TIME-RESOLVED RECOMBINATION DYNAMICS OF $IBr^-(CO_2)_n$ CLUSTERS

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We report the femtosecond dynamics of $IBr^-(CO_2)_n$ (n = 5, 6, 7, 8, 10) clusters. Excitation to the dissociative IBr^- $A'\ ^2\Pi_{1/2}$ state of the chromophore is achieved with a 180 fs 795 nm laser pulse. Dissociation from the A' state of the bare anion results in I^- and Br products. Solvent molecules surrounding the dihalide chromophore promote recombination of the dissociating IBr^-, in part through a solvent-induced well on the A' state that can trap the evolving cluster. The recombination time is determined by using a delayed femtosecond probe laser at the same wavelength, detecting recombined IBr^- cluster ions. In sharp contrast to previous I_2^- studies, the observed recombination times increase dramatically with increasing cluster size, from 15 ps for n = 5 to 900 ps for n = 10. Extensive electronic structure calculations and non-adiabatic molecular dynamics simulations provide a framework to understand this unexpected behavior.

Supported by NSF and AFOSR