The 11th Annual University of Waterloo **Symposium on Chemical Physics**

November 3-5, 1995

Acknowledgements

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Waterloo Symposium on Chemical Physics

November 3-5, 1995

at the University of Waterloo

REGISTRATION begins at 6:30 p.m., Davis Centre Room 1301

SESSION I: Friday, November 3, 1995 - P.M. Davis Centre 1351

Chair: **John Hepburn**

7:30 - 8:15 Jim Weisshaar (University of Wisconsin)
Understanding Methyl Rotor Barriers

8:15 - 8:30 M.A. Carpenter, M.T. Zanni, D.C. Sperry, S.R. Troutman and J.M. Farrar (University of Rochester)
Crossed Beam Studies of the $O^-+D_2 \rightarrow OD^-+D$ Reaction at Collision Energies Ranging from 0.25 eV to 1.2 eV: Anomalous Low Energy Results

8:30 - 8:45 M. Kolbuszewski and P.R. Bunker (NRC, Ottawa)
On the Proton Rearrangement Energy Levels and Spectrum of CH_5^+

8:45 - 9:00 F. Negri (Universita di Bologna, Italy) and M. Zgierski (NRC, Ottawa)
Vibronic Structure of the ZEKE Spectra of Naphthalene from Single Vibronic Levels of the S_1 Manifold. Theoretical Interpretation

SESSION II: Saturday, November 4, 1995 - A.M. Davis Centre 1351

Chair: **Bob Le Roy**

9:00 - 9:45 Terry Miller (Ohio State University)
Laser Spectroscopy of Cold Methoxy Radicals and its Derivatives: Molecules That Sometimes Fluoresce and Sometimes Don't

9:45 - 10:00 U. Marvet and M. Dantus (Michigan State University)
Bond Formation on the Femtosecond Time Scale; Time-resolved Photoassociation Studies of Mercury in the Gas Phase

10:00 - 10:15 E.W. Rothe, Y. Gu and G.P. Reck (Wayne State University)
Laser Induced Predissociative Fluorescence: Dynamics and Polarization. Effect of Lower-state Rotational Energy Transfer Upon Quantitative Diagnostics

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

10:45 -11:45 Bill Klemperer (Harvard University)
Spectroscopy, Structure and Dynamics of Molecular Complexes

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

11:45 - 12:00 M.M. Beaky and F.C. DeLucia (Ohio State University)
The Pressure Broadening and Center Frequency Shift of the J=0-1 and J=1-2 Transitions of CO in Collision with Helium

12:00 - 12:15 L.-H. Xu (University of New Brunswick), G.T. Fraser, S.C. Stone, J.-U. Grabow, F.J. Lovas, A.M. Andrews and B.H. Pate (National Inst. of Standards & Technology, Gaithersburg, MD)
Molecular Beam Spectroscopic Study of Fluorinated Ethanes: Vibration/Tunneling Dynamics

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

SESSION III: Saturday November 4, 1995 Davis Centre 1351

Chair: **Terry McMahon**

1:30 - 2:15 Martin Moskovits (University of Toronto)
Thinking Small -- Megascience with Nanostructures

2:15 - 2:30 C. Callegari, J. Higgins, G. Scoles (Princeton University), F. Stienkemeier (Univ. of Bielefield), W. Ernst (Penn State University) and M. Gutowsky (Univ. of Utah)
On the Quartet State of Alkali Trimers: Spectroscopy, Three Body Forces and Excited State Chemical Reactions

2:30 - 2:45 D.-S. Yang, D. Rayner, M. Zgierski, P. Hackett (Steacie Institute for Molecular Science, NRC, Ottawa), A. Martinez, P.-N. Roy, T. Carrington, Jr. and D. Salahub (Université de Montreal)
High Resolution Photoelectron Spectroscopy of Transition Metal Clusters

2:45 - 3:00 E. Rexer, T. Rycroft, M. Lyktey, B. DeLeon and J. Garvey (SUNY, Buffalo)
Novel Reactions of Acetone/Acetylene Cluster Ions

SESSION IV: Saturday, November 4, 1995 from 3:00 P.M. Davis Centre Lobby

POSTER SESSION AND MANUFACTURERS' 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

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

SESSION V: Sunday, November 5, 1995 - A.M. Davis Centre 1351

Chair: **Peter Bernath**

9:30 - 10:15 Tucker Carrington, Jr. (Université de Montreal)
A Time Dependent Multi-surface Calculation of the Orientation of Photofragments: The Photodissociation of ICN

10:15 - 10:30 M.A. White and D. Michalski (Dalhousie University)
Dynamical Disorder in Phase II of CBr_4

