UNRAVELING PROTON TRANSFER IN STEPWISE HYDRATED N-HETEROCYCLIC ANIONS

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Depending upon the number and location of nitrogen atoms in a N-heterocyclic azabenzene, the addition of a single water molecule can result in a positive electron affinity. The transfer of a proton from a solvating water azine base can be induced by excess electron attachment. Here we explore this phenomenon through the use of photoelectron spectroscopy and electronic structure theory. Carefully calibrated density functional theory (DFT) computations indicate that the excess electron predominantly resides in a π* orbital of the heterocycle.