

*The 13th Annual
University of Waterloo
Symposium
on
Chemical Physics*

October 24-26, 1997

Acknowledgements

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Waterloo Symposium on Chemical Physics

October 24-26, 1997

at the University of Waterloo

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

SESSION I: Friday, October 24, 1997 - P.M.

Davis Centre 1302

Chair: **John Hepburn**

- 7:30 - 8:15 T. Sears (Brookhaven National Laboratory)
Transient frequency modulation spectroscopy of simple carbenes
- 8:15 - 8:30 Q. Zhang, U. Marvet, E.J. Brown and M. Dantus (Michigan State University)
Femtosecond time-resolved studies of CH_2I_2 : Molecular photodetachment dynamics at high excitation energies
- 8:30 - 8:45 V. Blanchet and A. Stolow (NRC, Ottawa)
Non-adiabatic dynamics of the NO dimer studied by time-resolved photoelectron spectroscopy
- 8:45 - 9:00 M.W. Crofton (Aerospace Corporation)
Analysis and development of fullerene ion engines
- 9:00 - 9:15 D. Evard, A. Schiffman, B. Atherton and D. Nabors (Coherent Laser Group)
Recent work on the development of a high resolution continuous wave source in the infrared (1.5-4/ μ) using quasi phase matching in periodically poled lithium niobate
- 9:30 Grad Club

SESSION II: Saturday, October 25, 1997 - A.M.

Davis Centre 1351

Chair: **Peter Bernath**

- 9:00 - 9:45 J. Watson (SIMS, NRC, Ottawa)
The diffuse interstellar band problem
- 9:45 - 10:00 E. Hirota (Hyama, Japan) and Y. Kawashima (Atsugi, Japan)
Equilibrium Structure and Harmonic and Anharmonic Potential Functions of HBO and HCO⁺
- 10:00 - 10:15 R.J. Doerksen, N. El-Bakali Kassimi, V.J. Steeves and A.J. Thakkar (University of New Brunswick)
Quantitative aromaticity scales derived from accurate polarizabilities and bond orders

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**

10:45 - 11:45 T. Oka (The University of Chicago)
Detection of interstellar H_3^+ : Molecules in Astronomy

11:45 - 12:00 S. Miller and J. Tennyson (University College London, UK)
 H_3^+ as a probe - Astronomy's debt to Takeshi Oka

12:00 - 12:15 B. McCall (University of Chicago), T. Geballe (Joint Astronomy Centre), K. Hinkle (National Optical Astronomy Observatories) and T. Oka (University of Chicago)
The interstellar chemist's most insightful tool: H_3^+ observed in a variety of astronomical environments

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

SESSION III: Saturday, October 25, 1997

Davis Centre 1351

Chair: **Jim Sloan**

1:30 - 2:15 Y. Endo (The University of Tokyo, Japan)
Laser-induced fluorescence spectroscopy of carbon chain free radicals

2:15 - 2:30 D.P. Weliky and R. Tycko (National Institute of Health, Bethesda, MD)
Solid state NMR structural studies of an AIDS-related peptide/antibody complex in frozen solution

2:30 - 2:45 R.M. Dickson and W.E. Moerner (University of California, San Diego)
Single molecule motion and optical switching at room temperature

2:45 - 3:05 **Coffee Break**

3:05 - 3:20 R. Abusen, F. Bennett, I.R. McNab, D.N. Sharp, R.C. Shiell and C.A. Woodward (University of Newcastle Upon Tyne, UK)
The hyperfine resolved, infrared spectrum of the molecular dication, DCl^{2+}

3:20 - 3:35 N.R. Forde and L.J. Butler (University of Chicago)
*The effect of π delocalization on the photodissociation dynamics of *N,N*-dimethylformamide at 193 nm*

3:35 - 3:50 S.W. Joo, S.K. Kim (Seoul National University, Korea), D. Worsnop, C.E. Kolb (Aerodyne Research, Billerica, MA) and D.R. Herschbach (Harvard University)
Infrared spectroscopy of the A-X electronic transition of NaO

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

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

SESSION IV: Saturday, October 25, 1997 - from 3:50 P.M.

