CONTENTS

IMS 1998 -	Mitsuo Ito	iii
CONTENT	ΓS	V
	ZATION AND STAFF	
BUILDING	GS AND CAMPUS	-14
RESEARC	CH ACTIVITIES I	
Departn	nent of Theoretical Studies	-17
A. Deve	lopment of New Theoretical and Numerical Techniques e Study of Molecular Structures	
in the	Generalization of the Coupled-Cluster Response Theory to Multireference Expansion Spaces;	·17
1	an Application of the Coupled-Cluster Singles and Doubles Effective Hamiltonian	.17
2	Modified McMurchie-Davidson Method for the Calculation of the Two-Electron Integral and its Derivatives	
3		
4	Photodetachment Cross Section of Anions	
5		18
	er Clusters and Their Complexes with Atomic Ions	-18
1	Dipole-Bound and Interior Electrons in Water Dimer and Trimer Anions: Ab Initio MO Studies	1 0
2	A New Form of Stable Excess Electron: {e}·(HO) bonds	
3	Electronic Structure of Li(H_2O) _n and Na(H_2O) _n for $n = 3$, 4 and 5	-18
4	Ab-Initio Monte Carlo Simulation Using Multicanonical Algorithm:	
	Temperature Dependence of the Average Structure of Water Dimer	19
5	Theoretical Assignments of the Photo-Dissociation Excitation Spectra of Mg ⁺ Ion Complexes with Water Clusters: Multi-Reference CI Studies	-19
6		.19
C. Struc	ctures and Vibrational Frequencies of Infinite Polymer Chains	
2	Analytical Second Derivatives in Ab Initio Hartree-Fock Crystal Orbital Theory of Polymers Analytical Energy Gradients in Second-Order Møller-Plesset Perturbation Theory	-20
	Analytical Energy Gradients in Second-Order Møller-Plesset Perturbation Theory for Extended Systems	20
3	Ab Initio Hartree-Fock and Density Functional Studies on the Structures and Vibrations	
	of an Infinite Hydrogen Fluoride Polymer	20
D. Struc	ctures and Reactions of Atomic and Molecular Clusters	
1	Photodissociation Dynamics of Argon Cluster Ions	21
2 3	Theoretical Investigation of the Structure and Spectroscopy of Silicon-Carbon Mixed Clusters - Model Study of H-Bonded ROH (NH ₃) ₅ Clusters:	
4	A Search for Possible Ground-State Proton Transfer SpeciesAb Initio MO Studies of van der Waals Molecule (N ₂) ₂ :	-21
4	Potential Energy Surface and Internal Motion	21
5		.21
	rate Studies of Excited States of Small Molecules	-22
1	A Theoretical Study of the Electronic Structure and Spectroscopic Properties	
	of the Low-Lying Electronic States of the Molecule AlSi	22
2	The Variety of [Fe,N,O] Isomers. A Theoretical Study	.22
3	Theoretical Studies of Highly-Excited Valence States of N ₂ ⁺ Molecule Ion	23
4	Theoretical Study on Spectroscopic Properties of Positive, Neutral, and Negative Species	
-	of BCl ₂ and AlCl ₂ The Electronic Structures of HCCS and NCS	-23
5		
6 F Anni	ication of Ab Initio Molecular Orbital Methods to Experimentally Relevant Systems	
r. App i 1	Theoretical Studies of Geometric and Electronic Structures of Novel Molecular Anion	4
1	CH ₃ CO ₂ I ⁻	-24
2	Theoretical Studies of Internal Methyl Rotations in <i>m</i> -Xylene: Comparison of Franck-Condon	
	Factors with the Experimental Spectra	24
3	Theoretical Studies of Internal Methyl Rotations in <i>ο</i> -Xylene: Coupled Internal Rotation	-24
4	Reaction of OCrO ⁺ with a H ₂ Molecule	-24

G.	Predi	ction of Protein Tertiary Structures from the First Principles	-25
	1	Effects of Side-Chain Charges on -Helix Stability in C-Peptide of Ribonuclease A	
		Studied by Multicanonical Algorithm	-25
	2	Stochastic Dynamics Simulations in a New Generalized Ensemble	-25
	3	The Folding Funnel Landscape for the Peptide Met-Enkephalin	-26
	4	Finite-Size Scaling of Helix-Coil Transitions in Poly-Alanine Studied	
	•	by Multicanonical Simulations	-26
	5	Singular Behavior of the RISM Theory Observed for Peptide in Salt Solution	-26 -26
	6	Analysis on Conformational Stability of C-Peptide of Ribonuclease A in Water	20
	U	Using the Reference Interaction Site Model Theory and Monte Carlo Simulated Annealing	-26
	7	-Sheet Formation in BPTI(16-36) by Monte Carlo Simulated Annealing	
н	Theor	retical Studies of Chemical Reaction Dynamics	27
11.		Cumulative Reaction Probability without Absorbing Potentials	27
	1	Cumulative Reaction Probability Without Absorbing Potentials	-21
	2	Hyperspherical Elliptic Coordinates for the Theory of Light Atom Transfer Reactions in Atom-Diatom Collisions	27
	2		-21
	3	Quantum Mechanical Elucidation of Reaction Mechanisms of Heavy-Light-Heavy Systems:	27
		Role of Potential Ridge	-27
	4	Quantum Reaction Dynamics of Cl + HCl HCl + Cl: Vibrationally Nonadiabatic Reactions	-27
	5	Semiclassical Treatment of Resonances in the Collinear O + HO Exchange Reaction	-28
	6	Four Mathematical Dimensional Quantum Mechanical Studies of Tetra-Atom Systems:	
		State-to-State $J = 0$ Probabilities for the $H_2 + OH$ $H_2O + H$ Reaction	-28
I.	Theo	ry of Nonadiabatic Transitions	-28
	1		
		Nonadiabatic Tunneling Case	-28
	2	Semiclassical Theory of Nonadiabatic Transition in a Two-State Exponential Model	-28
	3	Improvement of the Adiabatic Phase Integral for the Landau-Zener-Type Curve Crossing	-28
	4	Patterns of Time-Propagation on the Grid of Potential Curves	-29
J.	New Y	Way of Controlling Molecular Nonadiabatic Processes	-29
	1		-29
	2	New Way of Controlling Molecular Processes by a Time-Dependent External Field	-29
K.		retical Studies of Characteristics and Dynamics of Superexcited States of Molecules	
		Characteristics and Dynamics of Superexcited States of Diatomic Molecules:	
	_	General Theoretical Procedure	-29
	2.	Analytical Treatment of Singular Equations in Dissociative Recombination	
		Electron Attachment and Vibrational Excitation in Hydrogen Iodide: Calculations	-
	5	Based on the Nonlocal Resonance Model	-30
Τ.	Siege	rt Pseude-State Formulation of Scattering Theory	-30
	1	C' D 1. Ct F 1	20
М	Theor	retical Studies of Ultrafast Nonlinear Optical Spectroscopy of Molecules ndensed Phases	-50
171.	in Co	ndensed Phases	30
		Fifth-Order Two-Dimensional Vibrational Spectroscopy of a Morse Potential System	-30
	1		20
	2	in Condensed Phases	-30
	2	Pump-Probe Spectra and Nuclear Dynamics for a Dissipative Molecular System	21
	2	in a Strong Laser Field: Predissociation Dynamics	-31
	3	Coherent Two-Dimensional Raman Scattering: Frequency-Domain Measurement	21
		of the Intra- and Intermolecular Vibrational Interactions	-31
	4	Sensitivity of Two-Dimensional Fifth-Order Raman Response to the Mechanism	
		of Vibrational Mode-Mode Coupling in Liquid Molecules	-31
	5	Two-Dimensional THz Spectroscopy of Liquids:	
		Nonlinear Vibrational Response to a Series of THz Laser Pulses	-31
	6	Optimized Perturbation Approach to a Dissipative System:	
		Correlation Functions of Anharmonic Oscillators	
N.	Theo	retical Studies of Molecular System Coupled to a Glass Environment	-32
	1	Spectral Random Walks and Line Broadening of Impurity Molecules	
		in an Ising Spin Glass Environment	-32
	2	Absorption Line Shape of Impurity Molecule Driven by a Fractal Noise	-32
0.	Ab In	itio Molecular Orbital studies of Organic Conductors	-32
	1	Ab Initio MO Studies on Electronic States of DCNQI Molecules	-32
	2	Theoretical Study on Electron Correlation of 1-D (DCNQI)2M (M = Li, Ag) Salts	-32
P.		ron and Positron Scattering from Polyatomic Molecules	-33
- •	1	A Comparative Study of Electron- and Positron-Polyatomic Molecule Scattering	-33
	2	Mode-Dependence in Vibrational Excitation of CO ₂ Molecule	
	_	by Electron and Positron Impacts	-33
		y recommendation of the recommendation of th	_

	3	Total Cross Sections of Electron and Positron Collisions with C ₃ F ₈ and C ₃ H ₈ Molecules, and Differential Elastic and Vibrational Excitation Cross Sections by Electron Impact	
		on These Molecules	-34
O.	Electi	onic Structure of a Molecule in Solution	-34
v.	1	Molecular Theory of Solvent Effect on keto-enol Tautomers of Formamide in Aprotic Solvents RISM-SCF Approach	:
	2	Theoretical Study of the Solvent Effect on Triiodie Ion in Solutions	_35 -35_
	3	Theoretical Study for Autoionization of Liquid Water:	
	3	Temperature Dependence of the Ionic Product (pK_w)	-35
	4	The Syn-/Anti- Conformational Equilibrium of Acetic Acid in Water	
	•	The Syn-/Anti- Conformational Equilibrium of Acetic Acid in Water Studied by the RISM-SCF/MCSCF Method	-35
	5	RISM-SCF Study for the Free Energy Profile of Menshutkin Type Reaction	
	_	$NH_3 + CH_3Cl$ $NH_3^+CH_3 + Cl^-$ in Aqueous Solution	-35
R.	Solva	tion Thermodynamics of Protein and Related Molecules	-36
	1	Calculation of Hydration Free Energy for a Solute with Many Atomic Sites	
		Using the RISM Theory: Robust and Efficient Algorithm	-36
	2	Solvation Structure and Stability of Pentides in Aqueous Solutions	
		Analyzed by the Reference Interaction Site Model Theory	-36
	3	First-Principle Determination of Pentide Conformations in Solvents:	
		Combination of Monte Carlo Simulated Annealing and RISM Theory	-37
	4	Calculation of Solvation Free Energy Using RISM Theory for Peptide in Salt Solution	-37
	5	Singular Behavior of the RISM Theory Observed for Peptide in Salt Solution	-37
	6	Analysis on Conformational Stability of C-Peptide of Ribonuclease A in Water	
		Using the Reference Interaction Site Model Theory and Monte Carlo Simulated Annealing	-37
	7	Molecular Theories of Partial Molar Volume	-38
S.	Spatia	al and Temporal Density Fluctuation in Molecular Liquids	-38
		Interaction-Site-Model Description of Collective Excitations in Classical Molecular Fluids	
		Dynamics of Solvated Ion in Polar Liquids: An Interaction-Site-Model Description	
		Interaction-Site Representation for Collective Excitations in Diatomic Dipolar Liquid	-39
	4	Effect of Molecular Symmetry on Electrical Potential Fluctuations of Solvent Around Solute	20
	~	in Polar Liquid	
	5	Mode-Coupling Theory for Molecular Liquids Based on the Interaction-Site Model	-39
	6	Time-Correlation Functions in Molecular Liquids Studied by the Mode-Coupling Theory Based on the Interaction-Site Model	20
Tr.	T !!	d-Solid Interface	-39
1.	Liqui 1	Theoretical Study for Water Structure at Highly Ordered Surface: Effect of Surface Structure -	
	2	Solution of the Three Dimensional DISM/UNC Equations for SDC Water	
	2	by the Modified Method of Direct Inversion in the Iterative Subspace	40
	3	Three-Dimensional Density Profiles of Water in Contact with a Solute of Arbitrary Shape:	-40
	3	A RISM Approach	_41
	4	Extended States of a Shallow Donor Located near a Semiconductor-Insulator Interface	
	5	The Structure and Adsorption of the Four Bonding Sites Model for Associating Fluids	
		in Disordered Porous Media from Replica Ornstein-Zernike Integral Equation Theory	-41
U.	Dime	nsional Crossovers in Doned Ladder Systems, Organic Conductors	
	and C	Cuprate Superconductors	-42
	1	Spin Gap and Superconductivity in Weakly Coupled Ladders:	
		Interladder One-Particle vs. Two-Particle Crossover	-42
	2	One-Particle vs. Two-Particle Crossover in Weakly Coupled Hubbard Chains and Ladders:	
		Perturbative Renormalization Group Approach	-42
	3	Dimensional Crossovers in the Doped Ladder System: Spin Gap, Superconductivity	
		and Interladder Coherent Band Motion	-42
	4	Antiferromagnetic Phase Transition and Crossover to Fermi Liquid Phase	
		in a Weakly Coupled Half-Filled Chain System	-42
	5	Effects of Dimerization and Interchain One-Particle Hopping	
		in a Weakly Coupled Dimerized Chain System at Quarter Filling	-43
	6	Geometry, Universality and Dimensional Crossovers in Weakly Coupled One-Dimensional Conductors	
	_	in Weakly Coupled One-Dimensional Conductors	-43
	7	Renormalization-Group Study of Competition between Density Waves and Pairing	
	_	in Quasi-One-Dimensional Electron Systems	-43
	8	Anisotropic Suppression of Quasiparticle Weight in Two-Dimensional Electron System	40
T 7	3.7	with Partially Flat Fermi Surface: Two-Loop Renormalization-Group Analysis	
٧.	- 7	etic Properties of Metal-Assembled Complexes with Two Different-Dimensional Bands	
	1	On the Effects of On-Site Coulomb Interaction in Strongly Dimerized Two Band Systems Possible Magnetic Phases in Two-Band Systems with Different Dimensionality	
	2	russide magnetic rhases in 1 wo-dand Systems with Different Dimensionality	-44

