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INTERNATIONAL CONFERENCE ON RADIATIONLESS TRANSITIONS  
HELD AT NEWPORT BEA. (U) CALIFORNIA UNIV IRVINE DEPT OF  
CHEMISTRY E K LEE ET AL. 31 DEC 84 N00014-83-G-0178

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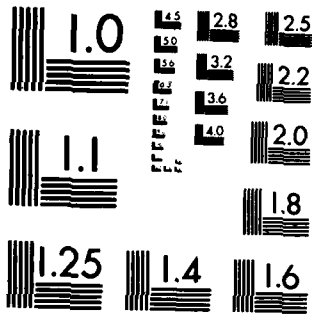
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FINAL REPORT

ON

International Conference on Radiationless Transitions

held at

The Hotel Newporter, Newport Beach, California

on

January 3-7, 1984

to

The Office of Naval Research

(N-00014-830G-0178)

Submitted by the Organizers:

Edward K.C. Lee

F. Sherwood Rowland

Max Wolfsberg

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Report Prepared on May 17, 1984

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FIELD	GROUP	SUB. GR.	
		Conference support	
19. ABSTRACT (Continue on reverse if necessary and identify by block number) International Conference on Radiationless Transitions was held at the Hotel Newporter, Newport Beach, California, on January 3-7, 1984. Thirty long invited talks (30-20 minutes), 13 short talks (15-10 minutes), and 26 poster papers were presented. Topics presented in 9 half-day sessions (besides 2 poster sessions) were laser multiphoton ionization, photo dissociation dynamics, theories on intramolecular dynamics, gas phase relaxation dynamics, condensed phase dynamics and laser-jet spectroscopy. The international scientists totaling 111 had exchanged recent scientific information and generated new ideas for future research with intense participation during the conference.			
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22a. NAME OF RESPONSIBLE INDIVIDUAL Professor Edward K.C. Lee		22b. TELEPHONE NUMBER (Include Area Code) 714-856-6021	22c. OFFICE SYMBOL

The Local Organizing Committee consisting of  
 M.A. El-Sayed, University of California, Los Angeles  
 E.K.C. Lee, University of California, Irvine  
 F.S. Rowland, University of California, Irvine  
 C. Wittig, University of Southern California, Los Angeles  
 M. Wolfsberg, University of California, Irvine  
 A.H. Zewail, California Institute of Technology, Pasadena

arranged the scientific program attached as Appendix A. Thirty long invited talks (30-20 min), 13 short talks (15-10 min), and 26 poster papers were presented. One invited talk by Dr. A. Tramer was cancelled. The following main topics were presented in half day sessions:

Half-day sessions

Topic

- |   |  |
|---|--|
| 1 | Laser multiphoton ionization             |
| 1 | Photodissociation and collision dynamics |
| 2 | Theories on intramolecular dynamics      |
| 2 | Gas phase relaxation dynamics            |
| 2 | Condensed phase dynamics                 |
| 1 | Laser jet spectroscopy                   |

Additionally, there were two afternoon poster sessions.



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On the last day, there was an open discussion of the intramolecular dynamics of pyrazine led by A.H. Zewail and D.W. Pratt. Recent scientific information and new ideas for future research were exchanged with intense participation during the conference.

The total number of participants was 111 including 25 post-doctoral research associates and 20 graduate students. The list is attached as Appendix B.

The federal agencies appropriated funds for partial reimbursement of travel expenses for some invited speakers as follows:

AFOSR	\$ 4,550
NSF	3,500
ONR	<u>4,030</u>
TOTAL	\$12,080

Of this sum, \$12,000 was spent for partial reimbursement of the travel expenses of ten invited foreign speakers (\$6800) and twelve invited domestic speakers (\$5200).

A total of \$9908 was collected through registration fees and food payments (the costs for breakfast were included in the regular registration fee). This sum plus the remaining \$80 from the federal grants was used to cover conference costs for books of abstracts, postage, conference secretary (Mrs. M. Pellman), poster stands, hotel facility charges, and breakfast/lunches.

