The 8th Annual

University of Waterloo

Symposium on Chemical Physics

November 6-8, 1992

Acknowledgements

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Waterloo Symposium on Chemical Physics

November 6-8, 1992

at the University of Waterloo

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

SESSION I: Friday, November 6, 1992 - P.M. Davis Centre 1351

Chair: **John Hepburn**

7:30 - 8:10 David Perry (University of Akron)
Infrared Molecular Eigenstate Spectroscopy: A Probe for the Rate and Mechanism of Intramolecular Relaxation

8:10 - 8:30 John W. Tromp and G.C. Corey (Université de Montréal)
Grid Methods in Sphirical Coordinates

8:30 - 8:50 David Cramb and S.C. Wallace (University of Toronto) and H. Bitto and J.R. Huber (University of Zurich)
Coherence Phenomena in Electronically Excited CS_2

8:50 - 9:10 Rebecca Settle and T. Rizzo (University of Rochester)
CO_2 Laser Assisted Vibrational Overtone Spectroscopy

SESSION II: Saturday, November 7, 1992 - A.M. Davis Centre 1351

Chair: **Terry McMahon**

9:00 - 9:40 Ajit Thakkar (University of New Brunswick)
Van der Waals Coefficients, Polarizabilities and Hyperpolarizabilities: Current Calculational Possibilities

9:40 - 10:00 Mark Thachuk and G.C. Schatz (Northwestern University)
Time Dependent Methods for Calculating Thermal Rate Coefficients Using Flux Correlation Functions

10:00 - 10.20 Elizabeth Bishenden, C.A. Bird and D.J. Donaldson (University of Toronto)
Near UV Photolysis of OC*l*O in Room Temperature Samples and in Supersonic Jet Expansions

10:20 - 10:40 **Coffee Break**

10:40 -11:40 W. Carl Lineberger (University of Colorado)
Time-Resolved Cage Recombination Dynamics in Large Molecular Cluster Ions

11:40 - 12:00 Gopalakrishnan Vaidyanathan, W.J. Herron and J. Garvey (SUNY at Buffalo)
Mass Spectrometric Investigations of 2-alkoxyethanol clusters. Reactivity, Magic Numbers and Structural Implications

12:00 - 12:20 David L. Phillips, Jon-Marc Rodier and Anne B. Myers (University of Rochester)
Picosecond Spectroscopy of Cis-Stilbene Photoproducts and Trans-Hexatriene

12:20 - 2:00 **Lunch** Davis Centre 1301

SESSION III: Saturday November 7, 1992 Davis Centre 1351

Chair: **Tong Leung**

2:00 - 2:40 Leon Sanche (Université de Sherbrooke)
Surface Reactions and Desorption Induced by Electron Attachment

2:40 - 3:00 Vladimir M. Shalaev, C. Douketis and M. Moskovits (University of Toronto)
Light Induced Drift of Electrons in Metals

3:00 - 3:20 Mario Morin, (University of Ottawa) and K. Kuhnke, A.L. Harris (AT&T Bell Labs)
Vibrational Dynamics of Hydrogen-Terminated Vicinal Si(111) Surfaces: Interadsorbate Energy Transfer

3:20- - 3:40 Stephen Urquhart, A.P. Hitchcock (McMaster University) and E.G. Rightor (Dow Chemical, Texas)
Core Excitation Spectroscopy for Microanalysis of Polymers

