Waterloo Symposium on Chemical Physics

November 4-6, 1994

at the University of Waterloo

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

SESSION I: Friday, November 4, 1994 - P.M. Davis Centre 1351

Chair: **Bob Le Roy**

7:30 - 8:10 Terry E. Gough (University of Victoria)
Infrared Spectroscopy of Molecular Microcrystallites

8:10 - 8:30 R.H. Lipson, S.S. Dimov, J.Y. Cai, P. Wang and H.A. Bascal (University of Western Ontario)
Two-Photon Time-of-Flight Mass Spectra of Rare Gas Excimers

8:30 - 8:50 J.W. Forsman, R. Berman, P. Duggan, S. Hamid Fakhr-Eslam, M. Le Flohic, Guy D. Sheldon, P.M. Sinclair, J.R. Drummond and A.D. May (University of Toronto)
A High Resolution Raman and Infrared Spectrometer for Line Shape, Molecular Dynamics and Atmospheric Sounding Studies: Accomplishments and a Perspective

8:50 - 9:10 R.J.C. Brown (Queen's University) and R.M. Lynden-Bell (University of Cambridge)
A Molecular Dynamics Study of Ammonium Perrhenate

SESSION II: Saturday, November 5, 1994 - A.M. Davis Centre 1351

Chair: **John Hepburn**

9:00 - 9:40 Jeremy M. Hutson (University of Durham, U.K.)
Additive and Non-additive Intermolecular Forces from the Spectroscopy of Van der Waals Complexes

9:40 - 10:00 Robert Weersink, D. Cramb, S.C. Wallace and R. Gordon (University of Toronto)
Torsion-Inversion Coupling in the S_1 State of Acetaldehyde

10:00 - 10:20 Piotr Piecuch and J. Paldus (University of Waterloo)
Coupled-Cluster Methods for Quasidegenerate States. Calculation of Potential Energy Surfaces and Molecular Properties Using the State-Universal Multi-Reference Coupled-Cluster Approach

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

10:40 -11:40 Giacinto Scoles (Princeton University)
Clusters Within Clusters: Matrix Isolation Spectroscopy in Condensed Helium Beams

11:40 - 12:00 John C. Shelley (Univ. of British Columbia), M. Sprik (IBM Research, Zurich) and M. Klein (Univ. of Pennsylvania)
Electrostatic Effects in Aqueous Ionic Surfactant Systems: Molecular Dynamics Simulations

12:00 - 12:20 David S. Perry, G.A. Bethardy and X. Wang (University of Akron)
The Acceleration of Vibrational Energy Flow in Flexible Molecules

12:20 - 1:40 **Lunch** Davis Centre 1301

SESSION III: Saturday November 5, 1994 Davis Centre 1351

Chair: **Jim Sloan**

1:40 - 2:20 A.R.W. McKellar (NRC, Ottawa)
Long-Path Infrared Spectra of Weakly-Bound Complexes

2:20 - 2:40 David S. Green and J.W. Hudgens (National Institute of Standards & Technology, Gaithersburg, MD)
Nonlinear Laser Diagnostics of Reactive Intermediates in Plasmas

2:40 - 3:00 Tamar Seideman (Steacie Institute of Molecular Science, NRC, Ottawa)
On the Dissociative Ionization of Diatomic Molecules in Intense Fields

3:00 - 3:20 B.N. Jagatap, W.J. Meath (University of Western Ontario), D. Tittelbach-Helmrich and R.P. Steer (University of Saskatchewan)
Multi-Photon Dynamics Related to Two-Colour Time-Delay and Polarization Effects in Laser-Molecule Interactions with Applications to α-NPO.

SESSION IV: Saturday, November 5, 1994 from 3:30 P.M. Davis Centre Lobby

POSTER SESSION AND MANUFACTURERS' DISPLAY

6:15 P.M. Bus departs from the Davis Centre for Golf's Steak House

7:00 P.M. **DINNER** Golf's Steak House

SESSION V: Sunday, November 6, 1994 - A.M. Davis Centre 1351

Chair: **Peter Bernath**

9:30 - 10:10 Roger E. Miller (University of North Carolina)
Photofragmentation of Oriented Molecules: New Insights into Photodissociation Dynamics from Pendular States

10:10 - 10:30 H. Palm (LPCR, France), Christian Alcaraz (University of Waterloo and LURE), O. Dutuit (LURE, LPCR, France) and P.M. Guyon (LCAM, France)
State-Selected Ion-Molecule Reactions