10:30 - 10:45 A. Berces (Steacie Inst. for Molecular Sciences, NRC, Ottawa)
Accurate Calculation of Vibrational Frequencies by Density Functional Methods: The Effect of Reference Geometry, Electron Correlation and Relativity

10:45 - 11:15 **Coffee Break**

11:15 - 12:00 Benoit Simard (Steacie Inst. for Molecular Sciences, NRC, Ottawa)
Experimental and Theoretical Studies of Cu-Group 13 and Al-Group 14 Diatomics

12:00 - 12:15 M.-A. Saberi, W. Hu and D. Jack (Concordia University)
Sub, Mono and Multilayer Structure of CO_2/NaCl(001)

12:15 - 12:30 Mushti Ramakrishna (New York University)
Chemical Reactions of Semiconductor Clusters

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 three time slots:

3:00 - 4:00 p.m. ***Those whose papers were given 1a, 2a, 3a, etc. should attend their posters.***

4:00 - 5:00 p.m. ***Those whose papers were given 1b, 2b, 3b, etc. should attend their posters.***

5:00 - 6:00 p.m. ***Those whose papers were given 1c, 2c, 3c, etc. should attend their posters.***

1a) K.L. Dunfield, C. Linton, C.A. Brodie and A.G. Adam (University of New Brunswick)
Laser Spectroscopy of Ytterbium Monohalides

1b) R.M. Lees, M. Mollabashi, A. Predoi, L.-H. Xu and S. Zhao (University of New Brunswick)
Do The Twist, The Rock, The Bend and the Stretch with Mighty Methanol and the Mode Mixers

1c) D. Moule (Brock University), H. Liu, E.C. Lim (University of Akron), C. Muñoz-Caro, A. Niño (Universidad de Castilla-La Mancha, Spain) and R.H. Judge (University of Wisconsin-Parkside)
The Torsion-Inversion Energy Levels in the $S_1(n,\pi^*)$ Electronic State of Acetaldehyde From High Resolution Jet-Cooled Fluorescence Excitation Spectroscopy

2a) D. Jelski (SUNY College at Fredonia), R.H. Haley (Georgia Institute of Technology) and J.M. Bowman (Emory University)
A New Vibrational Self-Consistent Field Program for Large Molecules

2b) F.P. Temme (Queen's University)
S-n Inner Plethyms and Use of Generalised High-n Weak-Branching Limits in Deriving Full Irrep Sets Over NMR Liouville Spin Space for Isotopomeric Clusters

2c) A. Czajkowski, W. Kedzierski, J.B. Atkinson and L. Krause (University of Windsor)
The Ro-vibronic $H1_u(v'=1) \leftarrow A0_g^{\pm}$ $(v''=0)$ Excitation Bands of $(^{202}Hg)_2$

3a) D. Gendron and J.W. Hepburn (University of Waterloo)
Photodissociation of HI in the First Continuum: H LIF Doppler Spectroscopy at Lyman α

3b) M.Y.M. Lyktey, T.R. Rycroft and J.F. Garvey (SUNY at Buffalo)
Tandem Mass Spectrometry of $(C_2H_4)^+_{n=2-9}$ Ions: Structures of Molecular Ions Formed by Uncatalyzed Cationic Polymerization within Ethylene Van der Waals Cluster Ions

3c) G.B. Clark and F.R.W. McCourt (University of Waterloo)
The Calculation of Transport Properties for H-N_2

4a) D.S. Perry (University of Akron), G.A. Bethardy, M.J. Davis (Argonne National Lab.) and J. Go (Sunchon National University, South Korea)
Energy Randomisation. How Much Rotational Phase Space is Explored? How Long Does It Take?

4b) I.P. Swainson (Atomic Energy of Canada), R.J.C. Brown (Queen's University)
Ammonium Perrhenate Powder Neutron Diffraction: A Refinement of the Crystal Stucture Using a Pseudo-spin Model

4c) M. Thachuk and D. Wardlaw (Queen's University)
A Classical Hopping Algorithm for Coupled, Time Dependent Potential Surfaces

5a) X.K. Hu, D.M. Mao, S.S. Dimov and R.H. Lipson (University of Western Ontario)
Mapping the Electronic Structures of the Heteronuclear Rare Gas Dimers

5b) J.T. Paci (Queen's University) and P. Brumer (University of Toronto)
Optimal Coherent Control of Na_2 Photodissociation

5c) M. Hepp, G. Winnewisser (Universitaet zu Koeln, Germany), W. Jaeger (University of Alberta) and I. Pak (Russian Academy of Science, Russia)
Direct Absorption Measurements of Ar-CO Rotational Transitions with a Supersonic Jet mm-Wave Spectrometer

