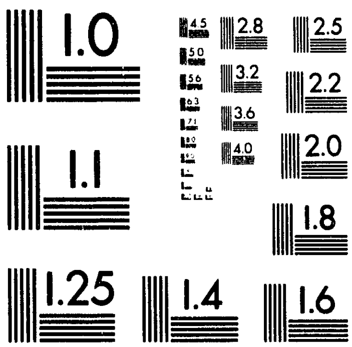
1.0
2.8
2.5
3.2
2.2
3.6
4.0
2.0
1.1
1.8
1.25
1.4
1.6

Quarterly Technical Progress Report to DOE
Fourth Quarter: 4/01/93-6/30/93

1. Principal Investigator: John W. Farley,
Associate Professor, Department of Physics, UNLV

2. Project Title: Studies of clusters

3. Accomplishments During the Interval:

This quarterly progress report should be read in conjunction with the previous quarterly progress reports. The overall goals are to establish a research group at UNLV working on molecular clusters, and to interact with other scientists in the same general research area. The clusters will then be used as "model systems" in order to test theories that purport to account for retardation factors in the migration of radionuclides. If the underlying theory can be verified, it will enhance confidence in the theory, and it may be possible to reduce the uncertainty in the retardation factors. In order to reach that goal, we need to fabricate a source of cluster ions, and to develop the laser techniques that will be used to probe the cluster ions.

In this quarter, we succeeded in producing positive cluster ions and measuring the mass spectrum using a radiofrequency quadrupole mass spectrometer. Mass spectrum are attached, showing the cluster ions produced using pure ammonia. They have the general formula $(NH_3)_nH_m^+$, where n and m are integers. [illegible] 1 shows n = 1-4, and Fig. 2 shows peaks with n=1-7. Peaks with [illegible]erent numbers of hydrogens (denoted by the integer m in the above formula) can barely be resolved. This is great news, because it shows that the ion source can produce cluster ions.

The development of sensitive laser techniques is necessary for probing the clusters. During this quarter, we succeeded in using a weak diode laser to probe a beam of negative molecular ions, NH^-. This is the first time that diode lasers have been used to perform autodetachment spectroscopy on a negative molecular ion. The resonance is shown in Fig. 3 below. This work will be written up for publication. We plan to submit it to Physical Review Letters, the most prestigious journal in physics.

The work on the visible absorption spectrum of D_2O^+ continues, and is now in the analysis phase. We expect to complete the assignment of quantum numbers and write it up for publication soon.

The work on the infrared vibrational-rotational spectrum of $H^{15}NO^-$ continues. The analysis is difficult. We are attempting to combine this data and our earlier data on $H^{14}NO^-$ in order to obtain a unique geometry for the ion.

In the second ion beam machine, a complete reworking of the voltages has been completed, and we are in the process of reassembling the apparatus. We expect to have new results on that apparatus in the early fall.

During the quarter, three presentations were made at the annual meeting of the Division of Atomic, Molecular and Optical Physics: one reporting our experimental measurements of the visible absorption spectrum of D_2O^+, one reporting our experimental measurements of the infrared vibrational-rotational spectrum of $H^{15}NO^-$, and one reporting the results of the theoretical calculation of the geometry of HNO^-.

The work on clusters cannot succeed without parallel theoretical work to guide the experiment and assist in interpreting the results. During the quarter, a manuscript was submitted to the Journal of Chemical Physics, reporting the results of the first calculation ever of the geometry of HNO^-. This is the first of what we expect will be a series of publications reporting the results of theoretical calculations, closely tied to experiment.

Also, during the interval, an article was published, reviewing our spectroscopic work on molecular ions: "High-Resolution Laser Spectroscopy of Molecular Ions." This is a conference proceeding, reporting the result of an invited talk given in January 1993.

Three undergraduates continued their progress in the laboratory: Mr. Ray Keeler, Ms. Debra Maxwell, and Mr. Umar Younas. They were joined by a fourth undergraduate, Mr. Andrew White, an undergraduate student from Reed College, who is working in the laboratory during the summer as part of the Research Experience for Undergraduates (REU) program, funded by the National Science Foundation. Mr. Wen Shen, a graduate special student, joined the group and began working on the cluster ion source.

