Symposium on Chemical Physics

at the University of Waterloo

October 31 – November 2, 2003

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

SESSION I: Friday, October 31, 2003 - P.M. Davis Centre Room 1351
Chair: **Terry McMahon**

7:30 – 8:15 Timothy Zwier (Purdue University)
Laser Probes of the Potential Energy Landscapes and Conformational Isomerization Dynamics of Flexible Biomolecules

8:15 – 8:30 M. O. Musa, G. Bussiere and J. Hepburn (University of British Columbia)
Experimental Study of the Dynamics of Water Dissociation on Crystalline Zr Surfaces

8:30 – 8:45 Zhen-Dong Sun[1], Qiang Liu[1], R.M. Lees[1], Li-Hong Xu[1], M.Yu. Tretyakov[2] and V. Dorovskikh[2] ([1]University of New Brunswick, [2]Russian Academy of Sciences)
Dual Mode CO_2 *Laser/MWSB Spectrometer with Broad Band and Precision Sub-Doppler Measurements for* CH_3OH *and* OCS

8:45 – 9:00 Tao-Nhan Nguyen, Qadir K. Timerghazin, Denise M. Koch, Holger Vach and Gilles H. Peslherbe (Concordia University)
Novel Cluster-Induced Reactions: Mechanisms of Silicon Surface Oxidation by $(O_2)_n$ *Cluster Beams*

9:15 Weaver's Arms (Phillip St., behind the Co-Op Residence) - Informal Discussions

SESSION II: Saturday, November 1, 2003 - A.M. Davis Centre Room 1351
Chair: **Peter Bernath**

9:00 – 9:45 William Meath (University of Western Ontario)
Mechanisms for Multiphoton Excitation of Molecules, and On the Enhancement of "Direct" Two- and Three-Photon Excitations

9:45 – 10:00 J. Tang and A.R.W. McKellar (Steacie Institute for Molecular Sciences, National Research Council)
Transition from an Individual Molecule to the Quantum Solvation Regime: IR Spectra of He_N *-*CO_2 *Clusters with N = 2 to 18*

10:00 – 10:15 Xiangzhu Li and Josef Paldus (University of Waterloo)
A General Multireference Coupled-Cluster Method

10:15 – 10:45 **Coffee Break**

SESSION III: Saturday, November 1, 2003 - A.M. Davis Centre Room 1351
Chair: **Bob Le Roy**

10:45 – 11:45 Moshe Shapiro (University of British Columbia)
Quantum Control of Chiral Conversion, Spontaneous Decay and Tunneling

11:45 – 12:00 David B. Pedersen, J. Mark Parnis, Rick D. Lafleur and David M. Rayner (Trent University, Queen's University and SIMS, National Research Council of Canada)
The Role of Entropy in Rate Determination for Barrierless Gas-Phase Metal Cluster-Alkane Complexation Reactions

12:00 – 12:15 Sergei Manzhos and Hans-Peter Loock (Queen's University)
Photoproduct Image Analysis: From Abel Integral to Pattern Recognition

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

SESSION IV: Saturday, November 1, 2003 - P.M. Davis Centre Room 1351
Chair: **James Martin**

1:30 – 2:15 Walter Balfour (University of Victoria)
The Challenging Playground of Transition Metal Diatomic Spectroscopy

2:15 – 2:30 Alexei Khalizov, Alexandre Zassetsky, Mike Earle and Jim Sloan (University of Waterloo)
A New Way to Approach the Ice Formation Mechanism in Aerosol Flow Tubes

2:30 – 2:45 Anirban Hazra and Marcel Nooijen (Princeton University, University of Waterloo)
The Vertical Franck-Condon Model: A General Adiabatic Approach for Calculating Electronic Absorption Spectra

2:45 – 3:00 Li-Hong Xu[1], Qiang Liu[1], R.D. Suenram[2], F.J. Lovas[2], D.F. Plusquellic[2], A.R. Hight Walker[2], J.O. Jensen[3] and A.C. Samuels[3] ([1]University of New Brunswick, [2]National Institute for Standards and Technology, Gaithersburg, MD, and [3]Passive Standoff Detection, Edgewood Chemical and Biology Center, Edgewood Area, Aberdeen Proving Ground, MD)
Rotational Spectra, Conformational Structures and Dipole Moments of Thiodiglycol ($HOCH_2CH_2SCH_2CH_2OH$)

