AD-A101 431 CALIFORNIA UNIV BERKELEY DEPT OF CHEMISTRY F/G 7/4
LASER STUDIES OF MOLECULAR COLLISION PROCESSES.(U)
JUL 81 C B MOORE DAAG26-77-G-0200
UNCLASSIFIED ARO-15131.23-P NL

ADA101431

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

ARO 19 16131.23-P

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER (6)	2. GOVT ACCESSION NO. AD-A102 432	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Laser Studies of Molecular Collision Processes. (12)	5. TYPE OF REPORT & PERIOD COVERED Final 8/15/77 - 3/31/81
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) (10) Professor C. Bradley Moore (15)	8. CONTRACT OR GRANT NUMBER(s) DAAG26-77-G-0200
9. PERFORMING ORGANIZATION NAME AND ADDRESS Regents of the University of California 118 California Hall Berkeley, CA 94720 (11) 15 Jul 82	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS (12) 61
11. CONTROLLING OFFICE NAME AND ADDRESS U. S. Army Research Office Post Office Box 12211 Research Triangle Park, NC 27709 (18) ARO	12. REPORT DATE July 15, 1981
	13. NUMBER OF PAGES 5
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office) (9) Final rept. 15 Aug 77-31 Mar 82	15. SECURITY CLASS. (of this report) Unclassified
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

LEVEL II

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

DTIC ELECTE JUL 21 1981 D C

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

NA

18. SUPPLEMENTARY NOTES

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Vibrational Energy Transfer

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

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UNCLASSIFIED 400373
SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

FINAL REPORT

ARO PROPOSAL NUMBER: RDRD-P-12224

PERIOD COVERED BY REPORT: August 15, 1977 - March 31, 1981

TITLE OF PROPOSAL: Laser Studies of Molecular Collision Processes

CONTRACT OR GRANT NUMBER: DAAG26-77-G-0200

NAME OF INSTITUTION: Department of Chemistry
University of California
Berkeley, CA 94720

PRINCIPAL INVESTIGATOR: Professor C. Bradley Moore

I. Statement of Problem:

The purpose of this research has been to determine the effect of selective electronic and vibrational excitation on energy transfer and reaction rates in simple molecular systems.

II. Principal Results:

A wide variety of behavior is exhibited in the competition between reaction and energy transfer for simple molecular systems. The principal results can be grouped into 3 categories.

(1) Relaxation of highly vibrationally excited species

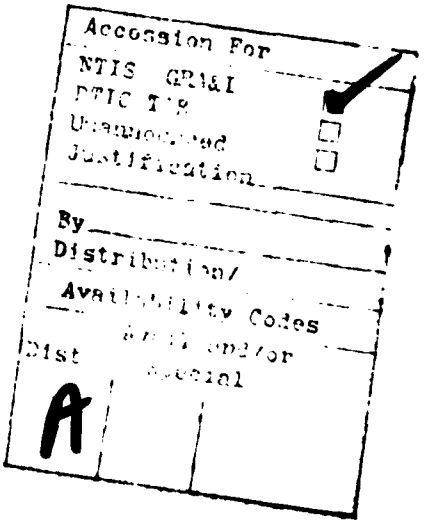
The competition between relaxation and reaction in collisions of a highly vibrationally excited diatomic with thermal molecules has been studied. The observation of multiquantum energy transfer upon collision infers the occurrence of a reaction. In studies of HF(v = 4) with a variety of collision partners, removal of the initially excited species is seen to occur via single quantum energy transfer implying that the relaxation channel dominates.

cont (2) Vibrational Relaxation in Polyatomic Systems:

Studies of vibrational relaxation pathways have been extended to the CH_4, NH_3, H_2O, D_2O, H_2Se, D_2S systems. It is shown that systems which interact via hydrogen bonding show increased V → T, R rates with negative temperature dependence near room temperature. The enhanced V → T, R rates and negative temperature dependence can be explained with a model in which orbiting collisions are most effective in causing relaxation.

3) Vibrational Relaxation in Condensed Media:

The vibrational spectroscopy and dynamics of matrix isolated HCl and CH_3F have been studied. At the cryogenic temperatures of these experiments, the attractive part of the intermolecular guest-host potential is seen to play an increasingly important role in causing vibrational relaxation. For those systems in which the attractive forces are known to be strong, as evidenced by the existence of van-der-Waals molecules in the gas phase, i.e. HCl-rare gas, relaxation rates correlate well with increasing intermolecular well depth. In all systems studied, there is a marked dependence of relaxation rates on host, spanning two orders of magnitude between Ar and Xe.



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IV. Personnel Supported and Degrees Granted:

Professor C. Bradley Moore

Cameron J. Dasch, Ph.D. 1978
Donald J. Douglas
Chang-Chi Mei, Ph.D. 1978
Peter Hess
Linda Young
Muhammad B. Zughul, Ph.D. 1978
Jay M. Wiesenfeld, Ph. D. 1978
Eliot Specht
Floyd E. Hovis, Ph.D. 1979
Scepan S. Miljanic
Zia Sabet Imani
David M. Goodall
Douglas Bamford
Pauline Ho
Andrew O. Langford
Michael R. Berman, Ph.D. 1981
Hai-Lung Dai, Ph.D. 1981
I.W.M. Smith
Chi-ke Cheng
Joseph Jasinski