TRANSITION STATE DYNAMICS OF $\mathrm{Ar}_n(\mathrm{ClHCl})$, (n = 0,...,5)

HOLLY B. LAVENDER, ANNE B. McCOY, *Department of Chemistry, The Ohio State University, Columbus, OH 43210*.

The effects of "microsolvation" on the transition state dynamics of the Cl + HCl reaction are investigated through time dependent quantum calculations of the photodetachment spectrum of $\mathrm{Ar}_n(\mathrm{ClHCl}^-)$, with n = 0,...,5. These systems were studied by propagating the ground state wave function of $\mathrm{Ar}_n(\mathrm{ClHCl}^-)$ on the $\mathrm{Ar}_n(\mathrm{ClHCl})$ surface, using a reduced dimensional approximation to the wave function. Our calculations show substantial differences in the projections of the probability density onto the coordinates of the hydrogen atom resulting from the presence of one or more argon atoms. The structure of the calculated spectra remains essentially the same, but we see a red shift as the size of the cluster increases. This talk will focus on the effects on the wave function and resulting calculated spectra as a result of adding argon atoms to the system. These calculations are of interest, because they provide insight into the nature of solvent effects on the transition state of the elementary Cl + HCl reaction.