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

POSTER SESSION AND MANUFACTURERS' DISPLAY

7:00 P.M. **DINNER** South Campus Hall

SESSION V: Sunday, November 8, 1992 - A.M. Davis Centre 1351

Chair: **Peter Bernath**

9:30 - 10:10	Phil Bunker (Herzberg Inst. of Astrophysics, NRC) The Infrared Spectrum, Torsional Barrier and Vibrational Motions in Dimethylacetylene
10:10 - 10:30	Terry E. Gough, J.A. Barnes and M. Stoer (University of Victoria) Stark Effect of Vibrationally Excited States
10.30 - 10:50	Man-Chor Chan, Takayoshi Amano and J.K.G. Watson (NRC, Ottawa) Infrared Absorptions of Deuterium Plasma in Hollow Cathode Discharges
10:50 - 11:10	**Coffee Break**
11:10 - 11:50	J. Bill McConkey (University of Windsor) Use of Laser Induced Fluorescence Techniques to Probe the Break Up of Simple Molecules Under Electron Impact
11:50 - 12:10	Raymond E. March, F.A. Londry and R.L. Alfred (Trent University) Quadrupole Ion Trap: Comparison of Simulation and Experimental Results
12:10 - 12:30	Albert Stolow and Y.T. Lee (University of California, Berkeley) Photodissociation Dynamics of CO_2 at 157nm

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:

4:00 - 5:15 p.m. ***Those whose papers were given even-number labels should attend their posters.***

5:15 - 6:30 p.m. ***Those whose papers were given odd-number labels should attend their posters.***

1) Cedric Accary, Philippe Barbarat and William L. Hase (Wayne State University)
A Preliminary Study of H-Atom Association with the (111) Surface of Diamond

2) Allan Adam, J.R.D. Peers, C. Linton, T.E. Clarke and S. Black (University of New Brunswick)
LIF and IMF Spectroscopy of Ytterbium Monofluoride: The $A^2\Pi_{1/2}$-$X^2\Sigma^+$ Band System

3) Kelly L. Akers and M. Moskovits (University of Toronto)
Raman Spectra of Potassium Doped C_{60} Films

4) Dominique R.T. Appadoo, J. Campbell, P.F. Bernath and R.J. Le Roy (University of Waterloo)
High Resolution Spectroscopy of the $A^3\Pi(1_u)$-$X^1\Sigma_g^+$ Transition of $I^{79}Br$ and $I^{81}Br$

5) Donald J. Arseneau, S. Baer, D.G. Fleming, M. Hahn, J. Pan, M. Senba and R. Snooks (University of British Columbia)
Isotope Effects and Muonium as a Probe of Chemical Reaction Dynamics (at TRIUMF)

6) Victoria Barclay, D.B. Jack, J.C. Polanyi and Y. Zeiri (University of Toronto)
Simulation of Hot H Atom Reactions in the Photolysis of HBr Aligned on the LiF(001) Surface

7) M. Keil, L.J. Rawluk, M. Alexander, H.R. Mayne and J.J.C. Barrett (University of New Hampshire)
Interference Effects in Ar+HF Scattering: A Mixed Quantum/Classical Study

8) John N. Beauregard and H.R. Mayne (University of New Hampshire)
Cluster Catalyzed Chemisorption of H_2 from Si(111)(1x1) - A Molecular Dynamics Study

9) Pamela A. Berg and J.J. Sloan (University of Waterloo)
The Effect of Reagent Translational Excitation on the Dynamics of the Reaction $H + Cl_2 \rightarrow HCl + Cl$

10) Matthew J. Bramley and N.C. Handy (Université de Montréal)
Converged Rovibrational Levels for 4-Atom Molecules with No Dynamical Approximations

11) Robert Callaghan, I. Lim, J.J. Sloan (University of Waterloo), D.J. Donaldson (University of Toronto) and T.E. Gough (University of Victoria)
Optical Measurements on Model Polar Stratospheric Clouds by FTIR Spectroscopy

12) Ruth E. Cameron, R.A. Holt, S.D. Rosner, T.J. Scholl and L. Zhang (University of Western Ontario)
High Resolution Study of the $B^2\Sigma$ - $X^2\Sigma$ System of SiO^+

13) Jenn M. Campbell and P.F. Bernath (University of Waterloo)
Rotation-Vibration Spectrum of IBr

14) Darryl Chartrand, R.J. Le Roy (University of Waterloo), A.Kumar and Wm. Meath (University of Western Ontario)
Effect of Three-Body Forces on the Statics and Dynamics of SF_6-$(Rg)_n$ and $(Rg)_{13}$ Clusters

