The 9th Annual

University of Waterloo

Symposium on Chemical Physics

November 5-7, 1993

Acknowledgements

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

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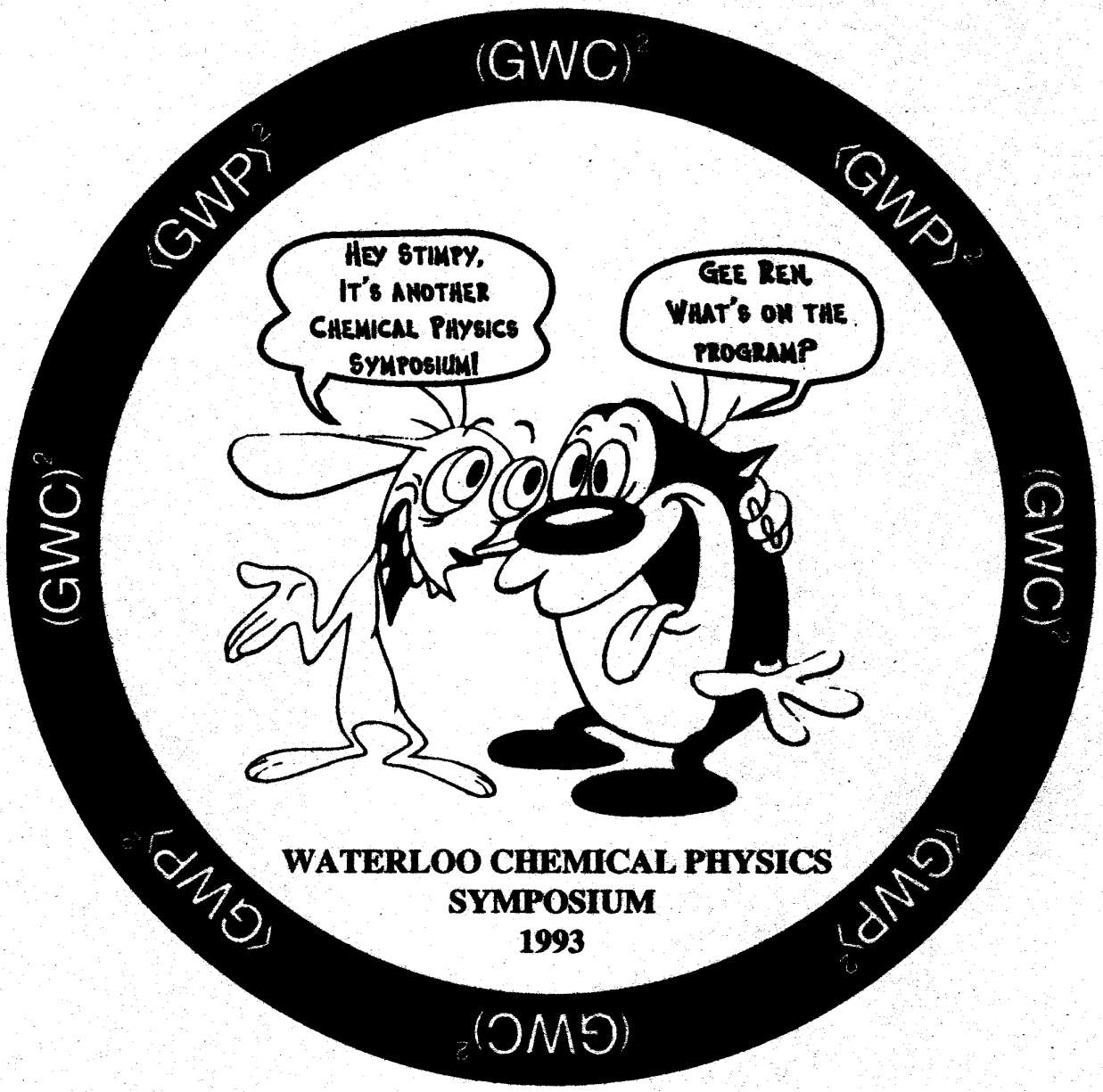
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HEY STIMPY, IT'S ANOTHER CHEMICAL PHYSICS SYMPOSIUM!
GEE REN, WHAT'S ON THE PROGRAM?
WATERLOO CHEMICAL PHYSICS SYMPOSIUM
1993