	3	Effective Exchange Interactions in Dimerized Systems	44
	4	From Possible Magnetic Orders to Quantum Disorder	44
W	.Metal	-Insulator and Superconducting Transitions in Strongly Correlated Electron Systems	
	Coup	led with Localized Spins or Phonons	44
		Conductivity and Magnetic Properties of One-Dimensional Heisenberg-Kondo Lattice	
	2	Superconductivity and Magnetism in Quasi-One-Dimensional Two-Band Systems	
3 7		Berry Phases and Pairing Symmetry in Holstein-Hubbard Polaron Systems	45
X.	Coexi	istence of or Competition between Different Density Waves ne-Dimensional Quarter-Filled Organic Conductors	15
	In On	Coexistence of SDW and Purely-Electronic CDW in Quarter-Filled Organic Conductors	45
		Coexistence of SDW and Purely-Electronic CDW in Quarter-Filled Organic Conductors Coexistence of SDW and Purely-Electronic CDW in Quarter-Filled Organic Conductors	40
	2	at Finite Temperatures	16
	3	Exact Diagonalization Study of (DCNQI) ₂ M (M = Li, Ag) Clusters	40
	3	Based on Ab Initio Molecular Orbital Parameters	16
V	Electr	ron Correlation and New Photoinduced Phenomenon in Polymers	40 46
1.	1	Effect of Electron Correlation on Competition between BOW and SDW in Polymer	
	2	Off-Diagonal Interactions and Spin-Density Waves in Polymers	47
	3	A Correlated-Basis-Function Study of SDW in Polymers	47
	4	Making a Molecule with Negative Polarizability	47
	5	Polarization and Dissociation of Exciton in Luminescent Polymers	47
		·	
RESE	ARC	H ACTIVITIES II	
Dep	artm	ent of Molecular Structure	48
_			
A.	. Labo	ratory and Astronomical Spectroscopy of Transient Molecules	48
	1		
		Spectroscopy	48
	2	Microwave Spectroscopic Detection of a New Transient Phosphorus-Bearing Molecule, H ₃ PO	
		Microwave Spectrum of Silicon Trifluoride, SiF ₃	49
	4	The Pure Rotational Spectra of $TiO(X^3)$ and $TiN(X^2)$ +	49
ъ	5	Microwave Spectrum of the PD ₂ Radical in the 2B_1 Ground Electronic State	
В.		opment of a Mt. Fuji Submillimeter-Wave Telescope	50
	1	Development of a Backend System for Mt. Fuji Submillimeter Wave Telescope: An IF Band Synthesis Unit and a New Data Accumulator	50
C	Locar	• Cooling and Trapping of Neutral Atoms	50
C.	Lasei 1	Isotopic Differences in Rate Coefficients of Cold Penning Collisions	51
	1	between Optically Trapped Metastable He Atoms	51
D	Spect	roscopy of Ions and Atoms in Liquid Helium	52
۵.	1	Laser Spectroscopy of Yb ⁺ Ions in Liquid Helium	52
	2	Laser Spectroscopy of Yb atoms in Liquid Helium	52
	3	Theoretical Analyses of the Spectrum of Mg Atoms in Liquid Helium	52
E.	Struc	ture and Function of Respiratory Terminal Oxidases	53
	1	Fluoride-Binding to the Oxidized <i>Escherichia coli bd</i> -Type Ubiquinol Oxidase	
		Studied by Visible Absorption and EPR Spectroscopies	53
	2	Azide- and Cyanide-Bindings to the <i>Escherichia coli bd</i> -Type Ubiquinol Oxidase	
		Studied by Visible Absorption, EPR and FTIR Spectroscopies	53
F.	Biom	olecular Science	54
	1	Resonance Raman Characterization of Nitrosylheme in Myoglobin and Its Mutants	54
	2	Infrared Evidence for Cu _B Ligation of Photodissociated CO of Cytochrome c Oxidase at	
	_	Ambient Temperatures and Accompanied Deprotonation of a Carboxyl Side Chain of Protein	54
	3	Interaction of Phosphatidylinositol 3-Kinase SH3 Domain with Its Ligand Peptide	
		Studied by Absorption, UV Resonance Raman and Circular Dichroism	54
	4	Quaternary Structure Sensitive Tyrosine Residues in Human Hemoglobin:	
	_	UV Resonance Raman Studies of Mutants at 140, 35 and 145 Tyrosine	55
	5	A Superoxodicopper(II) Complex Oxidatively Generated	
	-	by a Reaction of Di-µ-Hydroxodicopper(II) Complex with Hydrogen Peroxide	33
	6	Structural and Spectroscopic Characterization of a Mononuclear Hydroperoxo-Copper(II)	50
C	Foot 1	Complex with Tripodal Pyridylamine Ligands Dynamics of Photoproducts in Solution Phases	50 54
G		Photo-Induced Solvent Ligation to Nickel(II)-Octaethylporphyrin Probed	30
	1	by Picosecond Time-Resolved Resonance Raman Spectroscopy	56
	2	Time Resolved Resonance Raman Evidence for the Exciplex Formation of Free-Base Porphy	rin
	2	with an Electron Acceptor	
		··	50

	3	Comment on: Polarization Effects in Time Resolved Incoherent Anti-Stokes Raman	
	4	Spectroscopy	56
	4	Saturation Raman Spectrosocpy as a Tool for Studying the Excited States	57
п	Molor	of Complex Organic Molecules: Application to Nickel Octaethylporphyrin	31 57
11.		ENDOR Measurements of La@ C_{82}	
I.	Site S	elective Spectroscopy in Solid Crystals	57
1.	1	Coherent Raman Spectroscopy of Nuclear Quadrupole Resonance of La around Pr ³⁺ in LaF ₃ -	58
	2	Coherent Raman Scattering from a Delocalized Excitation in Molecular Crystal of 1,4-	50
	_	Dibromonaphthalene	58
J.	State	Correlated Raman Spectroscopy	58
	1	Polarized Raman Scattering Measurements of MHPOBC	59
K.	Doub	le Resonance Spectroscopy Using Two Phase-Locked Lasers	59
	1	Direct Observation of the Quantum Phase Induced by Third-order Nonlinear Susceptibility Using Phase-Locked OODR Spectroscopy	59
		H ACTIVITIES III	
Dep	artm	ent of Electronic Structure	61
Δ	Statos	s of Molecular Associates in Aqueous Environment	61
11.	1	Low Frequency Raman Spectra of Crystalline and Liquid Acetic Acid and its Mixtures	01
	1	with Water: Is the Liquid Dominated by Hydrogen-Bonded Cyclic Dimers?	61
	2	Effects of Intermolecular Hydrogen-Bonding Interactions on Raman Spectra of Crystalline	01
		and Liquid Acetic Acid: Ab Initio Molecular Orbital Study	61
	3	States of Acetic Acid and Water Molecules in Aqueous Mixture	
		Studied by Low Frequency Raman Spectroscopy	62
В.		roscopic and Dynamical Studies on Charge Delocalization and Charge Transfer	
	in Ar	omatic Molecular Clusters	63
	1	Vibrational Predissociation Spectroscopy of Phenol-Benzene Dimer Cation	63
	2	Electronic Structure of Solvent Benzene in (Phenol-Benzene) ⁺	63
	3	Photodissociation Dynamics of $(C_6H_6)_3^+$:	
		Role of the Extra Benzene Molecule Weakly Bound to the Dimer Core	64
	4	Photodissociation Spectroscopy of (Benzene-Toluene) ⁺ .	- 4
	_	Charge Delocalization in the Hetero-Dimer Ion	64
	5	Photodissociation Spectrum of Cyanobenzene Dimer Cation. Absence of Intermolecular Resonance Interaction	<i>(</i> =
C	Liltua	fast Dynamics of Photoexcited Molecules by Transient Absorption Spectroscopy	
C.	Unra	Construction of a Subpicosecond Time-Resolved Absorption Spectroscopy	03
	1	Using a Dye Amplifier	65
	2	Time-Resolved Absorption Studies on Photochromism of 2H-Chromene Derivatives	
D		chemistry on Well-Defined Surfaces	
υ.		Photodesorption of Xe Adsorbed on Clean and Oxidized Si(100) Surfaces	
E.	Photo	chemistry of Adsorbates on Thin Films and Clusters of Metals	67
	1	Photochemistry of Methane adsorbed on Pd/Al ₂ O ₃ Model Catalysts	67
F.	React	ion Dynamics on Well-Defined Surfaces	68
	1	Effective Conversion of CO ₂ to Carbonate in Surface Oxidation Processes at Si(100)	68
G.	Dyna	mical Behavior of Electronically Excited States	68
	1	Ultrafast Relaxation Processes from a Higher Electronically Excited State of a Dye Molecule	
		in Solution: A Femtosecond Time-Resolved Fluorescence Study	69
H.	Spect	roscopy and Dynamics of Vibrationally Excited Molecules and Clusters	69
	1	Nonresonant Ionization Detected IR Spectrum of Jet-Cooled Phenol	
		— Ionization Mechanism and Its Application to Overtone Spectroscopy	69
	2	Structure of 1-Naphthol-Water Clusters Studied by IR Dip Spectroscopy	
		and Ab Initio Molecular Orbital Calculation	69
I.	Large	Amplitude Motion in Molecular Cation Studied	
	by Pu	lsed Field Ionization - Zero Kinetic Energy Photoelectron Spectroscopy	70
	1	Internal Rotation of Methyl Group in Tolunitrile Cations	
_	_	Studied by Pulsed Field Ionization - Zero Kinetic Energy Spectroscopy	70
J.	_	Investigation of Molecular Photodissociation Dynamics	
	1	Quantal and Semiclassical Analysis of Vector Correlation in Molecular Photodissociation	70
	2	Geometrical Factors of Two-Photon Absorption for the Determination of Alignment	70
		and Orientation	/0

