THEORETICAL STUDIES OF THE PHOTOELECTRON SPECTROSCOPY OF $\mathrm{Ar}_n\cdot(\mathrm{IHI})^-$ $(n = 0 - 20)$

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In this talk we focus on a theoretical investigation of the effects of argon atoms on the transition state region of the I + HI reaction. To understand the effects of the introduction of argon atoms in our system, we construct potential energy surfaces for $\mathrm{Ar}_n\cdot(\mathrm{IHI})^-$ and $\mathrm{Ar}_n\cdot(\mathrm{IHI})$ and perform time–independent simulations of the photoelectron spectra of $\mathrm{Ar}_n\cdot(\mathrm{IHI})^-$ by calculating Frank–Condon overlaps between the anion and the neutral wave functions. Our results show more stabilization of the anionic species than the neutral complex with increasing number of argon atoms. Experimentally this stabilization leads to a shift of the photoelectron spectra of $\mathrm{Ar}_n\cdot(\mathrm{IHI})^-$ to lower electron kinetic energies.[a] Excellent agreement between the experimental and calculated shifts are found.[b] Finally, analysis of the resulting anion wave functions shows that the introduction of argon atoms limits the motion of the hydrogen atom causing a stronger localization of the hydrogen atom near the center of the complex.

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[a] Z. Liu, H. Gómez, and D. M. Neumark, Faraday Discuss. **118**, 221 (2001)

[b] J. G. López and A. B. McCoy, J. Phys. Chem. A, **109**, 1272 (2005)