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Hydration of the pyrimidine radical cation and stepwise solvation of protonated pyrimidine with water, methanol, and acetonitrile

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Abstract

Equilibrium thermochemical measurements using an ion mobility drift cell technique have been utilized to investigate the binding energies and entropy changes associated with the stepwise hydration of the biologically significant ions pyrimidine radical cation and protonated pyrimidine. The binding energy of the hydrated pyrimidine radical cation is weaker than that of the proton-bound dimer pyrimidineH(+) (H₂O) consistent with the formation of a weak carbon-based CH delta+ center dot center dot OH₂ hydrogen bond (11.9 kcal/mol) and a stronger NH+ center dot center dot OH₂ hydrogen bond (15.6 kcal/mol), respectively. Other proton-bound dimers such as pyrimidineH(+)(CH₃OH) and pyrimidineH(+)(CH₃CN) exhibit higher binding energies (18.2 kcal/mol and 22.8 kcal/mol, respectively) due to the higher proton affinities and dipole moments of acetonitrile and methanol as compared to water. The measured collisional cross sections of the proton-bound dimers provide experimental-based support for the DFT calculated structures at the M06-2x/6-311++G (d,p) level. The calculations show that the hydrated pyrimidine radical cation clusters form internally solvated structures in which the water molecules are bonded to the C₄N₂H₄ center dot+ ion by weak CH delta+ center dot center dot OH₂ hydrogen bonds. The hydrated protonated pyrimidine clusters form externally solvated structures where the water molecules are bonded to each other and the ion is external to the water cluster. Dissociative proton transfer reactions C₄N₂H₄ center dot+(H₂O)(n-1) + H₂O -> C₄N₂H₃ center dot + (H₂O)(n)H+ and C₄N₂H₅+(H₂O)(n-1) + H₂O -> C₄N₂H₄ + (H₂O)(n)H+ are observed for n >= 4 where the reactions become thermoneutral or exothermic. The absence of the dissociative proton transfer reaction within the C₄N₂H₅+(CH₃CN)(n) clusters results from the inability of acetonitrile molecules to form extended hydrogen bonding structures such as those formed by water and methanol due to the presence of the methyl groups which block the extension of hydrogen bonding networks. (C) 2013 AIP Publishing LLC.

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