10:30 - 10:50 Marc Vrakking and Y.T. Lee (University of California, Berkeley)
DC Electric Field Effects and Collisional Effects on the Lifetimes of High Principal Quantum Number Rydberg States of NO and Xe: Implications for Zero-Electron Kinetic Energy (ZEKE) Spectroscopy

10:50 - 11:10 **Coffee Break**

11:10 - 11:50 Mark S. Child (Oxford University, UK)
Inversion of Spectroscopic Data

11:50 - 12:10 Martin Poulin, M.J. Bramley and T. Carrington Jr. (Université de Montreal)
Calculated Spectrum of Polyatomic Molecules without Wavefunctions: Vibrational (J=0) Bands for Water and Formaldehyde, Using the RRGM

12:10 - 12:30 Albert Stolow (Steacie Institute for Molecular Science, NRC, Ottawa)
Femtosecond Pump-Probe ZEKE Photoelectron Spectroscopy

POSTER SESSION

Chair: **Terry McMahon**

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

3:30 - 4:20 p.m. ***Those whose papers were given 1a, 2a, 3a, etc. should attend their posters.***

4:20 - 5:10 p.m. ***Those whose papers were given 1b, 2b, 3b, etc. should attend their posters.***

5:10 - 6:00 p.m. ***Those whose papers were given 1c, 2c, 3c, etc. should attend their posters.***

1a) David Cramb and Stephen C. Wallace (University of Toronto)
Anomalous Surface Second Harmonic Generation: Results of 111-D at the Air-Toluene Interface

1b) S.D. Campbell, Lori A. Jones, F.-X. Wei and D.F. Thomas (University of Guelph)
Surface Structural Features of Chemically Etched Porous Silicon

1c) Michael Carpenter, M. Zanni and J. Farrar (University of Rochester)
Crossed Beam Studies of the $O^- + D_2 \rightarrow OD^- + D$ Reaction at Collision Energies Ranging from 0.25 eV to 1.2 eV.

2a) Jun Qian, T. Midey, S. Donnelly and J. Farrar (University of Rochester)
Photodissociation Study of $Sr^+(CH_3OH)_n$ and $Sr^+(H_2O)_n$ Systems

2b) J. Pan, A. Bahel and Mushti V. Ramakrishna (New York University)
Magic Numbers of Silicon Clusters

2c) Deqing Hu and W. Ho (Cornell University)
Translationally Activated Adsorption of CO on Si(100)2x1 Surface Using a Molecular Beam

3a) Paul Rowntree, D. Klyachko, W. Di and L. Sanche (Université de Sherbrooke)
Oxidation and Fluoridation of Silicon Surfaces Induced by Low-Energy Electron Beams

3b) Andrea McCormick, D. Thölmann and T.B. McMahon (University of Waterloo)
A Theoretical and Experimental Study of Radiative Stabilization and Unimolecular Dissociation of Chemically Activated Proton Bound Dimers

3c) Dennis Tokaryk, J.K.G. Watson, I. Dabrowski (Steacie Institute for Molecular Sciences, NRC, Ottawa) and M. Vervloet (Université de Paris Sud, Orsay)
Spectra of ArD Involving Rydberg Complexes

4a) Yunjie Xu, M. Fukushima, A. Taleb-Bendiab, T. Amano and A.R.W. McKellar (Steacie Institute for Molecular Sciences, NRC, Ottawa)
Infrared Absorption Spectroscopy of Molecular Ions in a Corona-Excited Slit Expansion

4b) Yunjie Xu, J.W.C. Johns and A.R.W. McKellar (Steacie Institute for Molecular Sciences, NRC, Ottawa)
High-Resolution Infrared Spectra of Formyl Fluoride, HFCO

4c) Mangala S. Krishnan, D. Wardlaw and N. Snider (Queen's University)
Collisional Redistribution of Internal States: Energy and Angular Momentum Dependent Transfer Probabilities for AR+H_2 System

5a) Mark Thachuk and D.M. Wardlaw (Queen's University)
Dissociation of Diatomic Molecules in Intense Laser Fields: Stormy Separation or Peaceful Parting?

