Theoretical Study on the Ground State Intramolecular Proton Transfer (IPT) in Two Schiff Bases Formed by 2-aminopyridine with 2-hydroxy-1- naphthaldehyde and 2-hydroxy Salicylaldehyde.

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Proton tautomerism is a general phenomenon in organic molecules and plays a vital role in many fields of chemistry and biochemistry. The study of ground state intramolecular proton (hydrogen) transfer (IPT) reactions has received increasing attention in the last few years aiming at the characterization of a large number of compounds in which rapid hydrogen migration occurs both in solution and in the solid state. Salicylidine aniline and its derivatives are among the earliest examples of a chemical system involving IPT. 2-hydroxy schiff base ligands and their complexes derived from the reaction of salicylaldehyde and 2-hydroxy-1-naphthaldehyde with amines have been extensively studied [1-3] and a number of them were usual as models for biological systems [4-5]. In the present work, we study IPT of the Schiff bases formed by 2-aminopyridine with 2-hydroxy-1- naphthaldehyde and 2-hydroxy salicylaldehyde in order compare the hydrogen bonding and tautomerism in those compounds in the gas phase and in solution. The results obtained from the ab initio calculations are compared with available experimental data.

Ab initio calculations suggest that the compound 1 exist mainly in the enol-imine form, and the compound 2 exist a mixture of enol and keto form in the gas phase. In polar solutions, Keto-amine form is dominant for molecule 2. All compounds were found to have planar structure in the gas phase and in solutions.

References