The 12th Annual
University of Waterloo

Symposium on Chemical Physics

November 1-3, 1996

Acknowledgements

We are very grateful to the following sponsors for their generous financial support of this conference.

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Waterloo Symposium on Chemical Physics

November 1-3, 1996

at the University of Waterloo

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

SESSION I: Friday, November 1, 1996 - P.M. Davis Centre 1302

Chair: **Jim Sloan**

7:30 - 8:15 Albert Stolow (NRC, Ottawa)
Time-resolved photoelectron/photoion spectroscopy

8:15 - 8:30 Allan L.L. East (NRC, Ottawa), B.J. Smith, (BMI, Australia and L. Radom (ANU, Australia)
Ab Initio thermodynamics: Application to proton affinity and proton transfer reactions

8:30 - 8:45 Steven M. Miller and Tucker Carrington (University of Montreal)
Time dependent methods for the cumulative reaction probability

8:45 - 9:00 Robert H. Lipson, P. Wang and S.S. Dimov (University of Western Ontario)
VUV laser/time-of-flight mass spectra of BrCl and Cl_2

SESSION II: Saturday, November 2, 1996 - A.M. Davis Centre 1351

Chair: **Bob Le Roy**

9:00 - 9:45 Dave Wardlaw (Queen's University, Kingston)
Molecular surface hopping in intense laser fields

9:45 - 10:00 M. Czajkowski and J. Koperski (University of Windsor)
Excitation spectrum of the B 1($5\ ^3P$) <-- X 0^+($5\ ^1S_0$) transition of CdXe van der Waals complex. Corrections to the CdXe (X 0^+) and CdXe (A 0^+) spectroscopic characterization

10:00 - 10:15 D. Cramb and S.C. Wallace (University of Toronto)
The behaviour of L-tryptophan at model membranes

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

10:45 - 11:45 D. Buckingham (University of Cambridge, U.K.)
Molecules in optical, electric and magnetic fields

11:45 - 12:00 Hans-Peter Loock, B. Simard (NRC, Ottawa) and C. Linton (Univ. of New Brunswick)
Towards an understanding of the chemistry of rare earth compounds: Photoionization spectra of Ytterbium carbides

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

12:00 - 12:15 Wolfgang Jaeger and Y. Xu (University of Alberta)
Evidence for large amplitude migration motion in RG-cyclopropane complexes (RG=Ne, Ar, Kr) from rotation-tunnelling spectroscopy

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

SESSION III: Saturday, November 2, 1996 Davis Centre 1351

Chair: **Peter Bernath**

1:30 - 1:45 Dan Matusek, M. Yu Ivanov and J.S. Wright (Carleton University)
The effect of intense infrared lasers on A+BC reaction dynamics

1:45 - 2:00 S. Mark Cybulski and J.S. Holt (Miami University)
Three-body interactions in complexes involving open-shell species

2:00 - 2:15 Sabrina J. Diol, Y. Gao (University of Rochester) and R.J.D. Miller (University of Toronto)
Femtosecond hot electron reaction dynamics at GaAs(100) surfaces

2:15 - 3:15 Robert Curl, (Rice University)
Infrared laser spectroscopy and Comments on the discovery of C_{60}

SESSION IV: Saturday, November 2, 1994 - from 3:30 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

SESSION V: Sunday, November 3, 1996 - A.M. Davis Centre 1302

Chair: **Terry McMahon**

9:30 - 10:15 Millard Alexander (University of Maryland)
Weakly bound complexes of atomic boron with argon and hydrogen

10:15 - 10:30 Robert J. Doerksen and A.J. Thakkar (University of New Brunswick)
Confrontation between theory and experiment for properties of aromatic molecules

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

10:30 - 10:45 Matthew D. Brookes, D.J. Hughes and B.J. Howard (Oxford University, U.K.)
Spectroscopy and dynamics of rare gas-spherical top complexes - understanding the infrared spectrum of the ν_3 band of Ne-SiH_4

