydberg Transitions -----	160
VI-M-7 Molecular Deformation in the O $1s^{-1}2\pi_u$ Excited States of CO_2 Probed by the Triple-Differential Measurement of Fragment Ions -----	160
VI-M-8 Resonant Auger Spectrum Following Kr:2p \rightarrow 5s Photoexcitation -----	160
VI-M-9 Angle-Resolved Electron and Ion Spectroscopy Apparatus on the Soft X-Ray Photochemistry Beamline BL27SU at SPring-8 -----	161
VI-M-10 Monochromator for a Soft X-Ray Photochemistry Beamline BL27SU of SPring-8 -----	161
VI-N Study on RF-Photocathode for Compact X-Ray Sources	
VI-N-1 Preliminary Study on Photoemission from Cesium Telluride Irradiated by Polarized Photon -----	162
RESEARCH ACTIVITIES VII -----	163

Coordination Chemistry Laboratories

VII-A New Insight into Mechanism of Oxygen Activation in Biological Oxygenases	
VII-A-1 Interaction between a Copper(II) Compound and Protein Investigated in terms of the Capillary Electrophoresis Method -----	163
VII-A-2 Contribution of a Metal-Peroxide Adduct to Neurodegeneration is due to its Oxidase Activity -----	163
VII-A-3 DNA Promotes the Activation of Oxygen Molecule by Binuclear Cobalt(II) Compounds -----	163
VII-A-4 Structure and Function of "Free Iron Ion" in Biological System and Their Model Compounds -----	164
VII-A-5 New Insight into Oxidative DNA Cleavage Reaction Catalyzed by Metal Chelates -----	164
VII-A-6 Cleavage of C-N bond of Peptide Group by Copper(II)-peroxide Adduct with η^1 -Coordination Mode -----	164
VII-A-7 Important role of Proton in Activation of Oxygen Molecule in Heme-Containing Oxygenases -----	164

