

Waterloo Symposium on Chemical Physics

October 25-27, 1991

at the University of Waterloo

REGISTRATION begins at 6:30 p.m., Davis Centre Room 1301

SESSION I: Friday October 25, 1991 - P.M.

Davis Centre 1302

Chair: John Hepburn

- 7:30 - 8:10 Takayoshi Amano (NRC, Ottawa)
The Dissociative Recombination Rate of H_3^+
- 8:10 - 8:30 Francis Markel (University of Rochester), N.S. Ferris (Eastman Kodak), I.R. Gould
(Eastman Kodak) and Ann B. Myers (University of Rochester)
Internal Reorganization Energies Accompanying Photoinduced Electron Transfer
- 8:30 - 8:50 Robert D.J. Froese and John D. Goddard (University of Guelph)
The Rejection of Oxygen Atoms with Carbon Disulfide: Potential Energy Surface
Features of a Preliminary Reaction for Carbon Monoxide Chemical Lasers.
- 8:50 - 9:10 Delmar N.S. Permann and Ian P. Hamilton (University of Ottawa)
Nonlinear Dynamics of Weakly Forced and Weakly Damped Oscillator Systems:
Complicated and Dissociative Dynamics for the Morse Oscillator and Self-similar and
Erratic Dynamics for the Simple Pendulum.

SESSION II: Saturday, October 26, 1991 - A.M.

Davis Centre 1302

Chair: Robert Le Roy

- 9:00 - 9:40 Tom Rizzo (University of Rochester)
Multiple Laser Probes of Intramolecular Dynamics.
- 9:40 - 10:00 Thomas L. Beck (University of Cincinnati)
Path Integral Quantum Generalization of Widom's Test Particle Method for Chemical
Potentials.
- 10:00 - 10:20 Yibing Fan and D.Jamie Donaldson (University of Toronto)
Laser-Induced Fluorescence Study of I_2 from $(CH_3I)_n$ Photodissociation.

- 10:20 - 10:40 **Coffee Break**
- 10:40 - 11:40 Richard N. Zare (Stanford University)
State-Selected and State-Detected Reaction Dynamics
- 11:40 - 12:00 Joseph M. Lanzafame, (University of Rochester), R.J.Dwayne Miller (University of Rochester), A.A. Muentert (Eastman Kodak) and B.A. Parkinson (Colorado State University)
Ultrafast Electron Dynamics at Dye-Sensitized SnS₂ Interfaces: Evidence for Continuum Delocalization.
- 12:00 - 12:20 Charles X.W. Qian (Steacie Inst. of Molecular Sciences, NRC Ottawa)
Spectroscopy and Dynamics of Fast Evolving States.
- 12:20 - 2:00 **Lunch** Davis Centre 1301

SESSION III: Saturday October 26, 1991

Davis Centre 1302

Chair: Tong Leung

- 2:00 - 2:40 Denis Roy (Universite Laval)
The Surface Chemistry of Silicon Investigated by Electron Spectroscopy:
Some New Results.
- 2:40 - 3:00 St.John Dixon-Warren, Erik Jensen and John C. Polanyi, (University of Toronto)
Direct Evidence for Charge-transfer Photodissociation at a Metal Surface:
CCl₄ on Ag(111).
- 3:00 - 3:20 M. Todd Coolbaugh, Gopalakrishnan Vaidyanathan, William R. Peifer and James F. Garvey (SUNY, Buffalo)
High Energy Reactions in Argon/Methanol and Argon/Water Heteroclusters.
- 3:20 - 3:40 Brent H. Besler and William L. Hase (Wayne State University)
A Theoretical Study of the Fundamental Growth Mechanism of the (110) Surface of
Diamond Films from Acetylene and Hydrogen Mixtures

SESSION IV: Saturday, October 26, 1991 from 4:00 P.M.

South Campus Hall

POSTER SESSION AND MANUFACTURERS' DISPLAY

7:00 P.M.

DINNER

South Campus Hall

SESSION V: Sunday, October 27, 1991 - A.M.

