
The 14th Annual
Symposium
on
Chemical Physics
at the
University of Waterloo
November 6-8, 1998

Symposium on Chemical Physics

at the University of Waterloo

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

SESSION I: Friday, November 6, 1998 - P.M. Davis Centre Room 1302

Chair: **Bob Le Roy**

7:45 - 8:30 Allan Adam (University of New Brunswick)
High Resolution Laser Spectroscopy of Diatomic Molecules Containing Cobalt

8:30 - 8:45 Matt L. Costen, Greg Hall and H. Katayanagi (Brookhaven National Laboratory)
Coincident State Distributions in the 308 nm Photolysis of Jet-Cooled Ketene

8:45 - 9:00 M.D. Brookes and A.R.W. McKellar (NRC, Ottawa)
Mysteries of the CO Dimer

9:15 Informal Discussion - Grad Club

SESSION II: Saturday, November 7, 1998 - A.M. Davis Centre 1351

Chair: **Jim Sloan**

9:00 - 9:45 Mark Johnson (Yale University)
Making and Breaking Water Networks Around Halide Ions: Ionic vs. Interwater Hydrogen Bonding

9:45 - 10:00 Randall S. Dumont, Rosa Assalone, Paul Hazendonk and Alex Bain
(McMaster University)
Simulation of Large Spin System Dynamics in Liquids and Rotating Solids

10:00 - 10:15 Ralph Shiell Matt Evans, Stephanie Stimson, Chai-Wei Hsu, Cheuk Ng and John Hepburn (University of Waterloo)
The Investigation of Correlation Satellites Using Pulsed Field Ionization-Zero Kinetic Energy Photoelectron Spectroscopy

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

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

10:15 - 10:45 **Coffee Break**

SESSION III: Saturday, November 7, 1998 - A.M.

Davis Centre 1351

Chair: **Bryan Henry**

10:45 - 11:45 Joshua Jortner (University of Tel Aviv, Plenary Lecturer)
On Dynamics. From Isolated Molecules to Biomolecules

11:45 - 12:00 C. Callegari, I. Reinhart, A. Conjusteau, K. Lehmann and G. Scoles
(Princeton University)
Recent Results of Infrared Spectroscopy in He Clusters

12:00 - 12:15 Gilles H. Peslherbe (Concordia University), Branka M. Ladanyi
(Colorado State University) and James T. Hynes (University of Colorado Boulder)
Photodissociation of NaI in Clusters

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

SESSION IV: Saturday, November 7, 1998 - P.M.

Davis Centre 1351

Chair: **John Hepburn**

1:30 - 2:15 Floyd Davis (Cornell University)
Transition Metal Chemistry in Crossed Beams

2:15 - 2:30 Emily J. Brown, Q. Zhang, Marcos Dantus (Michigan State University)
What Can We Learn From Transient Gratings in the Gas Phase?

2:30 - 2:45 Vladimir N. Markov, Yunjie Xu and Wolfgang Jaeger (University of Alberta)
A Microwave -Terahertz Double Resonance Spectrometer for The Investigation of Van der Waals Complexes

2:45 - 3:00 Adriana Predoi-Cross, R. Berman, J.R. Drummond and A.D. May
(University of Toronto)
Line mixing effects in pure CO₂ Q-branch spectra

3:00 - 3:15 K. Thomas Lorenz, David W. Chandler and George McBane
(Ohio State University)
Velocity Mapping of Inelastic Scattering in Crossed Beams: Experimental Results and Simulations for He-CO Collisions

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

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

SESSION V: Saturday, November 7, 1998 - from 3:30 P.M.

Davis Centre Lobby

POSTER SESSION AND SPONSORS' DISPLAY

6:00 P.M. Poster session ends.
Depart for Conrad Grebel College

6:30 P.M. Cash Bar

Conrad Grebel College

7:00 P.M. **DINNER**

Conrad Grebel College

SESSION VI: Sunday, November 8, 1998 - A.M.