VII-B Electronic Structure and Reactivity of Metal Cluster Complexes	
VII-B-1 A One-Step Synthesis of an Ir(II) Dinuclear Complex. Preparation, Structures and Properties of Bis(μ -acetato)dichlorodicarbonyliridium(II) Complexes -----	166
VII-B-2 Preparation and Structure of Bis(μ -acetato)dichlorodicarbonyliridium(II) Complexes with group 15 ligands, $[\text{Ir}_2(\mu\text{-O}_2\text{CMe})_2\text{Cl}_2(\text{CO})_2\text{L}_2]$ (L = PPh ₃ , PCy ₃ , P(OPh) ₃ , AsPh ₃ , SbPh ₃), and ESR and DFT Studies of Electronic Structure of Their Cationic Ra -----	166
VII-C Research on the Relationship between Structure of Vanadyl Complex and Insulin-Mimetic Activity	
VII-C-1 Stereospecific and Structure-Dependent Insulin-Mimetic Oxovanadium(IV) Complexes with N,N'-Ethylene-bis-amino Acids -----	167
VII-C-2 A New Type of Orally Active Insulin-Mimetic Vanadyl Complex: Bis(1-oxy-2-pyridinethiolate)oxovanadium(IV) with VO(S ₂ O ₂) Coordination Mode -----	167
VII-C-3 Evidence for the Improvement of Noninsulin-Dependent Diabetes Mellitus in KKAY Mice with Daily Oral Administration of Bis(6-methylpicolinato)oxovanadium(IV) Complex -----	167
VII-C-4 In vivo Coordination Structural Changes of a Potent Insulin-Mimetic Agent, Bis(picolinato)oxovanadium(IV), Studied by Electron Spin-Echo Envelope Modulation Spectroscopy -----	167
VII-C-5 Role of Vanadium in Treating Diabetes -----	168
VII-C-6 Ternary Complex Formation between VO(IV)-picolinic Acid or VO(IV)-6-Methylpicolinic Acid and Small Blood Serum Bioligands -----	168
VII-D-7 An Orally Active Antidiabetic Vanadyl Complex, Bis(1-oxy-2-pyridinethiolato)oxovanadium (IV), with VO(S ₂ O ₂) Coordination Mode; <i>In vitro</i> and <i>In vivo</i> Evaluation in Rats ---	168
VII-C-8 Interaction of Vanadyl Complexes with Biological Systems: Structure-Insulinomimetic Activity Relationship of Vanadyl-Picolinate Complexes -----	169
VII-C-9 Synthesis of New Vanadyl Complexes of Hydroxyazine-Type Heterocycles and Their Insulin-Mimetic Activities -----	169
VII-C-10 Speciation of Insulin-Mimetic VO(IV)-Containing Drugs in Blood Serum -----	169
VII-D Syntheses of Transition Metal-Sulfur Clusters and Development of Their Catalysis	
VII-D-1 Syntheses of a Dinuclear Ir Complex Containing Bridging Tetraselenide Ligands $[(\text{C}_5\text{Me}_5)\text{Ir}(\mu\text{-Se}_4)_2\text{Ir}(\text{C}_5\text{Me}_5)]$ and its Conversion into Ir ₂ Pd ₂ Se ₃ and Ir ₂ Pd ₃ Se ₅ Clusters -----	170
VII-D-2 Preparation of Sulfido-Bridged Di- or Trinuclear Pyrrolylimido and Diazoalkane Complexes Derived from a Tungsten Dinitrogen Complex -----	170
VII-E Reductive Activation of Carbon Monoxide derived from Carbon Dioxide and Oxidative Activation of Hydroxy- and Oxo-Groups Derived from Water	
VII-E-1 Oxidation of Hydrocarbon by Mono- and Dinuclear Ruthenium Quinone Complexes via Hydrogen Atom Abstraction -----	171
VII-E-2 Electrochemical Water-Oxidation to Dioxygen Catalyzed by Oxidized Form of Bis(ruthenium-hydroxo) Complex in H ₂ O -----	171
VII-E-3 Selective Production of Acetone in Electrochemical Reduction of CO ₂ Catalyzed by Ru-naphthyridine Complex -----	172
VII-E-4 Energy Conversion from Proton Gradient to Electricity Based on Characteristic Redox Behavior of an Aqua Ruthenium Complex -----	172
VII-E-5 Double Addition of CO ₂ and CH ₃ OH to Ruthenium Carbonyl Complex with Novel Mono-dentate Dithiolene -----	172
VII-E-6 Structural and Spectroscopic Characterization of Ruthenium(II) Complexes with Methyl, Formyl and Acetyl Groups as Model Species in Multi-Step CO ₂ Reduction -----	173
VII-F Synthesis of Transition-Metal Chalcogenido Complexes and Their Cluster-Forming Reactions	
VII-F-1 Synthesis of Bis{(2-dimethylphenylphosphino)ethane-1-thiolato}bis(tert-butylthiolato)molybdenum(IV) and Its Cluster-Forming Reactions with FeCl ₂ and CuBr -----	174
VII-F-2 Synthesis and Structure of a Triply-Fused Incomplete-Cubane Cluster $[(\eta^5\text{-C}_5\text{Me}_5)\text{WS}_3]_3\text{Cu}_7(\text{MeCN})_9(\text{PF}_6)_4$ and a 2D Polymer $[(\eta^5\text{-C}_5\text{Me}_5)\text{WS}_3\text{Cu}_3(\text{MeCN})(\text{pz})]\text{PF}_6$ (pz = pyrazine) -----	174
VII-F-3 Synthesis and Structures of the Halfsandwich W(VI) Triselenido and W(II) Selenolato Complexes -----	174
VII-G Artificial Photoreaction systems on a Protein Surface	
VII-G-1 Direct Observation of the Ferric-Porphyrin Cation Radical as an Intermediate in the Photo-Triggered Oxidation of Ferric- to Ferryl-Heme Tethered to Ru(bpy) ₃ in Reconstituted Myoglobin -----	176
VII-G-2 Construction of Artificial Photosynthetic Reaction Centers on a Protein Surface: Vectorial, Multistep, and Proton-Coupled Electron Transfer for Long-Lived Charge Separation -----	176
VII-G-3 Direct Comparison of Electron Transfer Properties of Two Distinct Semisynthetic Triads with Non-Protein Based Triad: Unambiguous Experimental Evidences on Protein Matrix Effects -----	176

VII-G-4 Cyclodextrin-Appended Myoglobin as a Tool for Construction of a Donor-Sensitizer-Acceptor Triad on a Protein Surface	177
---	-----

