

Regional Symposium on Chemical Physics

October 28-30, 1988

at the University of Waterloo

REGISTRATION begins at 6 p.m., Davis Centre Rm. 1301

SESSION I: Friday, October 28, 1988

Davis Centre 1302

Chairman: T.E. Gough

- 7:30 - 8:10 D. Rosner (University of Western Ontario).
Testing Quantum Electrodynamics with Lasers and Simple Atoms.
- 8:10 - 8:30 B. Simard, C. Masoni and P.A. Hackett (NRC, Ottawa).
Chemical Reactions in Laser-induced Plasma; A Route to High Resolution Spectroscopy of Refractory Diatomic Molecules.
- 8:30 - 8:50 A. Stolow, B.A. Collings and J.C. Polanyi (University of Toronto).
Direct Observation and Verification of the Transition State HD_2^+ in the Gas Phase Reaction $\text{H} + \text{D}_2 \rightarrow \text{HD} + \text{D}$.
- 8:50 - 9:10 C.R. Park and J.R. Wiesenfeld (Cornell University).
Reaction Dynamics of $\text{O}(^1\text{D})$ with HCl .
- 9:10 - 9:30 C.B. Cleveland and J.R. Wiesenfeld (Cornell University).
Observation of Highly Vibrationally Excited O_2 Resulting from the Reaction of $\text{O}(^1\text{D})$ with O_3 via $\text{O}_2(\text{B}^3\Sigma_u^- - \text{X}^3\Sigma_g^-)$ Schumann-Runge Laser Induced Fluorescence.

SESSION II: Saturday, October 29, 1988 A.M.

Davis Centre 1302

Chairman: K.T. Leung

- 9:00 - 9:40 R.F.W. Bader (McMaster University).
A Quantum Theory of Molecular Structure
- 9:40 - 10:00 J. Mark Parnis, S.A. Mitchell and P.A. Hackett (NRC, Ottawa).
Metal Atom and Metal Oxide Reaction Kinetics.
- 10:00 - 10:20 E.E. Aubanel and D.M. Wardlaw (Queen's University).
Experimental and Theoretical Rate Constants for $\text{CH}_3 + \text{H} \rightarrow \text{CH}_4$ and $\text{CH}_3 + \text{D} \rightarrow \text{CH}_3\text{D}$.
- 10:20 - 10:40 **Coffee Break**
- 10:40 - 11:20 M.J. Dignam (University of Toronto).
Spectroscopy of Ordered Molecular Assemblies.
- 11:20 - 11:40 W.K. Liu, Yuyi Shen and E. Altendorf (University of Waterloo).
A Numerical Study of Laser Excitation and Desorption of Adsorbates.
- 11:40 - 12:00 R.E. Gillilan and W.P. Reinhardt (Cornell University & Univ. of Pennsylvania).
Barrier Recrossing in Surface Diffusion: A Phase Space Perspective.
- 12:10 - 1:45 **Lunch** Davis Centre 1301

SESSION III: Saturday, October 29, 1988 P.M.

Davis Centre 1302

Chairman: R.J. Le Roy

- 2:00 - 3:00 R.S. Berry (University of Chicago).
How Good is Neil Bohr's Model of the Atom?
- 3:00 - 3:20 A. Myers and K.S. Pranata (University of Rochester).
Excited State Potential Surfaces and Dynamics of trans-1,3,5-hexatriene
from uv Resonance Raman Intensities.
- 3:20 - 3:40 C.L. Callender, S.A. Mitchell and P.A. Hackett (NRC, Ottawa).
Interatomic Potentials for Al- and In- Rare Gas Complexes.
- 3:40 - 4:00 L. Genberg, Q. Bao, S. Gracewski and R.J.D. Miller (University of Rochester).
Picosecond Transient Thermal Phase Grating Spectroscopy: A New Approach to the
study of Vibrational Energy Relaxation Processes in Proteins.

SESSION IV: Saturday, October 29, 1988 P.M.

Festival Room-SCH

POSTER SESSION

- 1) A. Janzen and J.E. Black (Brock University). Uniaxial Strain Events in Rafts of Xenon Physisorbed on Platinum, a Molecular Dynamics Study.
- 2) J. Bloch and J. Wiesenfeld (Cornell University). Photodissociation Dynamics of Cycloheptatriene using Lyman α Laser Induced Fluorescence.
- 3) P.J. Bruna (Carleton Univ.) and F. Grein (Univ. of New Brunswick). Electronic States of PS and AlP (neutral, positive and negative species).
- 4) B.I. Niefer, E.J. Kruus and J.J. Sloan (University of Waterloo). The Dynamics of Complex Gas Phase Reactions Measured by Time-Resolved Fourier Transform Spectroscopy.
- 5) H.F. Shurvell (Queens University) and F.J. Bergin (Shell Research Limited, UK). Fourier Transform Raman Spectroscopy.
- 6) D.J. Donaldson (University of Toronto), V. Vaida (Colorado), R. Naaman (Israel), and M.S. Child (Oxford). Cluster-Induced Potential Energy Shifts as a Probe for Intramolecular Predissociation Dynamics in Methyl Iodide, Acetone and Acetaldehyde.
- 7) M.P. Banjavcic, T.D. Pope, B.H. Watt, T.A. Daniels and K.T. Leung (University of Waterloo). Valence-Shell Electron Momentum Distributions of Cyclopropane by (e,2e) Spectroscopy.
- 8) L. Pylypow, J. Paldus and B. Jeziorski (University of Waterloo). Spin-Adapted Multi-Reference Coupled Cluster Formalism Including Non-Linear Terms and its Application to the H4 Model System.
- 9) X. Li and J. Paldus (University of Waterloo). Explicit Representation of Gelfand State in Clifford Algebra Unitary Group Approach.
- 10) A.T. Wen, E. Rühl and A.P. Hitchcock (McMaster University). Carbon K-Shell Excitation of Molecules by Electron Energy Loss Spectroscopy.
- 11) A. Damyanovich, J. Peternelj and M.M. Pintar (University of Waterloo). Aharonov-Bohm Effect on Protons in a State of Rotational Tunneling.

