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**Photophysical Properties for Excited-State Intramolecular Proton Transfer (ESIPT)
Reaction of *N*-Salicylidene-*o*-aminophenol: Experimental and DFT based approaches**

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Abstract

Photophysical properties for excited-state intramolecular proton transfer (ESIPT) reaction of *N*-salicylidene-*o*-aminophenol (SA) Schiff base were comprehensively studied based on experimental methods combined with theoretical calculations. The results revealed that the SA was mainly presented in enol form in acidic solutions while it was predominantly existed in keto form in basic solutions. From UV-vis absorption and fluorescence emission studies, it showed that the ESIPT could effectively take place in non-polar and aprotic polar solvents. By using the CAM-B3LYP/6-311G(d,p) level of theory, it was found that the intramolecular proton transfer could preferably occur through six-membered ring transition rather than through five-membered ring transition. The dynamics of the ESIPT reactions of enol and keto tautomers were studied using TD-CAM-B3LYP with 6-311G(d,p) basis set. The potential energy curves for the intramolecular proton transfer in the ground (GSIPT) and excited state (ESIPT) exhibited that the GSIPT could occur through a low activation barrier, whereas in the case of ESIPT, the process could arise via low energy barrier.

Keywords: enol-keto tautomerization, excited-state intramolecular proton transfer (ESIPT), density functional theory

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