Davis Centre 1302

Chair: **Peter Bernath**

9:15 - 10:00 Nick Westwood (University of Guelph)
Ground, Excited and Ionic States of Unstable Molecules: Experiment and Theory

10:00 - 10:15 Katherine Reid (University of Nottingham, U.K.)
Using Photoelectrons to Probe Dynamics

10:15 - 10:30 Trevor Sears, Phillip Johnson, Eileen Clifford and Craig Taatjes
(Brookhaven National Laboratory)
New Spectroscopic and Kinetics Measurements of Ethyl Radical

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

SESSION VII: Sunday, November 8, 1998 - A.M.

Davis Centre 1302

Chair: **Fred McCourt**

11:00 - 11:45 Dwayne Miller (University of Toronto)
Femtosecond Surface Reaction Dynamic Mapping the "Electron Trajectory"

11:45 - 12:00 Joanna Karczmarek, and Misha Ivanov
(Steacie Institute for Molecular Sciences, National Research Council)
Optical Twister

12:00 - 12:15 A. Alavi, R.M. Lynden-Bell and R.J.C. Brown (Queen's University)
Rotation of Ammonium Ions in Crystals: Is it Chemistry or Physics

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

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

POSTER SESSION

Chair: **John Hepburn**

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) B. Blicharska and M. Kluza (Jagellonian University)
The NMR Relaxation Study of The Hydration of Cellulose
- 1b) Kaley A. Walker and Michael C.L. Gerry (University of British Columbia)
Pure Rotational Spectroscopy of Aluminium and Indium Monocyanide Species
- 2a) David S. Perry, Andrei Chirokolava, Yongbin Ma, Xiaoliang Wang, Oleg Boyarkin and Thomas R. Rizzo (University of Akron)
Torsion-Vibration Coupling in Methanol
- 2b) Brant Billingham, Kathleen M. Gough, Henrik Kjaergaard and Geoffrey R. Low (University of Manitoba)
A Study of The Overtone Spectra of Trimethyl Amine and Dimethyl Sulfide
- 3a) D.M. Mao, X.K. Hu, Y.J. Shi, and R.H. Lipson (University of Western Ontario)
Mass-Resolved Vibrational Spectra of KrXe and ArXe Near the Highest Energy Level of Xe(5d) Manifold*
- 3b) M. Nezu, T. Amano, and K. Kawaguchi (Ibaraki University)
Ion-Beam and IR Matrix Isolation Spectroscopy for Determination of Branching ratios of Dissociative Recombination Reactions
- 4a) Patrick J. Pisano, Michael S. Westley, Michael A. Carpenter and Paul L. Houston (Cornell University)
A Crossed Molecular Beam Study of $O(^1D) + N_2O \rightarrow 2 NO$
- 4b) Dean Court and Wolfgang Jaeger (University of Alberta)
Ne-H₂CO Van der Waals Complex: ab initio Calculations and Rotational Spectra

- 5a) A.V. Fedorov and J.R. Cable (Bowling Green State University)
Structure and Properties of Water and Ammonia Clusters of Aromatic Amides in a Supersonic Jet Expansion
- 5b) A.V. Fedorov, D.L. Snavely (Bowling Green State University) and K.M. Gough (University of Manitoba)
Vibrational Overtone Spectroscopy of Cyclohexadiene Iron Tricarbonyl and 1,3-Cyclohexadiene
- 6a) Travis D. Fridgen and J. Mark Parnis (Trent and Queen's Universities)
1,2,-Proton-Transfer Catalysis by Ar, Kr, Xe and N₂: Theoretical Calculations and Possible Experimental Evidence
- 6b) David B. Pedersen, Rick D. Lafleur, J. Mark Parnis and David M. Rayner (Queen's and Trent Universities)
Experimental Evidence Supporting Ta Atoms as Reactive Sites in Ta Cluster Reactions
- 7a) Travis D. Fridgen and J. Mark Parnis (Trent and Queen's Universities)
(RgHRg')⁺ ions (Rg = Ar, Kr and/or Xe) isolated in rare gas matrices by electron bombardment matrix isolation: Experimental results and DFT calculations
- 7b) Jenning Seto and Robert Le Roy (University of Waterloo)
Development of a Computer Program to Fit Analytical Molecular Potentials Directly to Spectroscopic Data
- 8a) Randall Skelton, Treanna Parekunnel and Peter Bernath (University of Waterloo)
The Atmospheric Chemistry Experiment (ACE)
- 8b) Umesh A. Salain, Sudha Srinivas and Julius Jellinek (Argonne National Laboratory, IL)
Structural and Electronic Properties of Ag₃-C₂H₄ Complex
- 9a) Julius Jellinek and Alexander Golberg (Argonne National Laboratory)
Dynamics of Metallic Clusters: Unraveling the Complexity
- 9b) Ao Lin, Stiliana Antonova, Antonis P. Tsakotellis and George C. McBane (Ohio State University)
Lambda Doublet Propensities in Ar-NO Rotationally Inelastic Scattering at 220meV
- 10a) Antonis Tsakotellis, Ao Lin, Stiliana Antonova, and George C. McBane (Ohio State University)
State to State He-CO Rotationally Inelastic Scattering

