

# REPORT DOCUMENTATION PAGE

Form Approved  
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED FINAL 01 Jul 94 To 30 Nov 96	
4. TITLE AND SUBTITLE PHOTO-INITIATED ION-MOLECULAR REACTIONS IN SIZE-SELECTED CLUSTERS		5. FUNDING NUMBERS F49620-94-1-0412 3484/XS 61103D	
6. AUTHOR(S)  Dr Daniel M. Neumark			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) University of California Dept of Chemistry Berkeley CA 94720-1460		AFOSR-TR-97  0580	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NL 110 Duncan Ave Room B115 Bolling AFB DC 20332-8050  Dr Michael R. Berman		10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES			
12a. DISTRIBUTION/AVAILABILITY STATEMENT  <b>Approved for public release; distribution unlimited.</b>			
13. ABSTRACT (Maximum 200 words)  During the grant period, this work has focused on two research areas: zero electron kinetic energy (ZEKE) spectroscopy experiments on mass-selected cluster anions in which a halide ion (Cl or I) is solvated with a known number of rare gas atoms, and stimulated Raman pumping of negative ions. Negative ion ZEKE spectroscopy is a high resolution laser photodetachment experiment which yields information on the vibrational and electronic spectroscopy of both the anion cluster and the neutral species formed by photodetachment. By performing this experiment on a series of clusters (Ar <sub>n</sub> I, for example), one learns how the stepwise solvation of the halide ion affects the anion and neutral energetics and spectroscopy. We have measured ZEKE spectra of Ar <sub>n</sub> Cl, Ar <sub>n</sub> Br, Ar <sub>n</sub> I, and XenI clusters. In all cases, we obtain high quality intermolecular potentials for the diatomic neutral and anionic (i.e. n=1) clusters, and learn about the how the spin-orbit levels of the neutral halogen atom are perturbed by the rare gas atom. We have also performed stimulated Raman pumping in C <sub>2</sub> , the first such observation for a molecular negative ion.			
14. SUBJECT TERMS			15. NUMBER OF PAGES
			16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT (U)	18. SECURITY CLASSIFICATION OF THIS PAGE (U)	19. SECURITY CLASSIFICATION OF ABSTRACT (U)	20. LIMITATION OF ABSTRACT (UL)

19971106 165

Daniel M. Neumark

AFOSR/AASERT Grant Number F49620-94-1-0412

Photo-Initiated Ion-Molecular Reactions in Size-Selected Clusters

## FINAL TECHNICAL REPORT

AASERT funds have been used to support the research of a graduate student, Mr. Ivan Yourshaw, in conjunction with his efforts on my primary AFOSR grant (FR49620-94-1-0115). During the grant period, this work has focused on two research areas: zero electron kinetic energy (ZEKE) spectroscopy experiments on mass-selected cluster anions in which a halide ion ( $\text{Cl}^-$  or  $\text{I}^-$ ) is solvated with a known number of rare gas atoms, and stimulated Raman pumping of negative ions. Negative ion ZEKE spectroscopy is a high resolution laser photodetachment experiment which yields information on the vibrational and electronic spectroscopy of both the anion cluster and the neutral species formed by photodetachment. By performing this experiment on a series of clusters ( $\text{Ar}_n\text{I}^-$ , for example), one learns how the stepwise solvation of the halide ion affects the anion and neutral energetics and spectroscopy.

Thus far we have measured ZEKE spectra of  $\text{Ar}_n\text{Cl}^-$ ,  $\text{Ar}_n\text{Br}^-$ ,  $\text{Ar}_n\text{I}^-$ , and  $\text{Xe}_n\text{I}^-$  clusters. In all cases, we obtain high quality intermolecular potentials for the diatomic neutral and anionic (i.e.  $n=1$ ) clusters, and learn about the how the spin-orbit levels of the neutral halogen atom are perturbed by the rare gas atom. Using this information, we can then deduce the nature and extent of non-additive forces that play a role in the  $n>1$  clusters. We find the largest effects to be in the anion clusters, primarily through induction (i.e. the interaction between neighboring charge-induced dipoles) and exchange-induced quadrupole effects in the solvent atoms. Previously, many-body effects in clusters have been studied through the observation of small spectral shifts in high resolution spectra. Our results directly yield the solvent binding energies in these clusters, and this appears to be a clearer probe of non-additive forces in clusters.

The  $\text{Ar}_n\text{Cl}^-$  experiments are of particular interest because our results can be directly compared to detailed theoretical treatments of these clusters. The  $\text{Xe}_n\text{I}^-$  experiments are of interest in light of recent experiments by Cheshnovsky and co-workers in which the cluster analog of the charge-transfer-to-solvent (CTTS) band has been observed for these species. Our experiments will indicate whether this band lies above or below the adiabatic detachment energy for these clusters, a vital piece of information in the interpretation of the CTTS studies.

We have also performed stimulated Raman pumping in  $\text{C}_2^-$ , the first such observation for a molecular negative ion. In stimulated Raman pumping, a vibrational transition is pumped by two lasers, one tunable and one fixed in frequency, whose frequency difference equals the energy of the vibrational transition. In this case we pump the  $v=0, N=2$  level of  $\text{C}_2^-$  to the  $v=1, N=2$  level, and use resonant two-photon detachment (R2PD) to probe either depletion of the  $v=0$  level or gain in the  $v=1$  level resulting from stimulated Raman excitation. This bodes well for the primary goal of this research, in which stimulated Raman pumping will be used as a general means of vibrationally exciting negative ions and measuring their photoelectron spectra.