

Symposium on Chemical Physics

at the University of Waterloo

October 29 – 31, 2004

REGISTRATION begins at 7:00 p.m.

Davis Centre Room 1301

SESSION I: Friday, October 29, 2004 – P.M.

Davis Centre Room 1351

Chair: **Marcel Nooijen**

- 7:30 – 8:15 Timothy Steimle (Arizona State University)
Optical Stark and Zeeman Studies of Metal Containing Molecules
- 8:15 – 8:30 Yujun Shi, Christine Mah, and Benoit Simard (University of Calgary; Steacie Institute for Molecular Sciences, National Research Council of Canada)
Identification of Radicals in Hot Wire Decomposition of Tetramethylsilane Using Vacuum Ultraviolet Laser Single Photon Ionization
- 8:30 – 8:45 Jinhai Chen, Timothy C. Steimle, and Colan Linton (Arizona State University; University of New Brunswick)
Measurements of the Dipole Moment of Several Electronic States of Holmium Monoxide
- 8:45 – 9:00 Qadir K. Timerghazin, Denise M. Koch, and Gilles H. Peslherbe (Concordia University)
Ab Initio Studies of the $\text{Na}^+ \dots \text{I}^$ Complex*
- 9:15 Informal Discussions – “Grad House”

SESSION II: Saturday, October 30, 2004 – A.M.

Davis Centre Room 1351

Chair: **Peter Bernath**

- 9:00 – 9:45 Brenda Winnewisser (Ohio State University)
NCNCS: An Ideal Example of Molecular ‘Quantum Monodromy’
- 9:45 – 10:00 Richard Dawes and Tucker Carrington, Jr. (Université de Montréal)
How to Construct 1-D Basis Functions So That a Very Efficient Multidimensional Basis May Be Extracted From a Direct Product of the 1-D Functions: Energy Levels of Strongly Coupled Systems With as Many as 21 Coordinates
- 10:00 – 10:15 P. Ayotte, Martin Hébert, and Patrick Marchand (Université de Sherbrooke)
HF Adsorption on Ice: Whose Proton Is It Anyways?
- 10:15 – 10:45 **Coffee Break**

Invited talks are 45 min. including 5 min. for discussion

Contributed talks are 15 min. including 3 min. for discussion

SESSION III: Saturday, October 30, 2004 – A.M.

Davis Centre Room 1351

Chair: **Bob Le Roy**

10:45 – 11:45 William Miller - Plenary Lecturer (University of California, Berkeley)
Some Recent Applications of the Semiclassical Initial Value Representation

11:45 – 12:00 Stephen A. Cooke and Michael C. L. Gerry (University of British Columbia)
XeAuF: A New Molecule Containing a Xenon-Gold Covalent Bond

12:00 – 12:15 N. Blinov and P.-N. Roy (University of Alberta)
Quantum Solvation and Rotational Dynamics in Doped Helium Clusters

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

SESSION IV: Saturday, October, 2004 – P.M.

Davis Centre Room 1351

Chair: **James Martin**

1:30 – 2:15 John Coxon (Dalhousie University)
Some Modern Applications of Numerical Methods in the Interpretation of Rotational Structure in Band Spectra of Diatomic Molecules

2:15 – 2:30 Denise M. Koch, Qadir K. Timerghazin, Gilles H. Peslherbe, Branka M. Ladanyi, and James T. Hynes (Concordia University)
Photodissociation Dynamics of NaI in Water Clusters

2:30 – 2:45 James K. G. Watson (Steacie Institute for Molecular Sciences, National Research Council of Canada)
Different Forms of Effective Hamiltonians

2:45 – 3:00 Olga Pawluczyk and Romuald Pawluczyk (P&P Optica Inc., Kitchener, Ontario)
Applications of Multichannel VIS-NIR Imaging Spectrometers

3:00 – 3:15 A. R. W. McKellar and S. Moroni (Steacie Institute for Molecular Sciences, National Research Council of Canada; Universita di Roma La Sapienza, Rome, Italy)
Small Para-Hydrogen Clusters Doped With Carbon Monoxide: Quantum Monte Carlo Simulations and Infrared Spectroscopic Observations

3:15 **Refreshments and Poster Session**

Invited talks are 45 min. including 5 min. for discussion

Contributed talks are 15 min. including 3 min. for discussion

SESSION V: Saturday, October 30, 2004 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 "Bombshelter Pub" in the Student Life Centre (basement)

SESSION VI: Sunday, October 31, 2004 – A.M.

