

Symposium on Chemical Physics

at the University of Waterloo

October 28 – 30, 2005

REGISTRATION begins at 7:00 p.m.
1301

Davis Centre Room

SESSION I: Friday, October 28, 2005 — P.M.
1351

Davis Centre Room

Chair: **Terry McMahon**

- 7:30 – 8:15 Tomas Baer (University of North Carolina)
*PEPICO Studies of Energy Selected Sequential and Parallel Ionic
Dissociation Reactions*
- 8:15 – 8:30 Heekyung Han and David M. Wardlaw (Queen's University)
*Effects of Initial Coherence on the Stability of Chirality and the
Distinguishability of Pure/Mixed States in Open Chiral Systems*
- 8:30 – 8:45 B. Eustergerling, B. Lo, X. Li and Y.J. Shi (University of Calgary)
*Investigation of Gas-Phase Reactions and Chemical Species from the Hot-
Wire Decomposition of Silacyclobutane*
- 8:45 – 9:00 Jeffrey T. Paci, Ted Belytschko, and George C. Schatz
*The Mechanical Properties of Single-Crystal and Ultrananocrystalline
Diamond: A Theoretical Study*

SESSION II: Saturday, October 29, 2005 – A.M.

Chair: **Peter Bernath**

- 9:00 – 9:45 John Stanton (University of Texas at Austin)
The Unusually Complicated NO₃ Molecule
- 9:45 – 10:00 Li-Hong Xu (University of New Brunswick)
Conformational Isomerism in 1-Heptanal
 $H_3C-C(H_2)-C(H_2)-C(H_2)-C(H_2)-C(H)=O$
- 10:00 – 10:15 Mark Hoffman, Yury G. Khait, and Ajitha Devorajan (University of North
Dakota)
*Progress Towards a Size-Extensive, Incomplete Model Space Multi-
Reference Coupled Cluster Method*
- 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 29, 2005 – A.M.
1351

Davis Centre Room

Chair : **Marcel Nooijen**

10:45 – 11:45 Steve Leone (University of California Berkeley, and LBNL)
*Ultrafast Molecular Dynamics: Rydberg Wave Packets, Coherent Control,
and High-Harmonic Probing*

11:45 – 12:00 Xiaogang Wang and Tucker Carrington Jr. (Université de Montréal)
*A Parallel Strategy for Six-Atom Quantum Bending Dynamics: Application
to CH₅⁺*

12:00 – 12:15 Steven D. Chambreau, Sridhar A. Lahankar and Arthur G. Suits (Wayne
State University)
*Correlated State Distributions of j_{CO} and v_{H2} upon Photodissociation of
Formaldehyde: Molecular and Roaming H-Atom Channels*

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

SESSION IV: Saturday, October 29, 2005 – P.M.
1351

Davis Centre Room

Chair: **Robert Le Roy**

1:30 – 2:15 Raymond Laflamme (University of Waterloo)
Quantum Computer and NMR

2:15 – 2:30 Irina Paci, Igal Szleifer and Mark A. Ratner (Northwestern University and
Purdue University)
Chiral Resolution in Two-Dimensional Racemic Systems

2:30 – 2:45 Maria A. Gomez (Mount Holyoke College)
*Including Quantum Vibrational Character of a Small Molecular Subsystem
within Classical Equilibrium Simulations*

2:45 – 3:00 Zhen-Dong Sun, Kojiro Takagi and Fusakazu Matsushima
(Toyama University)
*Separation and Conversion Dynamics of Four Nuclear Spin Isomers of
Ethylene*

3:00 – 3:15 O. Pirali and D. Tokaryk (University of New Brunswick)
*Optogalvanic Detection of Quintet Transitions in N₂ Excited by a Corona Jet
Discharge*

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, October 29, 2005 from 3:30 P.M.
Lobby

Davis Centre

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, October 30, 2005 – A.M.

Chair: **Fred McCourt**

9:15 – 10:00 Pat Vaccaro (Yale University)
Lifting the Veil of Solvation: The Chiral-Optical Response of Isolated Molecules

10:00 – 10:15 Erin R. Johnson and Axel D. Becke (Queen's University)
Van der Waals Interactions from the Exchange Hole Dipole Moment

10:15 – 10:30 Alexander I. Pegarkov (University of Ottawa)
Phase Control Over Decaying Molecule States in Intense Laser Pulses

10:30 – 11:00 **Coffee Break**

SESSION VII: Sunday, October 30, 2005 – A.M.