5b) Laura M. Dobeck, W. Kong, P.L. Houston (Cornell University) and J.W. Hepburn (University of Waterloo)
Photodissociation Dynamics of Glyoxal: Searching of the Triple Whammy Channel

5c) Dierdre Belle-Oudry, T. Mussillon, S. Satyapal and P.L. Houston (Cornell University)
Detection of PO, P and Cl from the 193 nm Photolysis of $POCl_3$.

6a) Pascal de Sainte Claire and W.L. Hase (Wayne State University)
Classical Trajectory Simulations of the Collision-Induced Dissociation of Al_6 and Al_{13} by Argon

6b) Gilles H. Peslherbe and W.L. Hase (Wayne State University)
Direct Dynamics Simulations of SN_2 Nucleophilic Substitution

6c) Ki Song, P. de Sainte Claire and W.L. Hase (Wayne State University)
Comparison of Classical Trajectory and Canonical Variational Transition State Theory Rate Constants for H-Atom Association with the Diamond {111} Surface

7a) Christian Alcaraz, P. Brechignac, D. Dedonder-Lardeaux, A. Delboulbe, I. Dimicoli, O. Dutuit, D. Gauyacq, P.M. Guyon, J. Hepburn, C. Jouvet, S. Martrenchard, H. Palm, N. Shafizadeh, D. Solgadi, M. Vervloet, M. Richard-Viard (LURE, LCAM, LPPM, LPCR Orsay France ; CEN Saclay, France ; LCAR, IRSAMC Toulouse, France ; and University of Waterloo)
Photoionisation of Cold Species and Clusters Using Synchrotron Radiation in the 8-20 eV Range

7b) Dominique R.T. Appadoo, R.J. Le Roy (University of Waterloo), S. Gersternkorn and P. Luc (Lab. Aime Cotton, Orsay, France)
The First Comprehensive Analysis of the A-X IR Spectrum of I_2: An Application of the N-D Theory

7c) John N. Beauregard (University of New Hampshire) and D.L. Thompson (Oklahoma State University)
The Unimolecular Decomposition of Nitramines: Molecular Dynamics and Simulations

8a) Jennifer Busler, B. Guo, K.-Q. Zhang and P.F. Bernath (University of Waterloo)
New Assignments for Hot H_2O

8b) Christina Carere and J.J. Sloan (University of Waterloo)
The Dynamics of the Interaction Between Translationally Excited Hydrogen Atoms and Nitrous Oxide

8c) B. Guo, K.-Q. Zhang, Pina Colarusso, F. Charron and P.F. Bernath (University of Waterloo)
The High-Resolution Infrared Spectroscopy of the Alkaline Earth Fluorides

9a) P. Duggan, P.M. Sinclair, A.D. May and J.R. Drummond (University of Toronto)
Speed Dependent Collisional Inhomogeneities in Infrared Absorption Lineshapes of P and R Branches of CO Broadened by He, N_2 and Xe, Including Dicke Narrowed Doppler Broadening

9b) K.L. Dunfield, C. Linton, A.G. Adam and J.R.D. Peers (University of New Brunswick)
Laser Spectroscopy of Rare Earth Containing Diatomic Molecules: Recent Results

9c) S. Hamid Fakhr-Eslam, G.D. Sheldon, P.M. Sinclair, J.R. Drummond and A.D. May (University of Toronto)
Line Broadening and Shifting of the Raman Q-Branch in D_2 at Low Temperatures

10a) Sheldon Green (NASA/GSFC), L. Demeio and L. Monchick (Johns Hopkins University)
Lineshapes of HF in Ar: Effects of Velocity Changing Collisions

10b) Bujin Guo, S. Yost, K.-Q. Zhang, M. Dulick and P.F. Bernath (University of Waterloo)
High Resolution Emission Spectroscopy of LiH, LiD and LiI

10c) Bujin Guo, R. Ram and P.F. Bernath (University of Waterloo)
Fourier Transform Emission Spectroscopy of MgF_2

11a) Ju Guo, A. Mank and J.W. Hepburn (University of Waterloo)
Autoionization Dynamics of Rotationally Selected NO Rydberg States Probed by Energy- and Angle-Resolved Photoelectron Spectroscopy

11b) Photos G. Hajigeorgiou and R.J. Le Roy (University of Waterloo)
A Modified Lennard-Jones Oscillator Model for Diatomic Potentials

11c) V.J. Barclay, W.-H. Hung, William J. Keogh, R. Kuhnemuth, J.C. Polanyi, G. Zhang and Y. Zeiri (University of Toronto)
Photochemistry of Adsorbed Molecules: HI on LiF, HI on NaF; Theory and Experiment