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State to State He-CO Rotationally Inelastic Scattering

- 10b) Ryan Z. Hinrichs, Hans U. Stauffer, Peter A. Willis and H. Floyd Davis (Cornell University)
C-H Bond Activation of Ethane, Ethylene, and Acetylene by Ground State Yttrium Atoms
- 11a) Ruth Tanner, Scott Harris and N.P.C. Westwood (University of Guelph)
A Computational and Experimental Study of $B(NCO)_3$ and Related Intermediates
- 11b) Scott Harris, Ruth Tanner and N.P.C. Westwood (University of Guelph)
A Computation and Infrared Study of $BCl_x (OMe)_{3-x}$ Molecules
- 12a) Kenneth W. Chan, Trevor D. Power, Jaran Jai-nhuknan and Slawomir M. Cybulski (Miami University)
An Ab Initio Study of He-F₂, Ne-F₂ and Ar-F₂ Van der Waals Complexes
- 12b) Sophie Brunet, Tucker Carrington and S.V. Filseth (York University)
Rotational Relaxation in Collisions of CN with H₂ and D₂
- 13a) Jeff Paci and David Wardlaw (Queen's University)
The Strong Field Dissociation of H₂⁺ and HCl⁺
- 13b) R. Berman, P.M. Sinclair, J.R. Drummond and A.D. May (University of Toronto)
Direct Measurements of Line Mixing in Pure CO₂
- 14a) Zygmunt J. Jakubek, Benoit Simard (NRC, Ottawa), Hideaki Niki (Fuku University, Japan) and Walter J. Balfour (University of Victoria)
High Resolution Study of the $B(^2\Sigma^+)-X(^2\Sigma^+)$ (0,0,0 - 0, 0, 0) Band of Yttrium Imide ($Y^{14}NH$, $Y^{15}NH$ and $Y^{14}ND$).
- 14b) J. Guo, R. Eng, T. Carrington and S.V. Filseth (York University)
Energy Disposal in CN ($A^2\Pi$) Produced in the 157 nm Photodissociation of HCN
- 15a) L.M. Beaty, D.C. Moule (Brock University), R.H. Judge (University of Wisconsin-Parkside), H. Liu and E.C. Lim (University of Akron)
The S₁ - S₀ Fluorescence Excitation Spectrum of Formic Acid. A Rotational Analysis of the 9₀¹ Band. One-Dimensional Treatments of the Torsion and Wagging Vibronic Structure.
- 15b) James D.D. Martin and J.W. Hepburn (University of Waterloo)
Determination of Bond Energies by Threshold Ion-Pair Production Spectroscopy: An Improved D₀(HCl)
- 16a) X.K. Hu, D.M. Mao, Y.J. Shi, S.S. Dimiov and R.H. Lipson (University of Western Ontario, London)
Photoelectron Spectra of Xe(nf) Atomic States*

