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The order of multiple excited state proton transfer in ternary complex of norharmane and acetic acids

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ABSTRACT

Dolores Reyman *et al.* found the norharmane (9H-pyrindo [3,4-b] indole) (NHM) and two acetic acid molecules can form the ternary complex (NHM-2A) in component solvent of dichloromethane and acetic acid *via* the hydrogen bond chain (J. Lumin. 2014, 148, 64). But the specific reaction details during this process were rarely reported. In this study, we will give an insight into the reasons which promote the occurrence of this reaction as well as its reaction order. The hydrogen bond enhancing behavior in first excited state (S_1) is verified through the analysis of geometric configurations, infrared spectra, frontier molecular orbitals and potential energy curves. The absorption and fluorescence spectra we calculated are well coincident with the experimental results. Meanwhile, it is obvious that the hydrogen bond intensity is gradually enhanced from $N_1-H_2 \cdots O_3$, $O_4-H_5 \cdots O_6$ to $O_7-H_8 \cdots N_9$ by analyzing the reduced density gradient (RDG) isosurface. The hydrogen bond strengthening mechanism has been confirmed in which the hydrogen bond interaction acts as driving force for excited state proton transfer (ESPT) reaction. In order to provide a reliable description of the reaction energy profiles, we compare the barrier differences obtained by m062x and B3LYP methods. We might safely draw the conclusion that the multiple ESPT is a gradual process initiated by the proton transfer of $O_7-H_8 \cdots N_9$. And we further proof the ESPT process can be completed *via* the $NHM-2A \rightarrow NHM-2AS \rightarrow NHM-2AD \rightarrow NHM-2AT$ in S_1 state. Theoretical research of NHM-2A has been carried out by density functional theory (DFT) and time-dependent density functional theory (TDDFT). It is worth noting that we predicted that the fluorescence at 400 nm observed in experiment is more likely to be emitted by NHM-2AS in S_1 state.

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