

CONTENT

IMS 2002	iii
CONTENT	v
ORGANIZATION AND STAFF	1
COUNCIL	13
BUILDINGS AND CAMPUS	15
RESEARCH ACTIVITIES I	17

Department of Theoretical Studies

I-A Theoretical Study and Design of New Bonding, Structures, and Reactions	17
I-A-1 A Silicon-Silicon Triple Bond Surrounded by Bulky Terphenyl Groups	17
I-A-2 The Quest of Stable Silanones: Substituent Effects	17
I-A-3 Substituent Effects on Germanium-Germanium and Tin-Tin Triple Bonds	17
I-A-4 Theoretical Study of an Isolable Compound with a Short Silicon-Silicon Triple Bond; (<i>t</i> Bu ₃ Si) ₂ MeSiSi≡SiSiMe(Si <i>t</i> Bu ₃) ₂	17
I-A-5 Interesting Compounds Featuring Double Bonding between Heavier Group 15 Elements	17
I-A-6 The First Halogen-Substituted Cyclotrigermenes: A Unique Halogen Walk over the Three-Membered Skeleton and Facial Stereoselectivity in the Diels-Alder Reaction	18
I-A-7 Effects of the σ* Orbital of C-Apical O-Equatorial Spirophosphoranes on the Structure, Stereomutation, and Reactivity	18
I-A-8 Theoretical Calculations of Vibrational Modes in Endohedral Metallofullerenes: La@C ₈₂ and Sc ₂ @C ₈₄	18
I-A-9 A Stable Unconventional Structure of Sc ₂ @C ₆₆ Found by Density Functional Calculations	18
I-A-10 Theoretical Study of the Cations and Anions of La ₂ @C ₈₀ and Sc ₃ N@C ₈₀	18
I-A-11 Theoretical Identification of the Structures of C ₂₀ : Prevalence of the Monocyclic Isomer and Existences of the Smallest Fullerene and Bowl Isomers	18
I-A-12 The Size of Silicon Clusters Suitable for Endohedral Metal-Doping	19
I-A-13 What is the Smallest Metal-Encapsulated Germanium Clusters?	19
I-A-14 Host-Guest Interaction in Molecular Capsule Formation	19
I-A-15 Does the Axial Ligand of Iron (IV)-Oxo-Porphyrin Affect the Reactivity of Cytochrome P450?	19
I-A-16 A Nonspectroscopic Method to Determine the Photolytic Decomposition Pathways of 3-Chloro-3-Alkyldiazirine; Carbene, Diazo and Rearrangement in Excited State	19
I-A-17 Prediction of Molecular Crystal Structures by an Ab Initio Pair Potential Method	19
I-B Prediction of Protein Tertiary Structures from the First Principles	21
I-B-1 Replica-Exchange Monte Carlo Simulation of a Small Peptide in Aqueous Solution Based on the RISM Theory	21
I-B-2 Comparison of AMBER, CHARMM, OPLS, and GROMOS Force Fields by Generalized-Ensemble Simulations	21
I-C Development of Simulation Algorithms for Complex Systems	21
I-C-1 An Application of the Multicanonical Monte Carlo Method to the Bulk Water System	21
I-D Applications of the Zhu-Nakamura Theory to Electronically Nonadiabatic Chemical Reactions	23
I-D-1 Significant Improvement of the Trajectory Surface Hopping Method by the Zhu-Nakamura Theory	23
I-D-2 New Implementation of the Trajectory Surface Hopping Method with Use of the Zhu-Nakamura Theory. II. Application to the Charge Transfer Processes in the 3D DH ₂ ⁺ System	23
I-D-3 Elucidations of Nonadiabatic Tunneling Type and Conical Intersection Type Reactions with Use of the Zhu-Nakamura Theory	23
I-E Theory of Nonadiabatic Transitions	23
I-E-1 Nonadiabatic Transition: Concepts, Basic Theories and Applications	23
I-E-2 Semiclassical Theory of Nonadiabatic Transition and Tunneling	24
I-E-3 Analytical Solutions to Wave Packet Dynamics in a Laser Field	24
I-F Quantum Dynamics of Chemical Reactions	24
I-F-1 Accurate Quantum Dynamics of Electronically Nonadiabatic Chemical Reaction in the DH ₂ ⁺ System	24

I-F-2	Chemical Reactions in the $O(^1D) + HCl$ System I. Ab Initio Global Potential Energy Surfaces for the $1^1A'$, $2^1A'$, and $1^1A''$ States	24
I-F-3	Chemical Reactions in the $O(^1D) + HCl$ System II. Dynamics on the Ground $1^1A'$ State and Contributions of the Excited ($1^1A''$ and $2^1A'$) States	25
I-F-4	Chemical Reactions in the $O(^1D) + HCl$ System III. Quantum Dynamics on the Excited ($1^1A''$ and $2^1A'$) Potential Energy Surfaces	25
I-F-5	Use of Diabatic Basis in the Adiabatic-by-Sector R-Matrix Propagation Method in Time-Independent Reactive Scattering Calculations	25
I-G	Laser Control of Molecular Processes	25
I-G-1	Control of Photodissociation Branching Using the Complete Reflection Phenomenon: Application to HI Molecule	25
I-G-2	Control of Molecular Processes by a Sequence of Linearly Chirped Pulses	25
I-G-3	Selective Excitation among Closely Lying Multi-Levels	26
I-G-4	Photodissociation of H_2^+ and HD^+ in an Intense Laser Field	26
I-H	Theory of Multi-Dimensional Tunneling	26
I-H-1	Practical Implementation of the Instanton Theory for the Ground-State Tunneling Splitting	26
I-H-2	Instanton Theory for Multi-Dimension Decay through Tunneling	26
I-I	New Methods for Scattering Calculations	27
I-I-1	Regularization of Scattering Calculations at R-Matrix Poles	27
I-I-2	Calculation of Resonances <i>via</i> the R-Matrix Method	27
I-J	Theoretical Studies of Dissociative Attachment and Dissociative Recombination	27
I-J-1	Study of Dissociative Electron Attachment to HI Molecule by Using R-Matrix Representation for Green's Function	27
I-J-2	Analytical Treatment of the K-Matrix Integral Equation in the Dynamics of Superexcited Molecules	27
I-K	Theoretical Studies of Ultrafast Nonlinear Optical Spectroscopy of Molecules in Condensed Phases	29
I-K-1	Probing a Colored-Noise Induced Peak of a Strongly Damped Brownian System by One- and Two-Dimensional Spectroscopy	29
I-K-2	Vibrational Spectroscopy of a Harmonic Oscillator System Nonlinearly Coupled to a Heat Bath	29
I-K-3	Two-Dimensional Raman and Infrared Vibrational Spectroscopy for a Harmonic Oscillator System Nonlinearly Coupled with a Colored Noise Bath	29
I-K-4	Two-Time Correlation Function of a Two-Dimensional Quantal Rotator in a Colored Noise	29
I-K-5	Energy-Level Diagrams and Their Contribution to Two-Dimensional Spectroscopic Signal: Distinction between Relaxation Mechanisms by Two-Dimensional Spectroscopy	30
I-K-6	Two-Dimensional Spectroscopy for a Two-Dimensional Rotator Coupled to a Gaussian-Markoffian Noise Bath	30
I-K-7	Absorption Spectra for Two-Dimensional Rotator with Nonlinear System-Bath Coupling	30
I-L	The Condensed Phase Quantum Dynamics of Molecules and Atoms	31
I-L-1	The Energy Landscape for Solvent Dynamics in Electron Transfer Reactions: A Minimalist Model	31
I-L-2	A Quantum Master Equation with a Langevin Force; a Realization of a Real-Time Quantum Monte-Carlo Simulation in a Dissipative Environment	31
I-M	Theoretical Studies of Correlated Electron Systems	31
I-M-1	Biorthogonal Approach for Explicitly Correlated Calculations Using the Transcorrelated Hamiltonian	31
I-M-2	Application of the Transcorrelated Hamiltonian to the Linearized Coupled Cluster Singles and Doubles Model	31
I-N	Electronic Properties of Nanostructured Materials	33
I-N-1	Carbon Foam: Spanning the Phase Space between Graphite and Diamond	33
I-N-2	Electronic Structure of Ba_4C_{60} and Cs_4C_{60}	33
I-N-3	Geometric and Electronic Structure of New Carbon-Network Materials: Nanotube Array on Graphite Sheet	33
I-N-4	First Principles Study of H_2 and CH_4 Physisorption on Carbon Nanotubes	33
I-O	Simulation and Dynamics of Chemical Systems	34
I-O-1	Quasi-Degenerate Perturbation Theory with General Multiconfiguration Self-Consistent Field Reference Functions	34
I-O-2	A Highly Efficient Algorithm for Electron Repulsion Integrals over Relativistic Four-Component Gaussian-Type Spinors	34
I-O-3	Accurate Relativistic Gaussian Basis Sets Determined by the Third-Order Douglas-Kroll Approximation with a Finite-Nucleus Model	34
I-O-4	A Density Functional Study of van der Waals Interactions	34

