Symposium on Chemical Physics

at the University of Waterloo

November 9 - 11, 2001

REGISTRATION begins at 7:00 p.m., Davis Centre Room 1301

SESSION I: Friday, November 9, 2001 - P.M. Davis Centre Room 1351

Chair: **Peter Bernath**

7:30 – 8:15 Ronald Steer (University of Saskatchewan)

Explorations of the Photophysics of Higher Electronic Valence States of Large Molecules: From Spectroscopic Curiosity to Photonics Applications

8:15 – 8:30 Saba M. Mattar and Alyson D. Stephens (University of New Brunswick)

Description of a Novel Multi-Frequency Steady State and Pulsed Electron Paramagnetic Resonance Spectrometer

8:30 – 8:45 Rongzhu Wang and J. Hugh Horton (Queen's University)

Characteristics of Silver and Germanium Sulfide Films Studied by Nanoindentation Methods.

8:45 – 9:00 K.K. Lehmann, M.R. Radcliff and G. Scoles (Princeton University)

Charge Distribution Deformation in Van der Waals Complexes Involving Atoms With Low Ionization Potentials

9:15 Grad Club - Informal Discussions

SESSION II: Saturday, November 10, 2001 - A.M. Davis Centre 1351

Chair: **Jim Sloan**

9:00 – 9:45 Jonathan Abbatt (University of Toronto)

Interactions of Atmospheric Trace Gases with Ice: Adsorption and Reaction Studies

9:45 – 10:00 R.M. Lees, M. Mollabashi, Li-Hong Xu, M. Lock and B.P. Winnewisser (University

of New Brunswick)

Variations in torsion-vibration energy structure of CH_3OH from fundamental, overtone and combination bands of the CH_3-rocking and CO-stretching modes

10:00 – 10:15 S. Dobrin, J.B. Giorgi, T.G. Lee, F.Y. Naumkin, S.A. Raspopov, J.C. Polanyi and J. Wang (University of Toronto)

Dynamics of Charge-Transfer Reactions in the Adsorbed State

10:15 – 10:45 **Coffee Break**

Chair: **James Martin**

10:45 - 11:45 William C. Stwalley (University of Connecticut)

Making Molecules at MicroKelvin

11:45 - 12:00 Denise M. Koch and Gilles H. Peslherbe (Concordia University), Nihed Chaabane and Holger Vach (l'École Polytechnique, Palaiseau, France)

Rotational Hindrance and Cage Effects in $(N_2)_n$ Cluster Scattering

12:00 - 12:15 Li-Hong Xu, R.M. Lees, L. Brown and I. Kleiner (University of New Brunswick) (JPL, Pasadena; Orsay, France)

Positions and Intensities for the ν_8 and ν_3 Vibrational Systems of CH_3OH

12:15 - 1:30 **Lunch** - Davis Centre 1301

SESSION III: Saturday, November 10, 2001 - P.M. Davis Centre 1351

Chair: **Fred McCourt**

1:30 - 2:15 Herschel Rabitz (Princeton University)

Teaching Lasers to Control Molecules: The Molecule Knows Best

2:15 - 2:30 Alex Brown, W.J. Meath and A.E. Kondo (University of Western Ontario) (Indiana University of Pennsylvania)

Absolute Laser Carrier Phase Effects in the Two-Color Excitation of Dipolar Molecules

2:30 - 2:45 David B. Pedersen and Benoit Simard (National Research Council of Canada)

Electron Transfer Processes in Metal-DNA Base Complexes in the Gas Phase

2:45 - 3:00 Sophie M.K. Brunet, Tucker Carrington, Stephen V. Filseth (York University)

Rotational Energy Transfer in CN(X,v=2) with H_2 and with D_2

3:00 - 3:15 M.Czajkowski, M.Lukomski, J.Koperski (University of Windsor)

Laser Spectroscopy of CdKr Molecules of B1-X0 Transition-the Case of Double-Well Potential Energy Curve

3:15 **Refreshments and Poster Session**

SESSION IV: Saturday, November 10, 2001 - from 3:30 P.M. Davis Centre Lobby

POSTER SESSION AND SPONSOR'S DISPLAY

6:00 P.M.	Poster session ends.	
	Depart for Conrad Grebel University College	
6:30 P.M.	Cash Bar	Conrad Grebel University College
7:00 P.M.	**DINNER**	Conrad Grebel University College

SESSION V: Sunday, November 11, 2001 - A.M. Davis Centre 1351

Chair: **Bob Le Roy**

9:15 – 10:00 Gilles Peslherbe (Concordia University)