INTERNATIONAL CONFERENCE ON RADIATIONLESS TRANSITIONS

PROGRAM

MONDAY, JANUARY 2, 1984

2:00 P.M. Registration

6:00 P.M. Informal Reception

TUESDAY, JANUARY 3, 1984

8:30 A.M. - 12:00 Noon

OPENING REMARK

- A-1 (30 Min) E.W. Schlag  
"Multiphoton Mass Spectrometry, Some Recent Applications"
- A-2 (30 Min) M.A. El-Sayed, D.A. Gobeli, J.R. Morgan, and J. St. Pierre  
"The Mechanism of Laser Multiphoton Ionization Dissociation by Two-Color (Pump-Pump) Picosecond Laser-Mass Spectrometric Techniques"
- A-3 (30 Min) J. Troe, H. Hippler, K.H. Hoyerman, and K. Luther  
"Kinetics of Multiphoton Ionization in Toluene and Cycloheptatriene"
- A-4 (30 Min) S. Leach and G. Dujardin  
"Recent Studies on Radiationless Transitions and Dissociative Relaxation in Molecular Ions"

12:00 - 2:00 P.M. LUNCH

2:00 P.M. - 4:00 P.M. POSTER SESSION

- B-1 E.C. Apel and E.K.C. Lee  
"Rovibronic Emission Locked Fluorescence Excitation Spectroscopy: A Selective Probe for Coriolis Perturbation in Rovibronic Levels of  $S_1$   $H_2CO$ "
- B-2 R. Copeland and D.R. Crosley  
"Rotational Level Dependence of Electronic Energy Transfer in the  $A^2I^+$ ,  $v'=0$  State of OH and OD"
- B-3 D. Dlott, L. Schosser, T.J. Kosic and R.E. Cline, Jr.  
"Vibrational Relaxation in Molecular Crystals at Low Temperatures"

- B-4 G. Dujardin, T. Govers and S. Leach  
 "Complete Dissociation of a Triatomic Cation: Simultaneous or Sequential Process?"
- B-5 B. Fain and S.H. Lin  
 "Non-Equilibrium Phonons in Rate Processes"
- B-6 J. Shiraishi, Y. Fujimura and T. Nakajima  
 "Mechanism of Resonant Two-photon Transitions via Repulsive Intermediate States. An Experimental and Theoretical Study on I<sub>2</sub> in Vapor"
- B-7 S.A. Mitchell and Peter Hackett  
 "Pump and Probe Experiments on the Visible Dye Laser Induced MPD of Gallium Trimethyl"
- B-8 R.J. Brudzynski, P. Felder, R.J. Buss, and Y.T. Lee  
 "Molecular Beam Study of the Unimolecular Decomposition of Toluene"
- B-9 P. Felder, R.J. Brudzynski, R.J. Buss and Y.T. Lee  
 "Photodissociation of Isopropylcycloheptatriene at 266 nm"
- B-10 T.K. Minton, P. Felder, R.J. Brudzynski, and Y.T. Lee  
 "Photodissociation of 1,2-Chloroiodoethane"
- B-11 J.K. McVey  
 "Relaxation Dynamics in Isolated Hydrogen-Bonded Dimers"
- B-12 V. Lejeune, A. Despres, and E. Migirdicyan  
 "Site Selection Spectroscopy of the Non-Kekule m-xylylene Biradical and its Methylated Derivatives"
- B-13 Y. Matsumoto, L.H. Spangler, and D.W. Pratt  
 "Magnetic Field Effects on Intersystem Crossing"
- B-14 I. Oref  
 "Statistical transition Probabilities and the Dynamics of Vibrational Energy Transfer in Reacting Systems"

4:00 - 5:30 P.M.

- C-1 (30 Min) Y.T. Lee, D.M. Newmark, A.W. Wodtke, and G.N. Robinson  
 "The Observation of Dynamic Resonances in the F + H<sub>2</sub> Reaction"
- C-2 (30 Min) I. Tanaka, K. Tsukiyama, K. Shibuya, and K. Obi  
 "Photodynamics of NO<sub>2</sub> in the 1<sup>2</sup>B<sub>2</sub> and 2<sup>2</sup>B<sub>2</sub> States"

8:00 - 10:00 P.M.

