

Self-consistent reaction field calculations on the proton transfer in ammonia-formic acid systems as a model for hydrogen bonding in amino acids in solution

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The reaction field (RF) model of solvent effects, implemented within the SCF-CNDO/2 scheme of calculation, has been applied to analyze the proton transfer in the $\text{NH}_3\text{-HCOOH}$ system in the presence of several polarizable media. The aim of such a study was to characterize the tautomeric equilibrium between the neutral and zwitterionic forms of H-bonded amino acids in aprotic solvents. Qualitative results concerning the energetics of this equilibrium show the stabilization of two different H-bonded complexes, corresponding to two separate minima in the free energy surface. These well known double minima potentials are found to be dependent on both the intermolecular N \cdots O distance and the strength of the reaction field. The behavior of this model is qualitatively consistent with experimental observations of nitrogen-substituted amino acids in solution: both show, for low values of the dielectric constant, tautomeric equilibria where the H-bonded complexes appear to be more stable than the corr