Photochemistry in Diverse Environments

10:00 – 10:15 Jian Tang and A.R.W. McKellar (National Research Council of Canada)

High Resolution Infrared Spectra of Helium Clusters Seeded with OCS: He_2-OCS to He_6-OCS

10:15 – 10:30 Yunjie Xu and Wolfgang Jaeger (University of Alberta)

High Resolution Spectra of Helium Clusters Seeded with OCS: He_2-OCS to He_6-OCS

(Part II)

10:30 - 11:00 **Coffee Break**

Chair: **Bob Le Roy**

11:00 - 11:45 Tom McElroy (Meteorological Service of Canada)

The MAESTRO Instrument that will fly on SciSat I, the Atmospheric Chemistry Experiment (ACE)

11:45 - 12:00 Thomas Schultz, M. Schmitt, J.P. Shaffer, M.Z. Zgierski, Albert Stolow (National Research Council of Canada)

Isomerization Dynamics of Azobenzene: How Azobenzene Breaks Kasha's Rule

12:00 - 12:15 Zhaoguo Tong, Alison Gillies and Hans-Peter Loock (Queen's University)

Fiber Loop Ring-Down Spectroscopy: Absorption Spectroscopy on Pico-Litre Samples

POSTER SESSION

Chair: **James Martin**

To give 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:

3:30 - 4:45 Those whose papers were given (a) labels (1a, 2a, 3a, etc.) should attend their posters.

4:45 - 6:00 Those whose papers were given (b) labels (1b, 2b, 3b, etc.) should attend their posters.

1 a) Alex Brown, R.H. Tipping, J.-M. Hartmann, C. Brodbeck, P.-M. Flaud, C. Boulet, Q. Ma and J. Lièvin (University of Alabama) (Université Paris-Sud, Campus d'Orsay) (Columbia University and Institute for Space Studies) (Goddard Space Flight Center) (Université Libre de Bruxelles)

Collision-Induced Absorption in the ν_2 Fundamental Band of CH_4

1 b) Marian Kowalski and Geoffrey Hunter (York University)

Quantum and Electromagnetic Descriptions of Photon Emission from the Hydrogen Atom

2 a) Scott Hopkins and Allan G. Adam (University of New Brunswick)

High Resolution Laser Spectroscopy of Titanium Monobromide

2 b) Hans-Peter Loock, Sergei Manzhos (Queen's University)

Software for Comprehensive Analysis of Photofragment Images

3 a) David I. Kreller, Graham Gibson, Gary W. van Loon and J. Hugh Horton (Queen's University)

Chemical Force Microscopy Investigation of Phosphate Adsorption on the Surface of Iron (III) Oxyhydroxide Colloids

3 b) Delia Fernandez, Rafael Escribano and James J. Sloan (Inst. Estructura de la Materia, CSIC, Madrid, Spain) (University of Waterloo)

On the Use of Wavelets and Correlation Techniques Applied to Atmospheric Satellite Spectra

4 a) Jami L. Burkell, Travis D. Fridgen and Terry B. McMahon (University of Waterloo)

Gas Phase Acidity of Some 2-Alkanones: Stabilization of Anionic Centres by Chain Coiling

4 b) P. Crozet, A.J. Ross, F. Martin, C. Linton, M.J. Dick and A.G. Adam (University of Lyon) (University of New Brunswick)

Rotational Analysis of the Origin Band of the $A\,^2E$ - $X\,^2A_1$ Transition of Calcium Methoxide

5 a) M.J. Dick, C. Linton, A. Kristoffersen, A.G. Adam, J.L. McGregor, A.J. Ross and P. Crozet (University of New Brunswick)

Laser Spectroscopy of Holmium Monofluoride and Holmium Monochloride

5 b) P. R. Bunker, Per Jensen, W. P. Kraemer and Yuan-Pern Lee (SIMS, National Research Council) (Wuppertal University) (Max-Planck Institute for Astrophysics, Garching) (National Tsing Hua University)

The Matrix Isolation Spectra of CH_2^+ and CH_2 at 5 K

6 a) Kaley A. Walker and Peter Bernath (University of Waterloo)

The Waterloo Atmospheric Observatory

6 b) Keith Tereszchuk, Ted Diogenous, Robert Mitchel, Bhairavi Shanghavi and Peter Bernath (University of Waterloo)

FIR Fourier Transform Emission Spectroscopy of the Alkali Iodides

7 a) N. Siddique, R. Escribano and J.J. Sloan (University of Waterloo)

Speciation of Urban Particulate Matter by Raman Spectroscopy

7 b) Constantin Romanescu, Sergei Manzhos, Jennifer Clarke and Hans-Peter Loock (Queen's University)