Davis Centre 1302

Chair: Jim Sloan

- 9:30 - 10:10 William J. Meath (University of Western Ontario)
Effects of Permanent Dipoles on the Resonance Profiles and Dynamics Associated with Single- and Multi-Photon Laser Molecule Interactions.
- 10:10 - 10:30 Peter Dietrich and Paul B. Corkum (Steacie Inst. for Molecular Sciences, NRC Ottawa)
Ionization and Dissociation of Small Molecules Using High-intensity Laser Radiation.
- 10:30 - 10:50 Andre D. Bandrauk and S. Chelkowski (Université de Sherbrooke)
Control of Vibrational Excitation and Dissociation by Chirped IR Laser Pulses.
- 10:50 - 11:10 **Coffee Break**
- 11:10 - 11:50 Paul Houston (Cornell University)
The HCO Potential Energy Surface; Probes Using Molecular Scattering and Photodissociation.
- 11:50 - 12:10 Leslie D. Waits, Ronald J. Horwitz and Joyce A. Guest (University of Cincinnati)
Study of Anisotropic Ion Photofragments from CF_3I^+ Produced by Resonant Multiphoton Ionization.
- 12:10 - 12:30 Glen A. McRae (Atomic Energy of Canada Ltd.)
Resonance Polarization Spectroscopy of Atoms.

POSTER SESSION

To give those people presenting papers in this session an opportunity to both present their work and visit other posters, this session is divided into two time slots:

4:15 - 5:30 p.m. Those whose papers were given even-number labels should attend their posters.

5:30 - 6:45 p.m. Those whose papers were given odd-number labels should attend their posters.

- 1) Tung Nguygen-Dang and Hakima Abou-Rachid (Université Laval)
Radiative Transitions Induced by Short Laser Pulses in Atomic Collisions: Non-Perturbative Study of Pulse Shape Effects
- 2) Kelly Akers and Martin Moskovits (University of Toronto)
Surface Enhanced Raman Spectra of C₆₀ and C₇₀
- 3) M. Keil and L. Rawluk (University of Alberta) and James C. Barrett and Howard R. Mayne (University of New Hampshire)
Rotationally Inelastic Scattering in Ar + HF; An Experimental and Theoretical Study
- 4) John N. Beauregard and Howard R. Mayne (University of New Hampshire)
Scattering of Small and Medium-sized Clusters from Reactive and Nonreactive Surfaces
- 5) Elizabeth Bishenden and D. Jamie Donaldson (University of Toronto)
Resonance Enhanced Multiphoton Ionization Measurement of Cl(²P_{3/2} and ²P_{1/2}) Produced in the Photolysis of Tetrachloroethylene, Trichloroethylene, cis-Dichloroethylene and Trans-Dichloroethylene.
- 6) Mark Blitz, Peter Hackett and Steven Mitchell (Steacie Institute for Molecular Science, NRC)
Reactions of Nickel Atoms with Ethers, Alcohols and Water: Evidence for Sigma Complex Formation and Insertion Reactions
- 7) Carl E. Bonner, M. Aeschlimann, J. Cao, H. El-Sayed-Ali, Y. Gao, R.J.Dwayne Miller (University of Rochester) and D. Mantell (Xerox Research Center)
RHEED Studies of Photoinduced Molecular Dynamics at Single Crystal Surfaces
- 8) Mark E. Casida (Université de Montreal) and John E. Harriman (University of Wisconsin)
Extended Husimi Representation
- 9) Darryl J. Chartrand and Robert J. Le Roy (University of Waterloo) and William J. Meath (University of Western Ontario)
Effect of Three-Body Forces on Static and Dynamic Behaviour of SF₆-Ar_n Clusters
- 10) W. Chen, William L. Hase and H.B. Schlegel (Wayne State University)
Ab initio MO Calculations for the Reactions of BCl, BF, AlCl and AlF with O₂
- 11) Young June Cho, Scott Vande Linde and William L. Hase (Wayne State University)
Trajectory Studies of S_N2 Nucleophilic Substitution - Nonstatistical Barrier Recrossing in the Cl + CH₃Cl System