Davis Centre Room 1351

Chair: **Fred McCourt**

- 9:15 – 10:00 James Donaldson (University of Toronto)
Atmospheric Reactions at the Air-Water Interface
- 10:00 – 10:15 A. Y. Zasetzky, A.F. Khalizov, and J. J. Sloan (University of Waterloo)
Frequency Dependent Complex Refractive Indices of Supercooled Liquid Water and Ice
- 10:15 – 10:30 Robert C. Mawhinney, Gilles H. Peslherbe, and Heidi M. Muchall (Concordia University)
The ¹³C Chemical Shift Tensor in Nitrilimines: A Gauge Including Atomic Orbital/Density Functional Theory Study
- 10:30 – 11:00 **Coffee Break**

SESSION VII: Sunday, October 31, 2004 – A.M.

Davis Centre Room 1351

Chair: **Tong Leung**

- 11:00 – 11:45 Hans-Peter Loock (Queen's University)
Fibre-Optic Detectors and Sensors
- 11:45 – 12:00 Zhen-Dong Sun, Li-Hong Xu, R. M. Lees, Xing-Jie Jiang, Sean Perry, N. C. Craig, and A. R. W. McKellar (University of New Brunswick, Saint John)
Going Up in Smoke! High-Resolution Spectra of 1,3-Butadiene and Acrolein

Invited talks are 45 min. including 5 min. for discussion

Contributed talks are 15 min. including 3 min. for discussion

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) Yong Dong Liu and Pierre-Nicholas Roy (University of Alberta)
Energy Levels and Wave Functions of Weakly Bound Helium Containing Complexes
- 1b) T. Cheng, H. Darmawan, and A. Brown (University of Alberta)
Effects of Background States in Stimulated Raman Adiabatic Passage
- 2a) D. Lacey, X. Hu, and R.H. Lipson (University of Western Ontario)
118 nm VUV Post-Ionization MALDI Using a Triple Quadrupole Mass Spectrometer
- 2b) Anatoly V. Komissarov, Laura Fredriksen, Gregory E. Hall, and Trevor J. Sears (Brookhaven National Laboratory)
Collision-Induced Singlet-Triplet Crossing and Recrossing in CH₂
- 3a) S. Gakwaya, Z. Abusara, and N. Moazzen-Ahmadi (University of Calgary)
Vibrational Hot Bands of Linear C₄ and C₅ Arising from a Bending Vibration with Two Quanta in the Bend: The ($\nu_3 + 2\nu_5 - 2\nu_5$) Band of C₄ and the ($\nu_3 + 2\nu_7 - 2\nu_7$) of C₅
- 3b) M. Koshelev, M. Yu. Tretyakov, R.M. Lees, and Li-Hong Xu (Nizhny Novgorod, University of New Brunswick, Saint John)
Measurements of N₂- and O₂-Pressure Broadening and Pressure-Induced Shifts for OCS Transitions in the ν_3 Band
- 4a) W. S. Hopkins, A. G. Adam, C. Linton, D. W. Tokaryk, and A. Read (University of New Brunswick)
High Resolution Laser Spectroscopy of the B-X Transition of Strontium Methoxide
- 4b) Jennifer van Wijngaarden, Ivan Shnitko, Anton Batalov, Jan Fulara, Przemyslaw Kolek, and J. P. Maier (University of Basel; Mount Holyoke College)
Electronic Absorption Spectra of C₃Cl, C₃Cl⁺, C₄Cl and C₄Cl⁺ in Neon Matrices
- 5a) F. Magnus, A. Flodin, A. Boatwright, and R. C. Shnell (University of Sussex; Trent University)
Coherent Population Trapping on the D₁ and D₂ Lines of Lithium
- 5b) R. C. Shnell, E. Reinhold, F. Magnus, and W. Ubachs (University of Sussex; Vrije Universiteit; Trent University)
Coherent Evolution of Weakly-Bound Ion-Pair States of the HF Molecule

