



The excited-state intramolecular proton transfer in N–H-type dye molecules with a seven-membered-ring intramolecular hydrogen bond: A theoretical insight

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**Abstract**

Excited-state intramolecular proton transfer (ESIPT) reactions of a series of N(R)–H···N-type seven-membered-ring hydrogen-bonding compounds were explored by employing density functional theory/time-dependent density functional theory calculations with the PBE0 functional. Our results indicate that the absorption and emission spectra predicted theoretically match very well the experimental findings. Additionally, as the electron-withdrawing strength of R increases, the intramolecular H-bond of the N-S<sub>1</sub> form gradually enhances, and the forward energy barrier along the ESIPT reaction gradually decreases. For compound **4**, its ESIPT reaction is found to be a barrierless process due to the involvement of a strong electron-withdrawing COCF<sub>3</sub> group. It is therefore a reasonable presumption that the ESIPT efficiency of these N(R)–H···N-type seven-membered-ring H-bonding systems can be improved when a strong electron-withdrawing group in R is introduced.

**Keywords:** ESIPT; TD-DFT; topological analysis; potential energy curve

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