3:00 – 3:15 Alex Brown[1], B. J. Braams[2], Z. Jin[2] and J. M. Bowman[3] ([1]University of Alberta, [2]New York University, and [3]Emory University)
A New Approach to Obtain a Potential Energy Surface from Direct Dynamics: Application to the Vibrational Spectrum of

3:15 **Refreshments and Poster Session**

SESSION V: Saturday, November 1, 2003 – 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
9:30 P.M.	Informal Discussions	Grad House

SESSION VI: Sunday, November 2, 2003 – A.M. Davis Centre Room 1351
Chair: **Fred McCourt**

9:15 – 10:00 Michael Gerry (University of British Columbia)
Microwave Spectroscopy of Noble Gas-Coinage Metal Halide Complexes and the Nature of the Noble Gas-Coinage Metal Bond

10:00 – 10:15 F.R. Bennett, S.P. Lee, P. Jemmer, A.M. Juarez, F. Kemp, G.C. King, I.R. McNab and A. Yencha (University of Newcastle upon Tyne)
Vibrational Spectroscopy of the HBr *and* HI *Dications*

10:15 – 10:30 Mark Cybulski (Miami University)
A Critical Note on Density Functional Theory Studies of Intermolecular Interactions - Part 2

10:30 – 11:00 **Coffee Break**

SESSION VII: Sunday, November 2, 2003 - A.M. Davis Centre Room 1351
Chair: **Marcel Nooijen**

11:00 – 11:45 Krzysztof Szalewicz (University of Delaware)
Theoretical Spectroscopy of Van der Waals Molecules

11:45 – 12:00 Xiao-Gang Wang and Tucker Carrington Jr. (Université de Montreal)
Numerically Exact Variational Calculation of the Rovibrational Levels of Methane: Solving the Schrödinger Equation in Twelve Dimensions

12:00 – 12:15 Roger E. Miller (University of North Carolina)
Vibrational Spectroscopy of Biomolecules in Helium Nanodroplets: New Structural Tools

POSTER SESSION

Chair: **Bob Le Roy**

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.**

1a) Jean Christophe Tremblay and Tucker Carrington, Jr. (Université de Montreal)
A New Preconditioned Method for Computing Lifetimes of Metastable States Using Real Matrix-Vector Products

1b) Lori M. Anthony and John M. Roscoe (Acadia University)
A Kinetic Study of Some Reactions of Atomic Bromine With Polar Organic Compounds at Atmospheric Pressure

2a) Bill Poirier and Tucker Carrington (University of Montreal)
Optimized Complex Absorbing Potentials

2b) Nicholas P. Cosman and Sharon G. Roscoe (Acadia University)
Analysis of Protein Adsorption Using the Electrochemical Quartz Crystal Nanobalance

3a) Michael E. Earle and John M. Roscoe (Acadia University)
Photolysis of Methyl Vinyl Ketone at Ambient Temperature Under Atmospherically Relevant Conditions

3b) Christa Brosseau and Sharon G. Roscoe (Acadia University)
Analysis of the Adsorption Behaviour of Mandelate Racemase and its Substrate: Comparison of Chronocoulometry and EQCN Techniques

4a) Jeremy J. B. Wentzell and John M. Roscoe (Acadia University)
The Measurement of Absolute Rate Constants for Some Reactions of Atomic Bromine in a Flow System

4b) M.G.K. Thompson, and J.M. Parnis, (Trent University)
Reaction of Early Transition Metal Atoms with Ethene: Matrix Isolated Ethylidene?