15) C.V.V. Prasad and P.F. Bernath (University of Waterloo)
Fourier Transform Spectroscopy of the Swan System of C_2 and the Red System of CN

16) Claudio Chuaqui, T. Slee and R.J. Le Roy (University of Waterloo)
Determination of the He-CO Potential Energy Surface From High Resolution Spectroscopy

17) Ashok K. Dham, A.R. Allnatt and W.J. Meath (University of Western Ontario)
Multi-Damped Exchange-Coulomb Potential Energy Curves for Rare Gas Dimers

18) P. Dietrich, M. Laberge and P.B. Corkum (Steacie Institute, NRC)
Dissociative Multiphoton Ionization of Diatomic Molecules with Femtosecond High Power Laser Pulses

19) Stephen Donnelly, A. Midey, J. Qian, C. Schmuttenmaer and J.M. Farrar (University of Rochester)
Photodissociation Studies of Mass-Selected Solvated Metal Cation Clusters

20) Constantine Douketis, V.M. Shalaev, T. Haslett, and M. Moskovits (University of Toronto)
Energy Resolved One Photon and Two Photon Electron Emission from Silver Films

21) Mike Dulick and P.F. Bernath (University of Waterloo)
Direct Reduction of Spectroscopic Data by Fitting to Potential Curves

22) Tom H. Ellis (Universé de Montréal)
Interactions Between Coadsorbed Molecules on Metal Surfaces

23) Y.B. Fan, K.L. Randall and D.J. Donaldson (University of Toronto)
Photochemistry of Alkyl Iodide Dimers

24) R. Fei, H.M. Lambert, T. Carrington, C.H. Dugan, S.V. Filseth and C.M Sadowski (York University)
Rotational Energy Transfer in Single Rotational States of CN(X, v=2)

25) R. Fournier (Steacie Institute, NRC)
Density Functional Study of 1:1 Complexes of Nickel with Small Molecules

26) James T. Francis and A.P. Hitchcock (McMaster University)
Inner Shell Excitation Spectroscopy of some Aromatic and Cyclic Diketone Compounds

27) Kathleen Gough, H.K. Srivastava and K. Belohorcova (Brock University)
Experimental and Theoretical Investigation of Raman Trace Scattering Intensities in Alkanes

28) Mee Hahn, D. Arseneau, S. Baer, D.G. Fleming, J. Pan, M. Senba and R. Snooks (University of British Columbia)
Muonium Studies on Powder and Zeolite Surfaces (at TRIUMF)

29) Jerry A. Heal (University of Waterloo), M. Ramek (Technical University of Graz) and P. Mezey (University of Saskatchewan)
On the Use and Limitations of Atom-based Modeling of Molecules

30) William J. Herron, G. Vaidyanathan and J. Garvey (SUNY at Buffalo)
If One Hydroxyl Group Is Good, Is Two Better? A Review of Cluster Mass Spectra for Small Alcohols and Diols

31) Deqing Hu, C. MacPherson and K.T. Leung (University of Waterloo)
High-Resolution Energy Loss Spectroscopy for Surface Analysis

32) D.V. Heyd, Erik Jensen and J.C. Polanyi (University of Toronto)
Photoejection of CH_3Cl by CH_3X (X=Br,I) and U.V. Photons

33) Xue-Pei Jiang (University of Toronto)
Optimal Chirping in Pumping Up Diatomics: Approach by Classical Mechanics

34) Dmitri Klyachko and V. Krigel (University of Sherbrooke)
Surface Electromotive Forces in Semiconductors Induced by Electron Bombardment

35) Marcin Kolbuszewski and J. Wright (Carleton University)
Kinetic and Thermodynamic Stability of Diatomic Dications

36) Anne Kondo and W.J. Meath (University of Western Ontario)
On the Effects of "Permanent Dipoles" in Microwave Spectroscopy

