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

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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. Because of the large mass of the Cl atoms relative to that of hydrogen, they move very little over the timeframe of the calculation. Thus, the wave function in the Cl-Cl stretch coordinate can be described by a semiclassical approximation. In this work, we have used the Gaussian wavepacket propagation scheme of Heller, together with the mixed quantum/semi-classical time-dependent self-consistent field method (Q/SC-TDSCF) to couple the quantum modes with the semi-classical motion of the Cl atoms. 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. In addition, we see an increasing trend towards colinear dissociation of Cl-H-Cl as argon atoms are added to the system. This is in contrast to the dissociation of the bare Cl-H-Cl species, in which the hydrogen atom tends to rotate out of the center. 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, the reaction dynamics, 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.