



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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SHORT ABSTRACT

Proton transfer is a fundamental process that plays a vital role in several natural processes. Azole derivative are important class of organic molecule in material science and biology. Large number of azoles derivatives emit fluorescence and some of them can undergo proton transfer. In the present work, a few azole derivatives capable of undergoing intra or inter molecular proton transfer were investigated using absorption, steady state and time resolved emission techniques.

First, the molecule possessing single intramolecular proton transfer unit, 2-phenylamino-5-(2-hydroxybenzono)-1,3,4-thiadiazole and its methoxy derivative were studied in different solvents to ascertain the origin of the longer wavelength emission of its analogue, 2-(4-fluorophenylamino)-5-(2,4-dihydroxybenzono)-1,3,4-thiadiazole.

Then, 3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazole (bis-HPTA), the molecule possessing two intramolecular proton transfer units was examined in water, cyclodextrin, normal and reverse micelle. The studies were carried out to understand the effect of microheterogeneous environment on the proton transfer in general and proton transfer triggered proton transfer in specific. Interestingly, the anion of bis-HPTA undergoes intermolecular proton transfer in the excited state to form tautomer in the excited state in water. However, cyclodextrin and micelles arrest the intermolecular proton transfer in anion. Bis(2-ethylhexyl)sodium sulfosuccinate reverse breaks one of the intramolecular hydrogen bond by forming an intermolecular hydrogen bond, that restricts bis-HPTA to exhibit single intramolecular proton transfer.

The competition between the intramolecular and the intermolecular proton transfer of 2-(4'-amino-2'-hydroxyphenyl)-1H-imidazo-[4,5-c]pyridine (AHPIP-c) was studied theoretically to detect the cause of absence of intramolecular charge transfer emission from the molecule in methanol. Then we also observed that the intramolecular charge transfer emission was triggered in AHPIP-c by both protonation and deprotonation. The spectral characteristics of different prototropic species of AHPIP-c formed by intermolecular proton transfer were also studied in water, acetonitrile and methanol.