- 6a) Qing Wen and Wolfgang Jäger (University of Alberta)
Microwave and Ab Initio Studies of the Xe-CH₄ Van der Waals Complex
- 6b) A. G. Adam, S. A. Shepard, R. Li, and W. J. Balfour (University of New Brunswick; University of Victoria)
High Resolution Laser Spectroscopy of HfCl and RhCl
- 7a) Saba M. Mattar and Jacob Sanford (University of New Brunswick, Fredericton)
Multifrequency Electron Paramagnetic Spectroscopy I: Construction and Calibration of a Field and Phase Modulation P-band Spectrometer
- 7b) Sergei Manzhos, Jonathan Underwood, Constantin Romanescu, Hans-Peter Looch (Queen's University)
Quantification of Competing Excitation Channels in Multiphoton Dissociation from the Analysis of Photofragment Angular Distributions
- 8a) Saba M. Mattar, Jacob Sanford, and Alyson Goodfellow (University of New Brunswick, Fredericton)
Multifrequency Electron Paramagnetic Resonance II: The Spectra of Copper(II) Tetrasulfophthalocyanin and Mn(II):CaO at X- and P-band Frequencies
- 8b) I.E. Gordon, M. J. Dick, D. R. T. Appadoo, A. Shayesteh, K. A. Walker, J. Tang, P. F. Bernath, J.-H. Chen, and T.C. Steimle (University of Waterloo; Arizona State University)
Spectroscopy of Molecules in Electronic States of High Multiplicity: Infrared Spectra of MnH and Electronic Spectra of EuH
- 9a) Robert Nieckarz, M. Clements, T. Fridgen, G. Li, I. Hamilton, and T. McMahon (University of Waterloo)
Bihalide FHF⁻ vs. Pseudobihalide NNN⁻: An Experimental and Theoretical Study of the Solvation by n-ROH(R=H, CH₃, C₂H₅)
- 9b) Richard A. Marta, Travis D. Fridgen, Sabrina J. Lorenz, and Terry B. McMahon (University of Waterloo)
The Tetrafluorodimethyl Ether Catalyzed Formation of the Proton-Bound Dimer of Water at Very Low Pressure
- 10a) J. Najera, R. Pancescu, R. McPhail, and J. Sloan (University of Waterloo)
Deliquescence of Ammonium Sulfate Aerosol
- 10b) Ronghu Wu and Terry B. McMahon (University of Waterloo)
Study on Ion-Molecular Interaction and Structures of Some Clusters of Protonated Glycine and Ammonia by HPMS and Ab Initio Calculations
- 11a) W. Shi, X. K. Hu, J. A. Vanstone, and R. H. Lipson (University of Western Ontario)
Construction of an Apparatus to Study the Structure of Hydrogen-Bonded Liquids

