

Symposium on Chemical Physics

at the University of Waterloo

November 3 - 5, 2006

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

SESSION I: Friday, November 3, 2006 — P.M. Davis Centre Room 1351

Chair: **Marcel Nooijen**

- 7:30 – 8:15 Amanda Ross (Université Lyon 1 (LASIM))
Cavity-Enhanced Laser-Induced Emission Spectroscopy
- 8:15 – 8:30 J.R. Cooper, L.-H. Xu and N. Moazzen-Ahmadi (University of Calgary)
Ab Initio Determination of Spectroscopic Parameters for Ethane-Like Molecules in the Ground State
- 8:30 – 8:45 Sergei Manzhos and Tucker Carrington (Université de Montréal)
Using Redundant Coordinates to Represent Potential Surfaces with Lower-Dimensional Functions
- 8:45 – 9:00 Denise M. Koch, Sichuan Xu, Celine Toubin, Gilles H. Peslherbe and James T. Hynes (École Normale Supérieure and Concordia University)
On the Formation of Glycine in the Interstellar Medium

SESSION II: Saturday, November 4, 2006 – A.M.

Chair: **Terrance McMahon**

- 9:00– 9:45 Giacinto Scoles (Princeton University & University of Trieste)
HENDI Spectroscopy: the Genesis of an Idea and Some Recent Results
- 9:45 – 10:00 Dominique Appadoo (Canadian Light Source)
The Far-InfraRed Beamline at the Canadian Light Source
- 10:00 – 10:15 N. Blinov and P.-N. Roy (University of Alberta)
Solvation, Structure and Non-Classical Rotational Inertia of Doped Helium Clusters
- 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, November 4, 2006 – A.M.

Davis Centre Room 1351

Chair : **Robert Le Roy**

10:45 – 11:45 Rodney Bartlett (University of Florida)

Coupled-Cluster Theory for Large Molecules: The Natural Linear Scaled Coupled-Cluster Method

11:45 – 12:00 Scott Hopkins, Hans-Peter Loock, Mike Ashfold, Brid Cronin, Richard Dixon and Andrew Orr-Ewing (Queen's University and University of Bristol)

Photodissociation of Formaldehyde

12:00 – 12:15 Qadir K. Timerghazin, Gilles H. Peslherbe and Ann M. English (Concordia University)

Multireference Character of S-Nitrosothiols, Biological NO Carriers

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

SESSION IV: Saturday, November 4, 2006 – P.M.

Davis Centre Room 1351

Chair: **Peter Bernath**

1:30 – 2:15 Yunjie Xu (University of Alberta)

Exploring Chirality and Chiral Recognition Using Spectroscopic and Ab Initio Method

2:15 – 2:30 C. Linton,^a T. Ma,^b T. C. Steimle,^b V. Goncharov^c and M. C. Heaven^c (^a University of New Brunswick; ^b Arizona State University; ^c Emory University)

The Permanent Electric Dipole Moment and Magnetic g-factors of Uranium Monoxide, UO

2:30 – 2:45 Jeongho Kim, Cathy Y. Wong and Gregory D. Scholes (University of Toronto)

Selective Measurement of Ultrafast Exciton Spin Relaxation in Quantum Dots and Nanoroda

2:45 – 3:00 Michel Malick Thiam and Kam Tong Leung (University of Waterloo)

Glycine-Ice Nanolayers: an Infrared Study

3:00 – 3:15 Yangsoo Kim, Gregory E. Hall and Trevor Sears (Brookhaven National Laboratory)

AC Stark Detection of Optical-Optical Double Resonance in CH₂

3:15 **Refreshments and Poster Session**

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

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

SESSION V: Saturday, November 4, 2006 from 3:30 P.M.

Davis Centre Lobby

POSTER SESSION AND SPONSOR'S DISPLAY

6:00 P.M. Poster sessions ends
Depart for Festival Room, South Campus Hall

6:30 P.M. Cash Bar Festival Room, South Campus Hall

7:00 P.M. **DINNER** Festival Room, South Campus Hall

9:30 P.M. Informal Discussions "Graduate Club"

SESSION VI: Sunday, November 5, 2006 – A.M.

Chair: **Jim Martin**

9:15– 10:00 Takamasa Momose (University of British Columbia)
Spectroscopy and Dynamics of Molecules in Solid Parahydrogen and in He Droplets

10:00 – 10:15 Mark Thachuk and Nalantha Wanasundara (University of British Columbia)
Dissociation of Protein Complex Ions in the Gas Phase

10:15 – 10:30 Qing-Bin Lu (University of Waterloo)
Studies of the Molecular Reaction Mechanisms of Anticancer Drugs using Time-Resolved Femtosecond Laser Spectroscopy

10:30 – 11:00 **Coffee Break**

SESSION VII: Sunday, November 5, 2006 – A.M.