	_	D 11 11 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	
	3	Probing alignment of $NO(X^2)$ by [2+1] REMPI via C^2 state:	71
		A Test of Semiclassical Theory in 355 nm Photodissociation of NO ₂	/1
	4	Non-Adiabatic Bending Dissociation in 16 Valence Electron System OCS	71
		C-Br Bond Rupture in 193 nm Photodissociation of Vinyl Bromide	/I
	6	Energy Barrier for the C-C Bond Rupture in Acetyl Radical	7 1
	7	Studied by Nanosecond Photofragment Imaging	/1
	/	Dissociation of Metastable CH ₃ CO Radical	70
	0	Observed by Subpicosecond Time-Clocked Imaging	/2
	8	Sensitized Phosphorescence Detection of Metastable Triplet Acetylene Produced by Intersyste Crossing	em 72
	0	Predissociation of Acetylene from the $\tilde{A}(^{1}A_{u})$ State Studied by Absorption, LIF	/ 2
	9	Predissociation of Acetylene from the A('A _u) State Studied by Absorption, LIF	72
17	T	and H-Atom Action Spectroscopies	/ Z
K.	Laser	Investigation of Bimolecular Reaction Dynamics	/ 2
	1	High-Resolution Measurements of State-Resolved Differential Cross Sections in NO + Ar Inelastic Scattering at $E_{coll} = 65 \text{ meV}$	72
	2	Development of an Intense Atomic Beam Source of $O(^1D)$	12 72
T		roscopy and Excited State Dynamics in van der Waals Complexes	
L.	Speci	Electronic Spectroscopy and Pre-dissociation Mechanism of Ar-NO in the 3p Rydberg States	/4 71
		Photochemical Reaction Dynamics of O(¹ D) with Saturated Hydrocarbons,	/4
	2	CH. C.H. and C.H. under Pulk Conditions and in year der Weels Complexes	74
NЛ	Dhote	CH ₄ , C ₂ H ₆ , and C ₃ H ₈ , under Bulk Conditions and in van der Waals Complexeschemical Processes Studied by Time-Resolved ESR	71
WI.	PHOU	Exchange Interaction in Radical-Triplet Pair: Evidence for CIDEP Generation	/4
	1	by Level Crossings in Triplet-Doublet Interactions	74
	2	CIDED in Product Singlet Molecular Overson System	75
NT	Dymo	CIDEP in Radical-Singlet Molecular Oxygen System mics of Excited Electronic States of 4-Dimethylaminopyridine and Its Derivatives	13 75
11.	Dyna	Dual Fluorescence of 4-Dimethylaminopyridine and Its Derivatives in Solutions	13 75
^	Confe	ormation, Photoisomerization and Solvent Effect of Merocyanine Dyes	13 76
J .	1	Dispersed Fluorescence and Fluorescence Excitation Spectra of Merocyanine Dyes	/0
	1	in Low-Temperature Argon Matrices	76
		in 2011 Temperature in gent interest	, 0
		H ACTIVITIES IV ent of Molecular Assemblies	78
epa	artm	ent of Molecular Assemblies	
epa	artm Solid	ent of Molecular AssembliesState Properties of Phthalocyanine Salts and Related Compounds	
epa	artm	ent of Molecular Assemblies State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts	78
epa	artm Solid	ent of Molecular Assemblies	78
epa	artm Solid	ent of Molecular Assemblies State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine	78 78
epa A.	Solid 1 2	ent of Molecular Assemblies State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process	78 78 78
epa A.	Solid 1 2 Struc	ent of Molecular Assemblies State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors	78 78 78
epa A.	Solid 1 2 Struc	ent of Molecular Assemblies State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors	78 78 78
epa A.	Solid 1 2 Struc	ent of Molecular Assemblies State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition of Metallic DMTSA-BF ₄ Charge-Transfer Transition Polarized Perpendicular to the Molecular Stack	78 78 79 79
epa A.	Solid 1 2 Struce 1 2	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition of Metallic DMTSA-BF ₄ Charge-Transfer Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄	78 78 79 79
pa A.	Solid 1 2 Struc	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5}	78 78 79 79
epa A.	Solid 1 2 Struc 1 2 3	ent of Molecular Assemblies State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5}	78 78 79 79
epa A.	Solid 1 2 Struce 1 2	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5}	78 78 79 79 80
pa A.	Solid 1 2 Struce 1 2 3 4	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5}	78 78 79 79 80 80
pa A.	Solid 1 2 Struce 1 2 3 4 5	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5}	78 78 79 79 80 80
pa A.	Solid 1 2 Struce 1 2 3 4	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5}	78 78 79 80 81
epa A.	Solid 1 2 Struc 1 2 3 4 5 6	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition of Metallic DMTSA-BF ₄ Charge-Transfer Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄ Two-Dimensional Band Structure of Organic Metals (BDT-TTP) ₂ X (X = SbF ₆ , AsF ₆) Studied by Polarized Reflection Spectroscopy Band Structure of Organic Metal (BDT-TTP) ₂ ClO ₄ Studied by Polarized Reflection Spectroscopy Spectroscopic Study of Narrow-Band Organic Metal (BEDT-ATD) ₂ PF ₆ (THF) Charge Distribution in (Et ₄ N)(DMe-TCNQ) ₂ Crystal Studied by Raman and Reflection Spectroscopy	78 78 79 80 81
epa A.	Solid 1 2 Struce 1 2 3 4 5	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition of Metallic DMTSA-BF ₄ Charge-Transfer Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄ Two-Dimensional Band Structure of Organic Metals (BDT-TTP) ₂ X (X = SbF ₆ , AsF ₆) Studied by Polarized Reflection Spectroscopy Band Structure of Organic Metal (BDT-TTP) ₂ ClO ₄ Studied by Polarized Reflection Spectroscopy Spectroscopic Study of Narrow-Band Organic Metal (BEDT-ATD) ₂ PF ₆ (THF) Charge Distribution in (Et ₄ N)(DMe-TCNQ) ₂ Crystal Studied by Raman and Reflection Spectroscopy Phase Transition of '-(BEDT-TTF) ₂ IBr ₂	78 78 79 80 81 81
epa A.	Solid 1 2 Struc 1 2 3 4 5 6	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition of Metallic DMTSA-BF ₄ Charge-Transfer Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄ Two-Dimensional Band Structure of Organic Metals (BDT-TTP) ₂ X (X = SbF ₆ , AsF ₆) Studied by Polarized Reflection Spectroscopy Band Structure of Organic Metal (BDT-TTP) ₂ ClO ₄ Studied by Polarized Reflection Spectroscopy Spectroscopic Study of Narrow-Band Organic Metal (BEDT-ATD) ₂ PF ₆ (THF) Charge Distribution in (Et ₄ N)(DMe-TCNQ) ₂ Crystal Studied by Raman and Reflection Spectroscopy Phase Transition of '-(BEDT-TTF) ₂ IBr ₂ Studied by Polarized Reflection and Raman Spectroscopy	78787879808182
е ра А. В.	Solid 1 2 Struce 1 2 3 4 5 6 7 8	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition of Metallic DMTSA-BF ₄ Charge-Transfer Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄ Two-Dimensional Band Structure of Organic Metals (BDT-TTP) ₂ X (X = SbF ₆ , AsF ₆) Studied by Polarized Reflection Spectroscopy Band Structure of Organic Metal (BDT-TTP) ₂ ClO ₄ Studied by Polarized Reflection Spectroscopy Spectroscopic Study of Narrow-Band Organic Metal (BEDT-ATD) ₂ PF ₆ (THF) Charge Distribution in (Et ₄ N)(DMe-TCNQ) ₂ Crystal Studied by Raman and Reflection Spectroscopy Phase Transition of '-(BEDT-TTF) ₂ IBr ₂ Studied by Polarized Reflection and Raman Spectroscopy BEDT-TTF Being Inserted into a Layered MnPS ₃	78787980818282
е ра А. В.	Solid 1 2 Struce 1 2 3 4 5 6 7 8 Theri	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄ Two-Dimensional Band Structure of Organic Metals (BDT-TTP) ₂ X (X = SbF ₆ , AsF ₆) Studied by Polarized Reflection Spectroscopy Band Structure of Organic Metal (BDT-TTP) ₂ ClO ₄ Studied by Polarized Reflection Spectroscopy Spectroscopic Study of Narrow-Band Organic Metal (BEDT-ATD) ₂ PF ₆ (THF) Charge Distribution in (Et ₄ N)(DMe-TCNQ) ₂ Crystal Studied by Raman and Reflection Spectroscopy Phase Transition of '-(BEDT-TTF) ₂ Br ₂ Studied by Polarized Reflection and Raman Spectroscopy BEDT-TTF Being Inserted into a Layered MnPS ₃ modynamic Study of Organic Conductors	7878798081828383
е ра А. В.	Solid 1 2 Struc 1 2 3 4 5 6 7 8 Theri	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄ Two-Dimensional Band Structure of Organic Metals (BDT-TTP) ₂ X (X = SbF ₆ , AsF ₆) Studied by Polarized Reflection Spectroscopy Band Structure of Organic Metal (BDT-TTP) ₂ ClO ₄ Studied by Polarized Reflection Spectroscopy Spectroscopic Study of Narrow-Band Organic Metal (BEDT-ATD) ₂ PF ₆ (THF) Charge Distribution in (Et ₄ N)(DMe-TCNQ) ₂ Crystal Studied by Raman and Reflection Spectroscopy Phase Transition of '-(BEDT-TTF) ₂ Br ₂ Studied by Polarized Reflection and Raman Spectroscopy BEDT-TTF Being Inserted into a Layered MnPS ₃ modynamic Study of Organic Conductors Thermodynamics of BEDT-TTF Based Dimeric Salts	7878798081828383
е ра А. В.	Solid 1 2 Struce 1 2 3 4 5 6 7 8 Theri	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(ASF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition of Metallic DMTSA-BF ₄ Charge-Transfer Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄ Two-Dimensional Band Structure of Organic Metals (BDT-TTP) ₂ X (X = SbF ₆ , AsF ₆) Studied by Polarized Reflection Spectroscopy Band Structure of Organic Metal (BDT-TTP) ₂ ClO ₄ Studied by Polarized Reflection Spectroscopy Spectroscopic Study of Narrow-Band Organic Metal (BEDT-ATD) ₂ PF ₆ (THF) Charge Distribution in (Et ₄ N)(DMe-TCNQ) ₂ Crystal Studied by Raman and Reflection Spectroscopy Phase Transition of '-(BEDT-TTF) ₂ IBr ₂ Studied by Polarized Reflection and Raman Spectroscopy BEDT-TTF Being Inserted into a Layered MnPS ₃ modynamic Study of Organic Conductors Thermodynamics of BEDT-TTF Based Dimeric Salts Cooling Rate Dependence of Low-Temperature Specific Heat	787879808181828383
е ра А. В.	Solid 1 2 Struce 1 2 3 4 5 6 7 8 Theri	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition of Metallic DMTSA-BF ₄ Charge-Transfer Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄ Two-Dimensional Band Structure of Organic Metals (BDT-TTP) ₂ X (X = SbF ₆ , AsF ₆) Studied by Polarized Reflection Spectroscopy Band Structure of Organic Metal (BDT-TTP) ₂ ClO ₄ Studied by Polarized Reflection Spectroscopy Spectroscopic Study of Narrow-Band Organic Metal (BEDT-ATD) ₂ PF ₆ (THF) Charge Distribution in (Et ₄ N)(DMe-TCNQ) ₂ Crystal Studied by Raman and Reflection Spectroscopy Phase Transition of '-(BEDT-TTF) ₂ IBr ₂ Studied by Polarized Reflection and Raman Spectroscopy BEDT-TTF Being Inserted into a Layered MnPS ₃ modynamic Study of Organic Conductors Thermodynamics of BEDT-TTF Based Dimeric Salts Cooling Rate Dependence of Low-Temperature Specific Heat of Deuterated -(BEDT-TTF) ₂ Cu[N(CN) ₂]Br	7878787980818182838383
е ра А. В.	Solid 1 2 Struce 1 2 3 4 5 6 7 8 Theri	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition of Metallic DMTSA-BF ₄ Charge-Transfer Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄ Two-Dimensional Band Structure of Organic Metals (BDT-TTP) ₂ X (X = SbF ₆ , AsF ₆) Studied by Polarized Reflection Spectroscopy Band Structure of Organic Metal (BDT-TTP) ₂ ClO ₄ Studied by Polarized Reflection Spectroscopy Spectroscopic Study of Narrow-Band Organic Metal (BEDT-ATD) ₂ PF ₆ (THF) Charge Distribution in (Et ₄ N)(DMe-TCNQ) ₂ Crystal Studied by Raman and Reflection Spectroscopy Phase Transition of '-(BEDT-TTF) ₂ IBr ₂ Studied by Polarized Reflection and Raman Spectroscopy BEDT-TTF Being Inserted into a Layered MnPS ₃ nodynamic Study of Organic Conductors Thermodynamics of BEDT-TTF Based Dimeric Salts Cooling Rate Dependence of Low-Temperature Specific Heat of Deuterated -(BEDT-TTF) ₂ Cu[N(CN) ₂]Br melectron Spectroscopy of Organic Solids in Vacuum Ultraviolet Region	7878787980818182838383
A. B.	Solid 1 2 Struc 1 2 3 4 5 6 7 8 Therr 1 2 Photo	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition of Metallic DMTSA-BF ₄ Charge-Transfer Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄ Two-Dimensional Band Structure of Organic Metals (BDT-TTP) ₂ X (X = SbF ₆ , AsF ₆) Studied by Polarized Reflection Spectroscopy Band Structure of Organic Metal (BDT-TTP) ₂ ClO ₄ Studied by Polarized Reflection Spectroscopy Spectroscopic Study of Narrow-Band Organic Metal (BEDT-ATD) ₂ PF ₆ (THF) Charge Distribution in (Et ₄ N)(DMe-TCNQ) ₂ Crystal Studied by Raman and Reflection Spectroscopy Phase Transition of '-(BEDT-TTF) ₂ IBr ₂ Studied by Polarized Reflection and Raman Spectroscopy BEDT-TTF Being Inserted into a Layered MnPS ₃ modynamic Study of Organic Conductors Thermodynamics of BEDT-TTF Based Dimeric Salts Cooling Rate Dependence of Low-Temperature Specific Heat of Deuterated -(BEDT-TTF) ₂ ClN(CN) ₂]Br Policy of the Photoemission Intensity Oscillation of C ₆₀	78787879808181828383838484
ера А. В.	Solid 1 2 Struce 1 2 3 4 5 6 7 8 Thern 1 2 Photo 1 Electric	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0,5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition of Metallic DMTSA-BF ₄ Charge-Transfer Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄ Two-Dimensional Band Structure of Organic Metals (BDT-TTP) ₂ X (X = SbF ₆ , AsF ₆) Studied by Polarized Reflection Spectroscopy Band Structure of Organic Metal (BDT-TTP) ₂ ClO ₄ Studied by Polarized Reflection Spectroscopy Spectroscopic Study of Narrow-Band Organic Metal (BEDT-ATD) ₂ PF ₆ (THF) Charge Distribution in (Et ₄ N)(DMe-TCNQ) ₂ Crystal Studied by Raman and Reflection Spectroscopy Phase Transition of '-(BEDT-TTF) ₂ Br ₂ Studied by Polarized Reflection and Raman Spectroscopy BEDT-TTF Being Inserted into a Layered MnPS ₃ nodynamic Study of Organic Conductors Thermodynamics of BEDT-TTF Based Dimeric Salts Cooling Rate Dependence of Low-Temperature Specific Heat of Deuterated -(BEDT-TTF) ₂ Cu[N(CN) ₂]Br relectron Spectroscopy of Organic Solids in Vacuum Ultraviolet Region Origin of the Photoemission Intensity Oscillation of C ₆₀ rical Conduction and its Related Properties of Organic Solids	78787879808181828383838484
ера А. В.	Solid 1 2 Struc 1 2 3 4 5 6 7 8 Therr 1 2 Photo	State Properties of Phthalocyanine Salts and Related Compounds Optical Spectra of the Single Crystals of Phthalocyanine Charge-Transfer Salts Co _x Ni _{1-x} Pc(AsF ₆) _{0.5} Optical, EPR, and Structural Properties of Solid Platinum Phthalocyanine in the Different Oxidation States of Electrochemical Process ture and Properties of Organic Conductors Nature of the Phase Transition of Metallic DMTSA-BF ₄ Charge-Transfer Transition Polarized Perpendicular to the Molecular Stack in 1:1 Metallic DMTSA-BF ₄ Two-Dimensional Band Structure of Organic Metals (BDT-TTP) ₂ X (X = SbF ₆ , AsF ₆) Studied by Polarized Reflection Spectroscopy Band Structure of Organic Metal (BDT-TTP) ₂ ClO ₄ Studied by Polarized Reflection Spectroscopy Spectroscopic Study of Narrow-Band Organic Metal (BEDT-ATD) ₂ PF ₆ (THF) Charge Distribution in (Et ₄ N)(DMe-TCNQ) ₂ Crystal Studied by Raman and Reflection Spectroscopy Phase Transition of '-(BEDT-TTF) ₂ IBr ₂ Studied by Polarized Reflection and Raman Spectroscopy BEDT-TTF Being Inserted into a Layered MnPS ₃ modynamic Study of Organic Conductors Thermodynamics of BEDT-TTF Based Dimeric Salts Cooling Rate Dependence of Low-Temperature Specific Heat of Deuterated -(BEDT-TTF) ₂ ClN(CN) ₂]Br Policy of the Photoemission Intensity Oscillation of C ₆₀	7878787980818182838383848485

