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Experimental and Computational study of azobenzene and 2,2',6,6'-tetrafluoroazobenzene cation.[1] MOHAMMADREZA REZAEE, Department of Physics and Astronomy, Texas AM University, PETER B. ARMENTROUT, University of Utah — The electronic structure of the protonated azobenzene and it its derivative 2,2',6,6'-tetrafluoroazobenzene were studied using ab initio methods and the bond strength were measured utilizing the collision induced dissociation experiment. Several highly accurate multi-level schemes such as different variations of the Complete Basis Set (CBS) method and the Gaussian (G-n) theory along with DFT study employed to accurately compute the energies of the neutral and the parent cation as well as the fragment ions. The transition state were studied and the dissociation path was identified using B3LYP method along with aug-cc-pVTZ as the basis set. Thermochemical properties such as proton affinity, gas phase basicity and the bond dissociation energies were calculated. Molecular electrostatic potential analysis was performed to identify the charge distribution inside the molecule to study the effects of the protonation reaction.

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