Davis Centre Room 1351

Chair: **Tong Leung**

11:00 – 11:45 Alan Dickinson (University of Newcastle)
Transport Properties of Gases: Beyond Linear Molecules

11:45 – 12:00 Li-Hong Xu, Hongyu Shi, Jonathan Fisher, R.M. Lees, John C. Pearson and Brian J. Drouin (University of New Brunswick)
New Terahertz Methanol Spectroscopy for HIFI on the Herschel Space Observatory

12:00 – 12:15 A.R.W. McKellar (National Research Council)
High Resolution Infrared Spectra of Helium Clusters Doped with Carbon Dioxide

Invited talks are 45 min. including 5 min. for discussion
Contributed talks are 15 min. including 3min. for discussion

POSTER SESSION

Chair: **Robert 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) Pierre-Nicholas Roy, Javier Eduardo Cuervo and Massimo Boninsegn (University of Alberta)
Ultra-Cold Para-Hydrogen Clusters: Solids or Liquids?
- 1b) Liyan Zhao, Allan Chung-Lung Siu and Tong Leung (University of Waterloo)
A New Way to Deposit Nanostructured Metallic Mn Film onto Si(100) by Electrodeposition
- 2a) J. Carter, O. Cherry and J. Martin (University of Waterloo)
Study of Rydberg Atom Surface Interactions using Laser Cooled Atoms and Magnetic Microtraps
- 2b) Matthew A. Furzeczott, Jonathan K. Martens, Richard A. Marta and Terry B. McMahon (University of Waterloo)
Probing the Effect of Fluorination on Strong Hydrogen Bonding in 2,4-pentanedione Proton-Bound Dimers
- 3a) Jean Christophe Tremblay and Tucker Carrington, Jr. (Université de Montréal)
New Ideas for Computing the Cumulative Reaction Probability
- 3b) L. Hernández de la Peña,^a M.S. Gulam Razul^b and P.G. Kusalik
(^a Concordia University; ^b St. Francis Xavier University; ^c University of Calgary)
Quantum Effects in Ice-Ih
- 4a) S. Dobrin, K.R. Harikumar, R.V. Jones, I.R. McNab, J.C. Polanyi, Z. Waqar and J.S.Y. Wang (University of Toronto)
Molecular Dynamics of Haloalkane Corral-Formation and Surface Halogenation at Si(111)-7×7
- 4b) Zhen-Dong Sun, R.M. Lees and Li-Hong Xu (University of New Brunswick)
Saturation-Dip Measurements In The C-N Stretching Band Of Methylamine
- 5a) Debabrata Pradhan and K. Tong Leung (University of Waterloo)
Two Dimensional Zinc Oxide Nano Structure Material on ITO Substrate
- 5b) Zeng Su and Yunjie Xu (University of Alberta)
High Resolution Mid-infrared Spectroscopic Study of a Chiral Molecule: C-H Stretching of Propylene Oxide in the Gas Phas