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

11:15 - 12:00 Mike Duncan (University of Georgia)
Electrostatic bonding in gas phase metal atom complexes

12:00 - 12:15 Dong-Shen Yang, M. Zgierski, A. Berces (NRC, Ottawa), A. Martinez, P.-N. Roy (University of Montreal), R. Fournier (York University) , T. Carrington, Jr., D. Salahub (University of Montreal) and P. Hackett (NRC, Ottawa)
PFI-ZEKE photoelectron spectroscopy and density functional calculations of Nb_3C_2 and Nb_3N_2

12:15 - 12:30 R.J. Dwayne Miller, G. Dadusc and P. Schulenberg (University of Toronto)
Heme protein relaxation: The coupled reaction coordinate problem in molecular cooperativity

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 - 4:30 Those whose papers were given (a) labels (1a, 2a, 3a, etc.) should attend their posters.

4:30 - 5:30 Those whose papers were given (b) labels (1b, 2b, 3b, etc.) should attend their posters

1a) A.K. Bertram and J.J. Sloan (University of Waterloo)
The freezing of nitric acid aerosols measured by FTIR extinction spectroscopy

1b) V.J. Barclay (SCIEX, Concord, Ont.) and I.P. Hamilton (Wilfrid Laurier University)
Local and normal modes in water: a visual deconvolution of the Darling-Dennison resonance

2a) K.T. Nguyen and R.J.C. Brown (Queen's University)
Molecular dynamics simulations of the Wurtzite structure

2b) E. Bernard, P. Willis and F. Davis (Cornell University)
Unimolecular reaction dynamics of H_2CN radicals

3a) R.S. Dumont (McMaster University)
Sparse wave packet propagation and quantum sensitivity to initial conditions

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

3b) T.D. Fridgen and J.M. Parnis (Trent University and Queen's University)
Electron bombardment matrix isolation of oxalyl chloride and effects of adding a gas-phase quencher

4a) D.J. Gendron and J.W. Hepburn (University of Waterloo)
Determination of the electronic structure of HI in the A band by Doppler spectroscopy of the H-atoms photofragments

4b) B. Guo, J. Lotoski, C. Zhang and P. Bernath (University of Waterloo)
A bibliographic database for diatomic molecules

5a) K. Higgins, I. Ho and W. Klemperer (Harvard University)
Ab initio and experimental studies of rare gas - ClF_3 complexes: What can they tell us about electron distribution in ClF_3?

5b) T. Hoffman and T.B. McMahon (University of Waterloo)
A high pressure mass spectrometric study of certain oxygen bases

6a) X.K. Hu, D.M. Mao, S.S. Dimov and R.H. Lipson (University of Western Ontario)
(2+1) REMPI/Time-of-flight and photoelectron spectra of Xe_2 in the region of Xe(5d)*

6b) A.A. Ahari and G. Hunter (York University)
Molecular size and shape defined by the classical turning surface of the exact one-electron Schroedinger model of the many-electron molecule, and non-bonding interactions between molecular fragments

7a) J. Koperski, J.B. Atkinson and L. Krause (University of Windsor)
The vibrationally and isotopically resolved G 0^+_u ($6\,^1P_1$) $\leftarrow$ X 0^+_g excitation spectrum of Hg_2

7b) M. Kolbuszewski (NRC, Ottawa)
Chemical physics on the WWW: What is available and how to find it?