Waterloo Symposium on Chemical Physics

November 5-7, 1993

at the University of Waterloo

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

SESSION I: Friday, November 5, 1993 - P.M. Davis Centre 1351

Chair: **Bob Le Roy**

7:30 - 8:10 Edward C. Lim (University of Akron)
Excited-State Dynamics and Photochemistry of Van der Waals Dimers and Clusters of Aromatic Molecules

8:10 - 8:30 Xiaokui K. Zhang, J. M. Parnis, E.G. Lewars and R.E. March (Trent University and Queen's University)
Molecular Isomerization via Ionization-Neutralization Processes Occuring During Low-Temperature Matrix Condensation: Synthesis and FTIR Spectroscopy of Isomers of Dichloromethane, Benzene and Acetone.

8:30 - 8:50 Colan Linton, K.L. Dunfield, A.G. Adam, J.R.D. Peers, (University of New Brunswick), B. Simard and A.M. James (NRC, Ottawa)
Spectroscopy of Rare Earth Containing Diatomic Molecules: Recent Results

8:50 - 9:10 Lucjan Krause, W. Kędzierski, A. Czajkowski, J. Supronowicz, M.J. Hinek and J.B. Atkinson (University of Windsor)
The Rotationally Resolved $G(O_u^+) \leftarrow A(O_g^+)$ Electronic Spectrum of the $(^{202}Hg)_2$ Excimer

SESSION II: Saturday, November 6, 1993 - A.M. Davis Centre 1351

Chair: **John Hepburn**

9:00 - 9:40 Ray Kapral (University of Toronto)
The Structure and Dynamics of Binary Clusters

9:40 - 10:00 Hu Wang, T.H. Ellis and E.J. Kruus (Université de Montreal)
Modelling Electrochemical Interfaces in UHV: How do Adsorbate-Metal Bonds Change in the Presence of Water?

10:00 - 10:20 Michael G. Szarka, D.S. Green and S.C. Wallace (York University and University of Toronto)
Multiphoton Studies of Methyl Chloride Rydberg States

10:20 - 10:40 **Coffee Break**

10:40 -11:40 Ahmed Zewail, (California Institute of Technology)
Recent Advances in Femtochemistry

11:40 - 12:00 Matthew J. Bramley, J.W. Tromp, T. Carrington, Jr., and G.C. Corey (Université de Montreal)
Very Efficient Exact Quantum Calculation of Highly Excited Vibrational Energy Levels of Floppy Molecules: The Band Origins of H_3^+ up to 35000 cm^{-1}

12:00 - 12:20 Jianming Cao, Y. Gao, C.A. Schmuttenmaer, M.A. Aeschlimann, H.E. Elsayed-Ali, R.J.D. Miller (University of Rochester) and D.A. Mantell (Xerox Webster Research Center)
Femto-second Photoemission Studies of Hot Electron Relaxation Dynamics of Single Crystal Cu Surfaces: Implications for Surface Photochemistry

12:20 - 2:00 **Lunch** Davis Centre 1301

SESSION III: Saturday November 6, 1993 Davis Centre 1351

Chair: **Jim Sloan**

2:00 - 2:40 Anne Myers (University of Rochester)
Dissecting the Ensemble Average: Spectroscopy and Dynamics of Individual Molecules

2:40 - 3:00 Marek Z. Zgierski (NRC, Ottawa), B. Hudson (University of Oregon) and M. Pawlikowski (Jagiellonian University, Gracow, Poland)
Resonance Raman Study of Excited States of Benzene and its Derivatives

3:00 - 3:20 Marcin Kolbuszewski and J.S. Wright (Carleton University)
Thermodynamically Stable Diatomic Dications: Are There Any?