I-P Theoretical Studies of Quantum Effects in Chemical Reactions	35
I-P-1 Quantum Scattering Calculations of the $O(^1D) + N_2(X^1\Sigma_g^+) \rightarrow O(^3P) + N_2(X^1\Sigma_g^+)$ Spin-Forbidden Electronic Quenching Collision	35
I-P-2 Translational Energy Dependence of $NO + NO / N_2 + O_2$ Product Branching in the $O(^1D) + N_2O$ Reaction: a Classical Trajectory Study on a New Global Potential Energy Surface for the Lowest $^1A'$ State	35
I-P-3 A CASPT2 Study of the Doublet Potential Energy Surface for the $CH(X^2\Pi) + N_2(X^1\Sigma_g^+)$ Reaction	35
I-Q Electronic Structure of a Molecule in Solution	36
I-Q-1 Equilibrium and Nonequilibrium Solvation Structure of Hexaamineruthenium (II,III) in Aqueous Solution: Ab Initio RISM-SCF Study	36
I-R Solvation Thermodynamics of Protein and Related Molecules	36
I-R-1 Partial Molar Volumes and Compressibilities of Alkali-Halide Ions in Aqueous Solution: Hydration Shell Analysis with an Integral Equation Theory of Molecular Liquids	37
I-S Collective Density Fluctuations in Polar Liquids and Their Response to Ion Dynamics	37
I-S-1 Translational Diffusion and Reorientational Relaxation of Water Analyzed by Site-Site Generalized Langevin Theory	38
I-S-2 Interaction-Site Model Description of the Reorientational Relaxation of Molecular Liquids: Incorporation of the Interaxial Coupling into the Site-Site Generalized Langevin/Mode-Coupling Theory	38
I-S-3 Collective Density Fluctuations and Dynamics of Ions in Water Studied by the Interaction-Site Model of Liquids	38
I-T Developing Theories of Liquids and Liquid Mixtures	38
I-T-1 Buthanol-Water Mixture, Structure of <i>tert</i> -Butyl Alcohol-Water Mixtures Studied by the RISM Theory	39
I-T-2 Improvement of the Reference Interaction Site Model Theory for Calculating the Partial Molar Volume of Amino Acids and Polypeptides	39
I-T-3 Description of a Polar Molecular Liquid in a Disordered Microporous Material with Activating Chemical Groups by a Replica RISM Theory	39
I-T-4 Toward a Molecular Theory for the van der Waals-Maxwell Description of Fluid Phase Transitions	39
I-U Neutral-Ionic, Dimerization and Photoinduced Phase Transitions and Their Dynamics in Mixed-Stack Organic Charge-Transfer Complexes	41
I-U-1 Finite-Temperature Phase Diagram of Mixed-Stack Charge-Transfer Complexes	41
I-U-2 Lattice and Magnetic Instabilities near the Neutral-Ionic Phase Transition of the One-Dimensional Extended Hubbard Model with Alternating Potentials in the Thermodynamic Limit	41
I-U-3 Variation of Excitation Spectra in Mixed-Stack Charge-Transfer Complexes	41
I-U-4 Dynamic Spin Correlations near Neutral-Ionic Phase Transitions	42
I-U-5 Thermodynamics of Neutral-Ionic and Ferroelectric Phase Transitions in the Two-Chain System	42
I-U-6 Domain-Wall Dynamics after Photoexcitations near Neutral-Ionic Phase Transitions	42
I-U-7 Variation Mechanisms of Ground-State and Optical-Excitation Properties in Quasi-One-Dimensional Two-Band Electron Systems	42
I-U-8 Photoinduced Dynamics of Ionicity near the Neutral-Ionic Phase Boundary in a One-Dimensional Extended Peierls-Hubbard Model	42
I-V Self-Doping, Nonlinear Excitations and Photoinduced Transitions between Charge and Lattice Ordered Phases of Metal Complexes	43
I-V-1 Self-Doping Effect on the Mott Transition Accompanied with Three-Fold Charge Ordering in $(DCNQI)_2Cu$	43
I-V-2 Spin Solitons in the Alternate Charge Polarization Background of MMX Chains	43
I-V-3 Photoexcited States and Photoinduced Dynamics in Electronic Phases of MMX-Chain Systems	43
I-V-4 Electromodulation Spectra of Optical Absorption in One-Dimensional Strongly Correlated Systems	43
I-W Dimensional Crossovers in Electronic Phases and Their Excitation Spectra of Quasi-One-Dimensional Organic Conductors	44
I-W-1 Dimensional Crossovers and Phase Transitions in Strongly Correlated Low-Dimensional Electron Systems: Renormalization-Group Study	44
I-W-2 Correlation-Induced Dimensional Crossovers of Charge-Transfer Excitations in Quasi-One-Dimensional Organic Conductors	44

I-X Underlying Gauge Structure and Competing Orders in Underdoped Cuprate Superconductors	44
I-X-1 Signature of the Staggered Flux State around a Superconducting Vortex in Underdoped Cuprates	45
I-X-2 Underlying SU(2) Gauge Structure and Hidden Staggered Flux State in the Lightly Doped Spin Liquid	45
I-X-3 Coexistence of Staggered Flux and Antiferromagnetic States in Superconducting Vortices in the Lightly Doped Mott Insulator	45
RESEARCH ACTIVITIES II	47

Department of Molecular Structure

II-A Development of Near-Field Dynamic Spectroscopy and Application to Mesophase Systems	47
II-A-1 Development of an Ultrafast Near-Field Spectroscopy and Observation of Dynamic Processes in GaAs Crystal	47
II-A-2 Near-Field Autocorrelation Measurements of Femtosecond Light Pulses at a Tip of a 100-nm Apertured Probe by Two-Photon-Induced Photoconductivity	48
II-A-3 Structure and Photophysics of PIC J-Aggregates Studied by Scanning Near-Field Optical Microscopy	48
II-B Laser Cooling and Trapping of Metastable Helium Atoms	50
II-B-1 New Design for Efficient Magneto-Optical Trapping of Metastable Helium Atoms	50
II-C Spectroscopic Studies on Atoms and Ions in Liquid Helium	50
II-C-1 Laser Spectroscopy of Eu Atoms in Liquid ³ He and ⁴ He	50
II-D Electron Transfer Regulation in Tetraheme Cytochromes <i>c</i>	52
II-D-1 Redox-Coupled Conformational Alternations in Cytochrome <i>c</i> ₃ from <i>D. vulgaris</i> Miyazaki F on the Basis of its Reduced Solution Structure	52
II-D-2 A Role of the Aromatic Ring of Tyr43 in Tetraheme Cytochrome <i>c</i> ₃ from <i>Desulfovibrio vulgaris</i> Miyazaki F	52
II-D-3 A Directional Redox-Regulator Based on the Heme-Chain Architecture in the Small Tetraheme Cytochrome <i>c</i> from <i>Shewanella oneidensis</i>	52
II-E Studies on Higher-Order Gaussian Light Beams	54
II-E-1 Simple Generation of Higher-Order Gaussian Beams and the Application to Spectroscopy	54
II-F Ultrafast Dynamics of Surface Adsorbed Species	55
II-F-1 Time-Resolved Study of Formate on Ni(111) by Picosecond SFG Spectroscopy	55
II-F-2 SFG Spectroscopy of CO/Ni(111): UV Pumping and Transient Hot Band Transition of Adsorbed CO	55
II-F-3 Surface Hydroxyl Group and Adsorbed Water on γ -Al ₂ O ₃ Studied by Picosecond Infrared Pump-Probe Experiment	55
II-G Spin Reorientation Transitions of Ultrathin Magnetic Films Induced by Chemisorption	56
II-G-1 Perpendicular Magnetic Anisotropy in Co/Pd(111) Stabilized by Chemisorption of CO and NO	56
II-H Local Structures in Photoinduced States of Molecular-Based Magnetic Materials	57
II-H-1 Photoinduced Phase Transition of RbMnFe(CN) ₆ Studied by X-Ray-Absorption Fine Structure Spectroscopy	57
II-I Molecular and Electronic Structures of Metallofullerenes	58
II-I-1 Spin Dynamics of Lanthanum Metallofullerenes	58
II-I-2 Electronic State of Scandium Trimer Encapsulated in C ₈₂ Cage	58
II-I-3 Efficient Reduction of Metallofullerenes by Solvation of Pyridine and Dimethylformamide	59
II-J High Field and Pulsed Electron Spin Resonance Spectroscopy	59
II-J-1 High-Field/High-Frequency ESR Study of Gadolinium Metallofullerenes	59
II-J-2 A Bindschedler's Green-Based Arylamine: Its Polycations with High-Spin Multiplicity	60
II-K State Correlated Raman Spectroscopy	61
II-K-1 Molecular Ordering Deformation Induced by Externally Applied Electric Field in an Antiferroelectric Liquid Crystal	61

RESEARCH ACTIVITIES III	63
--------------------------------------	-----------

Department of Electronic Structure

III-A Synthesis and Characterization of Exotic Molecule-Based Nano-Clusters with Transition Metals : Behavior as Single Domain Magnets	63
III-A-1 Magnetic Behavior of Crude CoC ₂ Solid Synthesized in Acetonitrile Solution	63
III-A-2 Electron Microscope and EXAFS Study of Matrix Embedded (Co-C ₂) _n Nano-Cluster Magnets	63