12a) Henrik G. Kjaergaard, B.R. Henry (University of Guelph), T. Carrington Jr. (Université de Montreal), O. S. Mortensen (Odense University) and M.L. Sage (Syracuse University)
Calculation of Local Mode Vibration Band Intensities in H_2O: The Role of the Dipole Moment Function

12b) Anne E. Kondo, P. Piecuch and J. Paldus (University of Waterloo)
Orthogonally Spin-Adapted Single-Reference Coupled-Cluster Formalism: Linear Response Calculation of Static Properties

12c) Rick D. Lafleur, J.M. Parnis and D.M. Rayner (Trent University)
Gas Phase Nb Cluster Reactivity with Isobutane: Measurement of Absolute Rate Coefficients Using a Fast Flow Reactor

13a) Sebastien Lefebvre, T. Carrington, J. Guan, M. Cassida and D. Salahub (Université de Montreal)
Vibrational Effects on Polarizability of Sodium Trimer

13b) Colan Linton (University of New Brunswick), I. Russier, F. Martin, P. Crozet, A.J. Ross and R. Bacis (Université de Lyon, France)
Optical Optical Double Resonance Spectroscopy of Li_2

13c) Andreas Mank, J.W. Hepburn, H. Kerr and E. Weckman (University of Waterloo)
What Is In a Plasma Welding Arc? or Practical Uses for Atomic Spectroscopy

14a) James D.D. Martin, C. Alcaraz and J.W. Hepburn (University of Waterloo)
Delayed Pulsed Field Ion-Pair Formation

14b) Sean McDowell and W.J. Meath (University of Western Ontario)
On the Anisotropy of the Triple-Dipole Dispersion Energy For Interactions Involving Diatomic Molecules

14c) Zulfikar Morbi and P.F. Bernath (University of Waterloo)
Laser Induced Fluorescence Spectroscopy of the $C\ ^2A_1$-$X\ ^2A_1$ Transition of $CaNH_2$

15a) Carey Bissonnette, R.J. Le Roy (University of Waterloo), R.J. Wheatley and W.J. Meath (University of Western Ontario)
A New Strategy for Including Theoretical Constraints in Fits to Determine Potential Energy Surfaces from Experimental Data: Application to H_2-Argon

15b) John A. Niesse and H.R. Mayne (University of New Hampshire)
The Scattering of Protonated H_2O/Alcohol Clusters from Crystal Surfaces

15c) J. Mark Parnis, L.E. Hoover, D.B. Pedersen and D.D. Patterson (Trent University)
Methanol Production from Methane by Li-promoted Charge-transfer Photodissociation of N_2O in Ar Matrices

16a) A.G. Adam, L.P. Fraser, W.D. Hamilton, J.R.D. Peers and M.C. Steeves (University of New Brunswick)
Electronic Spectroscopy of CoF: Rotational and Hyperfine Structure

16b) Adriana Predoi and R.M. Lees (University of New Brunswick)
Fourier Transform Spectroscopy of the OH-Bending Band of C-13 Methanol in the Torsional Ground State

16c) Neil Snider (Queen's University)
Effect of Weak Collisions on Unimolecular Rate Coefficients

17a) Francis Temme (Queen's University)
Simple-Reducibility Over H_v Carrier Subspaces of v-recoupled Spin-tensorial su2xS_n Liouvillian NMR-Formalisms, From Racah Unit-tensors as Superbosons

17b) Dietrich Tittelbach-Helmrich and R.P. Steer (University of Saskatchewan)
Subpicosecond Pump Probe Measurements of S_1 Population Relaxation Times of Azulene and Pseudoazulene Derivatives

17c) David Villeneuve, I. Fischer, A. Zavriyev and A. Stolow (Steacie Institute for Molecular Science, NRC, Ottawa)
Space Charge Effects in Photoelectron and ZEKE Spectroscopy

18a) Feng Wang, F.R. McCourt and R.J. Le Roy (University of Waterloo)
Simulated IR Spectra as Tests of N_2-Ar Pair Potentials

18b) Hua Wei and T. Carrington (Université de Montreal)
The Orientation of Photofragments

18c) Hui Yu and K.T. Leung (University of Waterloo)
Observation of a "New" Electron-induced Temperature Dependent ν(C-O) Shift in C(2x2)CO/Cu(100)