Davis Centre Lobby

POSTER SESSION AND MANUFACTURERS' DISPLAY

- 6:15 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 V: Sunday, October 26, 1997 - A.M.

Davis Centre 1302

Chair: **Bob Le Roy**

- 9:15 - 10:00 R. Saykally (University of California, Berkeley)
Infrared cavity ring down laser absorption spectroscopy
- 10:00 - 10:15 T. Momose, Y. Zhang and T. Oka (University of Chicago)
Infrared spectroscopy of Gamma-ray irradiated solid parahydrogen
- 10:15 - 10:30 L.-H. Xu, J.T. Hougen and R.M. Lees (University of New Brunswick)
How does the structure of methanol change when the methyl group rotates? A step towards the understanding of the Torsion-Vibration dynamics.
- 10:30 - 10:45 E.C. Korolenko (Tokyo Institute of Technology, Japan and Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia) and K. Kitahara (Tokyo Institute of Technology, Japan)
Influence of the spin-selective recombination on the electron spin relaxation in radical pairs. A comparison of the Redfield theory with the fluctuating magnetic field approach.
- 10:45 - 11:15 **Coffee Break**
- 11:15 - 12:00 M. Okumura (California Institute of Technology)
Solvation and state-mixing in clusters
- 12:00 - 12:15 C. Pursell (Trinity University, Texas)
Atmospheric heterogeneous chemistry on ice: The ionization of HCl and HNO₃
- 12:15 - 12:30 J. Higgins, C. Callegari, J. Reho, F. Stienkemeier, W.E. Ernst and G. Scoles (Princeton University)
Helium cluster isolation spectroscopy of alkali dimers in the triplet manifold

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:

4:00 - 5:00 Those whose papers were given (a) labels (1a, 2a, 3a, etc.) should attend their posters.

5:00 - 6:00 Those whose papers were given (b) labels (1b, 2b, 3b, etc.) should attend their posters

- 1a) R.S. Ram, J.R.D. Peers, Y. Teng, A.G. Adam, A. Muntianu, P.F. Bernath and S.P. Davis, (University of Waterloo and University of New Brunswick)
High Resolution Spectroscopy of Transition Metal Halides: FTS and Laser Excitation Spectroscopy of TiF, and Laser Excitation Spectroscopy of CoCl
- 1b) T. Amano, K. Akao, H. Oka and A. Unno (Ibaraki University, Japan)
Sum-millimeter wave measurements of the pressure broadening of O_2 in the $^1\Delta_g$ state by O_2 and N_2
- 2a) J.B. Atkinson, J. Koperski and L. Krause (University of Windsor)
First observations of laser-excited Hg_3 and Hg_2 -RG spectra in a supersonic expansion beam
- 2b) C.D. Ball and F.C. De Lucia (Ohio State University)
Direct Measurement of Rotational Inelastic Collision Cross Sections at Low Temperatures
- 3a) T. Barckholtz (Ohio State University), S. Panov (MIT), D. Powers and T. Miller (Ohio State University)
ZEKE Spectroscopy of the Organometallic Radicals $MgCH_3$, $ZNCH_3$ and $CdCH_3$
- 3b) E. Bishenden, D. Gentleman and D.J. Donaldson (Scarborough College and University of Toronto)
Adsorption of volatile solutes at the air-water interface
- 4a) M.D. Brookes and A.R.W. McKellar (NRC, Ottawa)
Unravelling the mystery of the CO dimer
- 4b) E.J. Brown, I. Pastirk, Q. Zhang and M. Dantus (Michigan State University)
Rotational anisotropy of iodine: Pump laser intensity effects
- 5a) S. Brunet and S.V. Filseth (York University)
State to state rotational relaxation of CN in collision with hydrogen and deuterium
- 5b) A. Conjusteau, A. Callegari, H.K. Srivastava, P. Engels, S. Choi, K.K. Lehmann and G. Scoles (Princeton University)
Intramolecular vibrational energy redistribution in aromatic molecules of different symmetry: Benzene, triazine and pyrrole C-H stretch overtone

