PROBING REACTION CHANNELS OF CHLOROBENZENE-AMMONIA CLUSTERS: A TWO-COLOR STUDY.

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Noncovalent interactions including π-π stacking, CH/π interactions and halogen bonding play a significant role in many chemical and biological processes. Understanding their nature and behavior gives insight into how they influence processes such as protein folding, molecular self-assembly, and drug-substrate interactions. Using a combination of velocity mapped ion imaging, two-color photoionization, and theoretical calculations we probe the chlorobenzene-ammonia cluster system. From our previous studies, we have insight into the reactive pathways as well as the possible geometries of the σ-type reaction intermediate (Reid, et al. 2013 [a]). This study is focusing on probing the reaction pathways around the activation energy. The first photon is for excitation and a time delayed second photon is for ionization to initiate the radical reaction. The dimer cation radical reacts via Cl- atom or HCl loss pathways forming protonated aniline and aniline cation respectively or H-atom loss forming ortho-chloro protonated aniline. The energy of the photons can be controlled enabling the experiment to determine threshold energy of the reaction as well as confirm the primary reaction channel.

[a] S.A Reid, S. Nyambo, A. Kalume, B. Uhler, C. Karshenas, L. Muzangwa, J.Phys. Chem. A 2013, 117, 12429-12437