III-A-3	Magnetic Behavior of Matrix Embedded (Co-C ₂) _n Nano-Clusters as Single Domain Room-Temperature Magnets	64
III-A-4	Construction of Vacuum Apparatus for Mass-Resolved Spectroscopies of Non-Volatile Solid Samples	64
III-B	States of Neutral and Ionic Molecular Associates in Solutions	65
III-B-1	States of Molecular Associates in Binary Mixtures of Acetic Acid with Protic and Aprotic Polar Solvents: A Raman Spectroscopic Study	65
III-C	Ultrafast Dynamics and Scanning Tunneling Microscopy	66
III-C-1	Construction of an Apparatus for Direct Observation of Reactions Induced by Ultrafast Laser Pulses Using a Low Temperature STM	66
III-C-2	Construction of a Femtosecond Time-Resolved Ionization Detected Spectrometer	66
III-C-3	Picosecond Time-Resolved Raman Studies on the Photochromic Reactions of Diarylethenes	67
III-D	Spectroscopic and Dynamical Studies of Molecular Cluster Ions	67
III-D-1	Intermolecular Interactions in Aniline/Benzene Hetero-Trimer and Aniline Homo-Trimer Ions	68
III-D-2	Infrared Photodissociation Spectroscopy of Protonated Formic Acid-Water Binary Clusters, H ⁺ ·(HCOOH) _n ·H ₂ O (<i>n</i> = 1–5). Spectroscopic Study of Ion Core Switch Model and Magic Number	68
III-D-3	Infrared Photodissociation Spectroscopy of Aniline ⁺ -(Water) _{1,2} and Aniline ⁺ -(Methanol) _{1,2}	68
III-D-4	Intracluster Proton Transfer in Aniline-Amine Complex Ions	68
III-D-5	LIF and IR Dip Spectra of Jet-Cooled <i>p</i> -Aminophenol- <i>M</i> (<i>M</i> = CO, N ₂): Hydrogen-Bonded or van der Waals-Bonded Structure?	68
III-D-6	Structure and Intermolecular Hydrogen Bond of Jet-Cooled <i>p</i> -Aminophenol-(H ₂ O) ₁ Studied by Electronic and IR-Dip Spectroscopy and Density Functional Theory Calculations	69
III-D-7	Positive Charge Distribution in (Benzene) ₁ (toluene) ₂ ⁺ and (Benzene) ₂ (toluene) ₁ ⁺ Studied by Photodissociation Spectroscopy	69
III-D-8	Infrared Photodissociation Spectroscopy of [Aniline-(Water) _n] ⁺ (<i>n</i> = 1–8)	69
III-E	Spectroscopy and Dynamics of Vibrationally Excited Molecules and Clusters	70
III-E-1	Hydrogen Transfer in Photo-Excited Phenol/Ammonia Clusters by UV-IR-UV Ion Dip Spectroscopy and Ab Initio MO Calculations I: Electronic Transitions	72
III-E-2	Hydrogen Transfer in Photo-Excited Phenol/Ammonia Clusters by UV-IR-UV Ion Dip Spectroscopy and Ab Initio MO Calculations II: Vibrational Transitions	72
III-E-3	Picosecond Time-Resolved Infrared Spectra of Photo-Excited Phenol-(NH ₃) ₃ Cluster	72
III-E-4	Picosecond Time-Resolved Nonresonant Ionization Detected IR Spectroscopy on 7-Azaindole Dimer	73
III-E-5	Structure of Hydrogen-Bonded Clusters of 7-Azaindole Studied by IR Dip Spectroscopy and Ab Initio Molecular Orbital Calculation	73
III-E-6	Structures of Carbazole-(H ₂ O) _n (<i>n</i> = 1–3) Clusters Studied by IR Dip Spectroscopy and a Quantum Chemical Calculation	73
III-E-7	Structure of 1-Naphthol/Alcohol Clusters Studied by IR Dip Spectroscopy and Ab Initio Molecular Orbital Calculations	73
III-E-8	Pulsed Field Ionization Zero Kinetic Energy Photoelectron Study on Methylanisole Molecules in a Supersonic Jet	73
III-E-9	The PFI-ZEKE Photoelectron Spectrum of <i>m</i> -Fluorophenol and its Aqueous Complexes: Comparing Intermolecular Vibrations in Rotational Isomers	74
III-E-10	OH- and CH-Stretching Overtone Spectra of Catechol	74
III-F	Ultrafast Molecular Dynamics Studied by Time-Resolved Photoelectron Imaging	75
III-F-1	Ionization Dynamics of NO A (2Σ ⁺) State Studied by Time-Resolved Photoelectron Imaging	75
III-F-2	Theoretical Analysis of Rotational Revivals in Intersystem Crossing in Pyrazine	75
III-F-3	Femtosecond Photoelectron Imaging on Pyridazine: S ₁ Decay Rate and 3s and 3p Rydberg State Energetics	76
III-G	Non-Adiabatic Photodissociation Dynamics of Fundamental Molecules	76
III-G-1	Non-Adiabatic Bending Dissociation of OCS: The Effect of Bending Excitation on the Transition Probability	76
III-G-2	Velocity Map Fragment Imaging on 205 nm Photodissociation of Nitrous Oxide	77
III-H	Development of New Devices for Molecular Dynamics Experiments	77
III-H-1	Three Dimensional Photofragment Imaging Using a Fast Response Imager	77
III-H-2	High Repetition Rate Two Dimensional Imaging Using C-MOS Imager	77
III-H-3	Construction of a Rotating-Source Crossed Beam Apparatus	77

III-I Structure and Properties of Polyoxometalates with a Magnetic, Electronic, or Biological Significance	78
III-I-1 Synthesis and Crystal Structure of a Novel Vanadium-Containing Tungstobismutate(III) $K_{12}[(VO)_3(BiW_9O_{33})_2] \cdot 30H_2O$	78
III-I-2 Crystallization and Structural Characterization of Two Europium Molybdates, $Eu_4Mo_7O_{27}$ and $Eu_6Mo_{10}O_{39}$	78
III-I-3 Nanocluster Crystals of Lacunary Polyoxometalates as Structure-Design-Flexible, Inorganic Nonlinear Materials	78
III-I-4 A Three-Dimensional Inorganic/Organic Hybrid Vanadium Oxide Complex with Pentacoordinate Co^{II} , $[CoV_2O_6(4,4'-bipy)]$	78
III-I-5 $Tb_2Mo_4O_{15}$	79
III-I-6 H_2O_2 -Based Epoxidation of Bridged Cyclic Alkenes with $[P\{Ti(O_2)\}_2W_{10}O_{38}]^{7-}$ in Monophasic Systems: Active Site and Kinetics	79
III-I-7 Photochemical Formation of a Lacunary Tire-Shaped Anion, $[Mo_{142}O_{432}H_{26}(H_2O)_{58}]^{14-}$, through Degradative Self-Assembly of $[Mo_{36}O_{112}(H_2O)_{16}]^{8-}$: Topology of Ring-Structural Molybdenum Blues	79
III-I-8 Size-Dependent Population of Trivalent Rare Earth Cations (RE^{3+}) in $[(RE)_2(H_2O)_2(SbW_9O_{33})(W_5O_{18})_2]^{15-}$, and Structural Characterization of a Lutetium-Polyoxotungstate Complex $[Lu_3(H_2O)_4(SbW_9O_{33})_2(W_5O_{18})_2]^{21-}$	79
III-I-9 $Gd_4Mo_7O_{27}$, a Novel Phase in the Gd_2O_3 - MoO_3 System	79
III-I-10 Time-Resolved ESR-Spectroscopic Investigation of Polyoxometalate Photochemistry	79
III-J Electronic Spectroscopy and Excited-State Dynamics of Aromatics Clusters	81
III-J-1 S_1 - S_0 Vibronic Spectrum of the Benzene Tetramer	81
III-J-2 S_1 - S_0 Vibronic Spectrum of the Benzene Trimer	81
III-K Electronic Spectroscopy of Molecules in Pendular States	81
III-K-1 Construction of an Apparatus for Measurements of Fluorescence Excitation Spectra in a Strong DC Electric Field	82
III-K-2 Laser-Induced Fluorescence Spectra of Pendular-State Aromatics in a Strong DC Electric Field	82
III-L Wave Packet Engineering Using a Phase-Programmable Femtosecond Optical Source	83
III-L-1 Single Molecular Phase-to-Amplitude Converter	83

RESEARCH ACTIVITIES IV -----85

Department of Molecular Assemblies

IV-A Spectroscopic Study of Charge Carriers in Organic Conductors	85
IV-A-1 Raman Study of the Charge Ordering in α -(BEDT-TTF) $_2I_3$ at High Pressure	85
IV-A-2 Raman Study of the Charge Ordering in α' -(BEDT-TTF) $_2IBr_2$ at High Pressure	86
IV-A-3 Charge Ordering in θ -(BEDT-TTF) $_2TIM(SCN)_4$ ($M = Co$ and Zn) Studied by Vibrational Spectroscopy	86
IV-A-4 High-Pressure Raman Study on a 1/3-Filled System (BEDT-TTF) $_3CuBr_4$	87
IV-A-5 Infrared and Raman Studies of the Charge Ordering in the Organic Semiconductor κ - $[(Et)_4N](ET)_4Co(CN)_6 \cdot 3H_2O$	87
IV-A-6 Charge-Ordering and Magnetic Phase Transitions in θ -(BDT-TTP) $_2Cu(NCS)_2$	87
IV-A-7 Spectroscopic Studies of Charge-Ordering System in Organic Conductors	88
IV-A-8 Charge and Molecular Arrangement in (DI-DCNQI) $_2Ag$ Studied by Vibrational Spectra	88
IV-A-9 Charge Distribution and Molecular Arrangement in the Pressure-Induced Metallic Phase of (DI-DCNQI) $_2Ag$	89
IV-A-10 Study of the Phase Transitions of (DI-DCNQI) $_2M$ ($M = Ag, Li, Cu$) through the Analysis of the Temperature Dependent Vibronic and Vibrational Infrared Absorptions	89
IV-A-11 Development of a High-Pressure Cell for Raman Measurement Using Sapphire Anvil	90
IV-A-12 Optical Study of Two-Dimensional Organic Metal (EO-TTP) $_2AsF_6$ (EO-TTP=2-(4,5-ethylenedioxy-1,3-dithiol-2-ylidene)-5-(1,3-dithiol-2-ylidene)-1,3,4,6-tetrathiapentalene)	90
IV-B Microscopic Investigation of Molecular-Based Conductors	91
IV-B-1 EPR Investigation of the Electronic States in β' -type $[Pd(dmit)_2]_2$ Compounds (where dmit is the 1,3-dithia-2-thione-4,5-dithiolato)	91
IV-B-2 NMR Study of Charge Localized States of (TMTTF) $_2Br$	91
IV-B-3 Magnetic Investigation of Possible Quasi-One-Dimensional Two-Leg Ladder Systems, (BDTFP) $_2X(PhCl)_{0.5}$ ($X = PF_6, AsF_6$)	92
IV-B-4 Microscopic Investigation of a New Two-Component Organic Conductor with Itinerant and Localized Spins: (CHTM-TTP) $_2TCNQ$	92
IV-B-5 ESR Study of the Charge Ordering States in (TMTTF) $_2X$	93