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

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

- 6a) S.M. Cybulski (Miami University), R.A. Kendall (Pacific Northwest National Lab), G. Chalasinski (University of Warsaw) and M.W. Severson and M.M. Szczesniak (Oakland University)
Ab initio study of the $Ar(^1S) - O_2(X^3 \Sigma_g^-)$ complex
- 6b) A.L.L. East (NRC, Ottawa)
Theoretical prediction of rovibronic intensities in the fluorescence excitation spectrum of toluene
- 7a) A.P. Hitchcock, I.G. Eustatiu, J.T. Francis and C.C. Turci (McMaster University)
Electron impact core excitation of molecules: Non dipole spectroscopy and generalized oscillator strengths
- 7b) K.M. Gough, J.R. Dwyer and T.J. Gawlik (University of Manitoba)
Ab initio Raman trace scattering parameters for CH and CC stretching vibrations in straight chain, cyclo- and bicycloalkanes, and propellanes
- 8a) E. Hackl, S. Kornilova and Y. Blagoi (National Academy of Sciences of Ukraine)
Influence of water activity on binding constants of biologically active metal ions interacting with DNA
- 8b) Z.J. Jakubek (NRC, Ottawa), Q. Hui and M. Takami (RIKEN, Japan)
Excitation dynamics of Ag in gaseous and liquid helium
- 9a) S.P. Goldman and J.A. Kempe (University of Western Ontario)
Accurate modified configuration interaction calculation on H_2^+
- 9b) R.M. Lees and L.-H. Xu (University of New Brunswick)
Our knowledge on Torsion-Vibration coupling of methanol in the fundamental region
- 10a) H.-P. Loock, A. Berces and B. Simard (NRC, Ottawa), C. Linton (University of New Brunswick)
Laser spectroscopy of the $A_1(^2\Pi) - X(^2\Sigma^+)$ Transition of Ytterbium Monoacetylide
- 10b) H.-P. Loock and B. Simard (NRC, Ottawa) and C. Linton (University of New Brunswick), S. Wallin and O. Launila (Stockholm University)
Photoionization efficiency spectroscopy of TiO, YO, ZrO, NbO and MoO
- 11a) U. Marvet, Q. Zhang, E. Brown, P. Gross and M. Dantus (Michigan State University)
Femtosecond studies of concerted elimination from gem - dihaloalkanes
- 11b) A.R.W. McKellar (NRC, Ottawa)
A cosmic complex: High resolution infrared spectrum and energy levels of the CO- H_2 Van der Waals complex
- 12a) N. Moazzen-Ahmadi (University of Lethbridge)
Infrared diode laser spectroscopy of CCO near 1950cm^{-1}