37) Wei Kong, D. Rodgers and J.W. Hepburn (University of Waterloo)
High Resolution Photoelectron Spectroscopy Using Coherent XUV: Studies of Ionic Excited States

38) Greg K. Koyanagi and T.B. McMahon (University of Waterloo)
Laser Ablation High Pressure Mass Spectrometry Photoelectron Spectroscopy

39) Mangala S. Krishnan and T. Carrington, Jr. (Université de Montréal)
Effective Hamiltonians for Coriolis-Coupled Nearly Degenerate Vibrational Modes: Illustrative Examples

40) T.H. Ellis, Erik Kruus, D.R. Salahub and H. Wang (Université de Montréal)
The Coadsorption of Water and CO on Ni(100) - A Combined Experimental and Theoretical Study

41) Rick D. Lafleur, P. Montoya-Palaez and J.M. Parnis (Trent University)
Insertion and Addition Reactions of $O(^1D)$ Atoms with Simple Molecules in Solid Rare Gas Matrices: An FTIR Study of Primary Reaction Products

42) T. Carrington, C.H. Dugan, S.V. Filseth, H.M. Lambert and C.M. Sadowski (York University)
Cross-sections and Energy Disposal for CN(X) Produced in the H+HCN Reaction at 53 and 58 kcal mol^{-1} Collision Energies

43) Dale Levandier, D. Varley, M. Carpenter and J.M. Farrar (University of Rochester)
Crossed Beam Studies of Ion-Molecule Reaction Dynamics: Vibrational State-Resolved Scattering in the System O^- + HF

44) Ian Lim, R. Callaghan and J.J. Sloan (University of Waterloo)
Production and Characteristics of Model Polar Stratospheric Clouds

45) Charlie MacPherson, D.Q. Hu and K.T. Leung (University of Waterloo)
The Catalytic Dehydrogenation of Cyclic Hydrocarbons to Aromatic Compounds on Si(111) 7x7

46) Robert S. Maher and H. Mayne (University of New Hampshire)
A New Representation of Potential Energy Surfaces: Quantum and Classical Dynamics Study

47) A.R.W. McKellar (Herzberg Institute of Astrophysics, NRC)
Carbon Monoxide - Rare Gas Complexes: CO-He to CO-Xe

48) André McNichols and T. Carrington, Jr. (Université de Montréal)
A Lanczos/DVR Method for the Calculation of the Vibrational Energies of Formaldehyde

49) Arthur Mihill, H.P. Bluem, B.C. Craft, E. Morikawa, V. Saile, J. Scott, O. Vladimirsky and Y. Vladimirsky (Louisiana State University)
CAMD - The New Synchrotron Light Source in Louisiana

50) Jay Niesse, J. Beauregard and H. Mayne (University of New Hampshire)
A Classical Trajectory Study of Ar Clusters Scattered from a Purely Repulsive Surface

51) X. Zhang, E.G. Lewars, R.E. March and J. Mark Parnis (Trent University)
The FT-infrared Spectrum of the Acetone-Water Complex: An Experimental and Theoretical Study

52) A.G. Adam, J.R.D. Peers (University of New Brunswick), B. Simard, A. James and P.A. Hackett (Steacie Institute, NRC)
Spectroscopy of Laser-Ablated ZrN: An Update

53) Z. Ye, R. Tu and Peter Piercy (University of Ottawa)
Infrared Absorption Line Shapes at Surfaces: Theory of Photon-Induced Relaxation, Dephasing and the Temperature-Dependent Frequency Shift of Vibrational Modes of an Adsorbed Molecule

54) Martin Poulin and T. Carrington, Jr. (Université de Montréal)
Determination of the Potential Surface for Diatomics Using the Discrete Variable Representation

55) Michael G. Prisant, G. Kedem and M. Head (Duke University)
Application of Ray Casting to Problems of Protein Structure

56) H.-P. Loock, J. Cao and Charles X.W. Qian (University of Victoria)
Vibrational Modification of the Spatial Anisotropy Parameter in Photodissociation; A Classical Trajectory Study