5a) Li-Hong Xu, R.M. Lees, P. Wang, Linda Brown, Isabelle Kleiner and J.W.C. Johns
HITRAN Line Parameters of Methanol (CH_3OH) *at 10 µm*

5b) Po Shan Ng, Travis D. Fridgen and Terry B. McMahon (University of Waterloo and Wilfrid Laurier University)
Infrared Radiative Association and Dissociation of Gaseous Cluster Ions

6a) R. Nieckarz, T. Fridgen, G. Li, I. Hamilton and T.B. McMahon (University of Waterloo and Wilfred Laurier University)
Clustering/Solvation of XHX^- (X = F, Cl, CN) *with* ROH (R = H, CH_3, C_2H_5) *to Elucidate Thermochemical and Structural Data*

6b) Jeffrey T. Paci and David M. Wardlaw (Queen's University)
The $H^+ + H_2$ *Reaction in a Strong Laser Field*

7a) I. Paci and N. M. Cann (Queen's University)
The Impact of the Multipolar Distribution on Chiral Discrimination in Racemates

7b) Qichi Hu and John W. Hepburn (University of British Columbia)
Threshold Ion-Pair Production Spectroscopy

8a) A. Simon, K. C. Hadley and T. B. McMahon (University of Waterloo)
Equilibria of Association of Proton-Bound Clusters of Amino Acid Esters in the Gas Phase: Experiment and Theory

8b) Kourosh Afrousheh and James Martin (University of Waterloo)
Measuring Electron Temperature in an Ultracold Plasma using Stimulated Photoattachment

9a) Abdul H. Emwas, Jill Lushman, Meghan P. Lobsinger, Michael J. T. Ditty, Howard N. Hunter and William P. Power (University of Waterloo)
ROESY vs. NOESY for Conformational Information of a Peptide on Wang Resin

9b) Andrew B. Ryzhkov, Bertrand J. Revenaz and Parisa A. Ariya (McGill University)
Atmospheric Impact of Alkene Ozonolysis on Sulfur Oxidation in Sulfate Aerosols

10a) Abdul H. Emwas and Saba Mattar (University of New Brunswick)
A Tuneable Doubly Stacked Dielectric Resonator Housed in an Intact Te102 Cavity for Electron Paramagnetic Resonance Spectroscopy

10b) Zhaoguo Tong, Mike Jacubinek, Runkai Li, Janice Allan and Hans-Peter Loock (Queen's University)
The Fiber-Loop Ring-Down Technique: An Absorption Detector for Microfluidic Devices

11a) Saba M. Mattar and Abdul Hamid Emwas (University of New Brunswick)
Spectroscopic Studies of the Transient Intermediates of the 1,4,11,12-Tetrahydro-9,10-Anthraquinone to 9,10-Anthraquinone Reaction

11b) Qadir K. Timerghazin and Gilles H. Peslherbe (Concordia University)
Topological Approach to the Solvated and Dipole-Bound Election

12a) Qadir K. Timerghazin and Parisa A. Ariya (Concordia University, McGill University)
Atmospherically Important Reactions of Br Atoms with Alkenes: The Mechanism and Role of Spin-Orbit Coupling Effects

12b) Shucheng Xu and David S. Perry (University of Akron)
CW Infrared Cavity Ringdown Spectroscopy of Jet-Cooled Methanol and Propyne

13a) Constantin Romanescu and Hans-Peter Loock (Queen's University)
Photodissociation Dynamics of HBr *Via Rydberg and Ion-Pair States*

13b) Saba M. Mattar (University of New Brunswick)
Accurate and Efficient Hybrid Density Functionals for Computing the g-Tensor Components of

1,4-Benzosemiquinone Radical Anion

14a) T. D. Fridgen, T. B. McMahon, J. Troe, A. A. Viggiano, A. J. Midey and S. Williams (Wilfrid Laurier University, University of Waterloo, University of Gettingen, Hanscom Air Force Base)
Benzylium/Tropylium Ratios Following Charge Exchange Ionization of Ethylbenzene: Determination of Threshold Energies

14b) Saba M. Mattar and Abdul Hamid Emwas (University of New Brunswick)
A Tuneable Doubly Stacked Dielectric Resonator Housed in an Intact TE102 Cavity

15a) Saba Mattar and Jacob Sanford (University of New Brunswick)
A Novel Phase-Modulated Electron Paramagnetic Resonance Spectrometer

15b) Qing Wen, XiaoGeng Song and Wolfgang Jäger (University of Alberta)
Microwave Spectra of the Xe-N_2 *van der Waals Complex: A Comparison of Experiment and Theory*

