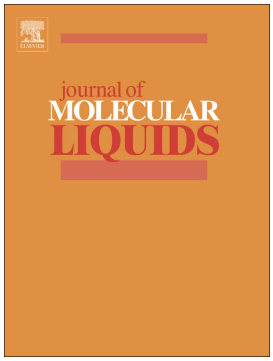


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# Explaining the excited state behavior of t-DMASIP-b sensor: A theoretical study

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**Abstract**

In this present work, we theoretically investigate the excited state dynamical mechanism of a novel sensor trans-2-[4'-(N,N-dimethylamino)styryl]imidazo[4,5-b]pyridine (t-DMASIP-b). Within the framework of density functional theory (DFT) and time dependent DFT (TDDFT) methods, we reasonably repeat the experimental electronic spectra, which further confirm the theoretical level used in this work is feasible. Given the best complex model, two methanol (MeOH) solvent molecules should be connected with t-DMASIP-b forming t-DMASIP-b-MeOH complex in both ground state and excited state. Exploring the changes about bond lengths and bond angles involved in hydrogen bond wires, we find the O5-H6···N7 one should be largely strengthened in the $S_1$ state, which might facilitate the excited state intermolecular proton transfer (ESIPT) process. In addition, the analyses about infrared (IR) vibrational spectra also confirm this conclusion. The redistribution about charges distinguished via frontier molecular orbitals (MOs) based on the photo-excitation, we do find tendency of ESIPT reaction due to the most charges located around N7 atom in the LUMO orbital. Even though some indications reveal the ESIPT, we find the moderate potential energy barriers in the $S_1$-state potential energy curves. The moderate potential energy barrier 12.89 kcal/mol along with O5-H6···N7 hydrogen bonding wire indeed hinders the proceeding of ESIPT, so only one fluorescence peak was reported in previous experiment, which has been reasonably explained in our work. As a whole, we deem our work not only successfully explains previous experimental work, but also paves the way for the further applications about t-DMASIP-b sensor in future.

**Keywords:** hydrogen bond; potential energy curves; IR spectra; electronic spectra.