RESEARCH ACTIVITIES VIII -----179

Laser Research Center for Molecular Science

VIII-A Developments and Researches of New Laser Materials

VIII-A-1 Intense THz Radiation from Femtosecond Laser Pulses Irradiated InAs in a Strong Magnetic Field	179
VIII-A-2 High-Repetition-Rate, High-Average-Power Mode-Locked Ti:Sapphire Laser with an Intracavity cw-Amplification Scheme	179
VIII-A-3 Compact THz-radiation Source Consisting of a Bulk Semiconductor, a Mode-Locked Fiber Laser, and a 2-T Permanent Magnet	180
VIII-A-4 Spectrum Control of THz Radiation from InAs in a Magnetic Field by Duration and Frequency Chirp of the Excitation Pulses	180
VIII-A-5 LiCAF Crystal as a New Vacuum Ultraviolet Optical Material with Transmission Down to 112 nm	181
VIII-A-7 THz Radiation from Intracavity Saturable Bragg Reflector in Magnetic Field with Self-Started Mode-Locking by Strained Saturable Bragg Reflector	181
VIII-A-8 High-Gain, Reflection-Double Pass, Ti:Sapphire Continuous-Wave Amplifier Delivering 5.77 W Average Power, 82 MHz Repetition Rate, Femtosecond Pulses	181

VIII-B Development and Research of Advanced Tunable Solid State Lasers

VIII-B-1 Performance of Widely Tunable Yb:YAG Microchip Lasers	182
VIII-B-2 High Average Power Diode-Pumped Composite Nd:YAG Laser with Cr ⁴⁺ :YAG Saturable Absorber for Passive Q-Switching	182
VIII-B-3 Optical Properties and Laser Characteristics of Highly Nd ³⁺ -Doped Y ₃ Al ₅ O ₁₂ Ceramics	183
VIII-B-4 Development of Multifunction Nonlinear Optical Wavelength Converter	184
VIII-B-5 Periodical Twinning in Crystal Quartz for Ultraviolet Nonlinear Optics	184

Research Center for Molecular Materials

VIII-C Development of Novel Heterocyclic Compounds and Their Molecular Assemblies for Advanced Materials

VIII-C-1 Preparation of New TTF Vinylogues Containing Substituents at the Vinyl Positions	186
VIII-C-2 Preparation, Structure, and Properties of 1,3-Bis(1,4-dithiafulven-6-yl)azulenes	186
VIII-C-3 Synthesis and Characterization of Novel Strong Electron Acceptors: Bithiazole Analogues of Tetracyanodiphenodimethane (TCNDQ)	186
VIII-C-4 Heterocyclic TCNQ Analogues Containing Thiophene and Benzothiadiazole Units	187
VIII-C-5 Crystal Engineering in π -Overlapping Stacks: Unusual One- and/or Two-Dimensional Stacking of π -System in the Crystal Structure of the Cation Radical Salts of Tetrathiafulvalene Vinylogues	187
VIII-C-6 One-Dimensional Supramolecular Tapes in the Co-Crystals of 2,5-Dibromo-3,6-dihydroxy-1,4-benzoquinone (Bromanilic Acid) with Heterocyclic Compounds Containing a Pyrazine Ring Unit	188
VIII-C-7 A Decamethylferrocene [Fe(C ₅ Me ₅) ₂] and Chloranilic Acid (CA) Complex with Hydrogen Bonded Supramolecular Structure between CA and H ₂ O	188
VIII-C-8 New Hydrogen Bond Donor-Acceptor Pairs between Dipyridylacetylenes and 2,5-Dichloro-3,6-dihydroxy-1,4-benzoquinone	188
VIII-C-9 Novel Synthetic Approach to 5–10 nm Long Functionalized Oligothiophenes	188

VIII-D Electronic Structures and Reactivities of Active Sites of Metalloproteins

VIII-D-1 Resonance Raman Spectra of Legitimate Models for the Ubiquitous Compound I Intermediates of Oxidative heme Enzymes	190
VIII-D-2 Spin Distribution in Low-Spin (meso-Tetraalkylporphyrinato)iron(III) Complexes with (dxz,dyz) ⁴ (dxy) ¹ Configuration. Studies by ¹ H-NMR, ¹³ C-NMR, and EPR Spectroscopies	190
VIII-D-3 Post-Assembly Insertion of Metal Ions into Thiol-Derivatized Porphyrin Monolayers on gold	190
VIII-D-4 Electron Spin-Echo Envelope Modulation Spectral properties of Amidate Nitrogen Coordinated to Oxovanadium(IV) Ion	191
VIII-D-5 Newly Designed Iron-Schiff Base Complexes as Models of Mononuclear Non-Heme Iron Active Sites	191
VIII-D-6 Synthesis and Characterization of High Valent Iron Porphyrin Complexes as Models for Reaction Intermediates of Cytochrome <i>c</i> Oxidase	191