6a) A.K. Bertram, D.D. Patterson and J.J. Sloan (University of Waterloo)
The Mechanisms and Temperatures for the Freezing of Model Sulfuric Acid Aerosols Measured by FTIR Extinction Spectroscopy

6b) C. Carere and J.J. Sloan (University of Waterloo)
Dynamics and Kinetics of H Atom Reactions with CF_xCl_{4-x}, O_3 and NO_2

6c) M. Peschke (University of Waterloo), M.L. McKee and A.J. Illies (Auburn University)
An Experimental and Theoretical Study of Thietane Radical Cation with Thietane

7a) J.W. Dolce, A. Callegari, H.K. Srivastava, K. Lehmann, G. Scoles (Princeton University) and B. Meyer (University of Bonn)
Eigenstate Resolved Intramolecular Vibrational Energy Relaxation in Methylsilane and Ethane

7b) D. Snavely (Bowling Green State University)
Vibrational Overtone Activation: Experiment and Simulation

7c) K.M. Gough (University of Manitoba) and H.K. Srivastava (Princeton University)
Analysis of Raman trace scattering intensities in alkanes: Why the bond polarizability model doesn't work

8a) S.G. Urquhart, A.P. Hitchcock (McMaster University) and M. Denk (University of Toronto)
Probing Delocalization in Stable Silylenes by Core Excitation Spectroscopy

8b) G. Eustatiu (McMaster University), F. Motte-Tollet (Université de Liége, Belgium), S. Lotfi and D. Roy (Université Laval)
Vibrational Excitation of Furane by Low Energy Electron Impact

8c) Y. Xu and A.R.W. McKellar (NRC, Ottawa)
Continuous Slit-Jet Infrared Spectrum of the CO-N_2 Complex

9a) Y. Xu and A.R.W. McKellar (NRC, Ottawa)
Comprehensive Analysis of the Ar-CO Complex, Including Intermolecular Stretching and Bending States

9b) J. Koperski (Jagiellonian University, Poland) and M. Czajkowski (University of Windsor)
Spectroscopic Characterization of the ZnRG (RG=Ne, Ar, Kr) Molecules in the D_1 and X_0^+ Energy States

9c) D.J. Levandier, R.A. Dressler (Hanscom AFB, MA) and E. Murad (Orion International Technologies, Albuquerque, NM)
Guided-Ion Beam Studies of Isotope Effects in the Reaction $O^+ + H_2O/D_2O \rightarrow OH^+/OD^+ + OH/OD$

10a) C. Zhao, J.W. Hepburn and P.F. Bernath (University of Waterloo)
High Resolution Spectroscopy of $SrNH_2$

10b) B. Guo, P.F. Bernath (University of Waterloo), T. Pasinszki and N. Westwood (University of Guelph)
Infrared Spectroscopy of New Nitrile Oxides

10c) A. Muntianu, B. Guo and P.F. Bernath (University of Waterloo)
High Resolution Infrared Emission Spectrum of NaF

11a) K. Higgins, F.-M. Tao and W. Klemperer (Harvard University)
HeClF and $(ClF)_2$: Potential Energy Surfaces and Spectroscopy

11b) D. Howard, H. Kjaergaard and B.R. Henry (University of Guelph)
Overtone Spectra of Vapour Phase Adamantane

11c) C. Zhu and B.R. Henry (University of Guelph)
Internal Rotation in Overtone Spectra - Fluorotoluenes

12a) H.G. Kjaergaard, D.M. Turnbull and B.R. Henry (University of Guelph)
Naphthalene: Subtle Differences in CH Bondlengths

12b) S.M. Ball, G. Hancock, J.C. Pinot de Moira (Oxford University), C.M. Sadowski (York University) and F. Winterbottom (AEA Technology)
Time-of-Flight Measurements of the Kinetic Energies of the $O_2(^1\Delta_g)$ Fragment from the Photolysis of Ozone Between 287-331 NM

12c) M.A. Lebeault-Dorget and B. Simard (NRC, Ottawa)
Preliminary Studies of Al-Group 14 Species

13a) K. Crowell, R.J. LeRoy, C. Bissonnette (University of Waterloo), T.H. Wu, W.J. Meath (University of Western Ontario) and A.R.W. McKellar (SIMS, NRC, Ottawa)
An Improved Three-Dimensional Potential Energy Surface for H_2-Ne from New Infrared Spectra

13b) F. Charron and P.F. Bernath (University of Waterloo)
Fourier Transform Infrared Emission Spectra of CuH, CuD, AgH and AgD

13c) Z. Morbi and P.F. Bernath (University of Waterloo)
High Resolution Laser Spectroscopy of the $\tilde{A}^2\Pi$-$\tilde{X}^2\Sigma^+$ Transition of CaCCH

