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Excited State (?) Proton Transfer in Benzimidazole Homodimer – An Experimental and Ab-Initio Study

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Abstract

Hydrogen bonds, which are abundant in nature give rise to a variety of phenomena that range from the anomalous behavior of water to the double helical nature of DNA. Further, these can play a decisive role in chemical reactions and could also be a gateway to proton transfer. Among the H-bonded systems, the N-H...N interactions are most interesting because of their abundance in the naturally occurring systems like the nucleic acids and proteins.

I will present our recent investigations on a model N-H...N hydrogen bonded dimer of benzimidazole (BIM) where we observe a proton transferred product at energies far below the thermochemical limit. Ion Depletion IR Spectroscopy was used to confirm that the dimer had an N-H...N hydrogen bonded structure. Mass selective excitation spectra, obtained using the two colour two photon resonantly enhanced ionization (2cR2PI), showed that the BIM dimer dissociates to give the protonated BIM fragment (H-BIM)⁺. Monitoring the fragment channel at various photon energies and supporting ab-initio calculations of the neutral ground, excited, and the cationic states has led us to believe that the proton transfer is a result of the relaxation of the electronically excited dimer into a charge transfer state and the subsequent dynamics. We present the experimental and computational observation of a proton transfer in the excited state of the BIM dimer.

Keywords: Excited State Proton Transfer, Benzimidazole dimer