19a) Keqing Zhang, B. Guo and P.F. Bernath (University of Waterloo)
Laboratory Evidence for Polycyclic Aromatic Hydrocarbon Molecules in the Interstellar Medium

19b) Chunfeng Zhao, P. Hajigeorgiou, J.W. Hepburn and P.F. Bernath (University of Waterloo)
High Resolution Spectra of SrOD by Supersonic Expansion

19c) Andrzej Czajkowski, W. Kedzierski, J.B. Atkinson and L. Krause (University of Windsor)
Rotationally Resolved $H1_u \leftarrow A0^{\pm}_g$ Vibronic Excitation Bands of the $(^{202}Hg)_2$ Excimer

20a) Pierre-Nicholas Roy and T. Carrington (Université de Montreal)
Direct Variational Calculation of Energy Levels and Wavefunctions in a Selected Spectral Window

20b) Denis J. Gendron, A. Mank and J.W. Hepburn (University of Waterloo)
Coherent Control in the Photodissociation of HI

20c) Marcin Kolbuszewski (Steacie Institute for Molecular Science, NRC, Ottawa)
Electronic States of Carbon Chains, Diffuse Interstellar Bands and Spectra of Carbon Vapour

21a) Vladmir Spirko and J. Cizek (University of Waterloo)
Non-adiabatic Corrections for Coupled Oscillators Using Hutson and Howard Perturbation Theory

21b) Xiangzhu Li and J. Paldus (University of Waterloo)
Accurate Quantum Chemical Computations for Excited States: Theory, Implementation and Applications of the Unitary Group Based Open-shell Coupled Cluster Method

21c) Philip R. Bunker (Steacie Institute for Molecular Sciences, NRC, Ottawa) and P. Jensen (Wuppertal University, Germany)
The Renner Effect in CH_2 and CH_2^+

22a) Randall S. Dumont, S. Jain and A.G. Basile (McMaster University)
Argon Cluster Evaporation Dynamics

22b) Allan Bertram, Dawn Patterson and J.J. Sloan (University of Waterloo)
Measurements of Temperature and Concentration Dependence of Phase Changes in Sulferic Acid Aerosols.

22c) Richard Brezina and W.-K. Liu (University of Waterloo)
Close-Coupling Calculation of Raman Lineshape for D_2-He

23a) Guy D. Sheldon, S. Hamid Fakhr-Eslam, P.M. Sinclair, J.R. Drummond and A.D. May (University of Toronto)
Low Temperature Line-Mixing in the Raman Q-Branch of D_2

23b) Richard Berman, P. Duggan, A.D. May and J.R. Drummond (University of Toronto)
Line Mixing in the 2076 cm^{-1} Vibrorotational Q Branch of Pure CO_2 Using High Resolution Infrared Spectroscopy

23c) S.S. Dimov, P. Wang and R.H. Lipson (University of Western Ontario)
High Resolution VUV Laser/Time-of-flight Spectroscopy of BrCl and Cl_2

24a) Mieczyslaw Czajkowski and J. Koperski (University of Windsor)
Spectroscopic Constants for ZnNe and ZnAr Van der Waals Clusters in $XO^+(4^1S_0)$ and $D1(4^1P_1)$ Molecular States

24b) Kelly Higgins, F.-M. Tao and W. Klemperer (Harvard University)
Ab Initio Potential Energy Surface and Molecular Dynamics for the HeClF Complex

24c) Fu-Ming Tao and W. Klemperer (Harvard University)
Ab Initio Potential Energy Surfaces for the HCl Dimer

25a) Robert C. Mawhinney (University of Guelph), P.J. Bruna, and F. Grein (University of New Brunswick)
An MRD-CI Study of the Dication BN^{2+} Potential Curves, Ionization Potentials, KER, and Lifetimes

25b) James Forrest, R.L. Brooks and J.L. Hunt (University of Guelph)
Spontaneous Optical Flashes in Proton-Irradiated Solid Deuterium

25c) Robert J. Le Roy (University of Waterloo), C.E. Chuaqui (University of British Columbia) and M. Thachuk (Queen's University)
CO-He: Do We Really Know How to Predict Very Low Temperature Line Broadening?

26a) Matthew M. Beaky, D.C. Flatin, T.M. Goyette and F.C. De Lucia (The Ohio State University)
Hydrogen and Helium Pressure Broadening of CO, CH_3F and H_2S Between 1K and 600K