

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 4.7 μ m 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 ensemble
- 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 $SO(3) \supset D_{\infty} \supset D_6 \supset D_2$ 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 measurements in the $A^3\Pi(1) \leftarrow X^1S^+$ 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 $H_2O_2 \rightarrow 2OH$: 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 CO₂⁺.
- 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.