Velocity-Map Imaging of the Superexcited States of HCl

8 a) Kirk Peterson and George C. McBane (Washington State University and Pacific Northwest National Laboratory) (Grand Valley State University)

He-CO 3D Potential Energy Surface at the Complete Basis Set Limit: Construction and Comparison with Experiments

8 b) Yiye Huang and Robert J. Le Roy (University of Waterloo)

Direct-Potential-Fit Determination of an Accurate Analytical Potential and Born-Oppenheimer Break-down Correction Functions for the $B\,^{1\Pi}{}_u$ "Barrier" State of Li_2

9 a) Jeff Paci and David M. Wardlaw (Queen's University)

Strong Laser Fields and the Molecular Keldysh Parameter

9 b) Hongwei Xie and William L. Hase (Wayne State University)

Effects of Pressure on Dynamics of Energy Transfer Between Hydroxylated Alumina Surfaces

10 a) Kihyung Song, William L. Hase and Reinhard Schinke (Wayne State University)

Role of State Specificity in the Temperature- and Pressure-Dependent Unimolecular Rate Constants: $HOCl \rightarrow OH + Cl$ Reaction

10 b) Hans Osthoff, Johnathon Walls, William van Wijngaarden and Wolfgang Jaeger (University of Alberta) (York University)

High Resolution Spectra of H_2-CO_2 and D_2-CO_2 van der Waals Complexes Measured With an Axial Molecular Beam Infrared Diode Laser Spectrometer

11 a) Marc Smits, Dave Rayner and Albert Stolow (National Research Council)

Ionization Dynamics of Metal Clusters in Strong Laserfields

11 b) R.J.C. Brown, M. Evans and Z. Tun (Queen's University) (Royal Military College) (National Research Council)

Neutron Scattering Study of Adsorption in Porous MCM-41 Silica

12 a) Lipeng Sun, Kihyung Song and W.L. Hase (Wayne State University)

Microscopic Mechanisms of the Gas-phase $OH^- + CH_3F \rightarrow CH_3OH + F^-$ S_N2

Reaction

12 b) L.M. Reynard and D.J. Donaldson (University of Toronto)

OH Production from the Reaction of Vibrationally Excited H_2 in the Mesosphere

13 a) Ray Nassar and Peter Bernath (University of Waterloo)

Hot Methane Spectra at the Temperature of a Brown Dwarf

13 b) Yanfei Wang, Kihyung Song and William L. Hase (Wayne State University)

Atomic Level Mechanisms for the $Cl^- + CH_3Br$ S_N2 Reaction

14 a) Jian Tang and A.R.W. McKellar (National Research Council)

Infrared spectra of OCS-H_2, OCS-HD, and OCS-D_2 complexes

14 b) I. Gordon, K. Tereszchuk, T.C. Melville, P.F. Bernath and J.A. Coxon (University of Waterloo) (Dalhousie University)

Fourier Transform Infrared Emission Spectroscopy of Gas-Phase YbO

15 a) A. Shayesteh, K. Tereszchuk and P. Bernath (University of Waterloo)

A New Discharge-Furnace Source: The $B^1 - X$ System of MgH

15 b) Andrew Janca, Keith Tereszchuk, Peter Bernath (University of Waterloo)

HDO and the Fate of the Universe

16 a) Jan K. Rainey and M. Cynthia Goh (University of Toronto)

Minimal Representations of Amino Acid Residue Functionality and Steric Bulk From Statistical Analysis of Culled High-Resolution Crystallographic Data

16 b) K.M. Poduska and S. Morin (York University)

Magnetic Characterization of Low-Dimensional, Electrodeposited Ni Structures

17 a) Erika F. Merschrod S. and M. Cynthia Goh (University of Toronto)

Surface-Mediated Collagen Fibril Growth

17 b) Shiliang Wang, Zygmunt J. Jakubek, Benoit Simard and Philip R. Bunker (SIMS, National Research Council)

(2+1) REMPI Spectra of Methylene Radical

18 a) D.W. Tokaryk and Tan-Trao Phi (Mount Allison University)

Is This a Mid-Infrared Band of HCN? A Rotationally Solved, Vibrationally Confusing Puzzle

18 b) Sanjay Nakhate, Zygmunt J. Jakubek and Benoit Simard (SIMS, National Research Council)

The SiP Molecule: First Observation and Spectroscopic Characterization

19 a) Zygmunt J. Jakubek, S.G. Nakhate and Benoit Simard (SIMS, National Research Council)