- 12) Claudio Chuaqui and Robert J. Le Roy (University of Waterloo)
Calculation of the Infrared Spectra of the H₂-CO Van der Waals Complex
- 13) Bruce Collings, David Rayner and Peter Hackett (Steacie Institute for Molecular Science, NRC)
Photodissociation and Photoionization Dynamics of Metal Cluster Beams: Time-resolved Thermionic Emission. The Vibrational Temperature of Supersonic Metal Clusters and the Question of Melting Prior to Ionization
- 14) Rogério Custodio and John D. Goddard (University of Guelph)
The Integral Version of the Hartree-Fock Equations and the Hellmann-Feynman Forces as Criteria for Improving Basis Sets
- 15) Zhongyi Deng and Donald E. Irish (University of Waterloo)
Surface Enhanced Raman Scattering from a Silver Electrode in a Methyl Acetate Solution Containing LiAsF₆, (CH₃)₄NBr
- 16) St. John Dixon-Warren, Erik T. Jensen and John C. Polanyi (University of Toronto)
Surface-aligned Charge-transfer Photodissociation and Ion-molecule Reaction in Adsorbates at a Metal Surface: Chloromethanes on Ag(111) and CH₃Br/CCl₄/Ag(111)
- 17) Stephen Donnelly and James Farrar (University of Rochester)
Photodissociation Studies of Mass Selected Solvated Metal Ion Clusters: Sr⁺(NH₃)_n, n = 1 to 6
- 18) Jack Barnes (University of Victoria), Constantine Douketis (University of Toronto), Terry Gough and Marcel Stoer (University of Victoria)
Absolute Transition Intensities from Intra-cavity Laser Photo-acoustic Spectroscopy
- 19) Dean R. Peterman, Robert G. Daniel and Joyce A. Guest (University of Cincinnati)
Characterization of Acetic Acid Photofragmentation Dynamics: Isotopic Substitution Effects
- 20) Phillip R. Bunker (Herzberg Inst. of Astrophysics), Per Jensen (Justus-Liebig-Universität) and Ian P. Hamilton (University of Ottawa)
Ab-initio Rotation-Vibration Energies and Intensities for the HO₂ Radical
- 21) William L. Hase (Wayne State University)
Stereochemistries of the Cl + CH₃Cl Association and Nucleophilic Substitution Reactions
- 22) Hartmut G. Hedderich, Peter F. Bernath (University of Waterloo), Corey I. Frum and R. Engleman Jr. (University of Arizona)
Fourier Transform Emission Spectroscopy of Metal Halides
- 23) William J. Herron, M. Todd Coolbaugh, Gopalakrishnan Vaidyanathan, William R. Peifer and James F. Garvey (SUNY, Buffalo)
Magic Numbers in Mixed Alcohol/Water Clusters: Implications for Cluster Ion Structure
- 24) Tim J. Scoll, S. David Rosner and Richard A. Holt (University of Western Ontario), N. Berrah Mansour, C. Kurtz, T.C. Steimle, G.L. Goodman and L. Young (Argonne National Lab)
Laser-rf-laser Measurement of Fine and Hyperfine Structure in N₂⁺

- 25) Deqing Hu, Charlie D. MacPherson and K. Tong Leung (University of Waterloo)
Room Temperature Adsorption of Six-membered Aromatic Hydrocarbons: Cyclohexene, 1,3-Cyclohexadiene, 1,4-Cyclohexadiene and Benzene on Si(111)7x7 by Thermal Desorption Spectrometry
- 26) Victoria J. Barclay, David B. Jack, John C. Polanyi and Yehuda Zeiri (University of Toronto)
Simulation of Hot H Atom Scattering from the Photolysis of HBr Aligned on the LiF(001) Surface
- 27) Andrew James, Benoit Simard and Peter Hackett (Steacie Institute for Molecular Science, NRC)
Molecular Beam Optical Laser Spectroscopy of Lanthanum Fluoride: Magnetic Hyperfine and Dipole Moment Determinations
- 28) John Hepburn, Mari-Noëlle Jégo, Andreas Mank and Caroline Starrs (University of Waterloo)
Dynamics of Photodissociation in CS₂: Evidence for Mode-Specific Chemistry in Predissociation of the ¹B₂ State
- 29) Kevin J. Jordan, Rob H. Lipson, N.A. McDonald and Dong-Shen Yang (University of Western Ontario) and Robert J. Le Roy (University of Waterloo)
Jet Emission Spectra of Group IIB Metal Monohalides
- 30) Wei Kong, David Rodgers and John W. Hepburn (University of Waterloo)
Dynamics of Molecular Autoionization Studied by Coherent Vacuum Ultraviolet Radiation
- 31) Mangala S. Krishnan and Tucker Carrington, Jr. (Université de Montréal)
Quantum Canonical Transformation of Coriolis and Centrifugal Terms in the Ro-vibrational Hamiltonian: A New Zeroth Order Hamiltonian for Spectroscopy of Excited States
- 32) Martin Leboeuf and Dennis R. Salahub (Université de Montréal)
LCGTO-NLDF Calculations on the Water Dimer: A Study of Hydrogen Bonding
- 33) Dale Levandier, David Varley and James Farrar (University of Rochester)
Reactive and Nonreactive Scattering in the Systems O⁻ + NH₃ and O⁻ + H₂O
- 34) Kevin Jordan, Dong Shen Yang, N.A. McDonald and Rob H. Lipson (University of Western Ontario)
Photodissociation of Metal Dihalides
- 35) Kun Liu, John C. Polanyi and Shi-He Yang (University of Toronto)
Photo-induced Charge-transfer with Van der Waals Complexes Na_n...(RX)_m, (RX = CH₃Cl, phF)
- 36) Peter McBreen, M. Ayyoob and S. Serghini Monim (Université Laval)
Adsorption Geometry Dependent Selective Bond Activation of CH₂N₂ on Pd(110)
- 37) Andreas Mank (University of Waterloo), M. Drescher (Universität Bielefeld), T. Huth-Fehre (SRI International, Menlo Park, CA), M. Buchner, A. Brockhinke, U. Heinzmann (Universität Bielefeld)
Rotationally Resolved Study of the HI(5pπ)-photoionization Using Angle- and Spin Resolved Photoelectron Spectroscopy
- 38) Robin L. Miller, Scott H. Kable and Paul L. Houston (Cornell University) and Itamar Burak (Tel Aviv University)
Product Distributions in the 157nm Photodissociation of CO₂