IV-C Magnetic Organic Superconductors and Related Systems	94
IV-C-1 An Indication of Magnetic-Field-Induced Superconductivity in a Bi-Functional Layered Organic Conductor, κ -(BETS) ₂ FeBr ₄	94
IV-C-2 Dual-Action Molecular Superconductors with Magnetic Anions	94
IV-C-3 A Series of Organic Conductors κ -(BETS) ₂ FeBr _x Cl _{4-x} (0 ≤ x ≤ 4) Exhibiting Successive Antiferromagnetic and Superconducting Transitions	95
IV-C-4 Magnetic Molecular Conductors Based on BETS Molecules and Divalent Magnetic Anions [BETS = Bis(ethylenedithio)tetraselenafulvalene]	95
IV-C-5 Crystal Structure of BETS ²⁺ Dication Salt (BETS)TlCl ₅ and Formal Charge Dependence of Bond Lengths of BETS ^{+Q} (Q = 0–2)	96
IV-C-6 Charge-Transfer Salt of [C ₁₂ H ₈ S ₄ Se ₄ Cl ₂]FeCl ₄ ·C ₆ H ₅ Cl	96
IV-C-7 A New Charge-Transfer Salt of (BETS) ₄ Fe ₂ (C ₂ O ₄) ₅	97
IV-D Development of New Conducting Molecular Materials	97
IV-D-1 Development of Conducting Crystals Based on Single-Component Transition Metal Complex Molecules with Extended-TTF Ligands	97
IV-D-2 A Conducting Crystal Based on a Single-Component Paramagnetic Molecule [Cu(dmdt) ₂] (dmdt = dimethyltetraathiafulvalenedithiolate)	98
IV-D-3 Novel π -Electron Donors for Magnetic Conductors Containing a PROXYL Radical	98
IV-D-4 Novel TTP Donors Containing a PROXYL Radical for Magnetic Molecular Conductors	99
IV-D-5 Synthesis and Physical Properties of New Molecular Conductors Based on Lanthanoid Nitrate Complex Anions	99
IV-E Control of Intermolecular Interactions with Chemical and Physical Methods	100
IV-E-1 Unique Structural and Physical Properties of Ni(dmit) ₂ Anion Radical Salts Characterized by Short Te...S Contacts, where dmit = 1,3-dithiole-2-thione-4,5-dithiolate	100
IV-E-2 Uniaxial Strain Effect in the Two-Dimensional Strongly Correlated System, β^{\prime} -(CH ₃) ₄ As[Pd(dmit) ₂] ₂ (dmit = 1,3-dithiol-2-thione-4,5-dithiolate)	100
IV-F Synthetic Approach Toward Single Molecular Transistors	102
IV-F-1 Synthesis of Novel Ruthenium Complexes Optimized for Molecular Single Electron Transistor	102
IV-F-2 Preparation of Porphyrin Wires Optimized for Molecular Field Effect Transistors	102
IV-F-3 Synthesis of Octopus Shaped Self Standing Molecular Jacks	102

RESEARCH ACTIVITIES V -----103

Department of Applied Molecular Science

V-A Synthesis of Chiral Molecule-Based Magnets	103
V-A-1 Structure and Magnetic Properties of a Chiral Two-dimensional Ferrimagnet with T_C of 38 K	103
V-B Hydrothermal Synthesis of Molecule-Based Magnets	104
V-B-1 Self-Organized Metallo-Helicates and -Ladder with 2,2'-Biphenyldicarboxylate (C ₁₄ H ₈ O ₄) ²⁻ : Synthesis, Crystal Structures, and Magnetic Properties	104
V-C Synthesis and Characterization of Quantum-Spin Systems	104
V-C-1 Magnetic Properties of Organic Two-Leg Spin Ladder Systems with $S = 1/2$ and $S = 1$	104
V-C-2 Low Dimensionality Observed by ESR Measurements in $S = 1$ Spin Ladder Substance BIP-TENO	105
V-D Organic Ferrimagnetism	105
V-D-1 Magnetic Properties on an Organic Ferrimagnetic Compound and Related Materials	105
V-E Pressure Effects on Molecular Magnetism	106
V-E-1 Pressure Effects on Molecular Magnets of Mn Complexes with Bisaminoxylbenzene Derivatives	106
V-E-2 Pressure-Induced Metamagnetic Behavior in a Quasi-One-Dimensional Molecule-Based Ferrimagnet	106
V-F Bioinorganic Studies on Structures and Functions of Non-Heme Metalloenzymes Using Model Complexes	107
V-F-1 Novel Phosphate Bond Formation in a Cobalt(III) Complex System	107
V-F-2 Syntheses and Structures of Tetrakis(1-methyluracilato)palladium Complexes Capturing Alkali Metal Ions. A New Type of Metallo-Podand	107
V-F-3 Investigations of the Effects of Intramolecular Hydrogen Bonding Networks on Tripodal Trihydroxamate-Type Artificial Siderophores	107
V-F-4 The Role of the Zn(II) Site in Cu,Zn SOD (1). Synthesis and Characterization of Novel Hydroperoxo-Zinc(II) Intermediates	108
V-F-5 Epoxidation Activities of Mononuclear Ruthenium-oxo Complexes with a Square Planar 6,6'-Bis(benzoylamino)-2,2'-bipyridine and Axial Ligands	108
V-F-6 Reactivity of Hydroperoxide Bound to a Mononuclear Non-Heme Iron Site	108

V-F-7	Reactivity Control for Epoxidation of Olefins and Dehydrogenation of Alcohols Catalyzed by Ruthenium-oxo Complexes	108
V-F-8	Crystal Structure and Solution Behavior of the Iron(III) Complex of the Artificial Trihydroxamate Siderophore with Tris(3-aminopropyl)amine Backbone	109
V-F-9	Reverse Reactivity in Hydroxylation of Adamantane and Epoxidation of Cyclohexene Catalyzed by the Mononuclear Ruthenium-oxo Complexes with 6-Substituted Tripodal Polypyridine Ligands	109
V-F-10	Characterization of an NH- π Interaction in Co(III) Ternary Complexes with Aromatic Amino Acids	109
V-F-11	The Role of the Zn(II) Site in Cu,Zn SOD. (2) Evidence of Superoxide Disproportionation Catalyzed by Sterically- and Electrostatically-Controlled Zinc(II) Complexes	110
V-F-12	SOD Activities of the Copper Complexes with Tripodal Polypyridylamine Ligands Having a Hydrogen Bonding Site	110
V-F-13	Site-Selective Recognition of Amino Acids by Co(III) Complexes Containing a (N)(O) ₃ -Type Tripodal Tetradentate Ligand	110
V-G	Probing Time-Dependent Processes in Solution with Time-Resolved Spectroscopic Methods	111
V-G-1	Femtosecond Time-Resolved Anisotropy Measurement of Biphenyl Fluorescence	111
V-G-2	Effect of Pump and Probe Light Field on Picosecond Time-Resolved Resonance Raman Spectra of <i>S</i> ₁ <i>trans</i> -Stilbene. Disagreement between Stokes- and Anti-Stokes Scattering Frequencies	111
V-G-3	Photoinduced Cl Transfer Reaction between Biphenyl and Carbon Tetrachloride Studied by Nanosecond Time-Resolved Infrared Spectroscopy and Picosecond Time-Resolved Fluorescence Spectroscopy	112
V-G-4	Analysis of the Solvent- and Temperature-Dependent Raman Spectral Changes of <i>S</i> ₁ <i>trans</i> -Stilbene and the Mechanism of the <i>Trans</i> to <i>Cis</i> Isomerization: Dynamic Polarization Model of Vibrational Dephasing and the C=C Double-Bond Rotation	112
V-G-5	Picosecond Dynamics of Stepwise Double Proton-Transfer Reaction in the Excited State of the 2-Aminopyridine/Acetic Acid System	113
V-H	Structures and Properties of Lanthanoid-Metallofullerenes	114
V-H-1	Spectroscopic Studies of Endohedral Metallofullerenes	114
V-H-2	Structural Study of Three Isomers of Tm@C ₈₂ by ¹³ C NMR Spectroscopy	114
V-I	Development of Organic Superconductors	114
V-I-1	New Organic Superconductors Consisting of an Unprecedented π -Electron Donor	114
V-I-2	Tetrachloroferrate (III) Salts of BDH-TTP and BDA-TTP: Crystal Structures and Physical Properties	115
V-J	Stereodynamics of Crossed Beam Reactions	116
V-J-1	Stereo-Selectivity in the Penning Ionization Reaction of CH ₃ X (X = Cl, Br, I) + Ar(³ P) \rightarrow CH ₃ X ⁺ + Ar + e ⁻	116
V-J-2	Evidence for the HCl ⁺ (A) Formation in the Reaction of Ne(³ P) with the Size-Selected HCl Dimer Using an Electrostatic Hexapole Field	116
V-K	Photodissociation Dynamics	116
V-K-1	Photodissociation of DCI Dimer Selected by an Electrostatic Hexapole Field Combined with Doppler-Selected TOF Technique: Observation of [CIDCI] Transient Species	117
V-K-2	A New Channel of Hydrogen Elimination in the 121.6-nm Photodissociation of Formic Acid Detected by a Doppler-Selected TOF Mass Spectrometry	117
V-L	Non-Destructive Structure Determination of Neural Clusters	117
V-L-1	Focusing and Selecting the Linear Type HBr-N ₂ O by Using a 2 m Long Electrostatic Hexapole Field	117
V-M	Reaction Dynamics at Surfaces	118
V-M-1	Hydrogen-Exchange Reactions <i>via</i> Hot Hydrogen Atoms Produced in the Dissociation Process of Molecular Hydrogen on Ir{100}	118
V-N	Simulation of Molecular Clusters	119
V-N-1	Characterization of Gel Using Modeled Radical Polymerization with Cross Linkers Performed by Monte Carlo Method	119
V-N-2	Analysis of Intra- and Inter-Linkers in Gels by Brownian Dynamics Simulation	119
V-N-3	Self-Assembly of Amphiphiles into Vesicles: a Brownian Dynamics Simulation	119
V-N-4	Fusion Pathways of Vesicles, a Brownian Dynamics Simulation	119
V-N-5	Adhesion of Nanoparticles to Vesicles: a Brownian Dynamics Simulation	119
V-N-6	Structural Changes of Pulled Vesicles: a Brownian Dynamics Simulation	119
V-O	Development of Broadband Solid-State NMR Spectroscopy	121
V-O-1	Numerical Simulations and Experiments on the Transmission Line Probe	121
V-O-2	Developments of Fast Digital RF Frequency Modulator	122