Electronic Structure of the YH and YN Molecules

19 b) Zygmunt J. Jakubek, Mirek Zachwieja, S.G. Nakhate and Benoit Simard (SIMS, National Research Council)

Investigation of the $\tilde{X}^2B_1$ Ground State of the PH_2 Radical by Stimulated Emission Pumping

20 a) Jason A. Barron, Samantha Glazier, Hector Abruna and Paul L. Houston (Cornell University)

Photophysics of PAMAM-Based Dendrimers of Polypyridyl Complexes of Ruthenuim

20 b) D.B. Dickens and J.J. Sloan (University of Waterloo)

Freezing of Dilute Nitric Acid Aerosols

21 a) Irina Paci and N.M. Cann (Queen's University)

The Impact of Molecular Shape and Polarity on Chiral Discrimination

21 b) Alvin C. Lin and M. Cynthia Goh (University of Toronto)

Fibrous Long Spacing Collagen: A New Interpretation of its Ultrastructure Through Parallel Atomic Force and Transmission Electron Microscopy

22 a) Denise M. Koch and Gilles H. Peslherbe (Concordia University)

A Rigorous Investigation of Halide-Water Clusters

22 b) Mark Cybulski (Miami University)

Nonadditive Effects in Open-Shell Clusters: Application to Ar_2-XH (X = F, O, N, C) Complexes

23 a) Travis D. Fridgen and Terry B. McMahon (University of Waterloo)

Experimental Energy Barriers for Methyl, Ethyl, and Propyl Cation Transfer Reactions by Temperature-Dependent Kinetics in an FTICR Cell

23 b) Travis D. Fridgen and Terry B. McMahon (University of Waterloo)

Binding Energies of Proton-Bound Ether/Alcohol Mixed Dimers Determined by FTICR Radiative Association Kinetics Measurements

24 a) F. Temme (Queen's University)

On Spin Irreps of (n= 8,12,20) -fold Uniform Higher (NMR) Spin Systems via Cλ Encoded Designs of Partition-based Statistical Frequencies over M: From Met-cars and 12-fold Polyhedral Boron Cage Ensembles / Isotopomers to the Polyhedral Combinatorics and S_n Invariants of $[^{14}N]_{20}$ (Schaefer) (Poly-Azo)-Dodecahedrane

24 b) Tianying Yan, William L. Hase and John R. Barker (Wayne State University) (University of Michigan)

Energy Transfer Dynamics Associated with Ne-Atom Collisions with the n-Hexylthiolate Self-Assembled Monolayer (SAM)/Au{111} Surface

25 a) Celine Toubin, David Y.-H. Yeung, Ann M. English and Gilles H. Peslherbe (Concordia University)

Theoretical Investigation of S-Nitrosothiols Degradation: Probing the Catalytic Role of Copper Metal Ions

25 b) Sean R. Hughes, Gilles H. Peslherbe and John A. Capobianco (Concordia University)

On the Nature of the Bonding Interactions in Metal Ion-Water Clusters

26 a) Qadir K. Timerghazin, Tao-Nhan Nguyen and Gilles H. Peslherbe (Concordia University)

Asymmetric Solvation Revisited: The Importance of Hydrogen-Bonding Iodide-Acetorntrile Clusters

26 b) Tao-Nhan V. Nguyen, Gilles H. Peslherbe and Holger Vach (Concordia University) (Ecole Polytechnique, France)

Molecular Vibrational Excitation in Surface-Induced Fragmentation of $(N_2)n$ and $(O_2)n$ Clusters

27 a) N. Moazzen-Ahmadi (University of Calgary)

A Combined Frequency Analysis of the ν_3, ν_9, $3\nu_4$ and the Far-Infrared Bands of Ethane: A Reassessment of the Torsional Parameters for the Ground Vibrational State

27 b) C.O. Uibel, R.J. Le Roy and E.H. Fink (University of Waterloo)

Simultaneous Analysis of 14 Data Sets Acquired by High-Resolution Fourier-Transform Spectroscopy Interconnecting 12 Electronic States of As_2

28 a) Wai-To Chan and I.P. Hamilton (Wilfrid Laurier University)

Possible Source of Atmospheric Epoxide in the Ozonolysis of Alkenes

28 b) Bernie D. Sattin, Andrew Pelling and M. Cynthia Goh (University of Toronto)

Single Molecule Explorations into the Mechanical Stability of DNA

29 a) Xiaojing Zhou, Marilyn Louie, Dilip Sarkar, and K. T. Leung (WATlabs, University of Waterloo)

Deposition of Copper Nanoparticles on Ultrathin Polypyrrole Films