REACTION DYNAMICS OF THE BROMINE-BROMOFORM COMPLEX IN SOLUTION

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We have followed the evolution of the bromine species that arise from the photolysis of bromoform in the condensed phase. Solvent caging promotes the formation of iso-bromoform (CHBr₂-Br), which can then release a Br atom by breaking the newly formed Br-Br bond. This ejected Br can form a van der Waals complex (Br-CHBr₃) with a nearby un-photolyzed bromoform molecule, which is stable during our 1 ns time-window. Using the van der Waals complex as a reservoir for Br atoms, we now proceed to drive hydrogen abstraction from CHBr₃ by Br. Estimates indicate that the barrier to this reaction is a few thousand wavenumbers. Our goal is to introduce excitation into the C-H stretching motion of a nearby solvent CHBr₃ to access the activated complex region of the bimolecular potential energy surface.