F.		conductivity and Antiferromagnetism of -Type BETS Conductors Evidence of the Bulk Superconductor-to-Insulator Transition	-85
	1	in -BETS ₂ Fe _x Ga _{1-x} Cl ₄ (x 0.45)	0/
	2	III -DE132Fe _X Ua _{1-X} U ₄ (X U.43)	00
	2	Superconductor-to-Metal Transition in -BETS ₂ Fe _x Ga _{1-x} BrCl ₃ (x 0.1-0.2)	-86 07
	3	Temperature-Composition Phase Diagram of -BETS ₂ Fe _x Ga _{1-x} Cl ₄	-87
	4	Antiferromagnetic Ordering of Diluted Fe ³⁺ Spins in -BETS ₂ Fe _x Ga _{1-x} BrCl ₃ (x 0.1)	-87
	5	The x-Dependence of Antiferromagnetic Interaction between Fe ³⁺ Ions	
		in -BETS ₂ Fe _x Ga _{1-x} Cl ₄	-88
	6	Easy Axis Rotation of Antiferromagnetic Structure and Phase Diagram of -BETS ₂ FeBr _x Cl _{4-x} -	-88
	7	Systematic x-Dependence of the Crystal Structure and Magnetic and Electric Properties	
		of -BETS ₂ GaBr _x Cl _{4-x}	-89
G.	Struc	tural Studies at Low Temperature and High Pressure	-89
		High Pressure Structure of $[(C_2H_5)_2(CH_3)_2N][Pd(dmit)_2]_2$	
		Low-Temperature Structural Analysis of -(BETS) ₂ Cu _{5-x} I ₆	
H.	Electr	ical Properties of Molecular Crystals at High Pressure	-90
	1	Pressure-Temperature Phase Diagram of (TMTTF) ₂ PF ₆	-91
I.	Devel	opment of New Molecular Conductors	-91
	1	Novel Stable Metallic Salts Based on a Donor Molecule Containing Peri-Ditellurium Bridges, TMTTeN	-92
	2	Synthesis and Properties of a New Organic Donor Containing an Organic Radical Part: TEMPOET	
	3	Synthesis, Structure and Physical Properties of Tetraalkylammonium	12
	3	Bis(5,6-dihydro-1,4-dithiin-2,3-diselenolato)-nickelate, (R ₄ N)[Ni(ddds) ₂]	
		$(R = Me, Et \text{ and } n-Bu)$ and Neutral Complex $[Ni(ddds)_2]_2$	03
	4	Synthesis, Structure and Properties of a New Derivative of Sulfur-Bridged TTF Dimer	03
	-1 -5	Synthesis, Structures and Properties of a New Derivative of Suntif-Bridged TT Diffier Synthesis, Structures and Properties of an Unsymmetrical Donor Containing Pyradino-Ring	-93
	3	(PEDTTSeF) and Its Cation Radical Salts	04
	6	Development of Novel Organic Conductors Based on Tellurium Containing Donor Molecules	04
т			
J.		opment of Pulsed Field Gradient NMR Spectroscopy	-93 05
	1	Înversion of Self-Diffusion Anisotropy within a Smectic A Phase of Liquid Crystal	95
T.	<i>Z</i>	Ion Dynamics in Superionic Glasses by ⁷ Li NMR	95
K.		Transitions and Dynamical Ordering in Liquid Crystals	-96
	1	Complete Assignment of ¹³ C NMR Spectra and Determination	
		of Orientational Order Parameter for Antiferroelectric Liquid Crystal MHPOBC	
	2	Freezing of Intramolecular Motion around the Chiral Center of Antiferroelectric Liquid Crystal	
	_	as Evidenced by Transient Oscillation in ¹³ C- ¹ H Cross Polarization Dynamics	
	3	Transient ¹³ C- ¹ H Nuclear Overhauser Effect in Liquid Crystal	-96
	4	Asymmetrical Hindrance of Methylene Group Rotations about the Chiral Alkyl Chain Axis	
		in the Smectic A Phase of an Antiferroelectric Liquid Crystal as Observed by ² H-NMR	-97
	5	Molecular Rotation in Antiferroelectric Liquid Crystal	
		Studied by ¹³ C-NMR Spin-Lattice Relaxation Time Measurement	97
		Neutron Diffraction Study of a Reentrant Liquid Crystal	
		¹³ C NMR Study of a Reentrant Liquid Crystal	
L.	Electi	onic Properties of Alkali-Hydrogen-Carbon Systems	-98
	1	First-Principles Study on Structure and Electronic State of NaH-Graphite Ternary	
		Intercalation Compound	-98
	2	¹ H NMR Study in Na ₄ HC ₆₀ Superconductor	-99
	3	Structural and Electronic Properties of Hydrogen-Absorbed Alkali-C ₆₀ Compounds	.99
	4	<i>In-Situ</i> NMR Study of the Reaction Process in Alkali-Hydrogen-C ₆₀ Compounds	
	5	Synthesis and Structural Study of New Alkali-Hydrogen-C ₆₀ Compounds	
Μ.		etic Local Structure and Magnetic Interactions in Molecule	
	Rased	and Organic-Inorganic Hybrid Magnets	00
	1	Solid State ¹ H-MAS-NMR and Spin Densities	.00
	1	on Protons of the Organic Ferromagnetic Tempo Derivatives	ሰሰ
	2	Solid State High Perclution NMP Studies of Floatron Spin Densities	.00
	2	Solid State High Resolution NMR Studies of Electron Spin Densities in Charge-Transfer Complex-Based Organic Ferromagnets	00
	2		UU
	3	Magic Angle Spinning ¹ H-NMR Study of the Spin Density Distribution	01
		of Pyridyl Nitronyl Nitroxides in the Crystalline Phase	UI
	4	Solid State High Resolution Deuterium NMR Study of Electron Spin Density Distribution	0.1
	_	of Hydrogen-bonded Organic Ferromagnetic Compound 4-Hydroxyimino-TEMPO1	
	5	Local Magnetic Structure of Layered Compounds Cu ₂ (OD) ₃ X with Exchangeable Acid Anion 2	
		Studied by Solid State High Resolution Deuterium NMR	01

N.	Proto	on Transfer Tunneling in Interacting Hydrogen Bonds in the Solid State	-102
	1	Observation of Thermal Tautomerism of Thermochromic Salicylidene-Aniline Derivatives	
	2	in the Solid State by ¹⁵ N CPMAS NMR down to Cryogenic Temperatures	-102
	2	Proton Dynamics in Interacting Hydrogen Bonds in the Solid State: Proton Tunneling in the NHO Hydrogen Bonds of N,N'-Di(2-hydroxy-1-naphthylmethylene)-p-phenylenediamine	102
		NHO Hydrogen Bonds of N,N -Di(z-nydroxy-1-naphunylmethylene)-p-phenylenediamine	-102
RESE	ARC	H ACTIVITIES V	
Dep	artm	ent of Applied Molecular Science	-103
	Molo	oular Machanisms of Ovygon Activation by Hama Engumes	102
Α.	1 v101e 0	cular Mechanisms of Oxygen Activation by Heme Enzymes On the Formation and Reactivity of Compound I of the His64 Myoglobin Mutants	-103
		Effects of the Location of Distal Histidine in the Reaction of Myoglobin	103
		with Hydrogen Peroxide	-103
	3	Mechanistic Studies of Suicidal meso-Oxidation of Novel Iron Porphyrin Complexes	
		as Models for the Formation of -Meso-Hydroxyheme by Heme Oxygenase	-104
	4		104
R	Mole	Generation and Stabilization of Transient Catalytic Intermediates at Low Temperaturecular Mechanisms of Substrate Metabolism by Heme Enzymes	104
ъ.	1	The Mechanisms of N-Demethylation Catalyzed by Heme Enzymes: Direct Observation of	-104
	•	N-Demethylation by Compound I of Horseradish Peroxidase and Its Model Complex	-104
	2	Effects of the Arrangement of a Distal Catalytic Residue on Regioselectivity and Reactivity	
		in the Coupled Oxidation of Sperm Whale Myoglobin Mutants	-105
C.		el Studies of Non-heme Proteins	
		A Model Complex for an Active Form of Soybean Lipoxygenase-1Functional Model Chemistry for Manganese(II)-Dependent Catechol Dioxygenases	
D		sition Metal Oxide Clusters	
Σ.	1	Direct Observation by Electrospray Ionization Mass Spectrometry of a Key Transient	100
		Intermediate in the Formation of a Double Bookshelf-Type Oxide Cluster	-106
Е.	Aque	ous Organometallic Chemistry	107
	1	Synthesis and Structure of a New Water Soluble Rhodium(III) Complex	-107
r.	Const	truction of New Molecule-Based Magnets Tacticity vs. Dimension of the Extended Structures in the Crystals of Heterospin Magnets	107
	1	Made of Transition Metal Complexes with Poly(aminoxyl) Radical	108
	2		100
		between the Trinitroxide Radical and Bis(Hexafluoroacetylacetonato)Manganese(II)	-109
	3	Magnetic Properties of Polymeric Chain Complex	
a	G 41	Made by 5-Bromo-1,3-Bis(<i>N</i> -tert-butyl- <i>N</i> -oxy-amino)benzene and Cu(II)(hfac) ₂	-109
G.		nesis of Chiral Molecule-Based MagnetsSynthesis and Magnetic Properties of Chiral Organic Triplet Bisaminoxyl Radical	-110
	1 2	A Chiral Molecule-Based Metamagnet	-110
	2	Made by Chiral Triplet Organic Radical and Manganese Ion	-111
Н.	Synth	nesis and Characterization of Light Induced Spin-Crossover Complexes	
	1	Synthesis and Magnetic Properties of Binuclear Iron(III) Complex	
_	G 43	Containing Photoisomerization Ligand	-112
I.	Synth	nesis and Characterization of Quantum-Spin Systems	-112
	1	Ground State Properties of One- and Two-Dimensional Antiferromagnetic Heisenberg Spin Systems Made of Stable Organic Biradicals	112
	2	Construction of One-dimensional Chain and Railroad-Trestle Using Organic Radicals	
J.	Press	ure Effects on Molecular Magnetism	113
	1	Pressure Effects on Organic Radicals with Ferromagnetic and Antiferromagnetic Interactions	-114
**	2	Pressure Effect on Mn Complexes of Bisaminoxyl Radicals	-114
K.		Charge-Transfer Complexes Exhibiting Novel Magnetic Properties	-114
	1	1:2 Dimethyl-Substituted Tetracyanoquinodimethane/Its Radical Anion Mixed Salts: Ferromagnetic Behavior and High Electrical Conductivity at Room Temperature	_115
	2	Room-Temperature Ferromagnetic Behavior in 2,5-Diethyltetracyanoquinodimethanide Salts	
	3		
		and Diethyl-Substituted Tetracyanoquinodimethanes, and Tetracyanonaphthoquinodimethane	
	4	Synthesis and Electrical Conducting Properties of Unsymmetrical Spiro Compounds	
	_	Bearing a Tetrathiafulvalenyl Group	-116
	5	Synthesis, and Electrical Conducting and Magnetic Properties of Neutral Bis(tetrathiafulvalenyldithiolato) Cobalt Complexes	_116
T	Desor	eption Induced by Electronic Transitions at the Surface of Van der Waals Condensates	
2.		Exciton Induced Desorption at the Surface of Rare Gas Solids	