Davis Centre Room

1351

Chair: **Bob LeRoy**

11:00 – 11:45 Pierre-Nicholas Roy (University of Alberta)
Molecular Dynamics in Doped Quantum Clusters: Rotations and Superfluid Response

11:45 – 12:00 J. Mark Parnis, Eric Escobar-Cabrera, Matthew G.K. Thompson, J. Paul Jacula, Rick D. Lafleur, Alfredo Guevara-García, Ana Martínez, and David M. Rayner
Cluster Size Selectivity in the Product Distribution of Ethene Dehydrogenation on Niobium Clusters

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) Helia Jalili, Nina Heinig, Liyan Zhao and K.T. Leung (University of Waterloo)
Pulsed Laser Deposition of Chromium Oxide Thin Films
- 1b) X. Li, B. Eustergerling and Y.J. Shi (University of Calgary)
Investigation of Gas-phase Chemistry in a Hot Wire Chemical Vapor Deposition Chamber Using Tetramethylsilane
- 2a) Rick A. Marta, Travis D. Fridgen, Matt A. Furzeczott and Terry B. McMahon (University of Waterloo)
Probing Strong Hydrogen Bonding in Gas Phase Association Reactions of Protonated 2-Pentanone and 2,4-Pentanedione with Their Neutral Counterparts via Mass Spectrometric and Computational Methods
- 2b) G.P. Li and I.P. Hamilton (Wilfrid Laurier University)
Complexes of Small Neutral Gold Clusters and Hydrogen Sulphide: A Theoretical Study
- 3a) Rob Nieckarz, Melisa Clements, Travis Fridgen, Guanping Li, Ian Hamilton and Terry McMahon (University of Waterloo; Wilfrid Laurier University)
An HPMS/Computational Study of the Solvation of FHF⁻ and NNN⁻ by H₂O, CH₃OH, and C₂H₅OH
- 3b) Matthew G.K. Thompson, Errol G. Lewar and J. Mark Parnis (Trent University and Queen's University)
FTIR Spectroscopic Evidence for the Water Diethene Complex, C₂H₄···HOH···C₂H₄
- 4a) Juan Casado, Rocio Ponce Ortiz, Victor Hernández, Juan T. López Navarrete, Enrique Orti, Petro M. Viruela, Begoña Milián, Shu Hotta, Sandro Zecchin, Barbara Vercelli and Gianni Zotti (University of Málaga)
Unexpected Magnetic Properties of Quinoidal Oligothiophenes. More than Good Candidates for Ambipolar Organic Semiconductors?
- 4b) Rouslan V. Olkhov, Chester M. Sadowski and Ian W.M. Smith (Cambridge University)
Total and State-to-State Rate Coefficients for Inelastic and Reactive Collisions for CN(X, v = 2) in Selected Levels in Collisions with N₂ and C₂H₂

- 5a) A.G. Adam, W.D. Hamilton, W. Sha, T. Ma and T.C. Steimle (University of New Brunswick and Arizona State University)
Fine and Hyperfine Structure and the Stark Effect in CoF
- 5b) David Pedersen, Mark Parnis, Greg Metha and Mark Buntine (Defence R&D Canada-Suffield; Trent University; Adelaide University)
ATR Spectroscopy of Benzene and Toluene on Nanogold
- 6a) Greg Bubnis and Howard R. Mayne (University of New Hampshire)
Composition-Induced Structural Changes in Mixed C₆₀, C₇₀ and C₈₄ Fullerene Clusters
- 6b) L.J. Neil, R.G. Remorov, W.J.W. Johnson, M.W. Bardwell and J.J. Sloan (University of Waterloo)
Uptake of OH Radicals by Surfactant Surface
- 7a) Dejian Fu, Kaley A. Walker, Keeyoon Sung, Chris Boone, Randall Skelton, Peter Bernath, Jeffrey R. Taylor, Debra Wunch, Kimberly Strong and James R. Drummond (University of Waterloo; University of Toronto)
PARIS-IR Ground-based Observation in Summer 2005
- 7b) Yoonjung Huh and P.-N. Roy (University of Alberta)
Inclusion of Inversion Symmetry in Centroid Molecular Dynamics
- 8a) Shanshan Yu, Iouli Gordon, Phillip Sheridan and Peter F. Bernath (University of Waterloo)
The Infrared Electronic Spectroscopy of CoS
- 8b) Jin-Guo Wang, Phillip Sheridan, Michael J. Dick and Peter F. Bernath (University of Waterloo)
Optical-Optical Double-Resonance Spectroscopy of SrOH: The C²Π(OOO)- \tilde{A} ²Π(OOO) Transition
- 9a) Sacha Zlatkova and Gilles Peslherbe (Concordia University)
An Ab Initio Characterization of the Electronic States of HBr in the Gas Phase and in Water Clusters
- 9b) Jack Barnes, Stephen Brown, Krista Laugesen, Hans-Peter Loock and Jun Zhang (Queen's University)
Measurement of Trace Organic Contaminants in Water Using Fibre-Loop Ring-Down Spectroscopy
- 10a) Qadir K. Timerghazin and Gilles H. Peslherbe (Concordia University)
Dynamics of Charge-Transfer-to-Solvent (CTTS) Excited States of Iodide-Solvent Clusters