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

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

- 12b) J.J. Neville , A. Hitchcock (McMaster University), A. Jurgensen and R.G. Cavelle, (University of Alberta)
Photoionization and photofragmentation spectroscopy of phosphorous compounds using synchrotron radiation and time-of-flight mass spectrometry
- 13a) J. Paci and D. Wardlaw (Queen's University, Kingston)
Strong field dissociation of HCl^+ - The calculation of kinetic energy distributions
- 13b) T. Parekunnel, T. Hirao, R.J. Le Roy and P.F. Bernath (University of Waterloo)
High Resolution IR spectra of DCl at high temperatures
- 14a) I. Pastirk, E.J. Brown, Q. Zhang and M. Dantus (Michigan State University)
Coherent control of the yield of chemical reactions
- 14b) J. Reho, C. Callegari, J. Higgins, K.K. Lehmann and G. Scoles (Princeton University)
Time-resolved spectroscopy of Na atoms and oligomers on the surface of He clusters
- 15a) Q. Gao, F.J. Morgan and C.M. Sadowski (York University)
State-to-state and total rotational energy transfer rate constants for $CN(B, V=0, N=11,13) + Ne$
- 15b) K. Higgins, I. Ho, and W. Klemperer (Harvard University)
Rg- ClF_3 Complexes: Further ab initio and experimental studies
- 16a) Y.J. Shi, X.K. Hu, D.M. Mao and R.H. Lipson (University of Western Ontario)
Qualitative and quantitative analysis of Xanthates by VUV laser/Time-of-flight mass spectrometry
- 16b) K. Takagi and F. Matsushima (Toyama University, Japan)
Rotational spectra of NeH^+ and NeD^+
- 17a) Q. Hui and M. Takami (RIKEN, Japan)
Phonon bands associated with narrow Eu atomic lines in liquid helium
- 17b) J. Miyawaki, K. Sugawara and H. Takeo (National Institute for Advanced Interdisciplinary Research, Japan)
Electronic Spectrum of $AgNH_3$
- 18a) J. Tang and T. Oka (University of Chicago)
Infrared spectrum of the η_1 fundamental band of H_3O^+
- 18b) R. Tanner and N.P.C. Westwood (University of Guelph)
Boron nitrogen compounds: Ab initio techniques and related spectroscopic results
- 19a) H. Wei and T. Carrington, Jr. (Université de Montréal)
Eckart frames and exact kinetic energy operators for triatomic and tetra-atomic molecules

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

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

- 19b) E. White, J. Tang and T. Oka (University of Chicago)
Observation of the C-H stretch band of CH_5^+
- 20a) R.P. White and H.R. Mayne (University of New Hampshire)
Some recent advances in global minimization techniques for atomic and molecular clusters
- 20b) D.-S. Yang, M.Z. Zgierski and P.A. Hackett (NRC, Ottawa)
Structure of gaseous zirconium-ether complexes
- 21a) Y. Zhang and T. Oka (University of Chicago)
 $v=1$ exciton hopping in solid para-hydrogen
- 21b) D.S. Tonner and T.B. McMahon (University of Waterloo)
Energetic bottlenecks in the infrared multi-photon dissociation of gaseous ions under collision-free conditions
- 22a) M. Czajkowski and J. Koperski (University of Windsor)
Excitation and fluorescence spectra of ZnAr and ZnKr molecules
- 22b) J.D.D. Martin and J.W. Hepburn (University of Waterloo)
Electric Field induced dissociation of molecules in Rydberg-like highly vibrationally excited ion-pair states
- 23a) R.C. Shiell, M. Evans, S. Stimson, C.-W. Hsu, C.Y. Ng and J.W. Hepburn
(University of Waterloo and Iowa State University)
A high resolution study of correlation satellites in xenon
- 23b) A. Beatty, R.C. Shiell and J.W. Hepburn (University of Waterloo)
A photodissociation study of CS_2
- 24a) R.J. Le Roy (University of Waterloo)
Uncertainty, sensitivity, convergence and rounding in performing and reporting least-squares fits
- 24b) E. Bernard, B. Strazisar and H.F. Davis (Cornell University)
Excited state dynamics of H_2CN radicals
- 25a) P.A. Willis, H.U. Stauffer, R.Z. Hinrichs and H.F. Davis (Cornell University)
Crossed beams study of C-H bond activation: $Mo(^5S_2) + CH_4 \rightarrow MoCH_2 + H_2$
- 25b) A.K. Bertram and J.J. Sloan (University of Waterloo)
The Freezing of Nitric Acid Aerosols
- 26a) J. Reho, J. Higgins, M. Radcliffe, K.K. Lehmann and G. Scoles (Princeton University)
Non-adiabatic processes in the photodissociation of quartet state Na trimer

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

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