Nutjarin Klinhom 2014: Ground State and Excited State Intramolecular Proton Transfer on the Enol-Keto Tautomerization of Salicylaldimine Based Chemosensor: Experimental and Theoretical Study. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Assistant Professor Songwut Suramitr, Ph.D. 107 pages.

Three Schiff base derivertives, 2-(2-hydroxybenzylideneamino)phenol, 2-(hydroxybenzylidene)aniline and (Benzylideneamino)phenol, were synthesized and characterized by ^{1}H-NMR and FT-IR spectrometer. The photophysical properties of these salicylaldimine derivertives were studied as a function of pH. The result showed the Enol-Keto tautomers in acid-base solution. The effect of solvent polarity on the absorption and fluorescence properties were analyzed as well and the result exhibited the excited state intramolcular proton transfer (ESIPT) in non-polar and aprotic polar solvents. Moreover, the geometries at the ground state were optimized using Density Functional Theory (DFT) calculations with the CAM-B3LYP/6-311G(d,p) level of approximation. The electronic properties were carried out using the Time Dependent Density Functional Theory (TDDFT) at the same method. The effects of the solvents (chloroform and acetonitrile) were added using the polarizable continuum model (PCM) to model the solvation effect. The calculated results were in good agreement with those obtained from the experimental observation. The potential energy profiles of the ground and the lowest excited singlet state were studied on 2-(2-hydroxybenzylideneamino)phenol. The results of potential energy curve showed low activation barrier on the ground state (8.6 kcal/mol), whereas barrierless proton transfers were observed in case of excited state, confirming that intramolecular proton transfer prefer in the first singlet excited states more than ground state. The calculations also indicated S_1/S_0 conical intersection (CI) which provided alternative channel for radiation-less decay to the ground state that was a complete cycle.

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