		Desorption of Metastable Particles Induced by Electronic Excitation	117
	•	at the Surface of Rare Gas Solid with Hydrogen Physisorbed	117/
	3	Desorption of an Excimer from the Surface of Solid Ne by Low Energy Electron	
		and Photon Impact	117/
Μ.	Synth	esis and Physical Properties of Novel Molecular Metals	117
	1	Structural Feature of Radical Cation Salts Based on TTP and Its Selenium Analogs	117
	2	Novel Oxygen Containing -Electron Donors for Organic Metals:	
		2-(1,3-Dithiol-2-ylidene)-5-(pyran-4-ylidene)-1,3,4,6-tetrathiapentalenes	118
	3	Structures and Physical Properties of TMEO-ST-TTP Salts	119
	4	Preparation and Properties of Gold Complexes with TTF-Dithiolato Ligands	119
N.	Theo	retical Study of the Electronic Structures of Weakly Bound Molecules	119
	1	Multi-Reference Coupled Pair Approximation (MRCPA) Calculations	
		for the Ground State of the ArI ₂ Complex	120
	2	Ab Initio Study of the Ground and Excited States of ArHF	120
	3	Ab Initio Molecular Orbital Study of Fe(CO) _n ($n = 1, 2, \text{ and } 3$)	120
		cular Dynamics Study Using Potentials by <i>Ab Initio</i> Molecular Orbital Calculations	120
J.	Mole		120
	1	Molecular Dynamics Study of Liquid Mercury in the Density Region between Metal and Nonmetal	100
	_		
	2	Molecular Dynamics Study for the Liquid-Vapor Coexistence Curve of Mercury	
	Struc	tures and Dynamics of Negatively-Charged Molecular Clusters	
	1	Formation of $N_3O_3^-$ anion in $(NO)_n^-$: Photoelectron Spectroscopy and <i>Ab Initio</i> Calculations	121
	2	Coexistence of Electronic Isomers in $[(CO_2)_nROH]^-$: Photoelectron Spectroscopy	
		and Ab Initio Calculations	122
	3	Relaxation of Photoexcited $(C_6F_6)_n$ Using Time-Resolved Photoelectron Spectroscopy	123
).		neter-Wave Spectroscopy Combined with Pulsed-Jet Expansion Technique	
		e Detection of the Novel Unstable Species	
	and t	he van der Waals Mode Transitions of Molecular Clusters	123
	and t	Direct Absorption Observation of the van der Waals Bending Band of the ArDCN Cluster by	123
	1	Direct Absorption Observation of the van der waats behalf the Proposition of the AIDCN Cluster by	100
	2	Millimeter-Wave Spectroscopy Combined with Pulsed-Jet Expansion Technique	123
	2	Millimeter-Wave Spectroscopy of the Iron Carbonyl Radical (FeCO) in the 2 State	124
•	Ion-N	Iolecule Reactions in the Troposphere	124
	1	Development of High-Resolution Ion Mobility/Mass Spectrometer	
E A	ARC	for the Study of Ion-Molecule Reactions in the Troposphere H ACTIVITIES VI	125
		H ACTIVITIES VI	
)	artm	H ACTIVITIES VI ent of Vacuum UV Photoscience	126
pa	artm Elect	H ACTIVITIES VI ent of Vacuum UV Photoscience conic Structure and Decay Mechanism of Inner-Shell Excited Molecules	126
)	artm	ent of Vacuum UV Photoscience ronic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the O1s 3p u Rydberg Excited States of CO2	126 126 126
pa	Electron 2	ent of Vacuum UV Photoscience	126 126 126
•	artm Elect	ent of Vacuum UV Photoscience	126 126 126
6	Electron 2	ent of Vacuum UV Photoscience	126 126 126
วล	Electron 2	ent of Vacuum UV Photoscience	126 126 126 126
pa	Electron 2 3	ent of Vacuum UV Photoscience	126 126 126 126
วล	Electron 2 3	ent of Vacuum UV Photoscience	126 126 126 127
pa	Electron 1 2 3 4	ent of Vacuum UV Photoscience	126 126 126 127
pa A.	Electron 1 2 3 4 5 5	ent of Vacuum UV Photoscience	126 126 126 127 127
р а Л.	Electron 1 2 3 4 5 5	ent of Vacuum UV Photoscience	126 126 126 127 127
pa A.	Electron 2 3 4 5 Soft 2 of Tra	ent of Vacuum UV Photoscience	126 126 126 127 127
р а Л.	Electron 1 2 3 4 5 5	ent of Vacuum UV Photoscience	12e 12e 12e 127 127 127
	Electron 2 3 4 5 Soft 2 of Tr. 1	ent of Vacuum UV Photoscience	12e 12e 12e 127 127 128 ra
	Electron 2 3 4 5 Soft 2 of Tr. 1 2	ent of Vacuum UV Photoscience Fonic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the O1s 3p u Rydberg Excited States of CO2 Renner-Teller Splitting in the C1s * Excited States of CS2, OCS, and CO2 Kinetic Energy Dependence of the Anisotropy Parameters for the Fragmentation of the C1s Excited States of C2H4 Kinetic Energy Dependence of Anisotropic Yields of Ionic Fragmentations Following S 1s Excitations of SO2 Direct Determination of Partial Waves Contributions in the * Shape Resonance in CO Molecules	126126127127127128128128
	Electron 2 3 4 5 Soft 2 of Tr. 1	ent of Vacuum UV Photoscience Conic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the O1s 3p u Rydberg Excited States of CO2 Renner-Teller Splitting in the C1s * Excited States of CS2, OCS, and CO2 Kinetic Energy Dependence of the Anisotropy Parameters for the Fragmentation of the C1s Excited States of C2H4 Kinetic Energy Dependence of Anisotropic Yields of Ionic Fragmentations Following S 1s Excitations of SO2 Direct Determination of Partial Waves Contributions in the * Shape Resonance in CO Molecules C-Ray Photoelectron-Photoabsorption Spectroscopy and Electronic Structure ansition Metal Compounds Metal-to-Ligand Charge Transfer Bands Observed in Polarized Ni 2p Photoabsorption Spectro of [Ni(mnt)2] ²⁻ Polarized Ni 1s and 2p, and S 1s Photoabsorption Spectra of [Ni(III)(mnt)2] ¹⁻ Strong Pre-Edge Peaks Found in Ni 1s Photoabsorption Spectra of Ni Planar Complexes	126126127127127128128128
	Electron 2 3 4 5 Soft 2 of Tr. 1 2	ent of Vacuum UV Photoscience Fronic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the O1s 3p u Rydberg Excited States of CO2 Renner-Teller Splitting in the C1s * Excited States of CS2, OCS, and CO2 Kinetic Energy Dependence of the Anisotropy Parameters for the Fragmentation of the C1s Excited States of C2H4 Kinetic Energy Dependence of Anisotropic Yields of Ionic Fragmentations Following S 1s Excitations of SO2	126126127127127128128129
	Electron 2 3 4 5 Soft 2 of Tr. 1 2 3	ent of Vacuum UV Photoscience Fonic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the O1s 3p u Rydberg Excited States of CO2 Renner-Teller Splitting in the C1s * Excited States of CS2, OCS, and CO2 Kinetic Energy Dependence of the Anisotropy Parameters for the Fragmentation of the C1s Excited States of C2H4 Kinetic Energy Dependence of Anisotropic Yields of Ionic Fragmentations Following S 1s Excitations of SO2 Direct Determination of Partial Waves Contributions in the * Shape Resonance in CO Molecules K-Ray Photoelectron-Photoabsorption Spectroscopy and Electronic Structure ansition Metal Compounds	126126127127127128128128129
	Electron 2 3 4 5 Soft 2 of Tr. 1 2 3	ent of Vacuum UV Photoscience Fonic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the O1s 3p u Rydberg Excited States of CO2 Renner-Teller Splitting in the C1s * Excited States of CS2, OCS, and CO2 Kinetic Energy Dependence of the Anisotropy Parameters for the Fragmentation of the C1s Excited States of C2H4 Kinetic Energy Dependence of Anisotropic Yields of Ionic Fragmentations Following S 1s Excitations of SO2 Direct Determination of Partial Waves Contributions in the * Shape Resonance in CO Molecules K-Ray Photoelectron-Photoabsorption Spectroscopy and Electronic Structure ansition Metal Compounds	126126127127127128128128129
р а А.	Electron 1 2 3 4 5 Soft 2 3 4 5 5	ent of Vacuum UV Photoscience Fonic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the O1s 3p u Rydberg Excited States of CO2 Renner-Teller Splitting in the C1s * Excited States of CS2, OCS, and CO2 Kinetic Energy Dependence of the Anisotropy Parameters for the Fragmentation of the C1s Excited States of C2H4 Kinetic Energy Dependence of Anisotropic Yields of Ionic Fragmentations Following S 1s Excitations of SO2 Direct Determination of Partial Waves Contributions in the * Shape Resonance in CO Molecules	126 126 127 127 127 128 a 128 129
pa A.	Electron 2 3 4 5 Soft 2 of Tron 1 2 3 4 5 Studi	ent of Vacuum UV Photoscience Fronic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the O1s 3p u Rydberg Excited States of CO2 Renner-Teller Splitting in the C1s * Excited States of CS2, OCS, and CO2 Kinetic Energy Dependence of the Anisotropy Parameters for the Fragmentation of the C1s Excited States of C2H4 Kinetic Energy Dependence of Anisotropic Yields of Ionic Fragmentations Following S 1s Excitations of SO2 Direct Determination of Partial Waves Contributions in the * Shape Resonance in CO Molecules Aray Photoelectron-Photoabsorption Spectroscopy and Electronic Structure ansition Metal Compounds Metal-to-Ligand Charge Transfer Bands Observed in Polarized Ni 2p Photoabsorption Spectro of [Ni(mnt) ₂] ²⁻ Polarized Ni 1s and 2p, and S 1s Photoabsorption Spectra of [Ni(III)(mnt) ₂] ¹⁻ Strong Pre-Edge Peaks Found in Ni 1s Photoabsorption Spectra of Ni Planar Complexes Effect of Intermolecular Interaction on Resonant Behavior of Satellite Photoelectrons in Ni Planar Complexes Resonant Photoelectron Spectra of Ni Metal Following the Ni 2p Excitation Beson Primary Photochemical/bhysical Processes	126126127127127128128128129
р а А.	Electron 1 2 3 4 5 Studi Using	ent of Vacuum UV Photoscience conic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the O1s 3p uRydberg Excited States of CO2 Renner-Teller Splitting in the C1s * Excited States of CS2, OCS, and CO2 Kinetic Energy Dependence of the Anisotropy Parameters for the Fragmentation of the C1s Excited States of C2H4 Kinetic Energy Dependence of Anisotropic Yields of Ionic Fragmentations Following S 1s Excitations of SO2 Direct Determination of Partial Waves Contributions in the * Shape Resonance in CO Molecules	126126127127127128128128129130
P a	Electron 1 2 3 4 5 Studi Using 1	ent of Vacuum UV Photoscience conic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the O1s 3p u Rydberg Excited States of CO2 Renner-Teller Splitting in the C1s * Excited States of CS2, OCS, and CO2 Kinetic Energy Dependence of the Anisotropy Parameters for the Fragmentation of the C1s Excited States of C2H4 Kinetic Energy Dependence of Anisotropic Yields of Ionic Fragmentations Following S 1s Excitations of SO2 Direct Determination of Partial Waves Contributions in the * Shape Resonance in CO Molecules	126126127127127128128129130
pa A.	Electron 1 2 3 4 5 Studi Using	ent of Vacuum UV Photoscience Fonic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the O1s 3p uRydberg Excited States of CO2 Renner-Teller Splitting in the C1s * Excited States of CS2, OCS, and CO2 Kinetic Energy Dependence of the Anisotropy Parameters for the Fragmentation of the C1s Excited States of C2H4 Kinetic Energy Dependence of Anisotropic Yields of Ionic Fragmentations Following S 1s Excitations of SO2 Direct Determination of Partial Waves Contributions in the * Shape Resonance in CO Molecules	126126127127127128128129130131
P a	Electr 1 2 3 4 5 Soft 2 of Tr. 1 2 3 4 5 Studi Using 1 2	ent of Vacuum UV Photoscience Fonic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the O1s 3p uRydberg Excited States of CO2 Renner-Teller Splitting in the C1s * Excited States of CS2, OCS, and CO2 Kinetic Energy Dependence of the Anisotropy Parameters for the Fragmentation of the C1s Excited States of C2H4 Kinetic Energy Dependence of Anisotropic Yields of Ionic Fragmentations Following S 1s Excitations of SO2	126126127127127128128129130131
	Electron 1 2 3 4 5 Studi Using 1	ent of Vacuum UV Photoscience Antisymmetric Stretching Vibrations in the O1s 3p u Rydberg Excited States of CO2	126126127127127128128129130131
ра А.	Electr 1 2 3 4 5 Soft 2 of Tr. 1 2 3 4 5 Studi Using 1 2	ent of Vacuum UV Photoscience Sonic Structure and Decay Mechanism of Inner-Shell Excited Molecules Antisymmetric Stretching Vibrations in the Ols 3p uRydberg Excited States of CO2 Renner-Teller Splitting in the Cls *Excited States of CS2, OCS, and CO2 Renner-Teller Splitting in the Cls *Excited States of CS2, OCS, and CO2 Renner-Teller Splitting in the Cls Excited States of CS2, OCS, and CO2 Renner-Teller Splitting in the Cls Excited States of C2H4 Kinetic Energy Dependence of the Anisotropy Parameters for the Fragmentation of the Cls Excited States of C2H4 Kinetic Energy Dependence of Anisotropic Yields of Ionic Fragmentations Following S 1s Excitations of SO2 Direct Determination of Partial Waves Contributions in the *Shape Resonance in CO Molecules K-Ray Photoelectron-Photoabsorption Spectroscopy and Electronic Structure ansition Metal Compounds Metal-to-Ligand Charge Transfer Bands Observed in Polarized Ni 2p Photoabsorption Spectr of [Ni(mnt)2] ² Strong Pre-Edge Peaks Found in Ni 1s Photoabsorption Spectra of Ni Planar Complexes Effect of Intermolecular Interaction on Resonant Behavior of Satellite Photoelectrons in Ni Planar Complexes Resonant Photoelectron Spectra of Ni Metal Following the Ni 2p Excitation ses on Primary Photochemical/physical Processes Femtosecond Time-Resolved Electronic Spectroscopy Generation of a Femtosecond Pulse in the Near- to Mid-Infrared Region Femtosecond Time-Resolved Electronic Spectroscopy Generation of Biblenyl Fluorescence by Carbon Tetrachloride	126126127127127128128129130131131
A.	Electron 1 2 3 4 5 Soft 2 3 4 5 Studi Using 1 2 3 3	ent of Vacuum UV Photoscience Antisymmetric Stretching Vibrations in the O1s 3p u Rydberg Excited States of CO2	126126127127127128128129130131131