- 6a) A.G. Adam,^a M.E. Slaney,^a D.W. Tokaryk,^a R. Li^b and W.J. Balfour^b
(^aUniversity of New Brunswick and ^bUniversity of Victoria)
Visible Laser Spectroscopy of Chromium Monophosphide
- 6b) A.R.W. McKellar, D.W. Tokaryk, Li-Hong Xu, D.R.T. Appadoo and T. May
(National Research Council, University of New Brunswick, and Canadian Light Source)
First Results from the CLS Far-Infrared Beamline: the ν_{12} and ν_{17} Bands of Acrolein CH_2CHCH
- 7a) Alex Brown,^a Audry Smolin,^b Oleg Vasyutinskii,^b and Gabriel G. Balint-Kurti^c
(^aUniversity of Alberta, ^bRussian Academy of Sciences, and ^cUniversity of Bristol)
Photodissociation of HBr and DBr: Vector Correlation Coefficients
- 7b) Amanda Ross,^a Houssam Salami,^a Pawel Kowalczyk,^b Wlodzomierz Jastrzebski,^c and Robert J. Le Roy^d (^aUniversité Lyon 1 (LASIM), ^bUniversity of Warsaw, ^cPolish Academy of Sciences, ^dUniversity of Waterloo)
An Analytical Potential Energy Curve for the Lowest Triplet State of KLi
- 8a) Avishek Chatterjee, K.T.Leung, Zhenhua He Liyan Zhao (University of Waterloo)
Carbon Nano-Clusters On a Si(111) Surface
- 8b) Chun-Rong Wang and Qing-Bin Lu (University of Waterloo)
Time-Resolved Femtosecond Laser Spectroscopic Studies of the Molecular Reaction Mechanism of Halopyrimidines as Candidate Drugs for Radiotherapy of Cancer
- 9a) David Pedersen and Shiliang Wang (Defence R&D Canada)
Ag@AgI Core-Shell Nanoparticles
- 9b) Deijan Fu, Kaley A. Walker, Keeyoon Sung, Chris D. Boone and Peter F. Bernath
(University of Waterloo)
Remote Sensing of Atmospheric Gases Using PARIS-IR
- 10a) Dominique Appadoo (Canadian Light Source)
The Far- and Mid-Infrared Beamlines at the Canadian Light Source
- 10b) George C. McBane and Reinhard Schinke (Grand Valley State University)
Trajectory Surface Hopping Study of the $H + NH(a)$ Reaction
- 11a) Hilke Bahmann, Alexander Rodenberg, Alexei V. Arbuznikov and Martin Knapp
(University of Wuerzburg)
A Thermochemically Competitive Local Hybrid Functional Without Gradient Corrections
- 11b) Hui Li and Robert J. Le Roy (University of Waterloo)
The Quadrupole Moment Function and Absolute Infrared Quadrupolar Intensities for N_2
- 12a) J.N. Philippson and R.C. Shiell (Trent University)
Predictions of Multi-Level Coherent Population Trapping in 7Li
- 12b) J.P. Brichta, S.J. Walker, R. Helsten and J.H. Sanderson (University of Waterloo)
Ultrafast Imaging of Multielectronic Dissociative Ionization of CO_2 in an Intense Laser Field

- 13a) L. Li, R.M. Lees and Li-Hong Xu (University of New Brunswick)
ECTDL Spectra of the $\nu_1+2\nu_4$ Combination Bands of ^{14}N and ^{15}N Ammonia
- 13b) L. Tong and Y.J. Shi (University of Calgary)
Study of the Filament Aging Process and the H_2 -etching Effect by SEM and AES
- 14a) Laura E. Downie, Julie M. Michaud and Wolfgang Jaeger (University of Alberta)
A Microwave Spectroscopic Study of the Inversion Motion in the Ne-NH₃ Van der Waals Bimer
- 14b) Leonardo Alvarez-Valtierra and David W. Pratt (University of Pittsburgh)
Rotationally Resolved Electronic Spectra of 9,10-dihydrophenanthrene in the Gas Phase. Potential Energy Surfaces Along Different Low Frequency Coordinates
- 15a) M. Ugray, J.E. Atfield, T.G. McCarthy and R.C.Shiell (Trent University)
A Microcontroller-Based Wavemeter Using Compression-Locking of an Internal Mirror Reference Laser
- 15b) Mark Cybulski (Miami University)
An Approach for Evaluating Dispersion Coefficients of Large Molecules
- 16a) Martin Losada and Yunjie Xu (University of Alberta)
Effect of Solute-Solvent Intermolecular Hydrogen Bonding on the Vibrational Absorption and Vibrational Circular Dichroism Spectra of (S)-(-)-Methyl Lactate in H_2O and in CH_3OH : Experimental and ab initio Analyses
- 16b) Maryam Ebrahimi and Kam Tong Leung (University of Waterloo)
Surface Chemistry of Carboxylic Acids on Si(100)2x1
- 17a) Michael Dick, Jin-Guo Wang, Phil Sheridan, Shanshan Yu and Peter F. Bernath (University of Waterloo)
Optical-Optical Double Resonance Spectroscopic Studies of SrOH and CaOH
- 17b) Nick Trefiak, Klaus Bescherer, Runkai Li, Jack Barnes, Hans-Peter Looock, James Fraser, Scott Yam and Richard Oleschuk (Queen's University)
Ringdown Spectroscopy in Optical Waveguides
- 18a) Nicole Borho and Yunjie Xu (University of Alberta)
Lock and Key Principle on a Microscopic Scale: The Case of the Propylene Oxide ...Ethanol Complex
- 18b) Qing Wen and Wolfgang Jaeger (University of Alberta)
Study of the Xe-NH₃ Van der Waals Bimer: High Resolution Microwave Spectra and ab initio Calculations
- 19a) Qing-Bin Lu, Saeed Kalantari, Chun-Rong Wang and Changnien Shi (University of Waterloo)
Time-Resolved Femtosecond Laser Spectroscopic Studies of the Molecular Reaction Mechanism of the Most Effective Chemotherapeutic Drug—Cisplatin

