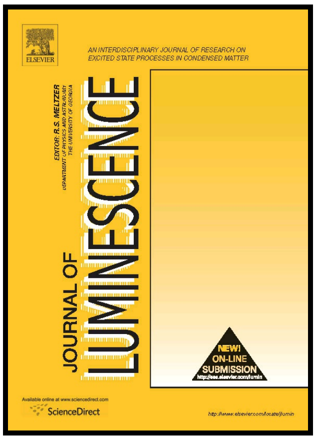

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Dapeng Yang, Guang Yang, Min Jia, Xiaoyan Song, Qiaoli Zhang

PII: S0022-2313(18)30385-5
DOI: https://doi.org/10.1016/j.jlumin.2018.06.027
Reference: LUMIN15689

To appear in: *Journal of Luminescence*

Received date: 1 March 2018
Revised date: 3 June 2018
Accepted date: 11 June 2018

Cite this article as: Dapeng Yang, Guang Yang, Min Jia, Xiaoyan Song and Qiaoli Zhang, Exploring excited state hydrogen bonding interactions and proton transfer mechanism for 2,2’-(thiazolo[5,4-d]thiazole-2,5-diyl)bis(4-tert-butylphenol), *Journal of Luminescence,* https://doi.org/10.1016/j.jlumin.2018.06.027

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Dapeng Yang[1,3,]*, Guang Yang[2], Min Jia[1], Xiaoyan Song[1], Qiaoli Zhang[1]
[1]School of Mathematics and Statics, North China University of Water Resources and Electric Power, Zhengzhou 450046, China
[2]Basic Teaching Department, Jiaozuo University, Jiaozuo 454000, China
[3]State Key Laboratory of Molecular Reaction Dynamics, Theoretical and Computational Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China
*Corresponding authors: Dapeng Yang, email: dpyang_ncwu@163.com.

Abstract

In this present work, combing density functional theory (DFT) and time-dependent DFT (TDDFT) methods, we investigate a novel white light material 2,2'-(thiazolo[5,4-d]thiazole-2,5-diyl)bis(4-tert-butylphenol) (t-HTTH) about its dual intramolecular hydrogen bonding behaviors and relative excited state intramolecular proton transfer (ESIPT) process in detail. Via testing functional and basis set, the DFT//TDDFT/MPW1PW91/6-311+G(d,p) theoretical level has been decided in three kinds of solvents (cyclohexane (CYH), dichloromethane (DCM) and toluene (Tol)), which can well reappear experimental phenomenon. Exploring molecular electrostatic potential (MEP), primary bond lengths, bond angles and infrared (IR) vibrational spectra for t-HTTH system in both S_0 and S_1 states, we find the double hydrogen bonds O1-H2···N3 as well as O4-H5···N6 should be strengthened in the S_1 state. Investigating the photo-excitation process, we find that the $S_0 \rightarrow S_1$ transition corresponds to charge transfer, which provides the driving force for ESIPT. And analyses about frontier molecular orbitals (MOs) and relative energy gaps between HOMO and LUMO orbitals, we deduced the ESIPT process may occur more likely in nonpolar solvents. Constructing potential energy curves, we reveal that the ESIPT reaction results in the dynamic equilibrium in S_1 state between forward and backward processes, which facilitates white light. We not only clarify the excited state hydrogen bond dynamical behavior of t-HTTH material, but also elaborate the ESIPT mechanism and explain previous experimental phenomenon reasonably.

Keywords: Intramolecular hydrogen bond; proton transfer; Infrared spectra; Frontier molecular orbital; Potential energy curves