VIII-E Molecular Mechanism of Heme Degradation and Oxygen Activation by Heme Oxygenase	
VIII-E-1 Participation of Carboxylate Amino Acid Side Chain in Regiospecific Oxidation of Heme by Heme Oxygenase -----	192
VIII-F Designing Artificial Photosynthesis at Molecular Dimensions	
VIII-F-1 Porphyrin Catalyzed Reductive Silylation and Acylation of Quinones under Irradiation of Visible Light -----	193
VIII-G Development of New Metal Complexes as Redox Catalysts	
VIII-G-1 Synthesis of Terpyridine-Based Binary Ligands and Their Metal Complexes -----	193
VIII-H Development of Organic n-Type Semiconductors for Molecular Thin-Film Devices	
VIII-H-1 Synthesis, Characterization, and Electron-Transport Property of Perfluorinated Phenylene Dendrimers -----	195
VIII-H-2 Perfluorinated Oligo(<i>p</i> -Phenylene)s: Efficient n-Type Semiconductors for Organic Light-Emitting Diodes -----	195
VIII-I The Effects of the 2D Spin-Echo NMR Experiment on a Solid-State Homonuclear Spin-1/2 Pair	
VIII-I-1 Real Figure of Two-Dimensional Spin-Echo NMR Spectra for a Homonuclear Two-Spin System in Rotating Solids -----	196
VIII-J The Applications of Double-Rotation NMR Method	
VIII-J-1 The Observation of REDOR Phenomenon for CH _x ($x \geq 2$) Spin Systems under DOR ----	196

Equipment Development Center

VIII-K Development of "IMS Machines"	
VIII-K-1 Vacuum-Chamber-Based High Voltage Application Apparatus to Fabricate Wide-Range Nonlinear Optical Wavelength Converters -----	197
VIII-L Development of New Laser Materials	
VIII-L-1 Deep-Ultraviolet Light Amplification within a Nanometer-Sized Layer -----	199

Ultraviolet Synchrotron Orbital Radiation Facility

VIII-M Development of the UVSOR Light Source	
VIII-M-1 New Lattice for UVSOR -----	200
VIII-M-2 Development of Longitudinal Feedback System for a Storage Ring Free Electron Laser -----	200
VIII-N Researches by the USE of UVSOR	
VIII-N-1 Photoelectron Spectroscopic Study on Photo-Induced Phase Transition in a Spin Crossover Complex [Fe(2-pic) ₃]Cl ₂ EtOH -----	200
VIII-N-2 Photo-Induced Change in Semiconductor-Vacuum Interface of p-GaAs(100) Studied by Photoelectron Spectroscopy -----	200
VIII-N-3 Excitation Spectra of a Long-Persistent Phosphor SrAl ₂ O ₄ :Eu,Dy in Vacuum Ultraviolet Region -----	200
VIII-N-4 Two-Dimensional Imaging Technique for Measuring Translational Energy and Angular Distribution of Ionic Photofragments -----	201
VIII-N-5 Angular Distribution Measurement of Auger Electrons from Fixed in Space Molecules	201
VIII-N-6 Construction of a Varied-Line-Spacing Plane Grating Monochromator at BL-4B -----	201

Computer Center

VIII-O Theoretical Studies on Electronic Structure and Dynamics of Electronically Excited States in Polyatomic Molecules	
VIII-O-1 Theoretical Study of the Potential Energy Surfaces and Bound States of HCP -----	202
VIII-O-2 A Comparative Study of the Quantum Dynamics and Rate Constants of the O(³ P) + HCl Reaction Described by Two Potential Surfaces -----	202
VIII-O-3 Determination of the Global Potential Energy Surfaces for Polyatomic Systems -----	202
VIII-O-4 Semiclassical Study of Nonintegrable Systems -----	202
VIII-O-5 Development of ab initio MD Method Based on the Direct Evaluation of CAS-SCF Energy Derivatives -----	203