RESEARCH ACTIVITIES VI -----123**Department of Vacuum UV PhotoScience**

VI-A Electronic Structure and Decay Mechanism of Inner-Shell Excited Molecules -----	123
VI-A-1 Spin-Forbidden Shake-Up States in the Valence Ionization of CS ₂ -----	123
VI-A-2 Spin- and Symmetry Forbidden Ionized States of OCS Molecule -----	123
VI-A-3 Measurements of Sulfur 2 <i>p</i> Photoelectron and Sulfur L-emission of SF ₆ at Sulfur 2 <i>p</i> Resonances -----	124
VI-A-4 N 1 <i>s</i> Photoabsorption of N ₂ Trapped in Rare Gas Matrices -----	124
VI-A-5 Ab Initio CI Calculation for O1 <i>s</i> → σ* Core-Excited States of Ozone: Difference in Direction between Transition Dipole Moment and Photodissociation -----	125
VI-B Soft X-Ray Photoelectron-Photoabsorption Spectroscopy and Electronic Structure of Transition Metal Compounds -----	126
VI-B-1 B 1 <i>s</i> - and La 4 <i>d</i> -Edge Photoabsorption and Resonant Photoelectron Spectroscopy of Rare-Earth Borocarbide LaB ₂ C ₂ -----	126
VI-C Observation of Vibrational Coherence (Wavepacket Motion) in Solution-Phase Molecules Using Ultrashort Pulses -----	127
VI-C-1 Excited-State Vibrational Coherence of Solution-Phase Molecules Observed in the Third-Order Optical Process Using Extremely Short Pulses -----	127
VI-D Studies of Primary Photochemical/Physical Processes Using Femtosecond Electronic Spectroscopy -----	127
VI-D-1 Femtosecond/Picosecond Time-Resolved Spectroscopy of Trans-Azobenzene: Isomerization Mechanism Following S ₂ (ππ*) ← S ₀ Photoexcitation -----	128
VI-D-2 Ultrafast Fluorescence of the Chromophore of the Green Fluorescent Protein in Alcohol Solutions -----	128
VI-D-3 Femtosecond Study of Solvation Dynamics of DCM in Micelles -----	128
VI-E Studies of Photochemical Reactions Using Picosecond Time-Resolved Vibrational Spectroscopy -----	129
VI-E-1 Picosecond Time-Resolved Raman Study of the Solvated Electron in Water -----	129
VI-E-2 Observation of Resonance Hyper-Raman Scattering from all-trans-Retinal -----	129
VI-F Synchrotron Radiation Stimulated Surface Reaction and Nanoscience -----	131
VI-F-1 Patterning SiO ₂ Thin Films Using Synchrotron Radiation Stimulated Etching with a Co Contact Mask -----	131
VI-G Noble Semiconductor Surface Vibration Spectroscopy -----	131
VI-G-1 Infrared Reflection Absorption Spectroscopy Using CoSi ₂ Buried Metal Layer Substrate Made by Wafer-Bonding -----	132
VI-G-2 Hydrogen Diffusion and Chemical Reactivity with Water on Nearly Ideally H-Terminated Si(100) Surface -----	132
VI-G-3 Atomic Hydrogen-Induced Oxidation on Water-Adsorbed Si(100)-(2×1) Surfaces -----	132
VI-H Integration of Bio-Functional Materials on Silicon -----	133
VI-H-1 Hydrophobic/Hydrophilic Interactions of Cytochrome <i>c</i> with Functionalized Self-Assembled Monolayers on Silicon -----	133
VI-H-2 Influence of Substrate Roughness on the Formation of Self-Assembled Monolayers (SAM) on Silicon(100) -----	134
VI-I Photoionization and Photodissociation Dynamics Studied by Electron and Fluorescence Spectroscopy -----	135
VI-I-1 Formation and Autoionization of a Dipole-Forbidden Superexcited State of CS ₂ -----	135
VI-I-2 Autoionization and Neutral Dissociation of Superexcited HI Studied by Two-Dimensional Photoelectron Spectroscopy -----	135
VI-I-3 Development of the Apparatus for High-Resolution Dispersed Spectroscopy and Fluorescence Excitation Spectroscopy at BL3A2 -----	135
VI-I-4 UV and Visible Dispersed Spectroscopy for the Photofragments Produced from H ₂ O in the Extreme Ultraviolet -----	136
VI-J Vacuum UV Spectroscopy Making Use of a Combination of Synchrotron Radiation and a Mode-Locked or Pulsed UV Laser -----	137
VI-J-1 Partial Photoionization Cross Sections for N ₂ ⁺ (X ² Σ _g ⁺ , ν _X = 0, 1) Measured by a Laser Synchrotron Radiation Combination Technique -----	137
VI-K Extreme UV Photoionization Studies by Employing a Dragon-Type Grazing-Incidence Monochromator -----	138
VI-K-1 Anisotropy of Fragment Ions from SF ₆ by Photoexcitation of a Valence- or Sulfur 2 <i>p</i> - Electron between 23 and 210 eV -----	138
VI-K-2 Construction of the Photoionization Spectrometer for Fullerenes and Metallofullerenes --	139
VI-K-3 Photoion Yield Spectra of C ₆₀ in the Region of 23–210 eV -----	139

RESEARCH ACTIVITIES VII -----141

Coordination Chemistry Laboratories

VII-A Development of Novel Transition Metal Complex Catalysts Having MOP Ligands -----	141
VII-A-1 Asymmetric Hydrosilylation of Styrenes Catalyzed by Palladium-MOP Complexes: Ligand Modification and Mechanistic Studies -----	141
VII-A-2 Modification of Chiral Monodentate Phosphine Ligands (MOP) for Palladium-Catalyzed Asymmetric Hydrosilylation of Cyclic 1,3-Dienes -----	141
VII-A-3 (<i>R</i>)-2-Diphenylphosphino-2'-methoxy-1,1'-binaphthyl -----	141
VII-B Green and Risk-Free Catalysis -----	142
VII-B-1 Amphiphilic Resin-Supported Rhodium-Phosphine Catalysts for C-C Bond Forming Reactions in Water -----	142
VII-B-2 Double Carbonylation of Aryl Iodides with Primary Amines under Atmospheric Pressure Conditions Using Pd/PPh ₃ /DABCO/THF System -----	142
VII-C Electrochemical Analysis of Biological Functions of Metalloproteins and their Mutated Molecules and its Applications to Coordination Chemistry for Catalysis -----	143
VII-C-1 Effects of Alkyl Chain as a Spacer on Electrochemical Reaction and SEIRA Spectra for Self-Assembled Monolayer Having Anthraquinone Redox Center -----	143
VII-C-2 Analysis of Biological Functions of Metalloproteins Using Biocompatible Modified Electrodes -----	143
VII-C-3 Interfacial Structures of Self-Assembled Monolayers of 2-Pyridinethiol on Au(111) Studied by In Situ Tunneling Microscopy -----	143
VII-C-4 NADP ⁺ Sensor on <i>Chrorella</i> Ferredoxin/Ferredoxin-NADP ⁺ -Reductase Modified Indium Oxides -----	143
VII-C-5 Surface pK _a of Amine-Terminated Self-Assembled Monolayers Evaluated by Direct Observation of Counter Anion by FT-Surface Enhanced Raman Spectroscopy -----	144
VII-C-6 Ion Selectivity for Electrode Reactions on Functionalized Monolayer Modified Electrode -----	144
VII-C-7 In-Situ STM Observation of Coronene Epitaxial Adlayers on Au(111) Surfaces Prepared by the Transfer of Langmuir Films -----	144
VII-C-8 New Route to Protoporphyrins III and XIII from Common Starting Pyrroles -----	144
VII-D Nano-Sciences of Advanced Metal Complexes -----	145
VII-D-1 Tuning of Electronic Structures of Quasi-One-Dimensional Bromo-Bridged Ni(III) Complexes with Strong Electron-Correlation by Doping of Co(III) Ions, [Ni _{1-x} Co _x (chxn) ₂ Br]Br ₂ -----	145
VII-D-2 Angle-Resolved Photoemission Study of the MX-Chain Compound [Ni(chxn) ₂ Br]Br ₂ : Spin-Charge Separation in Hybridized <i>d-p</i> Chains -----	145
VII-D-3 ESR Detection of Induced Spin Moments in Halogen-Bridged Mixed-Metal Complexes Ni _{1-x} Pd _x (chxn) ₂ Br ₃ -----	146
VII-D-4 A Chemical Modification of a Mn ₁₂ Single-Molecule Magnet by Replacing Carboxylate Anions with Diphenylphosphate Anions -----	146
VII-D-5 Construction of a One-Dimensional Chain Composed of Mn ₆ Clusters and 4,4'-Bipyridine Linker: The First Step for Creation of "Nano-Dots-Wires" -----	147
VII-D-6 Framework Engineering by Anions and Porous Functionalities Cu(II)/4,4'-bpy Coordination Polymers -----	147
VII-D-7 New Microporous Coordination Polymer Affording Guest-Coordination Sites at Channel Walls -----	147
VII-E Large Macrocyclic Formation Assisted by Coordination Bonds -----	148
VII-E-1 Solution and Solid-State Characterization of a Dicationic Receptor for Large Substrates --	148
VII-F Development of New Carbonylation Reactions -----	149
VII-F-1 Ru ₃ (CO) ₁₂ -Catalyzed Coupling Reaction of <i>sp</i> ³ C-H Bonds Adjacent to a Nitrogen Atom in Alkylamines with Alkenes -----	149
VII-F-2 Catalytic Carbonylation Reactions of Benzyne Derivatives -----	149
VII-G Development of Cycloisomerization Reactions -----	149
VII-G-1 Cycloisomerization of ω-Aryl-1-Alkynes: GaCl ₃ as a Highly Electrophilic Catalyst for Alkyne Activation -----	149
VII-H Multi-Electron Reduction of Carbon Dioxide through Metal-Carbonyl and Oxidative Activation of Water via Metal-Oxo Complexes -----	151
VII-H-1 Syntheses of New Ruthenium Carbonyl Terpyridine <i>o</i> -Phenylene Complexes: Strong Interaction between Carbonyl and <i>o</i> -Phenylene Ligands -----	151
VII-H-2 Synthesis and Redox Properties of Bis(ruthenium-hydroxo)complexes with Quinone and Bipyridine Ligand as a Water-Oxidation Catalysts -----	151
VII-H-3 Ruthenium Terpyridine Complexes with Mono- and Bi-Dentate Dithiolene Ligands -----	152