- 16b) Peter A. Willis, Ryan Z. Hinrichs, Hans U. Stauffer and H. Floyd Davis (Cornell University)
Reaction Dynamics of Zr and Nb with Ethylene
- 17a) Hans U. Stauffer, Ryan Z. Hinrichs, Peter A. Willis, H. Floyd Davis (Cornell University)
Oxidation of First Row Transition Metal Atoms
- 17b) Kathleen M. Gough, Pamela Bromberg, Jason Hein, Mandy Ogg, Marc de Bigio and Robert Julian (University of Manitoba and University of Wisconsin-Madison)
Synchrotron FT-IR Spectromicroscopy of Normal and Alzheimer Diseased Brain Tissue
- 18a) Nam-Anh Nguyen and T.T. Nguyen-Dang (Université Laval)
Symbolic Calculations in Quantum Molecular Dynamics
- 18b) Hakima Abou-Rachid, T. Tung Nguyen-Dang and Osman Atabek (Université Laval)
Dynamical Quenching of Laser-Induced Dissociation of Heteronuclear Diatomic Molecules in Intense IR Fields
- 19a) G. Eustatiu, T. Tyliczszak and A.P. Hitchcock (McMaster University)
Inner-shell Electron Energy-Loss Spectroscopy at High Momentum Transfer
- 19b) Li-Hong Xu and R.M. Lees (University of New Brunswick)
Methanol Studies at the University of New Brunswick
- 20a) L.M. Dobeck, W. Kong, H.M. Lambert and P.L. Houston (Cornell University)
Direct Evidence for the Triple Whammy Channel in the 440 nm Photolysis of Trans-Glyoxal: $(CHO)_2 \rightarrow 2CO + H_2$
- 20b) D.C. Sperry, J.I. Lee and J.M. Farrar (University of Rochester)
 $Sr^+(ND_3)_n D_m$ - - Novel Species Observed in the Ammonia Solvated Strontium Cation System
- 21a) S.T. Lee, E.S. Richards and J.M. Farrar (University of Rochester)
Reagent Rotational Energy Effects in the $O + D_2$ System
- 21b) J.I. Lee, D.C. Sperry and J.M. Farrar (University of Rochester)
Spectroscopy of $Mg^+(NH_3)_n$ and $Mg^+(CH_3OD)_n$
- 22a) Matt Costen, Simon North and Greg Hall (Brookhaven National Laboratory)
Multiple Surfaces But No Place To Hide: ICN Tells All to FM Doppler Spectroscopy
- 22b) Aaron S. Beatty, Ralph C. Shiell, Dongfang Chang and John W. Hepburn (University of Waterloo)
The (1+1) REMPI Spectra of Jet Cooled $^{12}C^{32}S_2$ and $^{12}C^{34}S^{32}S$ From 45500 to 48000 cm^{-1}

- 23a) N.S-K. Sze, Naila Siddique and J.J. Sloan (University of Waterloo)
Raman Spectroscopy to Characterize Tropospheric (Especially Urban) Aerosols and Particulate Matter
- 23b) Qing Xu, Allan Bertram, Jesse Rowsell, Mike DeWitte and J.J. Sloan (University of Waterloo)
Ph Effects on the Deliquescence of Sea Salt Aerosols
- 24a) Nilmadhab Chakrabarti, Tucker Carrington, Jr. and Benoit Roux (Université de Montréal)
A Rigorous and Practical Path-Integral Formulation for Calculating Rate Constants
- 24b) Pranab Sarkar, Nicolas Poulin and Tucker Carrington, Jr. (Université de Montréal)
A Theoretical Determination of the Ro-Vibrational Energy Levels of the Water Molecule
- 25a) Shiwei Huang and Tucker Carrington, Jr. (Université de Montréal)
Using Discrete-Variable-Representation Filtered Basis Functions to Calculate Vibrational Energy Levels in a Chosen Window of the Spectrum
- 25b) Dustin Dickens, Allan Bertram and J.J. Sloan (University of Waterloo)
Nucleation Kinetics of Nitric Acid and Water Aerosols
- 26a) G.P. Li and I.P. Hamilton (Wilfrid Laurier University)
The Low-Lying States of HF_2^+ : A Theoretical Study
- 26b) Edward G. Lee, Jenning Y. Seto, Tsuyoshi Hirao, Peter F. Bernath and Robert Le Roy (University of Waterloo)
FTIR Emission Spectra, Molecular Constants, and Potential Curve of Ground-State GeO
- 27a) Hua Wei and Robert J. Le Roy (University of Waterloo)
A New Potential Energy Surface of H_2 -Kr
- 27b) Patrick Ayotte, Gary H. Weddle, Christopher G. Bailey and Mark A. Johnson (Yale University), Fernando Vila, and Kenneth D. Jordan (University of Pittsburgh)
Infrared Spectroscopy of Negatively Charged Water Clusters: Evidence for a Linear Network