16a) Saba Mattar and Jacob Sanford (University of New Brunswick)
The Role of the Solvent and Geometry on the Accuracy of the 1,1'-Diphenyl-2-Picrylhydrazyl Computed Hyperfine and g Tensors

16b) Allan Adam, Scott Hopkins and Dennis Tokaryk (University of New Brunswick)
Visible Laser Spectroscopy of Hafnium Monofluoride

17a) Wen Li[1,2], Robert Lucchese[3], Adnan Doyuran[4], Zilu Wu[4], Henrik Loos[4], Gregory E. Hall[2] and Arthur G. Suits[1,2] ([1]Stony Brook University; [2]Brookhaven National Laboratory, [3]Texas A&M University, [4]National Synchrotron Light Source, Brookhaven National Laboratory)
Superexcited State Dynamics Probed with a XUV-FEL

17b) Allan Adam and Scott Shepard (University of New Brunswick)
Visible Laser Spectroscopy of Hafnium Monochloride

18a) Michael P. Minitti, Dave Townsend and Arthur G. Suits (SUNY Stony Brook, Brookhaven National Laboratory)
Spectroscopy using Direct Current (DC) Slice Imaging

18b) I. Gordon, A. Shayesteh, D. Appadoo and P. Bernath (University of Waterloo)
The Infrared Emission Spectra of MnH and MnD

19a) Michael Dick and Colan Linton (University of New Brunswick)
Laser Spectroscopy of Holmium Monochloride

19b) Ray Nassar, Kaley A. Walker, Chris Boone and Peter F. Bernath (University of Waterloo)
SCISAT-1/ACE: FTS Testing and Results

20a) Kaley A. Walker, Peter F. Bernath, Luc Levesque and Marc-Andre Soucy (University of Waterloo and ABB-Bomem, Quebec City)
The Portable Atmospheric Research Interferometric Spectrometer (PARIS-IR) for the Waterloo Atmospheric Observatory

20b) Hans Osthoff and Wolfgang Jaeger (University of Alberta)

Rotational and Ro-Vibrational Spectra of the Weakly Bound Complex CO_2-CH_4

21a) Dave Townsend, Suk Kyoung Lee and Arthur G. Suits (SUNY at Stony Brook)
Orbital Polarization from DC Slice Imaging: $S(^1D_2)$ *Alignment in the Photodissociation of Ethylene Sulfide*

21b) Myung Hwa Kim, Wen Li, Suk Kyoung Lee and Arthur G. Suits (State University of New York at Stony Brook)
Probing of the Hot Band Excitations from the Photodissociation of OCS *at 288 nm by DC Slice Imaging*

22a) Alireza Shayesteh, Dominique R. T. Appadoo, Iouli Gordon and Peter F. Bernath (University of Waterloo)
Fourier Transform Emission Spectroscopy of Group 2 and 12 Metal Hydrides

22b) Jian Tang and A.R.W. McKellar (Steacie Institute for Molecular Sciences, NRC of Canada)
Infrared Spectra of $(H_2)_N$ -N_2O *Clusters*

23a) Jin-Guo Wang (University of Waterloo)
Doppler-Free Two-Photon Absorption Spectroscopy on Deuterated Benzene

23b) Keeyoon Sung and Prasad Varanasi (University of Waterloo, MSRC/ITPA, State University at New York, Stony Brook)
Laboratory Measurement of Infrared Spectra of $^{12}C^{16}O$ *in the Fundamental and Overtone Bands at Various Temperatures Relevant to the Atmospheres of Jupiter, Saturn, Venus and Mars*

24a) Peter F. Bernath, Dominique R.T. Appadoo, Reginald Colin and Robert J. LeRoy (University of Waterloo)
Study of the Ground States of BeH *and* AgH *by Direct Potential Fitting of Spectroscopic Data*

24b) Jeff Seabrook and Dennis Tokaryk (University of New Brunswick)
Trace Gas Detection Using Integrated Cavity Output Spectroscopy

25a) Dmitrii Boldovsky, Constantin Romanescu and Hans-Peter Loock (Queen's University)
Photodissociation of BrCl *in the 380-440 nm Spectral Region*