Personnel

John W. Farley	Associate Professor of Physics
Daniel Cowles	Postdoctoral Research Associate
Ravi Marawar	Postdoctoral Research Associate
Qiang Tu	Graduate student, Physics
Wen Shen	Graduate special student, Physics
Umar Younas	Undergraduate student, Engineering
Ray Keeler	Undergraduate student, Physics
Debra Maxwell	Undergraduate student, Physics
Andrew White	Undergraduate student (Reed College), Physics

Presentations

"Experimental Determination of the Geometry of HNO^-," Daniel C. Cowles and John W. Farley, abstract submitted to DAMOP meeting, May 1993.

"Theoretical Study of the Geometry of HNO^-," Kathleen A. Robins, John W. Farley, and Joseph L. Toto, abstract submitted to DAMOP meeting, May 1993.

"Measurement of the visible absorption spectrum of D_2O^+ by velocity-modulation spectroscopy," Ravi Marawar and John W. Farley, abstract submitted to DAMOP meeting, May 1993.

Publications

"High-Resolution Laser Spectroscopy of Molecular Ions," John W. Farley, in Laser Techniques for State-Selected and State-to-State Chemistry, Proced. of Society of Photo-Optical Instrumentation Engineers, 1858 92 (1993).

"An Ab Initio Study of HNO^-, HNO and HO_2," K. A. Robins, J. W. Farley, and J. L. Toto, J. Chem. Phys. (submitted).

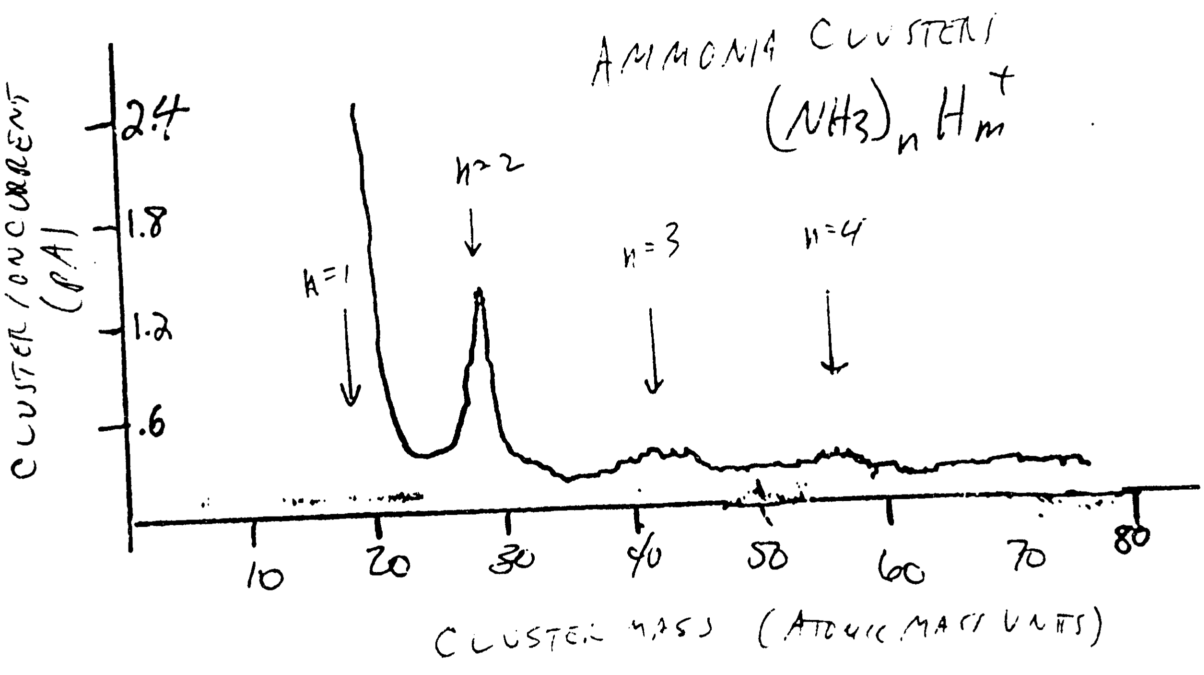

Fig. 1. Mass spectrum of cluster ions produced from ammonia, having the formula $(NH_3)_nH_m^+$. Peaks with n = 1-4 are visible.