57) Jun Qian, C. Schmuttenmaer, S. Donnelly and J.M. Farrar (University of Rochester)
The Time-Resolved Photodissociation Study of Mass-Selected Solvated Strontium Ion Clusters

58) L. Lian, R. Fournier, P. Hackett and David Rayner (Steacie Institute, NRC)
Gas-Phase Chemical Kinetics of Small Metal Clusters: Reactions of Cu_2

59) Jon-Marc Rodier and A.B. Myers (University of Rochester)
Photochemistry of Cis-Stilbene

60) Pierre-Nicholas Roy, J.W. Tromp and G.C. Corey (Université de Montréal)
Wave Packet Propagation in a Discrete Variable Representation Using the Split Operator Method

61) X. Luo, Tom Seckel and T.R. Rizzo (University of Rochester)
Rotationally Resolved Spectroscopy of Vibrational Overtone Levels in Hydrazoic Acid

62) Benoit Simard and Andrew James (Steacie Institute, NRC)
High Resolution Molecular Beam Spectroscopy of Yttrium Monosulfide

63) Caroline Starrs, M.N. Jego, A. Mank and J.W. Hepburn (University of Waterloo)
Mode Specific Photochemistry: Photofragment Spectroscopy of the Predissociating $^1B_2$ State of the CS_2 Molecule

64) James J. Stry, M.T. Coolbaugh, J.F. Garvey (SUNY at Buffalo)
Gas Phase Ion-Molecule Reactions of C_{60}^{++}

65) Marc ter Horst and C.J. Jameson (University of Illinois at Chicago)
Classical Trajectory Study of CO_2-Ar and Comparison with NMR Data

66) R.P. Steer and Brian D. Wagner (University of Saskatchewan)
Subpicosecond Pump-probe Studies of Azulene and Related Compounds in Solution

67) Haobin Wang and W.L. Hase (Wayne State University)
A Potential Energy Surface and Initial Dynamical Calculation for the Cl^-+CH_3 Br and $ClCH_3$ + Br^- Substitution Reaction

68) Robert A. Weersink and S.C. Wallace (University of Toronto)
Vibrational Spectroscopy and Quantum Interference Effects in N,N-Diethyl Aniline

69) Brad White and P.F. Bernath (University of Waterloo)
High Resolution Infrared Emission Spectra of High Temperature Gas Phase Molecules

70) Curtis Westerfield and Anne B. Myers (University of Rochester)
The 2^1A_g State of Cis-Hexatriene Vapor: Resonance Raman Spectra

71) F.R. McCourt, Clement Wong and E.E. Hanson (University of Waterloo)
Classical Trajectory Calculation of Transport and Relaxation Properties for Diatom-Diatom Mixtures

72) Mu-Liang Xu and M.J. Dignam (University of Toronto)
Calculations of SERS From a Pair of Coated Particles - CO and Benzene on Ag, Pt, Ge and SiO_2 - Showing Enhancements Exceeding 10^5

73) Tzyy-Schiuan Yang and A.B. Myers (University of Rochester)
Incoherent Four-wave Mixing Study of Dephasing in the B Electronic State of I_2 in Vapor and Solution Phases

74) Xiaoke Yang and C. Noda (University of New Hampshire)
Photoacoustic Detection of OCS Overtone Transitions in the Near-Infrared

75) Ji Feng Ying and K.T. Leung (University of Waterloo)
Observation of a "New" Dipole-forbidden Non-Rydberg State in CF_3Cl and CF_2Cl_2 by Momentum Transfer-Resolved Electron Energy Loss Spectroscopy

76) Ruihua Zhang and A.B. Myers (University of Rochester)
Ultrafast Dephasing and Modulation in Azulene

77) David Green, S. Williams, R.N. Zare, T. Owano and C.H. Kruger (Stanford University)
Degenerate Four-Wave Mixing Diagnostics in Hostile Environments: Boundary Layer Radical Profile in Reactive Plasmas