

Substituent Effect on Photophysical Properties of Salicylidene Schiff Base and Its Derivatives as Colorimetric Dyes: A TD-DFT Study

Amonchat Koonwong^{1,2}, Suwannee Sriyab^{1,2}, Supa Hannongbua^{1,2}, Songwut Suramitr^{1,2*}

¹ Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand

² Center for Advanced Studies in Nanotechnology for Chemical, Food and Agricultural Industries, KU Institute for Advanced Studies, Kasetsart University, Bangkok 10900, Thailand

*Corresponding author: fsciswsm@ku.ac.th (S. Suramitr)

Abstract

The effects of substitution groups on the photophysical properties and excited-state intramolecular proton transfer (ESIPT) of the salicylidene Schiff base derivatives (SA1, SA2, SA3 and SA4) were considered using density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations at CAM-B3LYP/6-311G(d,p) level. Geometries and absorption spectra of all derivatives were calculated at the same level of theory. The substitution of the salicylidene Schiff base derivatives resulted in the red shift spectra, which implies that the electron donor substituted has the effect on the π -conjugated system. In addition, results of molecular orbital analysis show that vertical $S_0 \rightarrow S_1$ transition of these molecules corresponds essentially excitable from HOMO (π) to LUMO (π^*). The potential energy curves (PECs) of selected derivatives were used to investigate the occurrence of ESIPT. The substitution of salicylidene Schiff base derivatives could easily facilitate the ESIPT process, because the electron donor substitution makes O-H bond of selected salicylidene Schiff base derivatives weaker than those of other derivatives and the hydrogen bond in N-H becomes stronger in the excited state, resulting in lower PT barrier. The obtained information of the electronic structure, the photophysical property and the chance of ESIPT of salicylidene Schiff base derivatives molecules is useful for molecular design of colorimetric molecular probes.

Keywords: Phototautomer, Schiff base derivatives, Time-dependent density functional theory (TD-DFT), Excited-state intramolecular proton transfer (ESIPT)