SOCIAL



WEDNESDAY, JANUARY 4

8:30 A.M. - 12:00 Noon

- D-1 (30 Min) R.M. Hochstrasser  
"Vibrational Energy Redistribution in Molecular Solids"
- D-2 (20 Min) S.H. Lin and H. Kono  
"Theoretical Studies of Photophysical Processes of  
Impurity Molecules in Solids"
- D-3 (10 Min) Raoul Kopelman  
"Fractal Energy Transport"
- D-4 (30 Min) V.E. Bondybey  
"Nonradiative Relaxation and Vibrational Energy Redistri-  
bution in Large Molecules"
- D-5 (15 Min) M. Kasha  
"Radiationless Mechanisms in Proton-Transfer  
Spectroscopy"
- D-6 (20 Min) D. Huppert, E. Helinski, and P.M. Rentzepis  
"Effect of Solvent Dielectric Relaxation on Intramole-  
cular Electron Transfer"

12:00 - 2:00 P.M.

LUNCH

4:00 - 6:00 P.M.

POSTER SESSION

- E-1 M. Noble and E.K.C. Lee  
"Vibrational Mode Specificity in the Nonradiative Decay  
Rates of Jet-Cooled  $S_1$  Acetaldehyde"
- E-2 A.E. Bruno and R.P. Steer  
"Radiationless Transitions on Thioformaldehyde, Thio-  
acetaldehyde and Thioacetone Excited to Single Vibronic  
Levels of Their First Excited Singlet States"
- E-3 P. Boczar, S.A. Schwartz, and M.R. Topp  
"Vibrational Relaxation Studies in Matrices and Jets"
- E-4 R.B. Weisman  
"Time-resolved Electronic and Vibrational Spectroscopy of  
Excited Azabenzenes"
- E-5 D.W. Boldridge, B.L. Justus, and G.W. Scott  
"Radiationless Decay Kinetics of the Lowest Energy  
Excited Singlet State ( $n\pi^*$ ) of the Naphthaldehydes"

- E-6 R.L. Whetten, C.E. Otis, K.-J. Fu, and E.R. Grant  
 "Measurements of Ultrafast Decay of Molecular Rydberg States"
- E-7 L. Bigio, R.L. Whetten, R.S. Tapper, and E.R. Grant  
 "Dynamics of Resonant Two-Photon Excitation: Evidence for the Effects of Intermediate Intramolecular Relaxation"
- E-8 I. Nadler, H. Reisler, and C. Wittig  
 "The Photodissociation of NCNO Following  $\pi^* \leftarrow n$  Excitation with a Tunable Dye Laser"
- E-9 D. Kelley  
 "Dynamics of Iodine Geminate Recombination via Excited Electronic States"
- E-10 J. Wessel, E.L. Loper, and D.M. Mordaunt  
 "Molecular Detection by Multiphoton Photoionization with Selective Ion Photofragmentation"
- E-11 D.M. Rayner and P.A. Hackett  
 "Investigation of IR MPD Dynamics by Time Resolved Multiphoton Ionization Techniques"
- E-12 S. Wallace

8:00 - 10:00 P.M.

- F-1 (30 Min) C.S. Parmenter, D.A. Dolson, R.A. Coveleskie, K.W. Holcelaw, and B. Stone  
 "The Dynamics of Vibrational Redistribution in Some Aromatic Molecules"
- F-2 (20 Min) E.C. Lim, S.L. Wang, and I.C. Khoo  
 "Dynamics of Coherent and Incoherent Emission from a Single Molecule"
- F-3 (30 Min) J. Kommandeur  
 "Molecular Eigenstates and Decays of Rotational States of Pyrazine"

10:00 P.M.

.SOCIAL

THURSDAY, JANUARY, 5

8:30 A.M. - 12:00 Noon

- G-1 (30 Min) R.D. Levine  
"Intramolecular Dynamics via the Algebraic Approach"
- G-2 (30 Min) D.A. Ramsay  
"The Application of Spectroscopy to the Study of  
Interstate Perturbations"
- G-3 (30 Min) M. Quack  
"Radiative and Radiationless Transitions in IR-Photo-  
chemistry and IR-Multiphoton Excitation"
- G-4 (30 Min) H.J. Neusser  
"Sub-Doppler Spectroscopy and Energy Randomization in  
Polyatomic Molecules"

12:00 - 2:00 P.M.

LUNCH

8:00 - 10:00 P.M.

- H-1 (30 Min) M.D. Fayer  
"Electronic Excitation Transport in Disordered Systems"
- H-2 (10 Min) D. Huppert and D. Rojansky  
"Picosecond Study of the Role of Electronic Excitation  
Diffusion in Energy Transfer Process in Solutions and  
Solids"
- H-3 (30 Min) K.B. Eisenthal  
"Chemistry on the Picosecond Time Scale"

10:00 P.M.

