Title : Influence of different heteroatom, pi-expansion, and additional proton transfer site for ESIPT of the 2-(2-hydroxyphenyl)benzazoles and their derivatives relieving antiaromaticity

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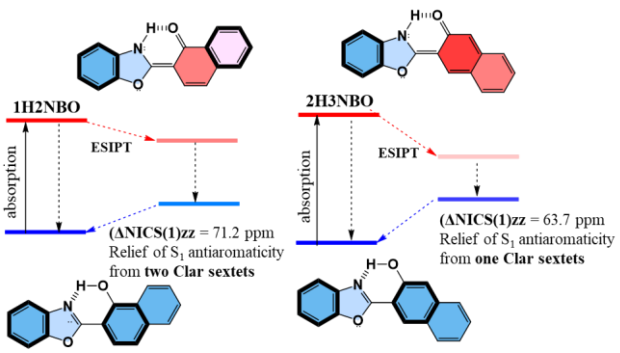
ABSTRACT

Excited state intramolecular proton transfer (ESIPT) process is one of the most important reactions in photochemistry and photobiology. The main driving force responsible for ESIPT process has been proposed including an increase in the acidity of the proton donor and basicity of the proton transfer, a difference in the character of the wavefunction or a change in aromatic character and recently as the relief of antiaromaticity in the photoexcited state. The aims of this work to understand the correlation of different heteroatom, pi-expansion, and addition PT sites on the ESIPT relieving antiaromaticity of the 2-(2-hydroxyphenyl)-benzazoles (HBX) and its derivatives. The correlation of such relieving antiaromaticity in term of computed nucleus-independent values in the singlet excited state with photophysical properties such Stokes shift, normal adsorption and tautomer emission in a longer wavelength were investigated using density functional theory. The red-shifts of normal absorption peaks are found for all HBX derivatives regardless of chemical structures, whereas the blue-shifts or red-shifts of tautomer emission peaks are dependent on the orientation of pi-expansion and the additional PT unit compared to HBX. Among designed HBX derivatives, a HBX having two PT units connected with pi-expansion along the nodal plane is the best candidate for fluorescent probes because of its tautomer emission at 942 nm with the largest Stokes shift. Moreover, computed NICS confirm that the emission of tautomers arising from ESIPT can be related to their inherent (anti)aromatic characters vary depending on the antiaromaticity of the photoinduced tautomers. Based on this theoretical investigation, the tautomer emission of HBX derivatives in NIR region can be achieved by the combination of pi-expansion along the nodal plane and additional PT unit.



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