3:20 - 3:40 Vladimir Spirko (University of Waterloo) and W.P. Kraemer (Max-Planck Institüt für Astrophysik, Garching Germany)
Vibrational Dynamics of H_5^+

SESSION IV: Saturday, November 6, 1993 from 4:00 P.M. Davis Centre Lobby

POSTER SESSION AND MANUFACTURERS' DISPLAY

6:00 P.M. Bus departs for the Transylvania Club

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

SESSION V: Sunday, November 7, 1993 - A.M. Davis Centre 1351

Chair: **Peter Bernath**

9:30 - 10:10 Peter Hackett (NRC, Ottawa)
Studies of the Structure and Reactivity of Small Metal Clusters

10:10 - 10:30 André D. Bandrauk and J. Zuo (Université de Sherbrooke)
Nonlinear Optical Properties of H_2^+ with Intense Femtosecond Pulses - Exact Calculations

10:30 - 10:50 Grant A. Bickel (AECL Research, Chalk River)
Laser Ablation with Resonance Ionization for Determination of H & D in Zirconium

10:50 - 11:10 **Coffee Break**

11:10 - 11:50 Peter Schultz (University of Western Ontario)
Probing Defects in Semiconductors with Slow Positrons

11:50 - 12:10 Rob Jackson, J.C. Polanyi and P. Sjövall (University of Toronto)
Photodissociation of $(NO)_2$ on LiF(100): Internal and Translational Energy Distributions

12:10 - 12:30 Dennis Salahub, V. Malkin, O. Malkina and D. Wei (Université de Montreal)
Modelling Complex Systems with Density Functional Theory: I- H-bonds and Solvation II - NMR Chemical Shifts

POSTER SESSION
Chair: **Terry McMahon**

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 p.m. ***Those whose papers were given even numbers should attend their posters.***

5:00 - 6:00 p.m. ***Those whose papers were given odd numbers should attend their posters.***

1) Mai Banh and David Wardlaw (Queen's University)
Flexible Transition-State Theory Rate Constants for H_2O_2

2) Victoria J. Barclay, W.-H. Hung, R. Kühnemuth, J.C. Polanyi, G. Zhang and Y. Zeiri (University of Toronto)
Hot H-atom Angular Distributions in HI/LiF(001) and HI/NaF(001) Photolysis

3) Oleg V. Boyarkin and T.R. Rizzo (University of Rochester)
Vibrational Overtone Spectroscopy of the CH Chromophore in Jet-Cooled CF_3H

4) Alexander Brown and W.J. Meath (University of Western Ontario)
On the Effects of Permanent Dipoles in the Phase Control of Two-Colour Multiphoton Processes

5) Michael A. Carpenter, M.T. Zanni, D.J. Levandier, D.F. Varley and J.M. Farrar (Univ. of Rochester)
Proton Transfer Dynamics on Highly Attractive Potential Energy Surfaces: Induced Repulsive Energy Release in O^-+HF at High Collision Energies

6) Ashok K. Dham and W.J. Meath (University of Western Ontario)
Exchange-Coulomb Potential Energy Models for the Kr-N_2 Interaction

7) S. Dénommée, M. DiRenzo, T.H. Ellis, E.J. Kruus and H. Wang (Université de Montreal)
Probing Chemical Reactions at Surfaces with Vibrational Spectroscopy

8) Robert Eng, H.M. Lambert, T. Carrington, S.V. Filseth and C.M. Sadowski(York University)
Multivariate Regression Analysis of Partially Resolved LIF Spectra. Application to the 157nm Photodissociation of C_2N_2

9) Ruian Fei, D.E. Adelman, T. Carrington and S.V. Filseth (York University)
Rotational Energy Transfer in CN(X,v=2) Induced by Collisions with Ar

10) James T. Francis and A.P. Hitchcock (McMaster University)
Vibrationally Resolved Triplet States in the Carbon 1s Spectra of CO and Benzene

11) Quishi (Joe) Gao and C.M. Sadowski (York University)
State-to-State Rotational Energy Transfer in Collisions of CN($B^2\Sigma^+$,v=0) with He and C_2N_2

12) Simon J. Garrett, V.P. Holbert, P.C. Stair and E. Weitz (Northwestern University)
Evidence for Competing Photoinduced Dissociation Mechanisms for CD_3I Adsorbed on TiO_2(110)

13) Denis J. Gendron, A. Mank and J.W. Hepburn (University of Waterloo)
Coherent Control in the Photodissociation of HI in the First Continuum

