The 6th Annual

University of Waterloo

Symposium on Chemical Physics

October 26-28, 1990

Acknowledgements

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Waterloo Symposium on Chemical Physics

October 26-28, 1990

at the University of Waterloo

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

SESSION I: Friday October 26, 1990 P.M. Davis Centre 1302

Chair: K.T. Leung

7:30 - 8:10	D.J. Donaldson (University of Toronto) Predissociation Dynamics of CS_2
8:10 - 8:30	T.T. Nguyen-Dang and S. Manoli (Université Laval) Adiabatic Laser-Induced Resonances and Photodissociation of H_2^+ in Intense Laser Fields
8:30 - 8:50	David L. Phillips and Anne B. Myers (University of Rochester) Photodissociation of Alkyl Iodides in Solution: Substituent Effects on the Early Time Dynamics
8:50 - 9:10	Sergio Paone and G.A. Kenney-Wallace (University of Toronto) Picosecond Pump-Probe Measurements of the Ground State Rotational Diffusion of Dyes (Resorufin and Nile Red) in Concentrated Electrolyte Solutions

SESSION II: Saturday, October 27, 1990 - A.M. Davis Centre 1302

Chair: J.W. Hepburn

9:00 - 9:40	K.C. Janda (University of Pittsburgh) Pump-probe Studies of the Structure and Dynamics of van der Waals Molecules and Small Clusters
9:40 - 10:00	R.S. Dumont (McMaster University) Nonstatistical Inversion Dynamics of T-Shaped Ar_3
10:00 - 10.20	I. Hamilton (University of Ottawa) Energy Level Statistics for the Regular Energy Spectrum of Nonlinear Triatomics: Nongeneric Aspects and Quantum Chaos
10:20 - 10:40	Mangala S. Krishnan and Tucker Carrington Jr., (Université de Montreal) On the Elimination of Coriolis Coupling Term(s) in the Rotation-Vibration Hamiltonian for Polyatomic Molecules
10:40 -11:00	**Coffee Break**
11:00 - 11:40	J. Barker (University of Michigan) Collisional Deactivation of Highly Excited Polyatomic Molecules
11:40 - 12:00	M. Pilling, N.J.B. Green and S.H. Robertson (Queens University) Approximate Diffusion Equation Description of Energy Transfer
12:00 - 12:20	Michael Ivanco and J.W. Goodale (Chalk River Laboratories) Dissociation of Highly Vibrationally Excited $CDCl_3$
12:20 - 2:00	**Lunch** Davis Centre 1301

SESSION III: Saturday October 27, 1990 Davis Centre 1302

Chair: J.J. Sloan

2:00 - 3:00 D. Truhlar (University of Minnesota)
The Calculation of Quantum Effects in Chemical Reaction Dynamics

3:00 - 3:20 V.J. Barclay, Bruce Collings, J.C. Polanyi and J.H. Wang (University of Toronto)
A Study of H+DCl as a Function of Collision Energy: Experiment"

3:20 - 3:40 V.J. Barclay, B.A. Collings, J.C. Polanyi and J.H. Wang (University of Toronto)
A Study of H+DCl as a Function of Collision Energy: Theory"

SESSION IV: Saturday, October 27, 1990 from 4:00 P.M. South Campus Hall

POSTER SESSION AND MANUFACTURERS' DISPLAY

1) T.T. Nguyen-Dang and H. Abou-Rachid (Université Laval).
Adaptation of exact adiabatic time evolution formalism to molecular excitations by an arbitrarily shaped laser pulse: A wavepacket propagation study

2) T.A. Daniels, M.P. Banjavcic and K.T. Leung (University of Waterloo).
Experimental momentum distributions of tetramethylsilane by (e, 2e) spectroscopy

→ 3) J.J. Barrett, H.R. Mayne, L.J. Rawluk and M. Keil (University of New Hampshire and University of Alberta).
Theoretical study of state to state differential cross sections for rotationally inelastic Ar + HF collisions - a comparison with experiment

4) John N. Beauregard and H.R. Mayne (University of New Hampshire).
A Trajectory study of the role of reactant rotation in promoting chemisorption reactions

5) Pamela Berg, Tari Kaye and J.J. Sloan (University of Waterloo).
The effect of reagent excitation on the dynamics of the reaction: $O(^1D_2)+H_2$ ---> $OH(X\ ^2\Pi) + H$

→ 6) Craig Bieler, Kevin Spence and Kenneth Janda (University of Pittsburgh).
The structure and reaction dynamics of the $KrCl_2$ and $XeCl_2$ van der Waals Isomers

7) Elizabeth Bishenden, Jennifer Haddock and D.J. Donaldson (University of Toronto).
Observation of $Cl(^3P_{3/2})$ from near-UV photolysis of OClO

8) P.J. Bruna and J.S. Wright (Carleton University).
Doubly-excited states of C_2, C_2^+ and C_2^{2+}

9) Xiaopei Ci, David L. Phillips and Anne B. Myers (University of Rochester).
Resonance Raman studies of short linear polyenes: Excited state geometry and dynamics of cis-1,3,5-hexatriene and 1,3-butadiene; Solvent effects on excited-state torsional motion of trans-1,3,5-hexatriene