14a) K.Q. Zhang, P. Colarusso, P.F. Bernath (University of Waterloo), T. Pasinszki and N. Westwood (University of Guelph)
The Infrared Spectroscopy of BrCNO and Br_2CNOH

14b) W.-T. Chan and I.P. Hamilton (Wilfrid Laurier University)
A Global Ab Initio Potential for HO_2^-/O_2H^- and Vibrational Splittings for Hydrogen Atom Transfer

14c) V.J. Barclay (PE Sciex) and I.P. Hamilton (Wilfrid Laurier University)
Application of Wavelet Transforms to Enhance Spectral Quality: Denoising, Smoothing and Dataset Compression

15a) H. Sabzyan, W.P. Power and F.R.W. McCourt (University of Waterloo)
NMR Spin-Lattice Relaxation Time Study of HD-Ar System

15b) P.-N. Roy and T. Carrington Jr. (Université de Montreal)
Selective Calculation of Eigenstates: Application to Vibrations (1-d and 3-d) and Reaction Rates

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16a) A. Midey, J. Qian, J. Lee, S. Donnelly and J.M. Farrar (University of Rochester)
Photodissociation Studies of Size-Selected Clusters of $Sr^+(CH_3OH)n$, $Sr^+(H_2O)_n$ and $Sr^+(D_2O)_n$

16b) D. Belle-Oudry (DAMAP, France), A. Jolly, D. Malmasson, A. Vient, J.-L. Lemaire, and F. Rostas (Cornell University)
High Resolution VUV Laser Measurements of the Absorption Cross Sections of the CO $A^1\Pi$ ($0<v'<17$) $\leftarrow$ $X^1\Sigma^+$ ($v' = 0$) Transition

16c) J.A. Mueller, S.A. Rogers, K.E. Trible and P.L. Houston (Cornell University)
ZKE Photofragment Spectroscopy of NO_2 Dissociation

17a) L.M. Dobeck, W. Kong, P.L. Houston (Cornell University) and J.W. Hepburn (University of Waterloo)
Photodissociation Dynamics of Glyoxal

17b) A. Kortyna, P. Willis, E. Bernard and H.F. Davis (Cornell University)
Photoinitiated Reactions of Nickel-Ethylene Complexes

17c) F. Wang and F.R.W. McCourt (University of Waterloo)
Potential Energy Surface and Pure Rotational Spectrum of the Rg-Cl_2 Van der Waals Complexes

18a) F. Wang, F.R.W. McCourt and R.J. Le Roy (University of Waterloo)
Tests of a Pure Multipolar Dispersion and Induction Dipole Moment Surface for Simulating the IR Spectra of N_2-Ar

18b) J.D.D. Martin, J.W. Hepburn (University of Waterloo) and C. Alcaraz (Centre Universitaire Paris-Sud, France)
PFI-ZEKE Photoelectron Spectroscopy of Highly Vibrationally Excited Molecular Hydrogen: Observation of ZEKE State Stabilization by Ions

18c) G. Hunter and A. Ahari (York University)
The Exact One-Electron Model of Molecular Structure - The Molecular Envelope - A Well-Defined Basis for Molecular Graphics

19a) J.B. Giorgi, R. Kühnemuth, J.C. Polanyi and J.-X. Wang (University of Toronto)
Photolysis of HX (X = Cl, Br, I) Adsorbed on LiF(001) Studied by H-Rydberg-Atom Time-of-Flight Spectroscopy

19b) R. Ehlich, A. Hudson, J.C. Polanyi, and J.-X. Wang (University of Toronto)
Photoinduced Charge-Transfer Dissociation in Van der Waals Complexes

19c) D. Routkevitch, C. Douketis, T.L. Haslett, L. Ryan and M. Moskovits (University of Toronto)
A^{II}-B^{VI} Nanowires - Fabrication and Resonance Raman Spectroscopy

20a) T.L. Haslett, S. Fedrigo and M. Moskovits (University of Toronto)
FTIR and SERS of Mass Selected Cluster Deposits

20b) T. Vu, A. Jakalian and D.B. Jack (Concordia University)
Phase Transition in Monolayer CO/NaCl(001)

20c) M. Ivanov, T. Seideman and P. Corkum (SIMS, N.R.C., Ottawa)
Explosive Multielectron Ionization of Diatomic Molecules

21a) D. Matusek, M. Ivanov and J.S. Wright (Carleton University)
Altered States: Lowered Barriers and Bound States Induced by Intense IR Laser Fields

21b) D. McKay and J.S. Wright (Carleton University)
Molecular Modelling Including Lone-Pair Interactions: Accurate Treatment of the Anomeric Effect and Conformation of Saturated Nitrogen Chains

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