		Femtosecond Fluorescence from the Higher Excited State of Tetracene	
	6	Ultrafast Relaxation Dynamics of Photoexcited Cu(II)(TMpy-P4) in Water	-134
D.		es on Photochemical Reactions	
	Using	Picosecond Time-Resolved Vibrational Spectroscopy	-134
	1	Vibrational Dynamics in the Lowest Excited Triplet State Immediately	
		after Intersystem Crossing	-134
	2	Cis-Trans Photoisomerization Mechanism of Retinal Studied by Picosecond Time-Resolved	
		Raman Spectroscopy	-135
	3	Vibrational Cooling Dynamics of Solvated Structures of para-Nitroaniline in Acetonitrile	
Ε.		opment of Time-Resolved Spectroscopy Using Synchrotron Radiation	-136
	1	Trial to Measure Time-Resolved Far-Infrared Spectra of '-(BEDT-TTF) ₂ ICl ₂	
		Using Synchrotron Radiation	-136
F.	Synch	rotron Radiation Stimulated Surface Reactions	-137
	1	The Direct Observation of Synchrotron Radiation Stimulated Desorption of Thin SiO ₂ Films	
		on Si (111) by Scanning Tunneling Microscopy	-137
	2	Chemisorption of Deuterium on an Ultrathin Ge Film Deposited over Si(100)-2×1:	
		Existence of a Dihydride Phase	-138
	3	Structure of Hydrogen Terminated Si(100) Surfaces and Modification	
		by Synchrotron Radiation Irradiation	-138
	4	Design and Performance of a Multilayered Mirror Monochromator in the Low Energy Region of Vacuum Ultra Violet	
	_	in the Low Energy Region of Vacuum Ultra Violet	-138
	5	Construction of the Multilayered-Mirror Monochromator and the Beam Line	
	_	for the Study of Synchrotron Radiation Stimulated Process	-139
~	6	Influence of Residual Fluorine Gases on the Adsorption of Atomic H on Si(100)-2×1 Surfaces	139
G.	Ion D	esorption Induced by Core-Electron Transitions Studied by Electron Ion Coincidence	4.40
		roscopy Combined with Synchrotron Radiation	-140
	1		
		with Synchrotron Radiation for the Study of Ion Desorption Mechanism in the Region of Resonant Transitions of Condensed H ₂ O	1.40
	2	in the Region of Resonant Transitions of Condensed H ₂ O	-140
	2	Study of Ion Desorption Induced by Resonant Core-Electron Excitation	
		of Isolated NH ₃ Monolayer Adsorbed on a Xe Film Using Auger Electron Photoion Coincidence Spectroscopy	1 / 1
	DI 4		-141
и			
Н.	Comb	ionization Dynamics Studied by Electron Spectroscopy	1./1
Н.	Comb	oined with a Continuous Synchrotron Radiation Source	-141
н.	Comb	bined with a Continuous Synchrotron Radiation Source	
	Comb	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141
	Comb 1 Laser	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141
	Comb 1 Laser	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142
	Comb	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142
	Comb	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142
I.	Comb	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142
I.	Combon 1 Laser 1 2 Vacua	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143
I.	Combon 1 Laser 1 2 Vacua	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS Photionization of Polarized Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization of Polarized Ar Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Mode-Locked or Pulsed UV Laser	-141 -142 -142 -143
I.	Combon 1 Laser 1 2 Vacua	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143
I.	Combon 1 Laser 1 2 Vacua	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143 -143
I.	Comband 1 Laser 1 2 Vacua and a 1	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143 -143
I.	Comband 1 Laser 1 2 Vacua and a 1	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143 -143
I.	Comband 1 Laser 1 2 Vacuand a 1 2 3	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143 -143 -144
I.	Comband 1 Laser 1 2 Vacuand a 1 2 3	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143 -143 -144
I.	Comband 1 Laser 1 2 Vacua and a 1 2 Mono	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143 -143 -144 -144 -144
I. J.	Comband 1 Laser 1 2 Vacua and a 1 2 3 Monoto 1	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143 -143 -144 -144 -145 -145
I. J.	Comband 1 Laser 1 2 Vacua and a 1 2 3 Monoto 1	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143 -143 -144 -144 -145 -145
I. J.	Comband 1 Laser 1 2 Vacua and a 1 2 3 Mono 1 Ultra	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143 -143 -144 -144 -145 -145
I. J.	Comband 1 Laser 1 2 Vacua and a 1 2 3 Mono 1 Ultra	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS Photionization of Polarized Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization of Polarized Ar Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Mode-Locked or Pulsed UV Laser Pump-Probe Spectroscopy of N2 and N2O by Using a Laser-Synchrotron Radiation Combination Technique Apparatus for Resonance Enhanced Multiphoton Ionization Spectroscopy of Neutral Fragments Produced by VUV Photoexcitation Laser Spectroscopy of Neutral Fragments from Superexcited States Prepared by Synchrotron-Radiation Photoexcitation Chromator Newly Developed on Beamline BL2B2 in UVSOR Design of an 18 m Spherical Grating Monochromator at UVSOR Posign of Spectroscopy on Organic Thin Films Using Synchrotron Radiation Angle-Resolved UV Photoelectron Spectra (UPS) of Thin Films of Perylene-3,4,9, 10- Tetracarboxylic Dianhydride on MoS2 Temperature Dependence of Photoelectron Angular Distribution	-141 -142 -142 -143 -143 -143 -144 -144 -145 -145 -145
I. J.	Comband 1 Laser 1 2 Vacuate and a 1 2 3 Monoral Ultra 1	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143 -143 -144 -144 -145 -145 -146
I. J.	Comband 1 Laser 1 2 Vacuate and a 1 2 3 Monoral Ultra 1	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS	-141 -142 -142 -143 -143 -144 -144 -145 -145 -146
I. J.	Comband 1 Laser 1 2 Vacuand a 1 2 3 Monoral Ultra 1 2	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS Photionization of Polarized Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization of Polarized Ar Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Mode-Locked or Pulsed UV Laser Pump-Probe Spectroscopy of N2 and N2O by Using a Laser-Synchrotron Radiation Combination Technique Apparatus for Resonance Enhanced Multiphoton Ionization Spectroscopy of Neutral Fragments Produced by VUV Photoexcitation Laser Spectroscopy of Neutral Fragments from Superexcited States Prepared by Synchrotron-Radiation Photoexcitation Chromator Newly Developed on Beamline BL2B2 in UVSOR Design of an 18 m Spherical Grating Monochromator at UVSOR Wiolet Photoelectron Spectroscopy on Organic Thin Films Using Synchrotron Radiation Angle-Resolved UV Photoelectron Spectra (UPS) of Thin Films of Perylene-3,4,9, 10- Tetracarboxylic Dianhydride on MoS2 Temperature Dependence of Photoelectron Angular Distribution from Thin Films of Chloroaluminum Phthalocyanine on MoS2 Photoemission Study of Pristine and Photodegraded Poly(Methyl Methacrylate) Site-Specific Chemical-Bond Scission in Poly(Methyl Methacrylate)	-141 -142 -143 -143 -143 -144 -144 -145 -145 -146 -146
I. J.	Comband 1 Laser 1 2 Vacuand a 1 2 3 Monoral 1 Ultra 1 2 3	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS Photionization of Polarized Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization of Polarized Ar Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Mode-Locked or Pulsed UV Laser Pump-Probe Spectroscopy of N2 and N2O by Using a Laser-Synchrotron Radiation Combination Technique Apparatus for Resonance Enhanced Multiphoton Ionization Spectroscopy of Neutral Fragments Produced by VUV Photoexcitation Laser Spectroscopy of Neutral Fragments from Superexcited States Prepared by Synchrotron-Radiation Photoexcitation Chromator Newly Developed on Beamline BL2B2 in UVSOR Design of an 18 m Spherical Grating Monochromator at UVSOR wiolet Photoelectron Spectroscopy on Organic Thin Films Using Synchrotron Radiation Angle-Resolved UV Photoelectron Spectra (UPS) of Thin Films of Perylene-3,4,9, 10- Tetracarboxylic Dianhydride on MoS2 Temperature Dependence of Photoelectron Angular Distribution from Thin Films of Chloroaluminum Phthalocyanine on MoS2 Photoemission Study of Pristine and Photodegraded Poly(Methyl Methacrylate) Site-Specific Chemical-Bond Scission in Poly(Methyl Methacrylate) by Inner Shell Excitation	-141 -142 -143 -143 -143 -144 -144 -145 -145 -146 -146
I. J.	Comband 1 Laser 1 2 Vacuand a 1 2 3 Monoral 1 Ultra 1 2 3	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS Photionization of Polarized Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization of Polarized Ar Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Mode-Locked or Pulsed UV Laser Pump-Probe Spectroscopy Making Use of a Combination of Synchrotron Radiation Mode-Locked or Pulsed UV Laser Pump-Probe Spectroscopy of N2 and N2O by Using a Laser-Synchrotron Radiation Combination Technique Apparatus for Resonance Enhanced Multiphoton Ionization Spectroscopy of Neutral Fragments Produced by VUV Photoexcitation Laser Spectroscopy of Neutral Fragments from Superexcited States Prepared by Synchrotron-Radiation Photoexcitation Lechromator Newly Developed on Beamline BL2B2 in UVSOR Design of an 18 m Spherical Grating Monochromator at UVSOR Violet Photoelectron Spectroscopy on Organic Thin Films Using Synchrotron Radiation Angle-Resolved UV Photoelectron Spectra (UPS) of Thin Films of Perylene-3,4,9, 10- Tetracarboxylic Dianhydride on MoS2 Temperature Dependence of Photoelectron Angular Distribution from Thin Films of Chloroaluminum Phthalocyanine on MoS2 Photoemission Study of Pristine and Photodegraded Poly(Methyl Methacrylate) by Inner Shell Excitation Study of Solid Surfaces by Metastable Electron Emission Microscopy: Energy-Filtered Image.	-141 -142 -143 -143 -143 -144 -145 -145 -146 -146 s
I. J.	Comband 1 Laser 1 2 Vacua and a 1 2 3 Mono 1 Ultra 1 2 3 4	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS Photionization of Polarized Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization of Polarized Ar Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Mode-Locked or Pulsed UV Laser Pump-Probe Spectroscopy of N2 and N2O by Using a Laser-Synchrotron Radiation Combination Technique Apparatus for Resonance Enhanced Multiphoton Ionization Spectroscopy of Neutral Fragments Produced by VUV Photoexcitation Laser Spectroscopy of Neutral Fragments from Superexcited States Prepared by Synchrotron-Radiation Photoexcitation Lochromator Newly Developed on Beamline BL2B2 in UVSOR Design of an 18 m Spherical Grating Monochromator at UVSOR wiolet Photoelectron Spectroscopy on Organic Thin Films Using Synchrotron Radiation Angle-Resolved UV Photoelectron Spectra (UPS) of Thin Films of Perylene-3,4,9, 10- Tetracarboxylic Dianhydride on MoS2 Temperature Dependence of Photoelectron Angular Distribution from Thin Films of Chloroaluminum Phthalocyanine on MoS2 Photoemission Study of Pristine and Photodegraded Poly(Methyl Methacrylate) Site-Specific Chemical-Bond Scission in Poly(Methyl Methacrylate) by Inner Shell Excitation Study of Solid Surfaces by Metastable Electron Emission Microscopy: Energy-Filtered Image and Local Electron Spectra at the Outermost Surface Layer of Silicon Oxide on Si(100)	-141 -142 -143 -143 -143 -144 -145 -145 -146 -146 s
I. J.	Comband 1 Laser 1 2 Vacua and a 1 2 3 Mono 1 Ultra 1 2 3 4	Spectator- and Participant-Like Behavior of a Rydberg Electron on Predissociation of Superexcited States of OCS Photionization of Polarized Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization of Polarized Ar Atoms Produced by Excitation with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Laser Photoionization Electron Spectroscopy of Polarized Kr Atoms Excited with Synchrotron Radiation Mode-Locked or Pulsed UV Laser Pump-Probe Spectroscopy Making Use of a Combination of Synchrotron Radiation Mode-Locked or Pulsed UV Laser Pump-Probe Spectroscopy of N2 and N2O by Using a Laser-Synchrotron Radiation Combination Technique Apparatus for Resonance Enhanced Multiphoton Ionization Spectroscopy of Neutral Fragments Produced by VUV Photoexcitation Laser Spectroscopy of Neutral Fragments from Superexcited States Prepared by Synchrotron-Radiation Photoexcitation Lechromator Newly Developed on Beamline BL2B2 in UVSOR Design of an 18 m Spherical Grating Monochromator at UVSOR Violet Photoelectron Spectroscopy on Organic Thin Films Using Synchrotron Radiation Angle-Resolved UV Photoelectron Spectra (UPS) of Thin Films of Perylene-3,4,9, 10- Tetracarboxylic Dianhydride on MoS2 Temperature Dependence of Photoelectron Angular Distribution from Thin Films of Chloroaluminum Phthalocyanine on MoS2 Photoemission Study of Pristine and Photodegraded Poly(Methyl Methacrylate) by Inner Shell Excitation Study of Solid Surfaces by Metastable Electron Emission Microscopy: Energy-Filtered Image.	-141 -142 -143 -143 -143 -144 -144 -145 -145 -146 -146 s

7	Photon Stimulated Ion Desorption of Deuterated Polystyrene Thin Films	
	Induced by Core Excitation	-147
8	Characterization of Self-Assembled Monolayer of Thiophenol on Gold	
	by Penning Ionization Electron Spectroscopy	-147
9	High-Resolution Electron Energy Loss Spectroscopy	
	of Chloroalminum Phthalocyanine Ultrathin Films	-147
10	Angle-Resolved UPS Study and Simulation with IAC Approximation	
	for Oriented Monolayer of Tetratetracontane (n-C ₄₄ H ₉₀) on Cu (100)	147
M. Form	ation of Nanometer-Scale InAs Island on GaP (001) Substrate	-148
	Nanometer-Scale InAs Islands Grown on GaP (001) by Organometallic Vapor Phase Epitaxy	-148
2	Effects of Post Annealing on Self-organized InAs Islands Grown on (001) GaP	
	by Organometallic Vapor Phase Epitaxy	-148
N. Desor	ption Induced by Electronic Transitions (DIET) from Cryogenic Surfaces	-149
1	Absolute Desorption Yield of Metastable Atoms from the Surface of Solid Rare Gases	
	Induced by Exiton Creation	-149
2	Long Lifetime Emission of the Excited Species Ejected from the Surface of Solid Ne	-149
	ture and Vibrational Spectra of Molecules Physisorbed on Metal Surfaces	
1	Upgraded Infrared Beamline BL6A1 at UVSOR	149
2	Development of High Sensitivity EELS	-150
3	Electronic Structure of a Pt(111)-Ge Surface Alloy and Adsorbed CO	-150
4	LEED and STM Measurement of NO /Pt(111) at Low Temperature	-150
RESEARC	H ACTIVITIES VII	
Coordina	ation Chemistry Laboratories	-151
A. Surfa	ce Coordination Chemistry towards Molecular Protonic Devices	-151
1	Proton-Coupled Electron Transfer Reaction of Self-Assembled Monolayer	
-	of Ruthenium(II) Complex Containing Tridentate 2,6-Bis(benzimidazol-2-yl)pyridine	-151
2	Proton-Coupled Electron Transfer Reaction of Langmuir-Blodgett Monolayer	131
_	of Ruthenium(II) Complex Containing Tridentate 2,6-Bis(benzimidazol-2-yl)pyridine	-152
3	Metal Coordination to Amphiphilic Ru Complexes at the Air-Water Interface	152
4	Synthesis and Characterization of Amphiphilic Ru Complex	.132
4	with 2,2':6',2"-Terpyridine-4'-phosphonic Acid at the Air-Water Interface	153
5	Metal-to-Ligand Charge Transfer (MLCT) Band of [Ru(L18)(tridentate ligand)] ²⁺	.133
3	as a Molecular Orientation Probe at the Air-water Interface	154
D Dodo	x Chemistry of Inorganic Metal Complexes	154
	1,8-Diphenyl-octa-1,3,5,7-tetraene Complexes of Ruthenium(II): Crystal Structures of $[\mu$ -(s- ci	
1	1,3-Diphenyi-octa-1,3,3,7-tetraene Complexes of Ruthendin(H). Crystal Structures of [μ-(s-cta-1,2,3,4- :s-cis-5,6,7,8PhCH=CHCH=CHCH=CHCH=CHPh)(RuClCp*) ₂] and [μ-(s-trans-	3-
2	1,2,3,4- :s-trans-5,6,7,8PhCH=CHCH=CHCH=CHCH=CHPh)-{Ru(acac) ₂ } ₂]	.133
2	Spectroelectrochemical Analysis of Intervalence Band	155
C N1	in Mixed-Valence Di- and Tetranuclear Ru Complexes by Flow-Through Method	150
C. New I	Insight into Mechanism of Biological Oxygenation Reactions	-150
1	Mechanism of Double-Strand DNA Cleavage Effected by Iron-Bleomycin	-130
2	Contribution of a Peroxide Adduct of Copper(II)-Peptide Complex to Modify the Secondary Structure of Albumin	150
D M ()	to Modify the Secondary Structure of Albumin	-150
D. Meta	l Ions in Biological Systems	-156
	Isolation and Characterization of Nitric Oxide Reductase from <i>Paracoccus halodenitrificans</i>	-156
2	Spectral Properties of Cytochrome c_{553} and a Membrane-Bound Cytochrome b	1.50
2	from Alcaligenes xylosoxidans GIFU 1051	-157
3	Observation of Cu-N ₃ - Stretching and N ₃ - Asymmetric Stretching Bands	
	for Mono-Azide Adduct of Rhus vernicifera Laccase	-157
4	Genomic Cloning of the Region Encoding Nitric Oxide Reductase	
	in Paracoccus halodenitrificans and a Structure Model Relevant to Cytochrome Oxidase	-157
5	Magnetic Studies of the Trinuclear Center in Laccase and Ascorbate Oxidase	
	Approached by EPR Spectroscopy and Magnetic Susceptibility Measurements	-157
6	Isolation and Characterization of Vanadium Bromoperoxidase from a Marine Macroalga,	
	Ecklonia stolonifera	-158
7	EPR and Magnetic Susceptibility Studies of the Trinuclear Copper Center	
	in Native and Azide-Reacted Zucchini Ascorbate Oxidase	-158
8	The Putative Proton-Transfer Pathway in Membrane-Bound Nitric Oxide Reductase	
	in Connection with Proton Transfers in Heme-Cu Terminal Oxidases	
9	Roles of Four Iron Centers in Paracoccus halodenitrificans Nitric Oxide Reductase	