→ 10) M. T. Coolbaugh, G. Vaidyanathan, W.R. Peifer and J.F. Garvey (SUNY, Buffalo).
Magic number behaviour in olefin cluster ions

→ 11) Linda K. Cooper (Université de Montreal).
Rotational energy transfer in a highly anisotropic System: Li_2-He ($A^1\Sigma_u^+$)

12) M.R. Davies and R.J. Le Roy (University of Waterloo).
Using Monte-Carlo simulations of matrix shifts to characterize trapping sites in rare gas matrices

13) T.R. Dickson and G.A. Kenney-Wallace (University of Toronto).
Ultrafast molecular dynamics of simple liquids by optical Kerr effects

14) R. Brosseau, T.H. Ellis and H. Wang (Université de Montreal).
The influence of water on the chemisorption of CO_2 onto Pd(110).

15) D. Gendron and J.W. Hepburn (University of Waterloo).
Coherence effects in photofragmentation reaction using Doppler spectroscopy in the VUV

16) M. Cynthia Goh (University of Toronto).
Studies of monolayers at the air/water interface by second harmonic generation

17) Ziya B. Guvenc and Julius Jellinek (Argonne National Laboratory).
Reactive and Inelastic Dynamics of the D_2 + Ni_{13} Collision System

18) Ernie Hanson and F.R. McCourt (University of Waterloo).
Thermal diffusion field effects in N_2-He mixtures

19) C.E.C.A. Hop and T.B. McMahon (University of Waterloo).
Identification of organometallic ions involving non-covalent bonds

20) P.M. Blass, R.C. Jackson, J.C. Polanyi and H. Weiss (University of Toronto).
Nitric oxide (dimers) adsorbed on lithium fluoride single crystals

21) A. Janza and T. Carrington (Université de Montreal).
Numerical implementation of pertubation theory for polyatomic molecules

22) E.T. Jensen (University of Toronto) and R.E. Palmer (University of Cambridge).
Transient negative ions in the spectroscopy and dynamics of molecules on surfaces

23) W.J. Keogh (University of Toronto), A. Boothroyd and P.G. Martin (Can. Inst. for Theoret. Astrophysics) and M.R. Peterson (University of Toronto).
Progress on an H_4 potential energy surface

24) C.A. Downie, L.A. Jones and D.F. Thomas (University of Guelph).
Ultrahigh vacuum scanning tunnelling microscopy at the University of Guelph: Recent progress and plans for the investigation of the Au/Si(100) and Au/GaAs(100) interfaces

25) M. Kolbuscewski (Carleton University).
Theoretical analysis of EPR spectra of monocrystals of low symmetry. Extension of Schonland procedure to systems of symmetry lower than rhombic

26) B. Leong Lan and R.F. Fox (Queen's University).
Quantum-Classical correspondence and quantum chaos in the periodically kicked pendulum

27) M. Shen, J.M. Farrar and D. Levandier (University of Rochester).
Photodissociation spectra of size-selected solvated metal ions: $Sr^+ (NH_3)_{n=1...4}$

28) B. Li and A.B. Myers (University of Rochester). *Emission polarization and raman lineshapes in the S_3 state of CS_2 vapor as a probe of predissociation: effect of finite bandwidth of the incident field*

29) Xiangzhu Li and J. Paldus (University of Waterloo).
PPP-VB theory of π-electron systems: Ground and excited states, resonance and geometric distortion, and spin properties

30) L. Liu and I. Hamilton (University of Ottawa).
Thermal dissociation of diatomics in inert gases: A Nosé equation approach

31) J. Yang, L. Lolle, J. Poll, B. Nickel and C. Gray (University of Guelph).
Theory of the high frequency wing in interaction-induced spectra

32) C. MacPherson, D. Hu and K.T. Leung (University of Waterloo).
Thermal desorption study of thiophene and related aromatics on Si(111) 7x7

33) A.R.W. McKellar (NRC Ottawa).
High resolution infrared spectra of the CO-H_2 and CO-D_2 Van der Waals complexes in the 4.7μm region.

34) A. McNichols and T. Carrington, Jr. (Université de Montreal).
Lanazos method for variational calculations with large sparse matrices to determine vibrational energy levels

35) M.E. Mandy and P.G. Martin (University of Toronto).
Some considerations in the calculation of rate constants from quasiclassical trajectory data

36) F. Markel, A.B. Myers (University of Rochester) and N.S. Ferris (Eastman Kodak & Co).
Optical and resonance raman studies of photoinduced electron transfer in hexamethylbenzene - tetracyanoethylene complexes in CH_2Cl_2 and CCl_4.

37) B. Meng, P.J. Bruna and J.S. Wright (Carleton University).
Ab-initio study of the Be_2^+ potential energy curves.