- 39) Arno Mann (Université de Sherbrooke) and F. Linder, Universitat Kaiserslautern)
Mode-selective Vibrational Excitation in Low-energy Electron Scattering from Halomethanes
- 40) Chris Mathers, Alex Brown and Neil R. Isenor (University of Waterloo)
Fragmentation of Seed Molecules in Rare Gas Clusters
- 41) Steven Mitchell, Carl Brown, Mark Blitz and Peter Hackett (Steacie Institute for Molecular Science, NRC)
Non-adiabatic Effects in Association Reactions of Nickel Atoms with Alkenes
- 42) John Muentzer (University of Rochester)
An Intermolecular Potential Function Model for Small Van der Waals Complexes
- 43) Anthony Muscat, Abdelilah Rjeb and Denis Roy (Université Laval)
A Low Cost UHV Sample Holder That Achieves 10 K/s Cooling Rates Between 1000k and 100k
- 44) Guijuan Nan and Paul L. Houston (Cornell University)
Doppler Profile Study of Velocity Relaxation for $S(^1D)$ from 222nm Photodissociation of OCS
- 45) David W. Neyer, Scott H. Kable, Jean-Christophe Loisson, Evelyn M. Goldfield and Paul L. Houston (Cornell University) and Itamar Burak (University of Tel Aviv)
Product Distributions from the Visible Photodissociation of HCO
- 46) Bernadette I. Niefer, Henrik Kjaegaard and Bryan R. Henry (University of Guelph)
Measured and Calculated Overtone Intensities in the Overtone Spectra of Cyclopropylamine and Cyclohexane
- 47) Rick D. Lafleur and J. Mark Parnis (Trent University)
Chemical Quenching of Excited-State Ga Atoms (2S) by Methane in Argon Matrices: Vibrational Spectra of Methylgallium Hydride
- 48) Marco A. Pereira, John Deak and R.J. Dwayne Miller (University of Rochester)
Evidence for Collective Modes and the Energy Relaxation in Biological Systems
- 49) Gilles H. Peslherbe and William L. Hase (Wayne State University)
Difficulties of Following the Reaction Path for Association Reactions
- 50) David L. Phillips and Anne B. Myers (University of Rochester)
Vapor and Solution Phase Resonance Raman Spectra of Photodissociating Nitromethane: Solvation and Solvent Effects
- 51) Prasad Chintalapati and Peter F. Bernath (University of Waterloo), Corey Frum and R. Engleman Jr. (University of Arizona)
Fourier Transform Jet Emission Spectroscopy of CN and C_2 Molecules
- 52) Charles X.W. Qian, M. Vasseur, David M. Rayner and Peter Hackett (Steacie Institute for Molecular Science, NRC)
Photofragment Translational Spectroscopy of Cl Atom

