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The Solvation and Photochemistry of $HI(H_2O)_n$ Clusters: Evidence of Excited State Biradical Formation and Implications to the Solvated Electron[1] NICHOLAS BIANCO, DARREN HYDUTSKY, A.W. CASTLEMAN, JR., Penn State University — The fundamental understanding of the dynamics of chemical reactions is an important step to a firm foundation of knowledge in many areas of science, including atmospheric chemistry. The dissolution of acids in water is one type of atmospheric reaction whose dynamics are in need of understanding, as this is a process which frees halogens, allowing them to react with and, as a result, break down ozone. In order to study this process, we employ a femtosecond laser system coupled to a time-of-flight mass spectrometer. This setup allows us to perform pump-probe experiments on a small cluster of molecules, thereby tracking the dynamics of the process. While investigating the $HI(H_2O)_n$ system, we observed unusual behavior associated with the iodine atoms. Upon further experimentation, we conclude that these findings provide experimental evidence for the biradical, a theoretically predicted species consisting of a halo-acid clustered to water molecules. In addition to its atmospheric relevance, the biradical is a structure that could better explain many phenomena currently thought to be the result of the cavity-bound hydrated electron.

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