- 10b) Zheng Su, wai Shun Tam and Yunjie Xu (University of Alberta)
High Resolution Infrared Spectroscopy and Ab Initio Studies of the Cyclopropane-Carbon Dioxide Interaction
- 11a) Sean M. Cleary and Howard R. Mayne (University of New Hampshire)
Novel High-Symmetry Mixed Ar-Xe Lennard-Jones Clusters
- 11b) Taiwang Cheng, Ryan Zaari, Jesse Kadosh and Alex Brown (University of Alberta)
Optimal Control of Vibrational Transitions
- 12a) H.M. Lambert, E.W. Davis, A.A. Dixit, Onur Tokel and P.L. Houston (Redeemer University College)
Product Imaging in the 130.2 nm Dissociation of Nitrous Oxide
- 12b) Myung Hwa Kim, Lei Shen, Brian D. Leskiw and Arthur G. Suits (Stony Brook University; Wayne State University)
Reflectron Multimass Velocity Map Imaging
- 13a) J.L. Ambrose, H.R. Mayne, J. Stutz, R.W. Talbot and B.C. Sive (University of New Hampshire)
Nighttime Oxidation of VOCs at Appledore Island, ME during ICARTT 2004
- 13b) Carl Shi and Allan L.L. East (University of Regina)
Theoretical Overview of the Ultraviolet Singlet Electronically Excited States of the NO Dimer
- 14a) Saba M. Mattar (University of New Brunswick)
First Principles Derivation of the Angular Dependence of Electron Paramagnetic Resonance Transition Probabilities for Doublet State Reactive Intermediates
- 14b) Nicole Borho, Cindy Lee, Wai Shun Tam and Yunjie Xu (University of Alberta)
High Resolution Mid-Infrared and Microwave Spectroscopy of Methyl Lactate
- 15a) Saba M. Mattar, Jacob Sanford and Alyson D. Goodfellow (University of New Brunswick)
g Tensor Computation of the Thiopheno- 1,3,2-dithiazolyl Radical by the Coupled-Perturbed Kohn-Sham Hybrid Density Functional Method
- 15b) X.J. Jiang, Li-Hong Xu and A.R.W. McKellar (University of New Brunswick; National Research Council)
10 μ m High-Resolution Spectra of Acrolein $H_2C=C(H)-C(H)=O$
- 16a) A.R.W. McKellar, (Steacie Institute for Molecular Sciences, National Research Council)
High Resolution Infrared Spectra of Larger Helium Clusters with N Up to 70
- 16b) Alireza Shayesteh, Robert J. Le Roy, Thomas D. Varberg and Peter F. Bernath (University of Waterloo; Macalester College)
New Infrared and Microwave spectra of ZnH and CdH

- 17a) Julie M. Michaud and Wolfgang Jäger (University of Alberta)
Doped Hydrogen Clusters: Rotational Spectroscopy of OCS Solvated with Ortho H₂ and para H₂
- 17b) Matthew A. Furzecott, Richard A. Marta, Travis D. Fridgen and Terry B. McMahon (University of Waterloo)
A Thermochemical Investigation of Ketone and Diketone Protonated Clusters in the Gas Phase via High Pressure Mass Spectrometry (HPMS)
- 18a) Rudolf Lehnig and Wolfgang Jäger (University of Alberta)
IR Spectroscopy of the Antisymmetric Stretching Mode of ¹⁶O C ¹⁸O in Superfluid Helium Nanodroplets
- 18b) Constantin Romanescu, Sumi Wren, Hans-Peter Looock and Sergei Manzhos (Queen's University; Université de Montreal)
Photodissociation from a Quantum-Selected State
- 19a) Nick Trefiak, Dan Courtney, Runkai Li, Richard Walford and Hans-Peter Looock (Queen's University)
Absorption Detector Using Fibre-Loop Ring-Down Spectroscopy
- 19b) N. Blinov and P.-N. Roy (University of Alberta)
Recurrences in Rotational Dynamics and Experimental Measurement of Superfluidity in Doped Helium Clusters
- 20a) Richard Dawes and Tucker Carrington Jr. (Université de Montréal)
Obtaining Good Basis Sets for Vibrational Hamiltonians Through Trace Minimization and Simultaneous Diagonalization
- 20b) Mark Cybulski (Miami University)
How Accurate are Popular Force Fields?
- 21a) Francis Temme (Queen's University)
In Search of Universal Determinancy in $SU(m) \times S_{2n} \downarrow G$ Direct Embeddings Defining NMR Spin Symmetries $\{\chi\}(C_i)$ Projective Modelling and Schur Hierarchical λ Decompositions for $SU(3(4)) \times S_{20} \downarrow A_5$
- 21b) Titus Sandu, (Université de Montréal)
Fast Calculation of Optical Matrix Elements in Density Functional Theory Methods and Beyond
- 22a) Jean Christophe Tremblay and Tucker Carrington Jr. (Université de Montréal)
Computing Resonance Energies, Widths, and Wave Functions Using a Lanczos Method in Real Arithmetic