- 12) N. Snider (Queen's University). Studies of a Model of Thermal Unimolecular Reactions with Slow Randomization.
- 13) C.M. Sadowski, J.K. Lai, F.J. Morgan and S.V. Filseth (York University). Quantitative Analysis of Environmental PAH's by Supersonic Jet-Cooled Laser Spectroscopy.
- 14) P. Piecuch (University of Waterloo and University of Wroclaw). Generalization of the Concept of Spherical Harmonic Expansions to Many-body Intermolecular Forces. Application to the Case of Fourth-order Induction Interactions in an Arbitrary Multimolecular System.
- 15) S. Zarrabian (University of Waterloo), C.R. Sarma (Indian Inst. of Tech.) and J. Paldus (University of Waterloo). Computational Schemes in Configuration Interaction Studies.
- 16) G. Hunter and R.L.P. Wadlinger (York University). Photons and Neutrinos as Axial Modes of the Maxwellian Field.
- 17) T. Daniels and K.T. Leung (University of Waterloo). An Advanced Multi-Purpose Electrostatic Optical System.
- 18) X. Hu and W.L. Hase (Wayne State University). General Properties of Variational Transition State Theory as Applied to Association Reactions without Potential Energy Barriers.
- 19) S.R. Vande Linde and W.L. Hase (Wayne State University). A Direct Mechanism for S_N2 Nucleophilic Substitution Enhanced by Mode Selective Vibrational Excitation.
- 20) X. Ci and A.B. Myers (University of Rochester). A Resonance Raman Study of Solvent and Temperature Effects on Potential Surfaces and Electronic Dephasing Times of trans-stilbene.
- 21) F.J. Schlenker, F. Bouchard, D.R. Cyr, I.M. Waller and J.W. Hepburn (Univ. of Waterloo). Dynamics of the Photofragmentation of $Ni(CO)_4$.
- 22) D. Milburn and J.W. Hepburn (Univ. of Waterloo). Vacuum Ultraviolet Laser Photoelectron Spectroscopy.
- 23) F. Bouchard, J.W. Hepburn and T.B. McMahon (Univ. of Waterloo). Clustering Reactions and Thermochemistry of Laser Ablated Metal Ions.
- 24) P. Piecuch and J. Paldus (Univ. of Waterloo). Orthogonally Spin-Adopted Coupled Cluster Equations. Comparison of Different Procedures for Spin-Adaptation.
- 25) D. Lemoine and B. Pouilly (Université de Montreal). Fully Adiabatic Description of Atomic and Molecular Collisions: Coupling Mechanisms for Inelastic Scattering.
- 26) T.H. Ellis and M. Morin (Université de Montreal). Structure and Dynamics of the H/Pd(110) System.
- 27) J.A. Barnes, T.E. Gough and M. Stoer (Univ. of Waterloo). Diffusive Trapping: An Alternative to Supersonic Jet Cooling for Spectroscopic Experiments?

7:00 P.M.

DINNER

Flamingo Room - SCH

Chairman: J.W. Hepburn

- 9:30 - 10:10 W. Siebrand (NRC, Ottawa). Tunnelling of Hydrogen and Heavier Atoms.
- 10:10 - 10:30 R.L.P. Wadlinger (Lewiston, N.Y.) and G. Hunter (York University). The Electrostatic Quantum of Action in the Quantum Hall Effect.
- 10:30 - 10:50 **Coffee Break**
- 10:50 - 11:30 S. Filseth (York University). Energy Disposal in CN Produced by Photodissociation and Reactions.
- 11:30 - 11:50 C. Douketis and J.P. Reilly (Indiana University). High Resolution Overtone Spectroscopy in the Bulk Gas and on Molecular Beams.
- 11:50 - 12:10 B. Li and A.B. Myers (University of Rochester). Predissociation Dynamics in the S_3 State of CS_2 from far-uv Resonance Raman Depolarization Dispersion Curves.
- 12:10 - 12:30 J.S. Wright and P.J. Bruna (Carleton University). Strongly Bound Doubly-Excited States of Diatomic Molecules.