- 53) Gomathi Ramachandran and Gregory S. Ezra (Cornell University)
Vibrational Deactivation in Kr/O_2^+ Collisions: The Role of Complex Formation
- 54) Jon-Marc Rodier, David Phillips and Anne B. Myers (University of Rochester)
Ultrafast Spectroscopic Studies of Trans-Hexatriene and Alkyl Iodides
- 55) G. Kim, L.M. Hitchcock, G.P. Reck and Erhard Rothe (Wayne State University)
Imaging of Total Densities, and of State Specific Densities, via LIF and Rayleigh Scattering of 193nm Light
- 56) Tom A. Seckel, Xin Luo and Tom R. Rizzo (University of Rochester)
Double Resonance Vibrational Overtone Spectroscopy of HN_3
- 57) Rebecca D.F. Settle and Tom Rizzo (University of Rochester)
 CO_2 Laser Assisted Vibrational Overtone Spectroscopy of Methanol
- 58) Vladimir Shalaev and Martin Moskovits (University of Toronto)
Optical Properties of Fractal Clusters
- 59) Benoit Simard, Andrew James and Peter Hackett (Steacie Institute for Molecular Science, NRC) and Walter Balfour (University of Victoria)
Optical Spectroscopy of Jet Cooled Yttrium Containing Compounds: Recent Progress on Yttrium Monohydride and Yttrium Monocarbide
- 60) Petra Swiderek and M. Michaud (Université de Sherbrooke), G. Hohlneicher (Universität zu Köln) and Leon Sanche (Université de Sherbrooke)
Electron Energy Loss Spectroscopy of Solid Phenanthrene: Search for the Low-lying Triplet States
- 61) Jan E. Szulejko and Terry B. McMahon (University of Waterloo)
A High Pressure Mass Spectrometric Determination of Proton Affinities of Compounds of Low Gas Phase Basicity Ranging from Nitrogen to Benzene (118 to 181 kcal mol⁻¹)
- 62) Daniel Tremblay (Université Laval), P.A. Thiry and J.J. Pireaux (FUNDP, Belgium)
Excitation Probability for Intramolecular Vibrations in a Uniform Dielectric Film Supported by a Metal Substrate. A Calculation in the Framework of the Dielectric Theory of Electron Energy Loss
- 63) John Tromp, Didier Lemoine and Gregory Corey (Université de Montréal)
Fourier Transform Wave Packet Propagation in Spherical Coordinates: In Search of the Holy Grail
- 64) D.P. Tsai and Martin Moskovits (University of Toronto)
Artifacts of STM Images
- 65) Peter J.M. van der Burgt and James W. McConkey (University of Windsor)
Time-of-flight Study of Electron-Impact Dissociation of SO_2
- 66) Kaley A. Walker, Hartmut G. Hedderich and Peter F. Bernath (University of Waterloo)
High Resolution Infrared Spectroscopy of BiH , BiD and BaH
- 67) WenGe Wang and Howard R. Mayne (University of New Hampshire)
A New Representation for Reactive Potential Energy Surfaces

- 68) Tzyy-Schiuan Yang and Anne B. Myers (University of Rochester)
Solvation Effects on the C^1B_2 and X^1A_1 States of SO_2 in Hexane Studied by Spontaneous Resonance Raman Scattering
- 69) Xiaobe Yang and Chifure Noda (University of New Hampshire)
Photoacoustic Detection of CO_2 and N_2O Overtone Transitions in the Near-IR Range
- 70) James Ying, Chris Mathers and K. Tong Leung (University of Waterloo)
K-dependent Electron Energy Loss Spectroscopy of SF_6 Molecules
- 71) Zhong Chen Zhang, Richard J. Wheatley, William J. Meath and A.R. Allnatt (University of Western Ontario)
Non-additive 3-body Interaction Energies for Closed Shell Atoms Using H_3 (Quartet Spin State) as a Model
- 72) Leegeng Zhao, William S. Neil and James J. Sloan (University of Waterloo)
Observation of HCN Chemiluminescence in Acrylonitrile Photodissociation at 193nm
- 73) Ling Zhu and William L. Hase (Wayne State University)
Study of Energy Transfer Pathways for $Li^+ + H_2O \rightarrow Li^+(H_2O)$ Association
- 74) Aaron W. Garrett, Daniel L. Severance and Timothy S. Zwier (Purdue University)
Immiscibility and Ion Chemistry in Molecular Clusters: $C_6H_6-(H_2O)_n$ and $C_6H_6-(CH_3OH)_n$