25b) L. Carsten Nielsen and Joeseph D. Geiser (University of New Hampshire)
Kinetic Study of Atmospherically Relevant Species Using Discharge Flow Mass Spectrometry

26a) F.P. Temme (Queen's University)
Augmented Weyl Time-reversal Invariance-based SU2 $\times S_{2n}$ *Invariants via Democratic Recoupling over Uniform* $(k_1..k_n)$*-defined Dual Tensorial (liquid state)* $[AX]_{2n}$ *NMR Spin Dynamics: Applications of Polyhedral Combinatorics over Erdos Lattice-points to Obtain SR Quasiparticle Carrier Spaces for* [redacted] *P Group Actions &* [redacted] *Completeness, for* [redacted] *Invariants as DR-based (Lie) Group Measures*

26b) C. Linton[a], C. Effantin[b], P. Crozet[b], J. d'Incan[b], A. J. Ross[b] and E. A. Shenyavskaya[c]
([a]University of New Brunswick, [b]Université de Lyon, France, [c]High Energy Density Research Center, Moscow)

Laser Spectroscopy of Neodymium Monoxide

27a) Nicholas Blinov and Pierre-Nicholas Roy (University of Alberta)
Path Integral Monte Carlo Simulations of Rotations in Doped Helium Clusters

27b) Serguei Raspopov and Terry McMahon (University of Waterloo)
Experimental and Computational Studies of the Proton-Bound Clusters and Dipeptide of Glycine. Possibility of Peptide Bond Formation by Gas Phase Ion-Molecule Reactions

28a) Dominika Zgid and Marcel Nooijen (University of Waterloo)
Density Matrix Renormalization Group in Electronic Structure Theory

28b) Marjan Mohammadi and Robert J. Le Roy (University of Waterloo)
Direct Potential-Fit vs. Mixed-Representation Analysis for the $A^3\Pi_{1u}$ *State of* I_2

29a) Denise M. Koch, Gilles H. Peslherbe and James T. Hynes (Concordia University; CNRS, Ecole Normale Supérieure, and University of Colorado)
Spectroscopy of $NaI(H_2O)_n$ *Clusters*

29b) Paul Moffatt and Pierre-Nicholas Roy (University of Alberta)
Calculation of Single-Particle Time Correlation Functions from Bose-Einstein Centroid Dynamics

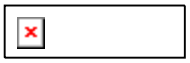
30a) Hannah Chang and Marcel Nooijen (Harvard University, University of Waterloo)
Van Vleck Transformations of Vibronic Hamiltonians

30b) Xiaojing Zhou and K.T. Leung (University of Waterloo)
The Adsorption and Thermal Desorption of Halogenated Ethylene on Si(100)2x1---cis-dichloroethylene vs. tetrachoroethylene

31a) Shihong Xu, Xiang Yang and K.T. Leung (University of Waterloo)
Room-Temperature Surface Chemistry and Spectroscopy of Chloroethylenes on Ni(100)

31b) Qiang Gao and K. T. Leung (University of Waterloo)
The Adsorption of Acetic Acid on Amorphous and Crystalline Ice by Fourier Transform Infrared Reflection Absorption Spectroscopy (FTIR-RAS)

32a) Sabrina Lorenz, Nina Heinig, Xiaojing Zhou, Osama Fouad and K.T. Leung (University of Waterloo)
Mesoscopic Chemical Physics of Ultra Thin Films of Metalloporphyrin-doped Polypyrrole

32b) Shanshan Yu, Xiaohua Yang, Benxia Li, Kakule Kaniki, Shenghai Wu, Yingchun Guo, Yuyan Liu and Yangqin Chen (University of Waterloo, East China Normal University)
Study of Hot Bands in the  *System Of Carbon Anion* 

33a) Dejian Fu, Shanshan Yu, Dominique Appadoo and Peter Bernath (University of Waterloo)
Study of the FTIR and Near-IR Emission Spectra of SbH

33b) Lixin Zhan, Bart Piwowar, Wing-Ki Liu, Jeff Z.Y. Chen (University of Waterloo)
Multi-Canonical Basin-Hopping: a New Global Optimization Method for Complex System