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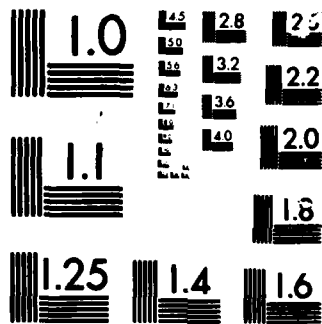
EXPERIMENTAL CHEMICAL PHYSICS: A 'NEXT GENERATION'
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ABSTRACT

An experimental arrangement is described which is used for studying gas phase elementary processes as well as gas/surface interactions. It consists of two separate parts: A photofragment spectrometer with LIF detection is used to study photoinitiated unimolecular and bimolecular reactions. An ultra high vacuum scattering chamber with MPI and mass spectrometric detection is used to probe fragments generated via molecule/molecule and molecule/surface interactions. A sophisticated data acquisition system is described based on LSI/11 23⁺ laboratory computers, that includes digital data collection, programmable pulse-and-delay generators, and simultaneously monitoring signals from several chemically distinct species.

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Final Report on Contract Research Entitled:

EXPERIMENTAL CHEMICAL PHYSICS: A 'NEXT GENERATION' MACHINE

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I. INTRODUCTION

This final report outlines our results obtained on AFOSR Grant number AFOSR-84-0294 during the period July 30, 1984 to July 29, 1985.

During this year we completed the assembly of an experimental arrangement that allows us to study elementary gas phase processes, as well as gas/surface interactions. Our philosophy was to direct a concerted effort into the study of all the facets of reaction dynamics, and to acquire facilities that will enable us to employ diverse excitation and diagnostic techniques. Our goal is to study the interactions of atoms and molecules that have defined energies and angular momenta with photons, isolated gas-phase molecules, clustered species, and surfaces. For these purposes we constructed the two experimental assemblies described below.

II. LIF PHOTOFRAGMENT SPECTROMETER

An LIF photofragment spectrometer was constructed for studies of unimolecular and bimolecular reactions. The emphasis here is on measuring vectorial as well as scalar properties (i.e. in addition to measuring E,V,R,T distributions in the fragments, Doppler shift measurements are used to determine the recoil anisotropies). This apparatus, which has 26 available ports, uses routinely 2 dye laser systems, 2 PMT's, and a pulsed nozzle for cooling the parent molecules. All signals are digitized and transferred to an LSI 11/23⁺ lab computer at 10 Hz, the repetition rate of the synchronized lasers. Digitizers with 10

ns (Transiac) or 50 ns (Nicolet, Explorer) resolution are interfaced with the computer, which averages the data as well as triggers the lasers, and the pulsed nozzle. All signals are normalized on a shot-to-shot basis to the lasers' intensities which are also monitored and stored by the computer.

In addition, we have developed a computer controlled pulse and delay board with 10 ns resolution and <2 ns jitter. The board has 5 pulse outputs with amplitudes of 5-20 V, which are used to trigger the lasers and the pulsed nozzle. The timing between the pulses can be programmed by the computer with variable delays of 10 ns - 1 s. We are presently preparing a manuscript that describes the design and operation of the pulse and delay board (see ref. 3 in publication list).

The LIF photofragment spectrometer has been used already in the studies of CN recoil anisotropies from ICN photolysis (ref. 1), and 2 photon LIF detection of $I(^2P_{1/2})$ and $I(^2P_{3/2})$ from ICN (ref.2). It is currently being used to study the reaction of H atoms with ClCN.

III. MPI-TOF ULTRA HIGH VACUUM SCATTERING CHAMBER

As we indicated in our original proposal, it may not be feasible to perform LIF and TOF-MPI experiments simultaneously. Therefore, we have built a separate ultra high vacuum chamber designed specifically for MPI-TOF detection of fragments. Using this experimental arrangement, we can probe molecule/molecule interactions in the gas phase, as well as molecular-beam/surface interactions. In order to work with molecular beams and clean single crystal surfaces, we constructed a UHV stainless steel

scattering chamber, capable of $< 10^{-9}$ Torr. A pulsed nozzle chamber pumped to $< 10^{-6}$ Torr is connected to the scattering chamber via one stage of differential pumping. Single crystal surfaces are mounted in the scattering chamber on a UHV manipulator, equipped with a sample heating assembly. Laser excitation of parent molecules in the incoming beam and/or fragments formed via surface collisions is achieved using the outputs of 2 dye laser systems through quartz windows. The fragments are probed via MPI and their E,V,R,T distributions can be obtained. A quadrupole mass spectrometer serves to characterize the molecular beam, and to determine the time-of-flight of the fragments and their angular distributions. The surface cleanliness is monitored before and during experiments by He or H₂ diffraction.

The data acquisition system is very similar to the one described for the LIF photofragment spectrometer described above. It consists of 2 laser systems, a quadrupole MS, a channeltron electron multiplier, digital scopes, a pulse-and-delay board, and a lab computer that controls the firing of the lasers and opening of the pulsed nozzle, averages the data and processes the results. This system is now nearing completion and preliminary results are anticipated soon.

PUBLICATIONS

1. I. Nadler, D. Mahgerefteh, H. Reisler, and C. Wittig, J. Chem. Phys. **82**, 3885 (1985).
2. S. Callister, H. Reisler, and C. Wittig, to be published.
3. C.X.W. Qian, F. Niertit, H. Reisler, and C. Wittig, to be published.

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