	10	Myrothecium verrucari MT-1 Bilirubin Oxidase and Its Mutants	
		for Potential Copper-Ligands	-159
Ε.	Homo	geneous Catalysis with Novel Reactivity	-159
	1	Palladium Complex Catalyzed Cyanation of Allylic Carbonates and Acetates	
		Using Trimethylsilyl Cyanide	-159
F.	Bio-Ir	nspired Molecular Architecture	-160
	1	Double-Strands Formation of Artificial DNAs Induced by Metal Complexation	
	2	Metal-Assisted Formation of Artificial Nucleic Acids	-160
	3	An Efficient Strategy for the Liquid-Phase Synthesis of Cyclic Metallopeptides	-161
	4	Highly Controlled and Hierarchical Assembly of Metal Complexes	-161
	5	Macrocyclic Metal Complexes for Selective Recognition of Nucleic Acid Bases	
		and Manipulation of Gene Expression	-161
	6	Macrocyclic Zinc(II) Complexes for Selective Recognition of Nucleobases	
		in Single- and Double-Stranded Polynucleotides	-162
G.	Stere	ochemistry of Coordination Compounds and Adsorption Phenomena of Various Gases	
	on Inc	organic Solids	-162
	1	Analysis of Active Sites on Copper Ion-Exchanged ZSM-5 for CO Adsorption	
		through IR and Adsorption-Heat Measurements	-162
	2	Preparative Study and Characterization of the Cis-Diamminetetranitro-Cobaltate(III) Ion	
		— A Missing Link in the Ammine-Nitro Cobalt(III) Series	-162
	3	Chromatographic Separation and Characterization of the Photoproduct of	
		Tris(L-cysteinesulfinato- <i>N</i> , <i>S</i>)cobaltate(III)	-162
	4	Stereochemistry of (R)-2 Methyl Aziridine Complex of Cobalt(III)	
		and Dimerization of the Ligand	-163
	5	Development of Site-Selective Copper-Ion-Exchanging Method of HZSM-5	
		by the Vapourization of Hexafluoroacetylacetonato-Copper Complex	-163
	6	A Stable Sulfonato-Cobalt(III) Complex: -[Co{OS(O) ₂ CH ₂ CH ₂ NH ₂ - <i>N</i> , <i>O</i> }(en) ₂](ClO ₄) ₂	-163
	7	Complete Chromatographic Resolution of Axially Chiral -Diketonate Complexes	
		on Cellulofine C-200	
Η.	Synth	eses of Transition Metal-Sulfur Clusters and Development of Their Catalysis	-163
	1		
		Clusters Derived from a Hydrosulfido-Bridged Diruthenium Complex	-164
	2	Syntheses of Ruthenium Hydridotris(1-pyrazolyl)borate Complexes	
	_	Having Sulfur-Donor Coligands	-164
	3	Unprecedented Conversion of Benzylideneanilines into Aryl Isocyanides	
		Promoted by a Low-Valent Molybdenum Complex. X-Ray Structure	
_		of trans-[Mo(CNPh)(N ₂)(Ph ₂ PCH ₂ CH ₂ PPh ₂) ₂]	-164
I.	Activa	ation of Carbon Dioxide and Energy Conversion	
	from	Proton Gradients to Electricity Mediated by Metal Complexes	-165
	1	Catalytic Generation of Oxalate through Activation of Two CO_2 Molecules on $[(IrC_p*)_2(Ir^4-C_p*CH_2CN)(\mu_3-S)_2]$	1.55
	2	on $[(IrC_p^*)_2(Ir- ^+C_p^*CH_2CN)(\mu_3-S)_2]$	-165
	2	Selective formation of HCOO and C ₂ O ₄ ²⁻ in Electrochemical Reduction of CO ₂	1
	2	Catalyzed by Mono- and Dinuclear Ruthenium Complexes	-166
	3	Stabilization of [Ru(bpy) ₂ (CO)(¹ -CO ₂)] and Unprecedented Reversible Oxide Transfer	1.00
	4	Reactions from CO_3^{2-} to $[Ru(bpy)_2(CO)_2]^{2+}$ and from $[Ru(bpy)_2(CO)(^{-1}-CO_2)]$ to CO_2	-100
	4	Synthesis and Characterization of Ruthenium Terpyridine Dioxolene Complexes:	100
	~	Resonance Equilibrium between Ru ^{III} -Catechol and Ru ^{II} -Semiquinone Forms	-166
	5	Novel Intramolecular Rearrangement of Hepta-Coordinate Rhenium(V) Complex	167
	(with Catecholato and Terpyridine Ligands	167
	6	First Artificial Energy Conversion from Proton Gradient to Electricity	-10/
	7	Two-Electron Reduction of [{(bpy) ₂ Ru(dmbbbpy)} ₃ Ru] ⁸⁺ from (BNA) ₂ via Photoinduced	1.00
	0	Electron Transfer [dmbbbpy = 2,2'-Bis(N-methylbenzimidazole-2-yl)-4,4'-bipyridine]	-108
	8	Selective Production of Acetone in Electrochemical Reduction of CO ₂	1.00
	0	Catalyzed by Ru-Naphthyridine Complex	-168
	9	Basicity of μ_3 -X and 1 -Y Ligands (X, Y = S, Se) of Reduced, Oxidized	1.00
•	C	and Super-Oxidized Forms of $[Fe_4X_4(YAd)_4]^{2-}$ (Ad = 1-adamantane) in Aqueous Solutions	-169
J.	_	molecular Self-Assembly through Coordination	-169
	1	Made-to-Order Assembling of [2]Catenanes	1.00
	2	from Palladium(II)-Linked Rectangular Molecular Boxes	-169
	2	Self-Assembled Molecular Ladders	-169
	3	Coordination Polymers Self-Assembling from Cadmium(II) Ions	1.00
	4	and Flexible Pyridine-Based Bridging Ligands	-109
	4	Nanometer-Sized Macrotricyclic Complexes Self-Assembled from Ten Small Component Molecules	170
		nom ten sman Component wiolecules	-1/0

	in a Self-Assembled Nanocage Incorporating Six Palladium(II) Ions	170
6	A Thermally Switchable Molecular Lock.	
	The Guest-Templated Synthesis of a Kinetically Stable Nano-Sized Cage	170
7	Spontaneous Assembling of Ten Small Components into a Three-Dimensionally Interlocked	
	Compound Consisting of the Same Two Cage Frameworks	171
8	A Nonometer-sized Hexahedral Coordination Capsule	
	Assembled from Eighteen Metal Ions and Six Triangular Organic Ligands	171
9	"Ship-in-a-Bottle" Formation of Stable Hydrophobic Dimers	
	of cis-Azobenzene and -Stilbene Derivatives in a Self-Assembled Coordination Nanocage	171
Svnth	esis and Reactivity of Complexes Containing Peculiar Bonds	
betwe	en Transition Elements and Main Group Elements of Group 14	172
1	Intramolecular Aromatic C-H Bond Activation by a Silylene Ligand	
1	in a Methoxy-Bridged Bis(silylene)-Ruthenium Complex	172
2	Quantitative Transfer of a Methyl Group from a Methyl(hydrido)iridium Complex to SiRH ₃	1/2
_	(R = n -butyl, pentyl or hexyl) to Give SiR(Me)H ₂ and a Dihydridoiridium Complex	172
2		
3	Thermal Reaction of Ethyl(hydrido){(2-phosphinoethyl)silyl}iridium(III) Complex —Formation of a {(2-Phosphinoethyl)}(ethene)iridium(I) Complex —	150
	—Formation of a {(2-Phosphinoethyl)}(ethene)iridium(1) Complex —	173
4	Synthesis of Cationic Germyleneiron Complexes and X-Ray Structure of [Cp*(CO) ₂ Fe	
	=GeMe ₂ ·DMAP]BPh ₄ ·CH ₃ CN (Cp* = C ₅ Me ₅ , DMAP = 4-(Dimethylamino)pyridine)	173
5	Thermal Reactions of Alkyl(hydrido)(hydrosilyl)iridium(III) Complexes:	
	Generation of a Hydrido(silylene)iridium(I) Species via the Reductive Elimination of Alkane	
	and 1,2-H-Shift from the Silicon Atom to the Ir(I) Metal Center	173
6	Synthesis, Structure, and Reactivity of a Bis(silylene)(carbonyl)ruthenium Complex	
O	and a Novel Addition Reaction of Photochemically Generated Dimethylsilylene	
	to Bis(silylene) Complexes $Cp(OC)M\{SiMe_2\cdots O(Me)\cdots SiMe_2\}\ (M = Ru, Fe)$	174
7	Synthesis and Properties of Intramolecularly Base-Stabilized Disilanyl(silylene)ruthenium	1/4
7	Synthesis and Properties of Inframolecularly Base-Stabilized Distranyi(shylene)ruthenium	174
	and -iron Complexes	1/4
8	Thermal and Photochemical Reactions of a Cationic Rhenocene-Acetonitrile Adduct:	
	The First C-H Bond Activation by Rhenocene Cation	175
9	Novel Reaction of Silyl Carbonyl Complexes with Hydride-Transfer Reagents:	
	Reduction of a Carbonyl Ligand and Coupling with a Silyl Group	175
	H ACTIVITIES VIII	
npute	er Center retical Studies on Electronic Structure and Dynamics of Electronically Excited States	176
pute Theor	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules	176 176
pute Theor in Pol	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS	176 176
pute Theor in Pol	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS	176 176
pute Theor in Pol	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited state	176 176 176
Theor n Pol 1 2	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited 1 state of HCP Molecule	176 176 176
heon Pol 1 2	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited 1 state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical	176 176 176 176
heon Pol	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited 1 state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO	176 176 176 176
heon Pol 1 2 3	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH	176 176 176 176 -176
Cheon Pol 1 2 3	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion	176 176 176 176 -176 -177
Theorem Pol 1 2 3 4 5 6	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited 1 state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems	176 176 176 176 176 177
heon 1 2 3 4 5	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion	176 176 176 176 -176 177
heori Pol 1 2 3 4 5 6 7	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers	176 176 176 176 -176 -177 177
heori Pol 1 2 3 4 5 6 7	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited 1 state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems	176 176 176 176 -176 -177 177
Theorem Pol 1 2 3 4 5 6 7	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers	176 176 176 176 -176 177 177
Theon 1 2 3 4 5 6 7 Re	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited 1 state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers Search Center for Molecular Science	176 176 176 176 -176 177 177
Theor n Pol 1 2 3 4 5 6 7 7 Re	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited 1 state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States	176 176 176 176 177 177 177 179 ates
Theor 1 2 3 4 5 6 7 Recent 2 2 4 2 4 4 5 6 7 4 4 5 6 7 4 4 5 6 7 4 6 6 7 6 7 6 7 7 Recent 2 4 6 7 6 7 7 Recent 2 4 6 7 6 7 7 8 7 8	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited 1 state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States and Waals Complexes	176 176 176 176 177 177 177 179 ates
Theorin Police 1 2 3 4 5 6 7 r Received and v	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited 1 state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States Energy Exchange between Electron and Ion Core in Very High-Lying Rydberg States	176176176176177177179 ates179
7 Record v	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited 1 state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH3CO CH3 + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH2O to t-OSiHOH Ab Initio Study of PH2 + O2 Reaction Relevant to the PH3 Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C84 Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States of Poliatomic Molecules Evidenced by Sweep-Off-Probe Pulsed-Electric-Field Ionization	176176176176177177179 ates179
Theorin Police 1 2 3 4 5 6 7 r Recard value 1	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States of Poliatomic Molecules Evidenced by Sweep-Off-Probe Pulsed-Electric-Field Ionization Cation Vibrational Spectra of Pyrimidine and Its van der Waals Complexes with Ar and N ₂	176176176176177177179 ates179
Theor in Pol 1 2 3 4 5 6 7 er Rec Zero and v 1 2	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States of Poliatomic Molecules Evidenced by Sweep-Off-Probe Pulsed-Electric-Field Ionization—Cation Vibrational Spectra of Pyrimidine and Its van der Waals Complexes with Ar and N ₂ by ZEKE Photoelectron Spectroscopy	176176176176177177179 ates179179
Theorin Police 1 2 3 4 5 6 7 7 Received and v 1 2	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States of Poliatomic Molecules Evidenced by Sweep-Off-Probe Pulsed-Electric-Field Ionization — Cation Vibrational Spectra of Pyrimidine and Its van der Waals Complexes with Ar and N ₂ by ZEKE Photoelectron Spectroscopy Topments and Researches of New Laser Materials	176176176176177177179 ates179179
Theorin Police 1 2 3 4 5 6 7 7 Received and v 1 2	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States of Poliatomic Molecules Evidenced by Sweep-Off-Probe Pulsed-Electric-Field Ionization — Cation Vibrational Spectra of Pyrimidine and Its van der Waals Complexes with Ar and N ₂ by ZEKE Photoelectron Spectroscopy Topments and Researches of New Laser Materials	176176176176177177179 ates179179
Theor in Pol 1 2 3 4 5 6 7 er Rec Zero and v 1 2 Devel 1	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States of Poliatomic Molecules Evidenced by Sweep-Off-Probe Pulsed-Electric-Field Ionization — Cation Vibrational Spectra of Pyrimidine and Its van der Waals Complexes with Ar and N ₂ by ZEKE Photoelectron Spectroscopy Spectrum Control of Intense THz-Radiation from InAs under Magnetic Field Irradiated with Stretched Femtoscoond Laser Pulses	176176176176177177179179179179
Theor in Pol 1 2 3 4 5 6 7 er Rec 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States of Poliatomic Molecules Evidenced by Sweep-Off-Probe Pulsed-Electric-Field Ionization — Cation Vibrational Spectra of Pyrimidine and Its van der Waals Complexes with Ar and N ₂ by ZEKE Photoelectron Spectroscopy Spectrum Control of Intense THz-Radiation from InAs under Magnetic Field Irradiated with Stretched Femtoscoond Laser Pulses	176176176176177177179179179179
Theor in Pol 1 2 3 4 5 6 7 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States and er Waals Complexes Energy Exchange between Electron and Ion Core in Very High-Lying Rydberg States of Poliatomic Molecules Evidenced by Sweep-Off-Probe Pulsed-Electric-Field Ionization — Cation Vibrational Spectra of Pyrimidine and Its van der Waals Complexes with Ar and N ₂ by ZEKE Photoelectron Spectroscopy opments and Researches of New Laser Materials Spectrum Control of Intense THz-Radiation from InAs under Magnetic Field Irradiated with Stretched Femtosecond Laser Pulses Estimation the Focusability of the THz Radiation	176176176176177177179179179179180180
Theor in Pol 1 2 3 4 5 6 7 7 Re Zero and v 1 2 Devel 1 2 3	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited 1 state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH3CO CH3 + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH2O to t-OSiHOH Ab Initio Study of PH2 + O2 Reaction Relevant to the PH3 Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C84 Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States of Poliatomic Molecules Evidenced by Sweep-Off-Probe Pulsed-Electric-Field Ionization — Cation Vibrational Spectra of Pyrimidine and Its van der Waals Complexes with Ar and N2 by ZEKE Photoelectron Spectroscopy opments and Researches of New Laser Materials Spectrum Control of Intense THz-Radiation from InAs under Magnetic Field Irradiated with Stretched Femtosecond Laser Pulses Estimation the Focusability of the THz Radiation Efficient, High Output Energy, Ultraviolet Ce:LiCAF Laser	176176176176177177179179179179180180
Theor in Pol 1 2 3 4 5 6 7 2 r Re Zero 2 and v 1 2 Devel 1 2 3	retical Studies on Electronic Structure and Dynamics of Electronically Excited States yatomic Molecules Wavepacket Study on the Photodissociation Dynamics of OCS Theoretical Study on the Predissociation Dynamics of Electronically Excited ¹ state of HCP Molecule Theoretical Study on the Unimolecular Reaction Dynamics of Acetyl Radical CH ₃ CO CH ₃ + CO Ab Initio Molecular Orbital Studies of Isomerization Reaction from c-OSiH ₂ O to t-OSiHOH Ab Initio Study of PH ₂ + O ₂ Reaction Relevant to the PH ₃ Combustion Semiclassical Study of Nonintegrable Systems A Theoretical Study on Structures and Vibrational Spectra of C ₈₄ Fullerene Isomers Search Center for Molecular Science Kinetic Energy Pulsed Field Ionization Spectroscopy of Very Highly Excited Rydberg States and er Waals Complexes Energy Exchange between Electron and Ion Core in Very High-Lying Rydberg States of Poliatomic Molecules Evidenced by Sweep-Off-Probe Pulsed-Electric-Field Ionization — Cation Vibrational Spectra of Pyrimidine and Its van der Waals Complexes with Ar and N ₂ by ZEKE Photoelectron Spectroscopy opments and Researches of New Laser Materials Spectrum Control of Intense THz-Radiation from InAs under Magnetic Field Irradiated with Stretched Femtosecond Laser Pulses Estimation the Focusability of the THz Radiation	176176176176177177179179179179180180