14) A.G. Adam, S.M. Mattar and William Hamilton (University of New Brunswick)
A Study of Cobalt-Fluoride LCAO-LDF Computations and Preliminary Laser Ablation - Laser Induced Fluorescence Results

15) S.J. Garrett, Darrick Heyd, E.T. Jensen and J.C. Polanyi (University of Toronto)
Evidence for Alignment of CH_3Br on LiF(100) and NaCl(100) from Photodissociation Dynamics

16) Deqing Hu, C.D. MacPherson and K.T. Leung (University of Waterloo)
The Proposed Binding Models and Dehydrogenation Mechanism for Six-membered Cyclic Unsaturated Hydrocarbons on Si(111)7x7

17) B.N. Jagatap and W.J. Meath (University of Western Ontario)
Probes of Molecular Orientations and Interactions Using One- Versus Two-Photon Transitions

18) Wei Kong, J. Martin, D. Rodgers and J.W. Hepburn (University of Waterloo)
PFI-ZEKE of Excited Ionic States of $N_2O^+(A^2\Sigma^+)$, $CO^+(A^2\Pi)$ and $O_2^+(X^2\Pi_g$, v>10) Using Coherent XUV

19) Jarek Koperski, J.B. Atkinson and L. Krause (University of Windsor)
Laser Spectroscopy of $A(O^+)$ - $X(O^+)$ and $B(1)$ - $X(O^+)$ Transitions in HgHe, HgNe, and HgAr, Excited in Supersonic Jets

20) Mangala S. Krishnan (Queen's University) and T. Carrington Jr. (Université de Montreal)
Isolated Effective Hamiltonians for Coriolis-Coupled Vibrational Modes

21) Rick D. Lafleur, J.M. Parnis and D.M. Rayner (Trent University and Queen's University)
Early Second-row Transition Metal Atom and Diatomic Transition Metal Oxide Reactions with Alkanes: A Fast-flow Reaction Kinetics Study

22) Dale J. Levandier and P.M. Johnson (State University of New York at Stony Brook)
Mass Analyzed Threshold Ionization Spectroscopy - A Mass Selective Method for the Determination of Optical Spectra of Molecular Ions

23) André McNichols, T. Carrington Jr. and G.C. Corey (Université de Montreal)
A Calculation of the Vibrational Energy Levels of Formaldehyde

24) Robert Maher and H.R. Mayne (University of New Hampshire)
A Comparison of Classical and Quantum Dynamics in the Cl+HCl System Using an Adiabatic Approximation

25) James D.D. Martin, T. Nguyen, A. Mank and J.W. Hepburn (University of Waterloo)
Molecular Beam Photoionization and Ion-Pair Formation Studies of HF and $(HF)_n$

26) Jifeng Ying, Chris P. Mathers and K.T. Leung (University of Waterloo)
Non-dipole Valence Transitions in CHF_2Cl by Angle-resolved EELS

27) Anthony Midey, S. Donnelly, J. Qian, C. Schmuttenmaer and J.M. Farrar (University of Rochester)
Frequency and Time Resolved Studies of Solvated Sr^+ Clusters

28) Zulfikar Morbi and P.F. Bernath (University of Waterloo)
High Resolution Laser Spectroscopy of BaS

29) David C. Moule (Brock University), A. Niño and C. Muñoz-Caro (Univ. de Castilla la Mancha, Spain)
A Study of Quadratic+Gaussian+Cosine Functions for the Simultaneous Description of Intramolecular Torsion and Inversion

30) John A. Niesse, J.N. Beauregard and H.R. Mayne (University of New Hampshire)
Geometry Dependent Trends in the Scattering of Van der Waals Clusters from Crystal Surfaces

31) J. Mark Parnis and L.E. Hoover (Trent University)
Alkali Metal Promoted, Visible Light Induced Photodissociation of Nitrous Oxide: Formation of Methanol from Methane and O atoms in Argon Matrices

32) A.G. Adam and James R.D. Peers (University of New Brunswick)
A Molecular Beam - Laser Induced Fluorescence Study of the $B(^1\Pi)$ - $X(^1\Sigma^+)$ Band of ScCl

