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STATE TO STATE STUDIES OF ENERGY TRANSFER PROCESSES.(U)
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FINAL REPORT

State to State Studies of Energy Transfer Processes

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Submitted by
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January 1981

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SUMMARY OF WORK ACCOMPLISHED

The work was carried out in the Research Laboratory of Electronics at M.I.T. In addition to the tunable single mode cw dye laser which was used in this experiment, this laboratory has a large assortment of equipment for research in atomic physics using optical techniques, including several spectrum analyzers, photomultiplier tubes, and miscellaneous optical and electronic equipment. The Research Laboratory of Electronics provides also a number of services and facilities essential to the work carried out, including glassblowing, machine shop, purchasing, drafting, photographic, and general administration.

In the first year of research we have made a clear-cut demonstration of the VSDS method by measuring the velocity dependence of the fine structure changing cross sections for two Na-rare gas systems. These were the first velocity dependent measurements in this system, and our measured velocity dependence has subsequently been confirmed by an independent mesurement in a crossed beams machine.

We have also, in the first six months, begun work on measurements of molecular energy transfer in collisions of Na_2 molecules with rare gases.

In the second year our studies of molecular energy transfer processes, including chemical reactions, were carried out using a new technique which permits measurement of the velocity dependence of the energy transfer cross sections in experiments conducted in gas cells. We used a tunable laser to excite molecules in a particular vibration and rotation state, and also to select their velocity by means of the Doppler shift, we studied the transfer and redistribution of initial translational and rotational energy when these molecules collide.

We continued our studies of collision processes by which an excited state molecule can transfer its energy to other atoms and molecules. We measured the influence of the initial electronic, vibrational, rotational and translational energy of the excited state molecule on the outcome of the collision. We made these measurements by using a tunable single-mode continuous wave due laser to excite the desired electronic, vibrational and rotational state of the molecule prior to the collision.

Atomic and molecular energy transfer processes were the object of considerable theoretical and experimental study. The primary stimulus for this research was the importance of these energy transfer processes to a number of devices and phenomena of practical interest in which a gas of atoms and/or molecules is found in thermal disequilibrium.

Another strong stimulus for the study of molecular energy transfer processes came from the fact that the problem was "ripe" for major scientific advances because of recent theoretical and experimental developments. The advent of tunable single-mode lasers made it possible to perform experiments with good signal-to-noise ratio in which the initial states, and the final states as well, of the colliding molecules were known exactly and chosen at will simply by tuning the laser to excited the desired state.

Rotational Energy Transfer (RET) for intensive study was selected for several reasons. Firstly, it is more rapid than any other energy transport process so that we have been able to study it in a single collision and without competition from other energy transfer processes (e. g. those involving the vibrational degree of freedom). Secondly, RET is a relatively simple collision process, governed by simple laws, which may be explained theoretically. Finally, because RET is so rapid, it is not possible to study other energy transfer processes in detail without encountering a great deal of RET; unless RET is already well understood it is difficult to understand these other processes completely.

We made a preliminary search for state-to-state anisotropies by looking for collision induced polarization of the Na_2 satellite lines. Any anisotropy of the collision cross-section produced anisotropy in the distribution of angular momenta of the collisionally populated rotational levels, thus causing satellite line polarization. We found less than 6% polarization of the satellite at high incident initial velocity, corresponding to a 30% anisotropy in the cross-section.

Experiments on Vibrational Rotational Energy Transfer (VRET) have been conducted under conditions where vibration changing collisions were relatively probable. Under these circumstances RET generally occured so fast that it smeared out the rotational distribution, rendering it impossible to study the influence of rotation in the vibrational energy transfer process. Our apparatus was sensitive enough to detect vib-rotational energy transfer at such low perturbed pressures that competition from RET collisions was minimized. Thus we were able to clearly see the effects of rotation on the vibrational energy transfer processes and vice versa.

Our studies of collisional energy transfer processes in molecules, with particular emphasis on Rotational and Vib-Rotational Energy Transfer (RET and VRET) were satisfactory. We have made progress with both our discovery of two simple three parameter fitting laws for RET processes, and our pioneering measurements of the velocity dependence of the RET cross sections in Na_2^*-Xe made by utilizing the Doppler shift to provide velocity selection of the molecules.

The work which we have accomplished is scientifically valuable in three major areas: technique, understanding, and application. Our techniques for careful gas cell measurements combined with those for Doppler velocity selection enable us to study energy transfer processes in great detail: we can select the initial level, rotational level, and kinetic energy, and monitor the final vibrational and rotational level. This amount of specificity is an advance in the number of controlled plus analyzed degrees of freedom over current state of the art for similar experiments. We believe that tunable lasers and Doppler velocity selection can give results whose scientific utility equals that of crossed molecular beams machines, and that they will be superior in productivity. Our experiments have also paved the way for future experiments in which Doppler velocity analysis techniques are used to determine the angular distribution of products of collisions.

Because our techniques are well suited to the study of energy transfer in atom-diatom collisions, we have made major contributions to the scientific understanding of these processes. Our power law for rotational energy transfer processes resulted from gathering data over a wide range of physical variables and then seeking the physical framework in which it could be represented most economically. This work has proved useful to people studying flames and to astrophysicists. We also are beginning to understand where the power law comes from theoretically, and why it fits RET data for so many systems.

Finally, our results will have practical value because the collisional transfer rates for molecular energy are an important parameter in many devices and processes of current importance: lasers, MHD generators, and combustion being but three examples. Our fitting laws are most useful in this regard because they form a valid basis for modeling such systems.

Results on the work accomplished are described in papers already published or accepted for publication.