- 19b) Qingxin Yang, Jack Barnes, Hans-Peter Looock and David Pedersen (Queen's University)
Time-Resolved Photoacoustic Spectroscopy using Fibre Bragg Grating Ultrasonic Transducers
- 20b) Raviraj M. Kulkarni, Waishun Tam, Zheng Su, Igor Leonov and Yunjie Xu (University of Alberta)
A Mid-Infrared Off-Axis Cavity Enhanced Absorption and Cavity Ring-down Spectrometer with a cw Quantum Cascade Laser
- 21a) Rick A. Marta, Travis D. Fridgen and Terry B. McMahon (University of Waterloo)
Probing Ion Molecule Reaction Mechanisms with Infrared Photo-Dissociation Spectra and ab initio Calculations: The Formation of the Protonated Water Dimer via Sequential Bimolecular Reactions with 1,1,3,3-Tetrafluorodimethyl Ether
- 21b) Ronghu Wu, Kris Eldridge and Terry B. McMahon (University of Waterloo)
Ion-Molecule Interaction and Conformation Change of the Clusters of Peptide and Ammonia/Ammonium by High Pressure Mass Spectrometry and Ab initio Calculations
- 22a) Rudolf Lehnig and Wolfgang Jaeger (University of Alberta)
The Tunneling Inversion Transition of Ammonia in Helium Nano-Droplets
- 22b) Saba M. Mattar (University of New Brunswick)
Determination of the Benzo-1,2:4,5-bis(1,3,2-dithiazolyl) Ground State Using the Broken Symmetry Technique and the Novel Spectroscopy Oriented Configuration Interaction Method
- 23a) Shanshan Yu, Jin-Guo Wang, Phillip M. Sheridan, Michael J. Dick and Peter F. Bernath (University of Waterloo)
Laser Spectroscopy of Alkaline-Earth Monohydroxides: the $A^2\Pi - X^2\Sigma^+$ and $C^2\Pi - A^2\Pi$ Transitions of SrOD and the $A^2\Pi - X^2\Sigma^+$ Transitions of BaOH
- 23b) Shiliang Wang, David B. Pedersen, Matt Paige and Adam Leontowich (Defence R&D Canada-Suffield)
Mind the Spacing: Coupling between Ag Nanoparticles and Observation of the Quadrupole Plasmon Resonance
- 24a) Vinay Venugopal, Z. H. He, and K.T. Leung (University of Waterloo)
Adsorption and Decomposition of Acetic Acid on Sputtered and Oxidized Si(111) Surfaces Characterized by EELS
- 24b) Wendy Topic and Wolfgang Jaeger (University of Alberta)
Rotational Study of He_n - Cyanoacetylene Isotopomers: $n = 1 - 18$ and $25 - 31$
- 25a) X.J. Jiang, Li-Hong Xu and A.R.W. McKellar (University of New Brunswick and National Research Council of Canada)
10 μ m High-Resolution Spectra of Acrolein
- 25b) Xiangzhu Li and Josef Paldus (University of Waterloo)
Application of the Newly Developed Reduced Multireference CCSD(T) Method to Transition Metal Complexes and Reaction Barriers

- 26a) Xiaogang Wang and Tucker Carrington, Jr. (Université de Montréal)
Vibrational Levels of Ar₄ : New Odd-Parity Bosonic States
- 26b) Andriy Plugatyr, Istok Nahtigal and Igor M. Svishchev (Trent University)
Hydration of Aromatic Molecules: Spatial Structure Analysis
- 27a) Julie M. Michaud and Wolfgang Jaeger (University of Alberta)
Solvation of OCS by {ortho}H₂ and {para}H₂ Molecules: A Microwave Spectroscopic Study
- 27b) K. R. Shamasundar and M. Nooijen (University of Waterloo)
State-Selective/State-Averaged Coupled-Cluster Method Using General Active Spaces : Pilot Application using Two-Body Transformed Hamiltonian
- 28a) Dominika Zgid and Marcel Nooijen (University of Waterloo)
Orbital Optimization with the Spin Adapted Density Matrix Renormalization Group Approach in the Active Matrix
- 28b) Yangsoo Kim, Gregory E. Hall and Trevor Sears (Brookhaven National Laboratory)
AC Stark Detection of Optical-Optical Double Resonance in CH₂

Notes