VII-H-4 A Ru-Carbene Complex with a Metallacycle Involving a 1,8-Naphthylidene Framework	152
VII-H-5 Ruthenium Oxyl Radical Complex Containing <i>o</i> -Quinone Ligand Detected by ESR Measurements of Spin Trapping Technique	152
VII-H-6 Multi-Electron Reduction of CO ₂ via Ru-CO ₂ -C(O)OH, -CO, -CHO, and -CH ₂ OH Species	153
VII-I Silanechalcogenolato Complexes	154
VII-I-1 Palladium Dimethylsilanedithiolato Complex: a Precursor for Ti-Pd and Ti-Pd ₂ Heterometallic Complexes	154
VII-I-2 Synthesis and Reactions of Triphenylsilanethiolato Complexes of Manganese(II), Iron(II), Cobalt(II), and Nickel(II)	154
VII-J Coordination Chemistry of New Multidentate Ligands and Activation of Small Molecules ---	155
VII-J-1 Binuclear Iron(II) Complex from a Linked-bis(amidinate) Ligand: Synthesis and its Reaction with Carbon Monoxide	155
VII-J-2 Synthesis and Structures of Ti(III) and Ti(IV) Complexes Supported by a Tridentate Aryloxy Ligand	155
VII-J-3 Dinitrogen-Bond Cleavage in a Niobium Complex Supported by a Tridentate Aryloxy Ligand	155
VII-K Synthesis of Compounds Having a Novel Bonding Containing Heavier Main Group Elements	156
VII-K-1 Syntheses and Crystal Structures of the First Disulfur and Diselenium Complexes of Platinum	156
VII-K-2 Synthesis and Structure of the First Stable Phosphabismuthene	156
VII-K-3 Synthesis of Kineically Stabilized Silaneselone and Silanetellone	157
VII-K-4 The First Stable 9-Silaanthracene	157
VII-K-5 Synthesis and Characterization of an Extremely Hindered Tetraaryl-Substituted Digermene and its Unique Properties in the Solid State and in Solution ..	158
VII-K-6 Syntheses, Structures and Properties of Kinetically Stabilized Distibenes and Dibismuthenes, Novel Doubly Bonded Systems between Heavier Group 15 Elements	158
VII-K-7 Synthesis and Properties of the First Stable Germabenzene	159
VII-K-8 Reactions of 2-Germanaphthalene with Elemental Sulfur and Selenium: Synthesis of Novel Cyclic Polychalcogenides Containing a Germanium, Trichalcogenagermolanes	159
VII-K-9 Synthesis and Properties of the First Stable 1-Silanaphthalene	160
VII-K-10 Synthesis and Isolation of the First Germacyclopropabenzene: A Study to Elucidate the Intrinsic Factor for the Ring Deformation of Cyclopropabenzene Skeletons	160
VII-L Precise Synthesis of Functional Macromolecules Using Organometallic Complexes	162
VII-L-1 Helical Poly(aryl isocyanide)s Possessing Chiral Alkoxy carbonyl Groups	162
VII-L-2 Formation of an Optically Active Helical Polyisocyanide Langmuir-Blodgett Film	162
VII-L-3 Helical Chiral Polyisocyanides Possessing Porphyrin Pendants: Determination of Helicity by Exciton Coupled Circular Dichroism	162

RESEARCH ACTIVITIES VIII

Laser Research Center for Molecular Science

VIII-A Developments and Researches of New Laser Materials	163
VIII-A-1 Ce ³⁺ :LiCaAlF ₆ Crystal for High-Gain or High-Peak-Power Amplification of Ultraviolet Femtosecond Pulses and New Potential Ultraviolet Gain Medium: Ce ³⁺ :LiSr _{0.8} Ca _{0.2} AlF ₆	163
VIII-A-2 Optical Fiber for Deep Ultraviolet Light	163
VIII-A-3 Crystal Growth of Fluorides for Optical Applications	163
VIII-A-4 Growth of Ce-Doped Colquirite- and Scheelite-Type Single Crystals for UV Laser Applications	164
VIII-A-5 High-Energy Pulse Generation from Solid-State Ultraviolet Lasers Using Large Ce:Fluoride Crystals	164
VIII-A-6 New Adjustment Technique for Time Coincidence of Femtosecond Laser Pulses Using Third Harmonic Generation in Air and its Application to Holograph Encoding System	165
VIII-A-7 Hybrid Time-Resolved Spectroscopic System for Evaluating Laser Material Using a Table-Top-Sized, Low-Jitter, 3-MeV Picosecond Electron-Beam Source with a Photocathode	165
VIII-A-8 Simultaneous Measurement of Thickness and Water Content of Thin Black Ink Films for the Printing Using THz Radiation	165
VIII-A-9 Far-Infrared Absorption Measurements of Polypeptides and Cytochrome <i>c</i> by THz Radiation	166

VIII-A-10	0.43 J, 10 Hz Fourth Harmonic Generation of Nd:YAG Laser Using Large $\text{Li}_2\text{B}_4\text{O}_7$ Crystals	166
VIII-A-11	Electron-Beam Excitation of a $\text{Ce}^{3+}:\text{LiCaAlF}_6$ Crystal for Future High-Peak-Power UV Lasers	166
VIII-B	Development and Research of Advanced Tunable Solid State Lasers	168
VIII-B-1	Thermal-Birefringence-Induced Depolarization in Nd:YAG Ceramics	168
VIII-B-2	Intrinsic Reduction of the Depolarization Loss in Solid-State Lasers by Use of a (110)-Cut $\text{Y}_3\text{Al}_5\text{O}_{12}$ Crystal	169
VIII-B-3	The Effect of Nd Concentration on the Spectroscopic and Emission Decay Properties of Highly-Doped Nd:YAG Ceramics	169
VIII-B-4	Spectroscopy and Laser Emission under Hot Band Resonant Pumping in Highly Doped Nd:YAG Ceramics	171
VIII-B-5	Efficient Laser Emission in Concentrated Nd Laser Materials under Pumping into the Emitting Level	172
VIII-B-6	1064-nm Laser Emission of Highly Doped Nd:Yttrium Aluminium Garnet under 885-nm Diode Laser Pumping	174
VIII-B-7	Diode Edge-Pumped Microchip Composite Yb:YAG Laser	175
Research Center for Molecular-Scale Nanoscience		
VIII-C	Development of Organic Semiconductors for Molecular Thin-Film Devices	177
VIII-C-1	Perfluoro-1,3,5-tris(<i>p</i> -Oligophenyl)benzenes: Amorphous Electron-Transport Materials with High Glass-Transition Temperature and High Electron Mobility	177
VIII-C-2	Synthesis and Properties of Iridium Complexes Bearing Perfluoroaryl-Substituted 2-Phenylpyridine	177
VIII-D	Field Effect Transistors with Organic Semiconductors	179
VIII-D-1	Electrical Characteristics of Phthalocyanine Films Prepared by Electrophoretic Deposition	179
VIII-D-2	BTQBT (bis-(1,2,5-thiadiazolo)- <i>p</i> -Quinobis(1,3-dithiole)) Thin Films; A Promising Candidate for High Mobility Organic Transistors	179
VIII-D-3	Field Effect Transistors of BTQBT and Its Derivatives	179
VIII-D-4	Preparation of Nanometer-Gap Electrodes for Field Effect Transistors by Electroplating	180
VIII-E	Preparation and Characterization of Highly Ordered Molecular Films on Silicon Bound with Si-C Covalent Bond	180
VIII-E-1	Force Curve Measurement of Self-Assembled Organic Monolayers Bound Covalently on Silicon(111)	180
VIII-E-2	Atomic Force Microscope Anodization of Si(111) Covered with Alkyl Monolayers	180
VIII-E-3	Nanopatterning of Alkyl Monolayers Covalently Bound to Si(111) with an Atomic Force Microscope	181
VIII-F	Development of Precisely-Defined Macromolecules and their Organization on Substrate Surfaces for Molecular-Scale Electronics Circuits	182
VIII-F-1	Design and Synthesis of Molecular Junction and Anchor Modules for Multi-Function Integrated Macromolecules	182
VIII-G	Development of Novel Heterocyclic Compounds and their Molecular Assemblies for Advanced Materials	182
VIII-G-1	Crystal Engineering Using Anilic Acids and Dipyriddy Compounds through a New Supramolecular Synthon	182
VIII-G-2	Bis(tetra- <i>n</i> -butylammonium) Bis(2-dicyanomethylene-4,5-dimercapto-1,3- dithiole)nickel(II)	183
VIII-G-3	^1H NMR Analysis and Crystal Structures of 1,1',3,3'-Tetramethyl-2,2'-bi-1 <i>H</i> - Imidazolium Bis(tetraphenylborate): Ion-Associative Interactions Containing Ketone, Aldehyde, and Nitrile	183
VIII-G-4	4,7-Diiodo-2,1,3-Benzothiadiazole and 7,7'-Diiodo-4,4'-bis(2,1,3-benzothiadiazole)	184
VIII-G-5	Synthesis and Properties of π -Extended TTF Analogues and Their Cation Radical and Dication Salts	184
VIII-G-6	Synthesis and Structure of Bi- and Terthiophene Derivatives Having 4-Pyridylethynyl Substituents	184
VIII-H	Designing Artificial Photosynthesis at Molecular Dimensions	185
VIII-H-1	Photoinduced Oxidation of Alcohols Catalyzed by Porphyrins and TEMPO	185
VIII-I	Development of New Metal Complexes as Redox Catalysts	186
VIII-I-1	Syntheses of a 6-(2-Pyrrolyl)-2,2'-Bipyridine Derivative and Its Ruthenium Complex	186
VIII-J	Electronic Properties of Monolayer-Protected Metal Clusters	187
VIII-J-1	Development of Mass Spectrometer for Clusters	187