RESEARCH FACILITIES -----205

Laser Research Center for Molecular Science -----	205
Research Center for Molecular Materials -----	205
Equipment Development Center -----	205
Ultraviolet Synchrotron Orbital Radiation Facility -----	205
Computer Center -----	207

SPECIAL RESEARCH PROJECTS -----209

(a) Chemical Reaction Dynamics	
Folding Mechanism of Protein Molecules Studied by Generalized-Ensemble Algorithms -----	209

Development and Applications of Basic Theories for Chemical Reaction Dynamics and Their Control -----	209
The Energy Landscape for Solvent Dynamics in Electron Transfer Reactions: A Minimalist Model -----	209
Constructing Molecular Theory of Chemical Processes in Solution -----	210
Imaging of Chemical Dynamics -----	210
Electronic Structure and Decay Mechanism of Inner-Shell Excited Molecules -----	210
Time-Resolved Spectroscopic Study of Photochemical Dynamics in Condensed Phase -----	210
Production of Optical Knife—Site-Specific Fragmentation Following Core-Level Photoexcitation	211
Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical $\text{CH}_3\text{CO} \rightarrow \text{CH}_3 + \text{CO}$ -----	211
(b) Molecular Photophysics and Science	
(1) Laser Cooling and Trapping of Metastable Helium Atoms -----	212
(2) Laser Spectroscopic Studies of Atoms and Ions in Liquid Helium -----	212
Structures of Reaction Intermediates of Bovine Cytochrome <i>c</i> Oxidase Probed by Time-Resolved Vibrational Spectroscopy -----	212
Laser Raman Beat Detection of Magnetic Resonance -----	212
Structure, Relaxation and Control of Reactive Cluster Studied by Two-Color Laser Spectroscopy	212
SR-Pump and Laser-Probe Experiments for the Photofragmentation Dynamics of Molecules -----	214
Electronic Structure and Optical Properties of III-V Nitrides -----	215
Decay and Dissociation Dynamics of Core Excited Molecules -----	215
(c) Novel Material Science	
Theory of Electronic Phases in Molecular Conductors and Insulators: Electron Correlations and Dimensional Crossovers -----	216
Size-Controlled Synthesis of Colloidal Metal Clusters -----	216
Spectroscopic and Physico-Chemical Studies of Organic Conductors -----	216
Broad-Line Solid State NMR Investigation of Electronic States in Molecular-Based Conductors -----	217
Development of New Organic Conductors and Their Physical Properties -----	217
Construction of a Catalase Active Site by Site Directed Mutagenesis of Myoglobin -----	217
Construction and Characterization of Chiral Molecule-Based Magnets in a Systematic Way -----	218
STM Study on Synchrotron-Radiation Stimulated SiO_2 Desorption on Si (111) Surface -----	218
Design and Construction of UVSOR-BL4A2 Beam Line for Nano-Structure Processing -----	218
Study on RF-Photocathode for Compact X-Ray Sources -----	218
Reductive Activation of Metal-Carbonyl Complexes Derived from Carbon Dioxide and Oxidative Activation of Metal-Hydroxy and -Oxo Complexes Derived from Water -----	219
Developments and Researches of New Laser Materials -----	219
New Advanced Organic Materials Based on Novel Heterocyclic Compounds -----	219
Molecular Mechanism of Oxygen Activation by Metalloenzymes -----	220
Generation of Reactive Species via Electron Transfer on Metal Complexes, as Basis of Chemical Energy Conversion Systems -----	220
Design and Synthesis of New Tellurium-Containing Donors -----	220
Ball on Disk Tribometer -----	220
Investigation of Dynamics on Photo-Excited Solids and Surfaces by Using the Combination of Synchrotron Radiation and Laser -----	221
OKAZAKI CONFERENCES -----	223
JOINT STUDIES PROGRAMS -----	225
(1) Special Projects	
(2) Research Symposia	
(3) Cooperative Research	
(4) Use of Facility	
(5) UVSOR	
FOREIGN SCHOLARS -----	233
AWARDS -----	237
LIST OF PUBLICATIONS -----	239
REVIEW ARTICLES AND TEXTBOOKS -----	255
AUTHOR INDEX -----	257

Abbreviations

IMS: Institute for Molecular Science
GUAS: The Graduate University for Advanced Studies