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SOLVATOCHROMIC SHIFTS: THE STUDY OF THE MEDIUM INFLUENCE ON BASE-FREE PORPHYRINS

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Resumo

The solvent's influence on molecular properties of materials has aroused great interest in spectroscopy due to the challenge to explain systematically the general (physical) and specific (chemical) effects caused by the solute-solvent interaction. In recent decades, significant progress has been correlating these effects semi-empirically with experimental and computational observations. However, it becomes clear that the interaction of solvent with molecules, ions, and radicals often cannot be explained satisfactorily by continuous properties of the solvent, such as the dielectric constant, refraction index, viscosity etc. Because of the presence of hydrogen bonding on a solvent that can be a donor (HBD) or acceptor (HBA). Many solvent scales had proposed to mitigate these undesirable solvation effects using a large number of solvents with a specific material. Although it's hard to believe that these scales will be precise by the change of the material. Then, this work investigated how solvents influence the absorption, emission, and constant rates of Tetraphenyl-porphyrin (TPP) and Tetracyanophenyl-porphyrin (TPCNP). We started our investigation through the solvent's relaxation theory proposed by Lippert and Mataga and other semi-empirical methods to explain the results. The results were obtained by measurements of stationary absorption, stationary fluorescence, and time-resolved emission (TCSPC technique). The porphyrins were dissolved in several aprotic and amphiprotic solvents. We identify solvatochromism on the absorption and emission spectra that displacement on the longer wavelength of B (380-450nm) and Q(460-700nm) bands and a change in a lifetime, radiative rates and quantum yield.

Palavras chave: Solvent Effects, Porphyrins, Lippert-Mataga.