Journal Papers

T. A. Brunner, R. D. Driver, N. Smith, and D. E. Pritchard, "Simple Scaling Law for Rotational Energy Transfer in Na_2^* - Xe Collisions," Phys. Rev. Lett. 41:13, 856-859 (1978)

T. A. Brunner, R. D. Driver, N. Smith, and D. E. Pritchard, "Rotational Energy Transfer in Na_2^* - Xe Collisions Level to Level Dynamics" J. Chem. Phys. 70, 4155-4167 (1979)

T. A. Brunner, N. Smith, and D. E. Pritchard, "New Experimental Evidence for the Energy Corrected Sudden Scaling Law," Chem. Phys. Lett. 71:2, 358-362 (1980)

T. A. Brunner, N. Smith, A. W. Karp, and D. E. Pritchard, "Rotational Energy Transfer in $Na_2^*(A\Sigma)$ Colliding with Xe, Kr, Ar, Ne, He, H_2, CH_4 and N_2: Experiment and Fitting Laws"(to be published in J. Chem. Phys.)

D. E. Pritchard, N. Smith, R. D. Driver, and T. A. Brunner, "Power Law Scaling for Rotational Energy Transfer," J. Chem. Phys. 70, 2112-2120 (1979)

N. Smith, T. A. Brunner, A. W. Karp, and D. E. Pritchard, "Velocity Dependence of Rotational Energy Transfer Rates in Na_2^* - Xe, " Phys. Rev. Lett. 43:10, 693-697 (1979)

N. Smith, T. A. Brunner, and D. E. Pritchard, "Velocity Dependence of Rates for Rotationally Inelastic Collisions in Na_2^* - Xe Using Velocity Selection by Doppler Shift" (to be published in J. Chem. Phys.)

N. Smith and D. E. Pritchard, "Simple Analytical Approximation for Rotationally Inelastic Rate Constants Based on the Energy Corrected Sudden Scaling Law," (to be published in J. Chem. Phys.)

M. Wainger, I. Al-Agil, T. A. Brunner, A. W. Karp, N. Smith, and D. E. Pritchard, "Power Law Scaling of Rotational Energy Transfer in $Na_2(A\Sigma)$ + He, H_2, CH_4 and N_2 (J. Chem. Phys. 71:4, 1977-1978 (1979)

Meeting Papers Presented

1978 Spring Meeting, American Physical Society, Washington, D.C.

April 24-27, 1978

R. D. Driver, T. A. Brunner, N. Smith, and D. E. Pritchard, Rotational Energy Transfer in $Na_2(A^1\Sigma)$ - Xe Collisions

Division of Physical Chemistry Meeting, American Chemical Society, Honolulu, Hawaii

April 1-6, 1979

T. A. Brunner, R. D. Driver, N. Smith, and D. E. Pritchard, Simple Scaling Law for Rotational-Energy Transfer in Na_2^* - Xe Collisions

T. A. Brunner, N. Smith, R. D. Driver, and D. E. Pritchard, Velocity Dependence of Rate Constants for Rotation Changing Collisions in Na_2^* - Xe

M. Wainer, I. Al-Agil, T. A. Brunner, A. Karp, N. Smith, and D. Pritchard, Rotational Energy Transfer (RET) of $Na_2^*[A^1\Sigma\ ]$ in Collision with He, Ne, Ar, Kr, H_2, N_2, and CH_4

Sixth International Conference on Molecular Energy Transfer, Comtral Center, Lionjas, Rodez, France

July 16-20, 1979

T. A. Brunner, N. Smith, R. D. Driver, and D. E, Pritchard. Rotational Energy Transfer in Na_2^* - Rare Gas Collisions Level to Level Dynamics

1980 March Meeting, AmericanPhysical Society, New York, New York

March 24-28, 1980

T. A. Brunner, M. Durand, N. Smith, and D. E. Pritchard, Rotational Energy Transfer in $I_2(B^3\Pi)$ - Xe

D. E. Pritchard, Scaling Laws for Rotational Energy Transfer: Experiment and "Theory" (Invited)

35th Annual Symposium on Molecular Spectroscopy, Columbus, Ohio

June 16-20, 1980

T. A. Brunner, N. Smith, and D. E. Pritchard, Fitting Laws for Rotational Energy Transfer

N. Smith, T. A. Brunner, and D. E. Pritchard, Velocity Dependence of Rotational Energy Transfer Rates in Na_2^* - Xe

XI International Quantum Electronic Conference, Boston, Massachusetts

June 23-26, 1980

T. A. Brunner, M. Durand, and D. E. Pritchard, Rotational Energy Transfer in $I_2^*(B^3\Pi)$ - Xe

Seventh International Conference on Atomic Physics, Cambridge, Massachusetts

August 4-8, 1980

T. A. Brunner, N. Smith, and D. E. Pritchard, Experimental Evidence for the Wide Applicability of Power Fitting Laws for Rotational Energy Transfer

N. Smith, T. A. Brunner, and D. E. Pritchard, Calculation of Rotational Energy Transfer Rate Constants for $j \rightarrow O$ Transitions

Division of Physical Chemistry Meeting, American Chemical Society, San Francisco, California

August 25-26, 1980

T. A. Brunner, N. Smith, and D. E. Pritchard, Power Laws for Fitting Rotational Energy Transfer Data: Theoretical Justifications

D. E. Pritchard, Rotationally Inelastic Collisions: Experiment and "Theory" (Invited)

We have given Seminars on this work at several industrial corporations and numerous universities.

Personnel

Dr. D. E. Pritchard	-	Professor
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