VIII-J-2 Formation of Pd _n (SR) _m Clusters (<i>n</i> < 60) in the Reactions of PdCl ₂ and RSH (R = <i>n</i> -C ₁₈ H ₃₇ , <i>n</i> -C ₁₂ H ₂₅)	187
VIII-J-3 Size-Selective Preparation of Water-Soluble Gold Clusters	188
VIII-J-4 Characterization and Purification of Pd:SR Nanoparticles by Gel Permeation Chromatography	188
VIII-K Structures and Dynamics of Molecular Cluster Ions	189
VIII-K-1 Structural Evolution of Large (CO ₂) _{<i>n</i>} ⁻ Clusters as Studied by Mass Spectrometry	189
VIII-K-2 Photochemistry of (NO) _{<i>n</i>} ⁻ as Studied by Photofragment Mass Spectrometry	190
VIII-L Rotational Echo Double Resonance (REDOR) Experiments with Overtone Adiabatic Inversion Pulses	191
VIII-L-1 The Observation of REDOR Phenomena for Solid-State ¹³ C- ¹⁴ N Spin Systems with the Help of Overtone Adiabatic Inversion Pulses	191
VIII-M Nanoscale Characterization of Heterogeneous Catalyst Surfaces	192
VIII-M-1 Determination of Extra-Framework Cation Positions and Their Occupancies on Heulandite(010) by Atomic Force Microscopy	192
VIII-M-2 Molecular Orbital Interpretation of Thymine/Graphite NC-AFM Images	192
VIII-M-3 Partial Reduction of Si(IV) in SiO ₂ Thin Film by Deposited Metal Particles —An XPS Study	192
VIII-M-4 Apparent Local Structural Change Caused by Ultraviolet Light on a TiO ₂ Surface Observed by Scanning Tunneling Microscopy	192
VIII-M-5 Various Phases on Natural Stilbite (010) Surface Observed by Atomic Force Microscopy under Aqueous Conditions	192
VIII-N Studies of Electronic Structure of Organic Thin Films and Organic/Inorganic Interfaces by Electron Spectroscopies	194
VIII-N-1 Low Energy Electron Diffraction of the System In-[perylene-3,4,9,10-tetracarboxylic Dianhydride] on MoS ₂	194
VIII-N-2 Electronic Structure and Molecular Orientation at Thin Film Surfaces of Pendant-Group Polymers Studied by Outermost Surface Spectroscopy Using Metastable Atoms	194
VIII-N-3 Photodegradation of Poly(tetrafluoroethylene) and Poly(vinylidene fluoride) Thin Films by Inner Shell Excitation	195
VIII-N-4 Intramolecular Energy-Band Dispersion in Oriented Thin Film of <i>n</i> -CF ₃ (CF ₂) ₂₂ CF ₃ Observed by Angle-Resolved UV Photoemission and its Theoretical Simulation	195
VIII-O Study on Compact X-Ray Sources	196
VIII-O-1 Study on Radiation Shielding for Small Synchrotron Radiation Facilities	196
VIII-P Syntheses of Fullerene-Based New Materials with Novel Physical Properties	197
VIII-P-1 Pressure and Temperature Dependences of the Structural Properties of Dy@C ₈₂ Isomer I	197
VIII-P-2 Ferromagnetism and Giant Magnetoresistance in the Rare-Earth Fullerides Eu _{6-x} Sr _x C ₆₀	197
VIII-P-3 Bridging Fullerenes with Metals	197
VIII-P-4 Structure and Physical Properties of Cs _{3+α} C ₆₀ (α = 0.0–1.0) under Ambient and High Pressures	197
VIII-P-5 Complex-Plane Impedance Study on a Hydrogen-Doped Copper Coordination Polymer: <i>N,N'</i> -bis(2-hydroxyethyl)dithiooxamidatocopper(II)	198
VIII-P-6 Crystal Structure and Electronic Transport of Dy@C ₈₂	198
VIII-P-7 <i>N</i> -Channel Field-Transistors with Thin Films of Fullerenes	198
VIII-P-8 STM Study of Dy@C ₈₂ on Si(111)-(7×7) Surface	198
VIII-Q Effects of High Magnetic Field on Chemical Process	199
VIII-Q-1 Magnetic Field Effects on Anodic Oxidation of Potassium Iodide	199
VIII-Q-2 High Magnetic Field Effect on the Growth of 3-Dimensional Silver Dendrites	199
VIII-R Theoretical and Computational Study on Gas Phase Reactions and Chromic Molecules	200
VIII-R-1 Polycyano–Polycadmiate Host Clathrates Including a Methylviologen Dication. Syntheses, Crystal Structures and Photo-Induced Reduction of Methylviologen Dication	200
VIII-R-2 IR Absorption Spectra of Electrochromic WO ₃ Films	200
VIII-R-3 A Local Interpolation Scheme Using No Derivatives in Potential Sampling: Application to O(¹ D) + H ₂ System	200
VIII-R-4 Theoretical Study on Photoinduced Color Change and Charge Transfer of Methylviologen	200
VIII-R-5 Potential Energy Surface Generation Using Ab Initio Calculations and IMLS/Shepard Interpolation for the LiH + H ⇌ Li + H ₂ Reactions	201
VIII-S Macromolecular Self-Assembly Opens a Way to the Development of Novel Materials that Have Characteristics of Cellular Systems	202
VIII-S-1 Fabrication of “Entropy-Saving” Nano-Solar-Cells	202

VIII-S-2 Model Study on Signaling Behaviors of Scaffold Proteins —Toward its Application to Novel Computing Devices—	202
VIII-S-3 Physicochemical Studies on the Molecular Mechanism of Photosynthesis	202

Equipment Development Center

VIII-T Development of “Special Machine”	204
VIII-T-1 Development of Twin-Probe Scanning Tunneling Microscope	204

Ultraviolet Synchrotron Orbital Radiation Facility

VIII-U Development of the UVSOR Light Source	205
VIII-U-1 Development of Lattice Components for UVSOR Upgrade Project	205
VIII-U-2 Storage Ring Free Electron Laser	205
VIII-U-3 Ion Trapping at UVSOR	205
VIII-U-4 Design Study of Vacuum System Improvement	205
VIII-V Researches by the USE of UVSOR	206
VIII-V-1 Non-Radiative Decay of the Core Excitons in Auger-Free Luminescence Materials, CsCl and BaF ₂	206
VIII-V-2 Photoelectron Spectroscopic Study on Photo-Induced Phase Transition of Spin-Crossover Complex	206
VIII-V-3 Surface-Photovoltage Effect in GaAs-GaAsP Super-Lattice Studied with Combination of Synchrotron Radiation and the Laser	206
VIII-V-4 Pump/Probe Experiments with FEL and SR Pulses at UVSOR	206
VIII-V-5 Angle-Resolved Photoion Spectra of SO ₂	207
VIII-V-6 The Measurement of Absorption Spectra of Trifluoromethyl Sulfur Pentafluoride in VUV Region	207
VIII-V-7 Symmetry-Resolved Cl 2 <i>p</i> Photoabsorption Spectra of Cl ₂	208
VIII-V-8 Dynamical Angular Correlation in Molecular Auger Decay	208
VIII-V-9 Nondipolar Electron Angular Distributions from Fixed-in-Space Molecules	209
VIII-V-10 Double and Triple Excitations Near the K-Shell Ionization Threshold of N ₂ Revealed by Symmetry-Resolved Spectroscopy	209
VIII-V-11 Optical and Magneto-Optical Studies on Electronic Structure of CeSb in the Magnetically Ordered States	209
VIII-V-12 Low Energy Electronic Structure of Ce _{1-x} La _x Sb (<i>x</i> = 0, 0.1) in the Magnetically Ordered States	209
VIII-V-13 Temperature Dependence of Low-Energy Optical Conductivity of Yb ₄ (As _{1-x} P _x) ₃ (<i>x</i> = 0, 0.05, 0.15)	209
VIII-V-14 Charge Ordering Effect of Electronic Structure of Yb ₄ (As _{1-x} Sb _x) ₃	210
VIII-V-15 Temperature-Induced Valence Transition of EuNi ₂ (Si _{0.25} Ge _{0.75}) ₂ Studied by Eu 4 <i>d-4f</i> Resonant Photoemission and Optical Conductivity	210
VIII-V-16 Optical Gap in the Diluted Kondo Semiconductors Yb _{1-x} Lu _x B ₁₂ : Lattice and Single-Site Effects	210
VIII-V-17 Magneto-Optical Study of the Colossal Magnetoresistance Pyrochlore Tl ₂ Mn ₂ O ₇	210
VIII-V-18 Influence of Electronic Structure of CeSbNi _{0.15} on its Optical Conductivity	210

Computer Center

VIII-W Computer Simulation of Quantum Systems in Condensed Phase	211
VIII-W-1 Vibrational Energy Transfer from Solute to Solvent: An Analysis Based upon Path Integral Influence Functional Theory and Mixed Quantum-Classical Molecular Dynamics Method	211
VIII-X Molecular Dynamics Study of Classical Complex Systems	211
VIII-X-1 A Molecular Dynamics Study of Water Penetration into Biomembrane	211
VIII-X-2 Molecular Dynamics Study of Mechanical Extension of Polyaniline by AFM Cantilever	211
VIII-Y Theoretical Studies on Electronic Structure and Dynamics of Electronically Excited States	212
VIII-Y-1 Chemical Reactions in the O(¹ D) + HCl System I. <i>Ab Initio</i> Global Potential Energy Surfaces for the 1 ¹ A', 2 ¹ A', and 1 ¹ A'' States	212
VIII-Y-2 Millimeter-Wave Spectroscopy of the Internal-Rotation Band of the He–HCN Complex and the Intermolecular Potential Energy Surface	212
VIII-Y-3 Determination of the Global Potential Energy Surfaces and Transition Wave Packet Dynamics for Polyatomic Systems	212
VIII-Y-4 <i>Ab Initio</i> Study of Conformers of <i>p-tert</i> -Butylcalix [4] Crown-6-Ether Complexed with Alkyl Ammonium Cations	213

VIII-Y-5 <i>Ab Initio</i> Study of the Complexation Behavior of Calix[5]arene Derivative toward Alkyl Ammonium Cations	213
VIII-Y-6 Formation of $\text{HCl}^+(\text{A}^2\Sigma^+)$ and $\text{HBr}^+(\text{A}^2\Sigma^+)$ Resulting from $\text{He}(2^3\text{S})$ Penning Ionization of HCl and HBr	213
VIII-Y-7 Theoretical Study of Vibrational States for AINC/AICN	213
VIII-Y-8 Boundary Expansion in Time-Dependent Nonadiabatic Problems	213
VIII-Y-9 Optimal Control of Random Matrix Systems with a Parameter	214

