ENERGETICS OF THE GAS PHASE MONOHYDRATES OF TRANS-FORMANILIDE : A MICROSCOPIC APPROACH TO THE HYDRATION SITES OF THE PEPTIDE BOND

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The energy of binding a water molecule to two H-bonded sites of trans-N-phenyl formamide (formanilide), an amide molecule that mimics the planar -NH-CO- peptide bond, has been measured in the gas-phase and calculated by an ab initio study. For the first time, the D0 dissociation energies of two 1:1 complexes, simultaneously observed in a supersonic expansion, is measured experimentally. They are found to be very similar. At the CO site, the water molecule acts as a proton donor and the H-bond has a energy of 5.40 +/- 0.28 kcal/mol. At the NH site, the water acts as an acceptor and the binding energy is 5.65 +/- 0.30 kcal/mol. Comparison of IR shifts with binding energies shows that they do not always correlate when the donor groups are different.