- 22b) Wen Li, Cunshun Huang and Arthur G. Suits (Wayne State University; Stony Brook University)
State-Resolved Reactive Scattering by Slice Imaging: A New View of the $Cl+C_2H_6$ Reaction
- 23a) Sergei Manzhos, X. Wang, R. Dawes and T. Carrington, Jr. (Université de Montréal)
Improved Neural Network Methods as Molecule-Independent Multidimensional Potential Energy Surface Builders. Application to the Vibrational Spectroscopy of H_2O , H_2CO , and H_2O_2
- 23b) Kaley A. Walker, Keeyoon Sung, Dejian Fu, Ian Young, Yony Bresler, Michelle Seguin and Peter F. Bernath (University of Waterloo)
Recent Atmospheric Measurements Obtained with the Portable Atmospheric Research Interferometric Spectrometer (PARIS-IR)
- 24a) Keeyoon Sung, Chris Boone, Kaley A. Walker, Richard Mittermeir, Hans Fast and Peter F. Bernath (University of Waterloo; Meteorological Service of Canada, Environment)
Comparison of Measurements of the Arctic Atmosphere by Two Fourier Transform Infrared Spectrometers
- 24b) Radu Iftimie (Université de Montréal)
The Molecular Origin of the “Continuous” Infrared Absorption in Aqueous Solutions of Acids: A Computational Approach
- 25a) J.P. Brichta, A. Trottier, A.A. Zaidi, W.-K. Liu, D. Strickland and J.H. Sanderson (University of Waterloo)
Vibrational State Dependence of Ionisation Rate Using Laser-Induced Field Ionisation and Tunneling Approach
- 25b) Jun Zhang, Jack Barnes, Krista Laugesen, Stephen Brown and Hans-Peter Looock (Queen’s University)
Modified EVA Film for Organic Contaminants Sensings
- 26a) Steven D. Chambreau, Sridhar A. Lahankar and Arthur G. Suits (Wayne State University)
Correlated State Distributions of H_2 and CO from Formaldehyde Photodissociation Using High Resolution DC Slice Imaging: Molecular Elimination Versus the “Roaming” H-atom Channel
- 26b) Yu-Jong Wu, R.M. Lees, Li-Hong Xu, Jon T. Hougen and Yuan-Pern Lee (University of New Brunswick; NIST; National Chiao Tung University)
Internal rotation of CH_3OH in Solid Para-Hydrogen
- 27a) L. Carsten Nielsen, Howard Mayne, Barkely C. Sive, Bob Talbot, Ruth Varner, Yong Zhao and Rachel Russo (University of New Hampshire)
Detection and Quantification of Atmospheric Oxygenated Volatile Organic Compounds by Proton Transfer Reaction Mass Spectrometry

- 27b) Irina Paci, Igal Szleifer and Mark A. Ratner (Northerwestern University and Purdue University)
Chiral Resolution in Two-Dimensional Racemic Systems
- 28a) Michael Dick, Phillip Sheridan, Jin-Guo Wang and Peter Bernath (University of Waterloo)
High Resolution Laser Spectroscopy of SrCH₃, CaBH₄ and SrBH₄
- 28b) C. Linton, A.J. Ross, P. Crozet, W.S. Hopkins and A.G. Adam (University of New Brunswick; Université Lyon I)
Structure and Spectra of the CaOCH₃ Radical
- 29a) A.G. Adam, J.G. Crouse, L.E. Downie, W.S. Hopkins, C. Linton, A. Read and D.W. Tokaryk (University of New Brunswick)
High Resolution Laser Spectroscopy of Strontium Monomethoxide
- 29b) Ronghu Wu and Terry B. McMahon (University of Waterloo)
Ion-molecular Interactions of Protonated Nucleic Acid Bases (Cytosine, Uracil, Thymine and Adenine) and Ammonia by High Pressure Mass Spectrometry and Ab initio Calculations
- 30a) Dominika Zgid and Marcel Nooijen (University of Waterloo)
Orbital Optimization in the Density Matrix Renormalization Group
- 30b) Aneta Chmielewski and Marcel Nooijen (University of Waterloo)
Analysis of the Time-Dependent Wavefunction in a Vibronic System