SOCIAL

FRIDAY, JANUARY 6

8:30 A.M. - 12:00 P.M.

- I-1 (30 Min) R.W. Field  
"A Time Independent View of Intramolecular Vibrational  
Redistribution: Coriolis Perturbations in Formaldehyde  
and Quantum Chaos in Acetylene"
- I-2 (30 Min) A.H. Zewail  
"Picosecond Dynamics of IVR: Quasiperiodic and  
Statistical Behavior"
- I-3 (30 Min) R.A. Marcus  
"Review of Some Concepts of Quasiperiodicity and Chaos"
- I-4 (15 Min) F.S. Rowland and P.J. Rogers  
"Non-RRKM Decomposition Reactions Following Halogen Atom  
Additions to Allylic Metallo-organic Compounds"
- I-5 (20 Min) C.B. Moore, D.J. Bamford, S.V. Filseth, and  
M.F. Foltz  
"Product Energy Distribution for Formaldehyde  
Photofragmentation"

12:00 - 2:00 P.M.

LUNCH

2:00 - 5:00 P.M.

- J-1 (30 Min) R.N. Zare  
"The Ebb and Flow of Energy in the Near UV Photolysis of  
trans-HONO\*"
- J-2 (30 Min) C. Wittig  
"The Development of Product States During Dissociation"
- J-3 (30 Min) R.N. Dixon  
"The Influence of Rotational Angular Momentum on the  
Predissociation of Some Small Polyatomic Molecules"
- J-4 (15 Min) H.S. Taylor and G. Hose  
"Implications of the Existence of Quantum Analogue of  
Classical Regular Motion on Molecular and Atomic  
Spectra"
- J-5 (15 Min) S. Mukamel  
"Anharmonic Molecular Spectra - Self Consistent Mode  
Coupling, Nonlinear Maps and Quantum Chaoses."

7:00 P.M.

RECEPTION

8:00 P.M.

BANQUET

SATURDAY, JANUARY, 7

8:30 A.M. - 12:00 P.M.

- K-1 (30 Min) A. Tramer, C. Jouvét, J.M. LeBars, and P. Millie  
"Intermediate Case in Vibrational Energy Redistribution."
- K-2 (10 Min) E.R. Grant, R.L. Whetten, and G.S. Ezra  
"Inverse Electronic Relaxation and Nonradiative Decay in the Jahn-Teller Conical Intersection: Exact Nonadiabatic Calculations in the Classical Limit"
- K-3 (10 Min) E.K.C. Lee, N.L. Garland, and E.C. Apel  
"SRL Fluorescence Emission Studies of Vibrational Mixing Induced by Coriolis Interaction: The Region of  $E_{\text{vib}} = 2200 - 3000 \text{ cm}^{-1}$  in  $S_1 \text{ H}_2\text{CO}$ "
- K-4 (10 Min) A.E.W. Knight and W.D. Lawrance  
"Vibronic Perturbations in Electronic States and the Manifestations of State Mixing"
- K-5 (30 Min) D.H. Levy, C.A. Haynam, C. Morfitt, and L. Young  
"The Photophysics and Photochemistry of Molecular Clusters"
- K-6 (20 Min) A. Amirav, M. Sonnenschein and J. Jortner  
"Absorption Spectroscopy Fluorescence Spectroscopy and Emission Quantum Yield Measurements of Large Molecules in Planar Supersonic Expansions"
- K-7 (10 Min) R.P.H. Rettschnick, J.J.F. Ramaekers, J. Langelaar, and H.J. Lips  
"Dynamics of the Dissociation of Electronically Excited Complexes of s-Tetrazine and Argon"

12:00 - 2:00 P.M.

LUNCH

2:00 - 4:00 P.M.

- L-1 (30 Min) R.E. Smalley  
"Photoionization Probes of Radiationless Transitions"
- L-2 (15 Min) D. Phillips, A. Autry, and A. Jones  
"Time Resolved Fluorescence from a Jet-Cooled Bridged Aromatic Molecule"
- L-3 (15 Min) M. Wolfsberg, C.L. Chen and B. Maessen  
"Variational Calculations of Rotational-Vibrational Energy Levels of Polyatomic Molecules"
- L-4 (30 Min) S.A. Rice and T.A. Stevenson  
"Energy Redistribution in Electronically Excited He-Benzene and Ar-Benzene van der Waals Molecules"

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