38) K.G. Lohn, H. Mizes and R.J.D. Miller (University of Rochester).
Atomic force microscopy (AFM) studies of Van der Waals and electrostatic contributions to attractive surface potentials

39) C. Douketis, M. Moskovits and T. Stuckless (University of Toronto).
Two-photon-electron spectroscopy of aromatic molecules adsorbed onto silver films

40) T.T. Nguyen-Dang (Université Laval).
Adiabatic representations for molecular dynamics in intense laser fields

41) J.M. Parnis (Trent University) and S.A. Mitchell and P.A. Hackett (NRC, Ottawa).
Gas-phase transition metal atom reaction kinetics: The Cr + O_2 and Cr + NO ground state association reactions over a wide pressure range

42) D. Permann and I. Hamilton (University of Ottawa).
Nonlinear dynamics of model systems

43) P. Piecuch, S. Zarrabian, J. Paldus and J. Cizek (University of Waterloo).
Account of higher than pair cluster contributions in single reference coupled cluster theory

44) Lynn Richard, L. Genberg, J. Deak and R.J.D. Miller (University of Rochester).
Direct observation of global protein motion: Evidence for collective modes in biomechanics

45) P.T. Rieger and R.J.D. Miller (University of Rochester).
Exact numerical solution to the incoherent limit of energy transport in random ensembly

46) A.B. Myers and J.-M. Rodier (University of Rochester).
A resonance raman study of 4a,4b-dihydrophenanthrene (the photocyclization product of cis-stilbene).

47) D. Sadovskii (NRC, Ottawa).
The $SO(3)>D_\infty>D_6>D_2$ irreducible tensors as applied to the problem of Rydberg states of the H_3 molecule. Calculation of spectroscopic transition frequencies and probabilities

48) S.P. Sapers, N. Anotos and D.J. Donaldson (University of Toronto).
S_2 from the reaction $S(^1D) + CS_2$

49) Michel Dupuis (IBM Corp.) and Fiona Sim (Université de Montreal).
Ab initio calculations of non-linear polarisabilities in para-nitroaniline including electron correlation treated by Moller-Plesset theory

50) K. Sinniah, W.D. Sands, J. Hrbek, J.T. Yates Jr., and K.C. Janda (University of Pittsburgh).
Isotope mixing between CO molecules on K/Ni(111) surface: An LITD study

51) T. Slee, C. Chuaqui and R.J. Le Roy (University of Waterloo).
Calculating the vib-rotational spectra of Van der Waals complexes. A new method and application to helium-acetylene complex

→ 52) T.J. Slotterback (University of Pittsburgh), C.M. Western (University of Bristol), J.R. Johnson (Texas Instruments, Dallas) and K.C. Janda and D.W. Pratt (University of Pittsburgh).
Hyperfine structure measurments in the $A^3\Pi(1)$ <--- X^1S^+ electronic transition of $I^{35}Cl$ near the dissociation limit: measurement of the ^{35}Cl atom hyperfine structure

53) M. Szarka and S. Wallace (University of Toronto).
Spectroscopy and photodissociation of Rydberg states of N_2O

54) M. Thachuk and F.R. McCourt (University of Waterloo).
The corrected coupled states (CCS) approximation: How good is it?

55) R. Weersink and S. Wallace (University of Toronto).
The roll of conformational changes in the photophysics of dimethyl amino benzoate (DMAMB) and $(DMAMB)_2$

56) Clement Wong and F.R. McCourt (University of Waterloo).
Classical trajectory calculation of transport and relaxation properties for O_2-He mixtures.

57) A. Wortman and D.M. Wardlaw (Queen's University).
Microscopic rate constants for H_2O_2 ---> 2OH: Comparison of flexible transition state theory and trajectory results

58) S.-H. Yang and M. Knicklebein (Argonne National Laboratory).
Near-threshold ionization of transition metal clusters

59) H. Zhu, J. Ying, M.P. Banjavcic and K.T. Leung (University of Waterloo).
Preliminary investigation of electronic structures for a series of molecules (iso-, cis-, and trans-butene) in valence orbitals by an (e, 2e) coincidence method

7:00 P.M. **DINNER** South Campus Hall

SESSION V: Sunday, October 28, 1990 A.M. Davis Centre 1302

Chair: R.J. Le Roy

9:30 - 10:10	B. Henry (University of Guelph) Sources of Intensity for Local Mode Overtones.
10:10 - 10:30	J. Rostas, D. Klapstein, M. Vervloet and J.K.G. Watson (NRC Ottawa) The Low-J perturbations of the B(000) State of CO^{2+}.
10.30 - 10:50	C. Frum, R. Engleman and P. Bernath (Arizona University) Fourier Transform Emission Spectroscopy.
10:50 - 11:10	**Coffee Break**
11:10 - 11:50	D. Salahub (Université de Montreal) Density Functional Theory and the Quantum Chemistry of Transition Metal Systems.
11:50 - 12:10	G. Vaidyanathan, M.T. Coolbaugh, W.R. Peiter and J.F. Garvey (SUNY, Buffalo) Novel Ion-Molecule Reactions in Argon-Methanol Heteroclusters.
12:10 - 12:30	P. Rowntree, L. Parenteau and L. Sanche (Université de Sherbrooke) Electron Stimulated Desorption of H^- (D^-) from Amorphous Ice *via* Core-Excited Anion States.