- 11b) P. Crozet, A. J. Ross, C. Linton, A. G. Adam, W. S. Hopkins, and R. J. Le Roy (Université Lyon I; University of New Brunswick; University of Waterloo)
Geometry of the CaOCH₃ Radical from Isotope Effects in the A²E–X²A₁ Transition
- 12a) Wendy C. Topic and Wolfgang Jäger (University of Alberta)
Solvating Cyanoacetylene with Helium-Atoms: A Rotational Spectroscopic Study
- 12b) R. Lehnig, D. Bremm, and W. Jäger (University of Alberta)
Spectroscopy in Superfluid ⁴Helium Droplets: Investigation of the Interaction between the Dopant Molecule and the Surrounding Helium
- 13a) Ian P. Hamilton and Jim Li (Wilfrid Laurier University)
Complexes of Small Gold Clusters and Hydrogen Sulphide
- 13b) Sacha Zlatkova and Gilles H. Peslherbe (Concordia University)
Computational Study of HCl and HBr Ionization in Water Clusters: Thermochemistry and Spectroscopy
- 14a) Po Shan Ng, Richard A. Marta, Travis D. Fridgen, and Terry B. McMahon (University of Waterloo; Wilfrid Laurier University)
Experimental and Theoretical Study of Ion-Molecule Reactions in the Gas Phase
- 14b) Cheng Lu, Xiaokun Hu, and Robert Lipson (University of Western Ontario)
Diffraction Holography for the Fabrication of Photonic Crystal Structures
- 15a) Zheng Su, Waishun Tam, and Yunjie Xu (University of Alberta)
Theoretical Studies of Chiral Discrimination
- 15b) Dejian Fu, Kaley Walker, Ian J. Young, Yony Bresler, and Peter F. Bernath (University of Waterloo)
Preparation of the PARIS-IR Instrument for Balloon-Based Measurements
- 16a) G. Dufour, S. Payan, F. Lefevre, C. Camy-Peyret (LPMA, CNRS/Université Paris 6 France) (University of Waterloo)
LPMA-Balloon Measurement Analysis and Applications to Chemical Modeling and Satellite Validation
- 16b) Waishun Tam, Igor Leonov, and Yunjie Xu (University of Alberta)
Construction of a Mid-infrared Cavity Ringdown Spectrometer with a Lead Salt Diode Laser
- 17a) X.-G. Wang and T. Carrington Jr. (Université de Montréal)
Quantum Calculation of Rovibrational Energies of He₂-OCS and He₂-N₂O
- 17b) Jean Christophe Tremblay and Tucker Carrington Jr. (Université de Montréal)
Using Preconditioned Adaptive Step Size Runge-Kutta Methods for Solving the Time-Dependent Schrödinger Equation

- 18a) Shanshan Yu, Alireza Shayesteh, Dejian Fu, and Peter F. Bernath (University of Waterloo)
Emission Spectroscopy of TeH, TeD and HZnCl
- 18b) Keeyoon Sung, Kaley Walker, Chris Boone, and Peter F. Bernath (University of Waterloo)
Atmospheric Absorption Measurements Made With PARIS-IR During the ACE Arctic Validation Campaign
- 19a) Alireza Shayesteh, Dominique R. T. Appadoo, Iouli E. Gordon, and Peter F. Bernath (University of Waterloo)
The Vibration-Rotation Emission Spectra of Gaseous ZnH₂ and ZnD₂
- 19b) P. Marchand and P. Ayotte (Université de Sherbrooke)
A New Way to Perform Diffusion in Ice Studies
- 20a) Runhua Li and Walter J. Balfour (University of Victoria)
Transition Metal Monophosphides: Electronic Spectra of TiP, VP and CrP
- 20b) Michael Dick, Iouli Gordon, Jin-Guo Wang, Peter Bernath, Tim Steimle, and Jinhai Chen (University of Waterloo; Arizona State University)
Europium Monofluoride: Recent Advances
- 21a) Jen Nicole Landry and Wolfgang Jäger (University of Alberta)
Rotational Spectra of the N₂O-paraD₂ van der Waals Complexes
- 21b) Jin-Guo Wang (University of Waterloo)
Perturbations in the 14₀¹ and 1₀¹14₀¹ Bands of the S₁←S₀ Transition of C₆D₆ Studied by Doppler-Free Two-Photon Excitation Spectroscopy
- 22a) Louis Wong, N. Heinig, X. J. Zhou, and K. T. Leung (University of Waterloo)
Electrochemical Fabrication of Magnetic Nanomaterials: Cobalt Nanostructures on H-terminated Si(100)
- 22b) M. E. Earle, A. Khalizov, A. Yu Zasetsky, B. Pinto, and J. J. Sloan (University of Waterloo)
Local Order and Nucleation of Ice in Supercooled Water
- 23a) R. G. Remorov, A. Yu. Zasetsky, M. Bardwell, and J. J. Sloan (University of Waterloo)
Uptake of Acetone by Water Aerosols Measured in a Low Pressure Aerosol Flow Reactor
- 23b) Joe Petrus, M. Thiam, N. Heinig, X. J. Zhou, and K. T. Leung (University of Waterloo)
Chemical Physics of Nanoscale Particles of Noble Metals: Effects of Morphology on Work Function Shifts
- 24a) Q. Gao, M. Thiam, and K. T. Leung (University of Waterloo)
Nanodeposits of Acetic Acid on Noncrystalline and Polycrystalline Ice: Hydrogen-bonding Interactions

