The 6th Annual

University of Waterloo

Symposium on Chemical Physics

October 26-28, 1990

Acknowledgements

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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.