5	Broad-Band Gain Demonstration of New Yb:Glass	-181
6	Strong Enhancement of THz-Radiation Power from Femtosecond-Laser	
	Irradiated InAs Clean Surface and Its Temperature Dependence	-182
D. Devel	lopment and Research of Advanced Tunable Solid State Laser Sources	-182
1	Întracavity Frequency Doubled Yb:YAG Miniature Laser	-182
2	Design of Longitudinally Solid-State Lasers by Using M ² Pump-Beam Factor	-183
3	Diode-Pumped Nd:YAG Ceramics Lasers	-183
_	-	
Research	n Center for Molecular Materials	-185
E. Devel	lopment of Novel Heterocyclic Compounds for Advanced Materials	-185
1	Synthesis and Characterization of New Electron Donors	
	Containing 1,2,5-Thiadiazole and 1,1'-Dihydro-4,4'-bi(pyridylidene) Units	-185
2	Synthesis and Properties of Bis(1,3-dithiol-2-ylidene) Compounds	
	Containing a 2,2'-Bithienyl Unit	-185
3	Synthesis and Properties of Novel Tetrathiafulvalene Vinylogues	-185
4	Molecular and Crystal Structure of Novel Tetrathiafulvalene Vinylogues	
	and Their Cation Radical Salts	186
5	New Electron Acceptors Containing Thieno[3,4-b]pyrazine Units	186
6	Design of Novel 4-Terminal Molecular Switching Unit Based on Multi-Stage Redox System -	-187
	tonic Structures and Rectivities of Active Sites of Metalloproteins	
1	Imidazole and p-Nitrophenolate Complexes of Oxo Iron(IV) Porphyrin -Cation Radicals	
	as Models for Compounds I of Peroxidase and Catalase	-187
2	Electron Configuration and Spin Distribution in Low-Spin (meso-Tetraalkylporphyrinato)-	
	iron(III) Complexes Carrying One or Two Orientationally Fixed Imidazole Ligands	-188
3	Raman Signature of the Fe ₂ O ₂ "Diamond" Core	
4	⁶³ Cu-NMR Study of Copper(I) Carbonyl Complexes with Various Hydrotris(pyrazolyl)borates	s:
	Correlation between ⁶³ Cu Chemical Shifts and CO Stretching Vibrations	-189
G. Mole	cular Mechanism of Heme Degradation and Oxygen Activation by Heme Oxygenase	
1		
	Cobalt Porphyrin Heme Oxygenase Complex. EPR Evidences for the Distal Heme Pocket Hydrogen Bonding	-189
2	The Oxygen and Carbon Monoxide Reactions of Heme Oxygenase	-190
3	Identification that Histidine 45 is the Axial Heme Iron Ligand of Heme Oxygenase-2	-190
H. Desig	ning Artificial Photosynthesis at Molecular Dimensions	-191
1	Synthesis and Characterization of Manganese Complexes	
2	Synthesis and Photophysical Properties of Porphyrin-Dimanganese Composite Molecules	
I. Orga	nic Molecular Materials with Novel Electronic Properties	-192
1	Functionalization of C ₆₀ by Acetylenes	-192
2	New Electron-Transporting Materials for Organic EL Devices	-192
J. Studi	es of Nanoscale Carbons	-192
1	Effect of Environment Temperature for Synthesizing the Single Wall Carbon Nanotubes	
	by Arc Vaporization Method	-193
2	Radial Thermal Expansion of Purified Multiwall Carbon Nanotubes	
	Measured by X-Ray Diffraction	-193
3	Effect of the Growth Temperature on the Diameter Distribution and Chirality	
_	of Single Wall Carbon Nanotubes	-193
4	Purification and Magnetic Properties of Carbon Nanotubes	-193
5		194
6	The Structure and Electronic Properties of Graphite Nano-Particles	-194
	Measurement of Dipolar Interactions under Magic-Angle Sample Spinning	-194
1	Dipolar Interactions between ¹³ C and ¹⁵ N	-194
Equipme	ent Development Center	-195
=qa.p	on Boyers pinette conter	1,0
L. Deve	lopment of "IMS Machines"	-195
1	Multi-Channel Detector for Mid-Infrared Light	
2	Programmable Micro Current Source	-196
	lopment of Experimental Devices	196
	Prototype Apparatus for Synthesizing the Single Wall Carbon Nanotubes by Arc Discharge	170
1	at High Temperature Environment	-196
N Dave	lopment of Spectroscopic System with Combination of Synchrotron Radiation and Laser	
1 l	Time-Gated Photon Counting Method for Two-Photon Spectroscopy	171
1	Using Synchrotron Radiation and Laser	107
	Osing Dynomotion Radiation and Laser	171

Ultr	aviolet Synchrotron Orbital Radiation Facility	198
0	Development of the UVSOR Light Source	109
O.	1 Non-linear Calibration of Beam Position Monitors	100
D	Researches by the USE of UVSOR	108
1.	1 Time Response and Temperature Dependence of Photo-Stimulated Desorption	190
	of Sodium Atoms from Sodium Halides	198
	2 Laser-Induced Fluorescence Study of Fast Desorption of Ground-State K Atoms	170
	from Potassium Halides Excited by Synchrotron Radiation	198
	3 Circular Dichroism in the Angular Distribution of Core-Level Photoelectrons	170
	from GaAs (111)	198
	4 Simultaneous Measurements of Photoelectron and Luminescence of Barium Halides	
	5 Temperature Dependence of Auger-Free Luminescence in Alkali and Alkaline-Earth Halic	
	6 Combinational Use of Synchrotron Radiation and Laser for Two-Photon Spectroscopy of BaF ₂ ¹	199
	7 Direct Excitation of Tl ⁺ Impurity Ions by Hot Photoelectrons in Wide-Gap Crystals	199
	8 Study of Ion Desorption Induced by the Core-Level Excitation on the CaF ₂ (111) Surface -	
	9 Observation of the Surface States on CuCl(100)	
	10 Electronic Structures of Organic Salts (DI-DCNOI) ₂ M (M = Cu and Ag)	
	Using Photoelectron Spectromicroscopy	200
	11 Resonant Photoemission Study of Temperature-Induced Valence Transition Material	
	$EuNi_2(Si_{1-x}Ge_x)_2$	200
	12 Study of Magnetic Linear Dichroism (MLD) for Different Thickness of Ni-Thin Film	
	Grown on Ferromagnetic Co (100) in Element Specific Photoemission	201
	13 Tm5p Resonant Photoemission Study of TmX (X=S, Se and Te) around 4d-Excitation Reg	ion 202
	14 Photodissociation of Ozone in the K-Edge Region	203
DECE	A D CHI D A CHI IMIDO	
RESE	ARCH FACILITIES	
	Computer Center	
	Laser Research Center for Molecular Science	
	Research Center for Molecular Materials	204
	Equipment Development Center	204
	Ultraviolet Synchrotron Orbital Radiation Facility	205
SDEC	AL RESEARCH PROJECTS	207
	Development of Microscopic Environments with Functionality	207
(1,	and Quantum Steering for Reactions	207
	Structures, Reactions and Spectroscopies of Molecules and Clusters	207
	Folding Simulations of Protein Molecules by Generalized-Ensemble Algorithms	207
	Quantum Mechanical and Semiclassical Studies of Chemical Dynamics	207
	Quantum Fokker-Planck Equation Approach to Electron Transfer Problem	207
	in Two-Dimensional Displaced Potential Surfaces	208
	Constructing Molecular Theory of Chemical Processes in Solution	208
	High-Resolution Terahertz Spectroscopy by a Compact Radiation Source	200
	Based on Photomixing with Diode Lasers in a Photoconductive Antenna	208
	(1) Studies on Laser Cooling and Trapping of Neutral Atoms	200
	(2) Laser Spectroscopic Studies of Atoms and Ions in Liquid Helium	209
	Structure and Function of Transmembrane Electron Transfer System	207
	in Neuroendocrine Secretory Vesicles	210
	Time-Resolved Resonance Raman Study on Mechanism of Oxygen Reduction	210
	by Cytochrome c Oxidase	210
	Laser Raman Beat Detection of Magnetic Resonance	210
	Studies of Laser-Induced Photochemistry on Solid Surfaces, Thin Films, and Clusters	210
	Hydrogen Bond Network Fragmentation and Its Detection	
	by Low Frequency Raman Spectroscopy	211
	Higher Vibrational States of Molecules and Clusters as Studied by Nonresonant Ionization	
	Detected IR Spectroscopy	211
	Laser Investigation of Elementary Reactions in the Gas Phase	212
	Theoretical Study on the Electronic Structures of Atoms, Molecules, and Clusters	212
	Preparation of Pt-Pd Bimetallic Clusters by Solvent Extraction	
	Development of Pulsed-Jet Millimeter-Wave Spectrometer for the Detection	
	of the Novel Unstable Species and the van der Waals Mode Transitions of Molecular Clusters	213
	Experimental Study of Ion-Induced Nucleation	

Time-Resolved Spectroscopic Studies on Chemical Reactions	212
Using Ultrafast Laser and Synchrotron Radiation	213
Development of Scanning Tunneling Microscopy System for the Study	21.4
of the Synchrotron-Radiation Stimulated Desorption of SiO ₂ Films on Si(111) Surface	214
Pump-Probe Spectroscopy of Atoms and Molecules	214
with a Combination of Synchrotron Radiation and a Mode-Locked or Pulsed Laser	
Vibrational Spectroscopy on Cryogenic Surfaces using Synchrotron Radiation	215
Formation of Ordered Array of Quantum Dots	215
Using Synchrotron Radiation-Stimulated Etching and Selective Growth	215
Similarity Transformed Preconditioners for Green Function Evaluation in Cumulative Reaction Probability Calculations	216
Developments of Advanced Lasers for Chemical Reaction Controls	216
Developments of Advanced Lasers for Chemical Reaction Controls Developments and Researches of New Laser Materials	216
Development and Research of Advanced Tunable Solid State Lasers	216
UHV Tribometer	210 217
Investigation of Electronic Structures of Solid/Surface by Using Synchrotron Radiation	
Non-Linear Phenomena and Related Beam Physics in Storage Ring Free Electron Lasers -	
Studies of Solids and Surfaces by Photoelectron Spectroscopy	
(2) Study of Molecular Solid toward Molecular Electronics	
Theory of Electronic Phases in Molecular Conductors and Insulators: Electron Correlations	210
and Dimensional Crossovers	218
-d Interaction in Molecular Metals	
Search for Negative-U Materials in Molecular Solid	
Exploring Novel Electronic Phases in Molecular-Based Conductors	219
Development of New Organic Metals and Superconductors	219
NMR Studies of Liquid Crystals	220
Construction and Characterization of Chiral Molecule-Based Magnets	220
Quantitative Analysis of Organic Thin Films Using Angle-Resolved UPS	220
New Advanced Organic Materials Based on Novel Heterocyclic Compounds	221
Design and Synthesis of New Tellurium-Containing Donors	221
(3) Material Control in Multi-Reaction Centers	222
Asymmetric Oxidation Catalyzed by Myoglobin Mutants	
Two Dimensional Coordination Chemistry at the Interface towards Molecular Protonic De	
Peroxide Adduct of Hydroxo(oxo)iron Clusters as a Cause of Neurodegenerative Diseases	222
Assembled Metal Centers in Enzymes	222
Novel Phosphorus Ligands for Supramolecular Catalyst System	223
Bio-Inspired Molecular Architecture	223
Stereochemistry of Six-Coordinated Octahedral Silicon(IV) Complexes	
Containing 2,2'-Bipyridine	223
Activation of Carbon Dioxide Directed toward Carbon-Carbon Bond Formation	
and Energy Conversion from Proton Gradients to Electricity	223
Self-Assembling Molecular Systems	224
Molecular Mechanism of Heme Degradation and Oxygen Activation by Heme Oxygenase Generation of Reactive Species on Multinuclear Metal Complexes as Molecular Componer	224 its
in Energy Conversion Systems	225
OVAZAVI COMBEDENICEC	
OKAZAKI CONFERENCES	226
JOINT STUDIES PROGRAMS	
(1) Special Projects	229
(2) Research Symposia	
(3) Cooperative Research	
(4) Use of Facility	
(5) UVSOR	234
FOREIGN SCHOLARS	236
AWARDS	
LIST OF PUBLICATIONS	
REVIEW ARTICLES AND TEXTBOOKS	258
AUTHOR INDEX TO RESEARCH ACTIVITIES AND SPECIAL RESEARCH PROJECT	Γ S 261