8a) D. Lacombe, R. Shiell, A. Beatty and J.W. Hepburn (University of Waterloo)
The continuing evolution of a H-atom photofragment spectrometer

8b) J.Y. Li, W.S. Neil, F. Kong and J.J. Sloan (University of Waterloo)
H+$N_2$0 collision dynamics, kinetics and energy transfer studied by time-resolved FTIR spectroscopy

9a) D.M. Mao, X.K. Hu, S.S. Dimov and R.H. Lipson (University of Western Ontario)
(1+1') VUV laser/time-of-flight spectra of Xe_2 in the vicinity of Xe + Xe(5d)*

9b) J.D.D. Martin and J.W. Hepburn (University of Waterloo)
Effects of ion-density on the ZEKE spectra of argon

10a) R.A. McAloney and M.C. Goh (University of Toronto)
Tapping mode atomic force microscopy: Phase detection imaging of solvent cast polymer films

10b) Z. Morbi and P.F. Bernath (University of Waterloo)
Laser spectroscopy of Ca and Sr derivatives

11a) F.Y. Naumkin and F.R.W. McCourt (University of Waterloo)
Sensitivity of microwave spectra of $ArCl_2$ to the relative stability of its isomers

11b) M.F. Paige and M.C. Goh (University of Toronto)
The adsorption behaviour of Bovine Serum Albumin on mica and highly ordered pyrolytic graphite

12a) F.Y. Naumkin (University of Waterloo)
Anisotropic atom-atom potentials for representing intermolecular interactions of Rg atoms with molecules

12b) R.D. Lafleur, J. M. Parnis (Trent University) and D.M. Rayner (NRC, Ottawa)
Gas phase niobium cluster reactivity with isobutane

13a) D.B. Pedersen, J.M. Parnis (Trent University) and D.M. Rayner (NRC, Ottawa)
Cyclopropane reactivity on tungsten nanosurfaces

13b) G. McGibbon, M. Peschke, J. Szulejko and T.B. McMahon (University of Waterloo)
Thiazole - A combined experimental and computational study of its proton affinity and its protonated association chemistry

14a) M. Petryk and B. Henry (University of Guelph)
Local modes: Probing highly excited vibrational states of deuterated neopentanes with the photoacoustic effect

14b) J.M. Roscoe (Acadia University), I.S. Jayaweera, A.L. MacKenzie and P.D. Pacey (Dalhousie University)
The mechanism of ethylene pyrolysis at small conversions

15a) F.P. Temme (Queen's University)
Natural embedding in determinable (NMR) spin algebras: Role of Schur-fn and S-n democratic Yamanouchi-Chain invariants in defining dual-group tensors (via Latin-sq formalisms)

15b) Y. Xu and W. Jaeger (University of Alberta)
Spectroscopic investigation of additive and non-additive interactions in a RG-RG'-molecule system: Ne-Ar-CO_2

16a) S. Xu, C.C. Miller, S.J. Diol, Y. Gao (University of Rochester), D.A. Mantell (Xerox Canada), M.G. Mason, A.A. Muenter (Kodak Co.), B.A. Parkinson (Colorado State University) and R.J.D. Miller (University of Toronto)
Femtosecond photoemission studies on the ultrafast electron dynamics in dimensional layered semiconductor SnS_2

16b) K. Zhang, P. Bernath (University of Waterloo), T. Pasinszki and N. Westwood (University of Guelph)
High resolution spectra of cyanoformyl bromide

17a) C. Zhao, J.W. Hepburn and P.F. Bernath (University of Waterloo)
High resolution spectroscopy of $CaOCH_3$

17b) D. Davydov, D. Routkevitch, J. Chan and M. Moskovits (University of Toronto)
Field emission and single wire resistance measurements on nanowire arrays

18a) F. Blais, D. Davydov, T. Haslett and M. Moskovits (University of Toronto)
Laser effects on tunneling in vacuum STM of thin silver films

18b) P. Zhang, T. Haslett, C. Douketis and M. Moskovits (University of Toronto)
Localization in self-affine films observed by near-field scanning optical microscopy

19a) J. Paci and D. Wardlaw (Queen's University)
The dissociation of small molecules in strong laser fields

19b) V. Staroverov and S.M. Rothstein (Brock University)
Variational Monte Carlo study of core-valence separation schemes

20a) P. Langfelder and S.M. Rothstein (Brock University)
Sampling algorithms for quantum Monte-Carlo simulations