Excited state proton transfer reaction of two new intramolecularly hydrogen bonded Schiff bases at room temperature and 77K.

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Two new orthohydroxy Schiff bases, 7-phenylsalicylidene benzylamine (PSBA) and 7-ethylsalicylideneaniline (ESA) have been synthesized. The excited state intramolecular proton transfer (ESIPT) and the structure of PSBA and ESA in its crystalline form and in the solvents n-hexane, n-heptane and 1,4-dioxane have been investigated by means of absorption, emission and nanosecond spectroscopy at room temperature and 77K. One ground state species has been detected both in neutral and basic solutions of both PSBA and ESA: the cis-enol form with an intramolecular hydrogen bond. The ESIPT and formation of keto tautomer are evidenced by a large Stokes shifted emission (approximately 12000 cm(-1)) at room temperature only in the case of ESA. On the other hand the keto tautomer is the predominant species at 77K in a solid matrix and as a solid sample at room temperature both in the case of ESA and PSBA. In the case of both ESA and PSBA the more intense, higher energy emission is due to the species which has not undergone ESIPT and attributed mainly due to cis-enol form. The trans-enol form is also observed by changing the excitation wavelength. Both the compounds are found to undergo a structural change to a zwitterionic and intermolecular hydrogen bonded form in the presence of a strong base like triethylamine. From the nanosecond measurements and quantum yield of fluorescence we have estimated the decay rates of proton transfer reaction in the case of PSBA. Our theoretical calculation at the AM1 level of approximation shows that the ground singlet state has a rather large activation barrier both in the case of PSBA and ESA. The barrier height is much lower on the corresponding excited singlet surface only in the case of ESA. The process is predicted to be endothermic in the ground state and exotherrmic in the excited singlet state.

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