- 24b) Mark Cybulski and Christopher E. Seversen (Miami University)
Critical Examination of the Supermolecule Density Functional Theory Calculations of Intermolecular Interactions
- 25a) Mark Pynenburg, N. Heinig, N. Kharbanda, X. J. Zhou, and K. T. Leung (University of Waterloo)
Deposition of Ni Nanoparticles on Ultrathin Polypyrrole Films: Effects of the Substrate
- 25b) Constantin Romanescu, Dmytro Grebennikov, and Hans-Peter Loock (Queen's University)
Photoelectron Imaging Study of Multiphoton Ionization of HBr in the 250 - 265 nm Region
- 26a) Travis D. Fridgen (Wilfrid Laurier University)
Structures of Asymmetric Proton-Bound Dimers With a Large Dipole Moment Monomer: Covalent vs. Electrostatic Interactions
- 26b) Dominik Bremm and Wolfgang Jäger (University of Alberta)
Ab Initio Calculation of Some Interaction Induced Electric Properties of Mixed Rare Gas Dimers
- 27a) Nicholas Trefiak, Zhaoguo Tong, Ian Adams, Richard Walford, Jack Barnes, and Hans-Peter Loock (Queen's University)
Phase-Shift Fiber-Loop Ring Down Sensing
- 27b) Travis D. Fridgen, Luke MacAleese, Terry McMahon, Joel Lemaire, and Philippe Maitre (Wilfrid Laurier University; University of Waterloo)
Infrared Spectra of Gaseous Proton-Bound Dimers from 600 cm⁻¹ to 1800 cm⁻¹
- 28a) F.P. Temme (Queen's University)
Role of Analytic $\phi_{\pm 1}^1(1..1)$ Coherences in Broken Permutational Spin Symmetry for Isochronous $X^{(1)} AX'^{(1)}$ bis-(Spin-One) NMR Systems under CP/CPT Invariance
- 28b) S. C. Ross and K. Tsukiyama (University of New Brunswick)
Lifetimes of Rovibration Levels of Outer Well \bar{H} State of H₂: Preliminary Theoretical Results Compared with Experiment. Fluorescence, Non-Adiabatic Dissociation, and Ionization Are All Involved
- 29a) Jun Zhang, Nicholas Trefiak, Krista Laugesen, Jack Barnes, Emily K. Gibb, Hans-Peter Loock, and Stephen Brown (Queen's University)
Development of a New Laser Refractometer
- 29b) Grygoriy A. Dolgonos and Gilles H. Peslherbe (Concordia University)
C₂ Fragmentation Energy of C₈₀: A Computational Study
- 30a) Xiaojing Zhou, Q. Li, and K. T. Leung (University of Waterloo)
Di-halogenated Benzenes on Si(100) Surfaces: Competition between Associative and Dissociative Adsorption

- 30b) David S. Perry, Lou Degliumberto, Robert L. Sams, Georg O. Sorensen, and Howard D. Mettee (University of Akron)
The Asymmetric N-O Stretch Fundamental Band of Nitromethane: FTIR Jet Spectra and Assignments of the Lowest 4 Internal Rotor States
- 31a) Q. Li and K. T. Leung (University of Waterloo)
Diffusion-mediated Kinetic Models of Hydrogen Evolution of Hexacyclic Aromatic Hydrocarbons on Si(100)
- 31b) Etienne Garand and Paul Rowntree (Université de Sherbrooke)
The Mechanism for the Production of Hydrogen During the Low-Energy Irradiation of Alkanethiol SAMs
- 32a) K. Afrousheh, P. Bohlouli-Z., D. Vagale, A. Mugford, M. Fedorov, and J. D. D. Martin (University of Waterloo)
Spectroscopic Observation of Resonant Electric Dipole-Dipole Interactions Between Cold Rydberg Atoms
- 32b) K. R. Shamasundar and Marcel Nooijen (University of Waterloo)
Internally Contracted State-Selective Multi-Reference Methods Based on the Equation-of-Motion Coupled-Cluster Approach.
- 33a) Tao Peng and Robert J. Le Roy (University of Waterloo)
Monte Carlo Simulation and Frequency Shifts of SF₆ in an Ar Matrix