RESEARCH ACTIVITIES IX

Center for Integrative Bioscience

IX-A Molecular Mechanisms of Oxygen Activation by Heme Enzymes	215
IX-A-1 Asymmetric Sulfoxidation and Amine Binding by H64D/V68A and H64D/V68S Mb: Mechanistic Insight into the Chiral Discrimination Step	215
IX-A-2 Molecular Mechanism of the Catalase Reaction Studied by Myoglobin Mutants	215
IX-B Model Studies of Non-Heme Proteins	216
IX-B-1 Reactivity of Hydrogenperoxide Bound to a Mononuclear Non-Heme Iron Site	216
IX-B-2 Synthesis, Structure, and Properties of A Novel Mononuclear Iron(III) Complex Containing Peroxocarbonate Ligand	216
IX-B-3 Structural and Spectroscopic Features of a <i>cis</i> (Hydroxo)- Fe^{III} -(Carboxylato) Configuration as an Active Site Model for Lipoxygenases	217
IX-C Aqueous Organometallic Chemistry	217
IX-C-1 pH-Dependent H_2 -Activation Cycle Coupled to Reduction of Nitrate Ion by Cp^*Ir Complexes	217
IX-C-2 pH-Dependent Cross-Coupling Reactions of Water-Soluble Organic Halides with Organoboron Compounds Catalyzed by an Organometallic Aqua Complex $[(\text{SCS})\text{Pd}^{\text{II}}(\text{H}_2\text{O})]^+$ {SCS = C_6H_3 -2,6-(CH-SBu^t) $_2$ }	217
IX-C-3 pH-Dependent Transfer Hydrogenation of Ketones with HCOONa as a Hydrogen Donor Promoted by $(\eta^6\text{-C}_6\text{Me}_6)\text{Ru}$ Complexes	218
IX-D Single-Molecule Physiology	219
IX-D-1 Myosin V Is a Left-Handed Spiral Motor on the Right-Handed Actin Helix	219
IX-D-2 Pause and Rotation of F_1 -ATPase during Catalysis	219
IX-D-3 F_1 -ATPase Changes its Conformations upon Phosphate Release	219
IX-E Bioinorganic Chemistry of Heme-Based Sensor Proteins	221
IX-E-1 Ligand-Switching Intermediates for the CO-Sensing Transcriptional Activator <i>CooA</i> Measured by Pulse Radiolysis	221
IX-E-2 Conformational Dynamics of the Transcriptional Regulator <i>CooA</i> Protein Studied by Subpicosecond Mid-Infrared Vibrational Spectroscopy	221
IX-E-3 Resonance Raman and Ligand Binding Studies of the Oxygen Sensing Signal Transducer Protein <i>HemAT</i> from <i>Bacillus subtilis</i>	221
IX-F Electronic Structure and Reactivity of Active Sites of Metalloproteins	223
IX-F-1 Trigonal Bipyramidal Ferric Aqua Complex with Sterically Hindered Salen Ligand as a Model for Active Site of Protocatechuate 3,4-Dioxygenase	223
IX-F-2 ^{13}C -NMR Signal Detection of Iron Bound Cyanide Ions in Ferric Cyanide Complexes of Heme Proteins	223
IX-G Molecular Mechanism of Heme Degradation and Oxygen Activation by Heme Oxygenase	224
IX-G-1 Catalytic Mechanism of Heme Oxygenase through EPR and ENDOR of Cryoreduced Oxy-Heme Oxygenase and Asp 140 Mutants	224
IX-H Biomolecular Science	225
IX-H-1 Stationary and Time-Resolved Resonance Raman Spectra of His77 and Met95 Mutants of the Isolated Heme Domain of a Direct Oxygen Sensor from <i>E. coli</i>	225
IX-H-2 Resonance Raman Studies on Xanthine Oxidase: Observation of the Mo^{VI} -Ligand Vibration	225
IX-H-3 Changes in the Abnormal α -Subunit upon CO-Binding to the Normal β -Subunit of Hb M Boston: Resonance Raman, EPR, and CD Study	226
IX-H-4 Coordination Geometry of Cu-Porphyrin in Cu(II)-Fe(II) Hybrid Hemoglobins Studied by Q-Band EPR and Resonance Raman Spectroscopies	226
IX-H-5 Fine-Tuning of Copper(I)-Dioxygen Reactivity by 2-(2-Pyridyl)ethylamine Bidentate Ligands	226
IX-H-6 Modulation of the Copper-Dioxygen Reactivity by Stereochemical Effect of Tetradentate Tripodal Ligands	227
IX-H-7 Reactivity of Hydroperoxide Bound to a Mononuclear Non-Heme Iron Site	227
IX-H-8 A New Mononuclear Iron(III) Complex Containing a Peroxocarbonate Ligand	227

IX-H-9 Formation, Characterization, and Reactivity of Bis(m-oxo)nickel(III) Complexes Supported by a Series of Bis[2-(2-pyridyl)ethyl]amine Ligands -----	227
IX-H-10 UV Resonance Raman and NMR Spectroscopic Studies on the pH Dependent Metal Ion Release from Pseudoazurin -----	228
IX-I Fast Dynamics of Photoproducts in Solution Phases -----	228
IX-I-1 Time-Resolved Resonance Raman Study on Ultrafast Structural Relaxation and Vibrational Cooling of Photodissociated Carbonmonoxy Myoglobin -----	228
IX-I-2 Vibrational Energy Relaxation of Metalloporphyrins in a Condensed Phase Probed by Time-Resolved Resonance Raman Spectroscopy -----	229
IX-I-3 Mode Dependence of Vibrational Energy Redistribution in Nickel Tetraphenylporphyrin Probed by Picosecond Time-Resolved Resonance Raman Spectroscopy: Slow IVR to Phenyl Peripherals -----	229
RESEARCH FACILITIES -----	231
Laser Research Center for Molecular Science -----	231
Research Center for Molecular-scale Nanoscience -----	231
Equipment Development Center -----	231
Ultraviolet Synchrotron Orbital Radiation Facility -----	231
Computer Center -----	232
SPECIAL RESEARCH PROJECTS -----	233
(a) Chemical Reaction Dynamics -----	233
Folding Mechanism of Protein Molecules Studied by Generalized-Ensemble Algorithms -----	233
Nonadiabatic Chemical Dynamics -----	233
Imaging of Chemical Dynamics -----	233
Stereodynamics and Active Control of Chemical Reactions by Using Electrostatic Hexapole State-Selector and Polarized Laser Excitation -----	234
Monte Carlo Simulation of Chemical Gel -----	234
Electronic Structure and Decay Mechanism of Inner-Shell Excited Molecules -----	234
Computational Study of Quantum Dynamics of a Solute in Solution -----	235
Photodissociation of 16 Valence Electron Systems, OCS and N ₂ O -----	235
Development of Single-Molecule Physiology -----	235
Ultrafast Protein Dynamics Probed by Time-Resolved Resonance Raman Spectroscopy -----	235
(b) Molecular Photophysics and Science -----	237
Development of Dynamic Spectroscopy Apparatus Having Nanometer Spatial Resolution -----	237
(1) Laser Cooling and Trapping of Metastable Helium Atoms -----	237
(2) Laser Spectroscopic Studies of Atoms and Ions in Liquid Helium -----	237
Structure, Relaxation and Control of Reactive Cluster Studied by Two-Color Laser Spectroscopy -----	237
Dynamics of Molecular Superexcited States Studied by Electron and Fluorescence Spectroscopy -----	237
Decay and Dissociation Dynamics of Core Excited Molecules -----	238
(c) Novel Material Science -----	239
Calculations of Large Molecular Systems -----	239
Response of Protein Conformation to Pressure: Theoretical Study on Partial Molar Volume -----	239
Theory for Equilibrium and Non-Equilibrium Properties of Low-Dimensional Molecular Materials with Strong Electron Correlation -----	239
UHV System for MOKE Measurements -----	240
Pulsed Methods of Electron Spin Resonance Spectroscopy -----	240
Spectroscopic Studies of Organic Conductors -----	240
Broad-Line Solid State NMR Investigation of Electronic States in Molecular-Based Conductors -----	241
Development of New Organic Conductors -----	241
Design and Synthesis of Organic Spin-Ladder Systems -----	241
Construction of BL-7A at UVSOR for STM Observation of SR Irradiation Induced Photochemical Reaction on Si Surfaces -----	242
Catalytic Oxidation of Alcohols in Water under Atmospheric Oxygen by Use of an Amphiphilic Resin-Dispersion of Nano-Palladium Catalyst -----	242
Reductive Activation of Carbon Dioxide and Oxidative Activation of Water Aimed at Energy Conversion -----	242
Coordination Chemistry of New Multidentate Ligands and Activation of Small Molecules -----	243
Developments and Researches of New Laser Materials -----	243
Development and Research of Advanced Tunable Solid State Lasers -----	243
Synthesis of Oligonaphthalenes and Oligoanthracenes and Applications for Organic Field-Effect Transistors -----	243
Field Effect Transistors of BTQBT and Its Derivatives -----	244

Generation of Reactive Species via Electron Transfer on Metal Complexes, as Basis of Chemical Energy Conversion Systems -----	244
Electronic Structures and Reactivities of Organic/Metal Clusters -----	244
Local Distribution of Photoexcited States on a Semiconductor Surface as Observed by Scanning Tunneling Spectroscopy -----	244
Electronic Structures and Surface Molecular Orientation of Organic Thin Films and Interfaces by Various Surface Sensitive Spectroscopies -----	245
Development of "Entropy-Saving" Nano-Materials -----	245
Investigation of Dynamics on Photo-Excited Solids and Surfaces by Using the Combination of Synchrotron Radiation and Laser Light -----	246
Construction and Commissioning of In-Vacuum Undulator -----	246
Optical Investigation on Fermiology of Strongly Correlated Electron Systems -----	246
Preparation of Artificial Metalloenzymes by Insertion of Chromium(III) Schiff Base Complexes into Apo-Myoglobin Mutants -----	246
Molecular Mechanism of Oxygen Activation by Metalloenzymes -----	247
OKAZAKI CONFERENCE -----	249
JOINT STUDIES PROGRAMS -----	251
(1) Special Projects -----	251
(2) Research Symposia -----	258
(3) Cooperative Research -----	259
(4) Use of Facility -----	259
(5) Invited Research -----	259
(6) Use of UVSOR Projects -----	259
(7) Use of Facility Program of the Computer Center -----	259
FOREIGN SCHOLARS -----	261
AWARDS -----	265
LIST OF PUBLICATIONS -----	269
REVIEW ARTICLES AND TEXTBOOKS -----	291
AUTHOR INDEX -----	295

Abbreviations

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