33) Martin Poulin, M.J. Bramley and T. Carrington Jr. (Université de Montreal)
Calculation of Vibrational Energies and Intensities for Water with a Discrete Variable Recursive Residue Generation Method (RRGM)

34) Charles Qian and Y. Wang (University of Victoria)
Nonadiabatic Photodissociation dynamics of ICN in the A Continuum: A Semiclassical Study

35) Kelly L. Akers and M. Moskovits (University of Toronto)
Raman Studies of Fullerenes

36) M.L. Senent, D.C. Moule (Brock University) and Y.G. Smeyers (Inst. de Estructura de la Materia, Spain)
Theoretical Two-dimensional Analyses of the Torsional Spectra of G_{36} Molecules with Two Methyl Groups

37) Rebecca D.F. Settle and T.R. Rizzo (University of Rochester)
Vibrational Overtone Spectroscopy of the $4\nu_{OH}$ and $5\nu_{OH}$ Bands of Jet-Cooled Methanols

38) Lubosh Skala (University of Waterloo)
Size Dependence of Properties of Finite Systems

39) Caroline Starrs, A. Mank, M.N. Jego and J.W. Hepburn (University of Waterloo)
Photodissociation Dynamics of the $(^1B_2)$ $^1\Sigma_u^+$ State of CS_2

40) O. Abou-Zied, H.K. Sinha and Ronald P. Steer (University of Saskatchewan)
Structures and Laser-Induced S_2-S_0 Fluorescence Excitation Spectra of Van der Waals Clusters of Azulene and Xanthione

41) Mark Thachuk, G.C. Schatz (Northwestern University) and H. Mayne (Univ. of New Hampshire)
Evaluation of Thermal Rates for Reactions with Intermediate Wells: Removal of Bound State Contributions to Quantum Flux Correlation Functions

42) Li-Hong Xu and R.M. Lees (University of New Brunswick)
High Resolution Spectroscopic Studies of Large-Amplitude Motions

43) Xiaoke Yang and C. Noda (University of New Hampshire)
Vibrational Overtone Transitions of ND_3 in the Near Infrared

44) Chunfeng Zhao and P.F. Bernath (University of Waterloo)
High Resolution Spectroscopy of Metal-containing Free Radicals Produced by Supersonic Expansions

45) M. Czajowski and L. Krause (University of Windsor)
Laser Spectroscopy of CdNe, CdAr and ZnAr Van der Waals Molecules

46) Christina Carere, P.A. Berg, J.J. Sloan and W.S. Neil (University of Waterloo)
The Reaction of Translationally Excited Hydrogen Atoms with Freons CCl_3F, CC_2F_2 and $CClF_3$

47) Pamela A. Berg and J.J. Sloan (University of Waterloo)
Translational Excitation of Reagents on a Repulsive Surface: $H+Cl_2 \rightarrow HCl(v',J')+Cl$

48) V.J. Barclay (Univ. of Toronto), C.E. Dateo (NASA, Ames, Iowa) and Ian P. Hamilton (Wilfrid Laurier University)
Ab Initio Vibrational Splittings for Hydrogen Atom Exchange in HO_2

49) Ingo Fischer (NRC, Ottawa), A. Strobel and V.E. Bondybey (Munich, Germany)
Photodissociation Dynamics of CH_3I and CD_3I Probed by Zero Kinetic Energy Photoelectron Spectroscopy

50) P.M. Sinclair, J.W. Forsman, J.R. Drummond and A. David May (University of Toronto)
Line Mixing and State-to-State Rotational Relaxation Rates in O_2 Determined from the Raman Q Branch

51) Joseph T. Buontempo, S. Palese and R.J.D. Miller (University of Rochester)
Femtosecond High-Order Nonlinear Raman Spectroscopy of Water: Computer Simulations and Experiments

52) David T. Cramb and S.C. Wallace (University of Toronto)
Spectroscopy and Dynamics of Ammonia Near the Ionization Threshold

53) Robert Weersink and S.C. Wallace (University of Toronto)
Anomalous Red-shifted Fluorescence in Clusters of N,N-Dimethyl Amino Methyl Benzoate

54) Karen L. Randall and D.J. Donaldson (University of Toronto)
Photochemistry and Spectroscopy of Halogen Containing Clusters