# Basicity and solvent effects on hydrogen bonding in NR3 ? HCOOH (R = H, CH3) model systems

Pérez, Patricia

Zapata-Torres, Gerald

Parra-Mouchet, Julia

Contreras, Renato

The effect of the basicity of methyl-amines on hydrogen bonding (HB) with HCOOH is examined in both gas and solution phases. In the gas phase, the strength of HB may be related to the proton affinity (PA) difference between the carboxylate anion and the methyl-amine, ?PA = PA(HCOO-) - PA(NR3). The changes in the driving potential ?PA are explained on the basis of electronic substituent effects. The electronic substituent effects are rationalized in terms of local reactivity indices such as the Fukui function and the local hardness and softness at the basic center. A simple model is then proposed to explain the enhancement HB in the solution phase. The HB pattern in the solution phase is changed by electrostatic and nonelectrostatic solvation of the zwitterionic and neutral species in equilibrium. 