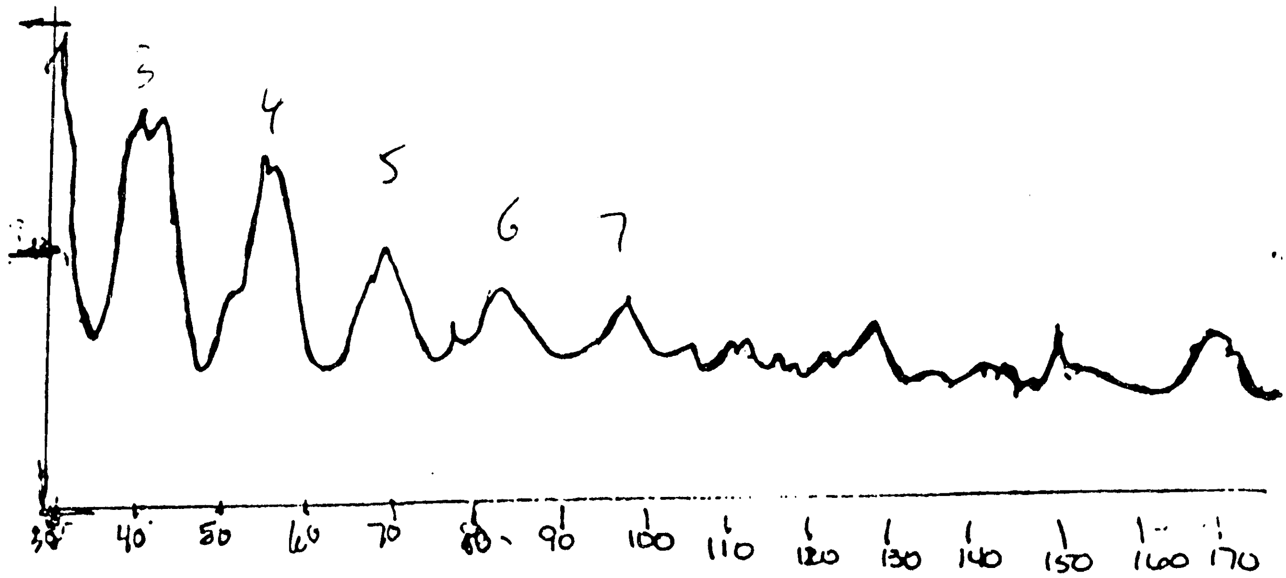

Fig. 2. Mass spectrum of cluster ions produced from ammonia, showing n = 3-7.

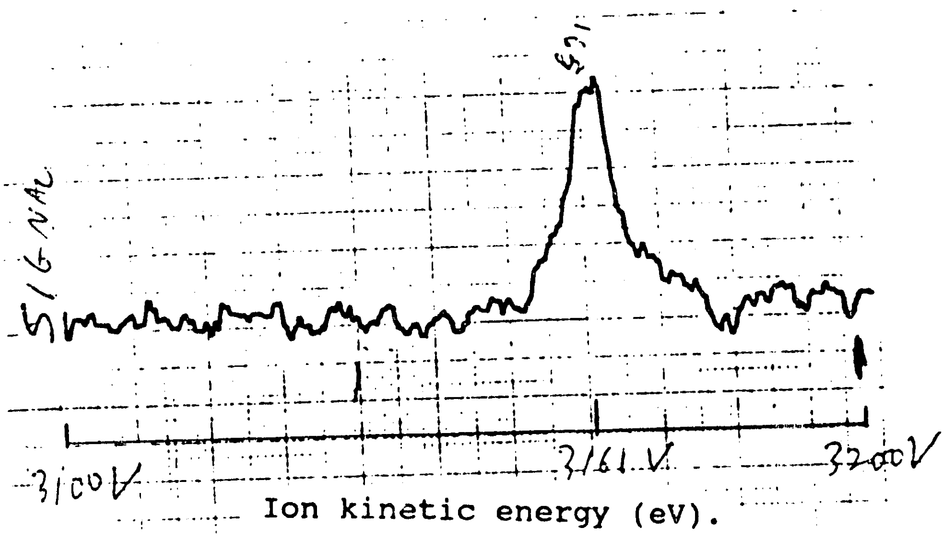

Fig. 3. First observation of the P_1 (6.5, e->e) transition in NH^-. The diode laser is tuned into coincidence with a reference line in neutral N_2O at 2807.84266 cm^{-1}, denoted by R_{11} (0111E-0000E). The ion transition is observed when the kinetic energy of the ions is 3161 keV. In the rest frame of the ion, the laser has a frequency of 2805.983 cm^{-1}. The lock-in time-constant is 30 seconds, and the entire scan takes 30 minutes.

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