## Accepted Manuscript

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

Huijuan Yuan, Songyan Feng, Keke Wen, Xugeng Guo, Jinglai Zhang

PII: S1386-1425(17)30853-3

DOI: doi:10.1016/j.saa.2017.10.048

Reference: SAA 15554

To appear in: Spectrochimica Acta Part A: Molecular and Biomolecular

Spectroscopy

Received date: 23 August 2017 Revised date: 9 October 2017

Accepted 15 October 2017

date:

Please cite this article as: Huijuan Yuan, Songyan Feng, Keke Wen, Xugeng Guo, Jinglai Zhang, The excited-state intramolecular proton transfer in N-H-type dye molecules with a seven-membered-ring intramolecular hydrogen bond: A theoretical insight. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Saa(2017), doi:10.1016/j.saa.2017.10.048

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



## CCEPTED MANUSCRIPT

The excited-state intramolecular proton transfer in N–H-type dye

molecules with a seven-membered-ring intramolecular hydrogen

bond: A theoretical insight

Huijuan Yuan, Songyan Feng, Keke Wen, Xugeng Guo\* and Jinglai Zhang\*

College of Chemistry and Chemical Engineering, Henan University, Kaifeng 475004,

P. R. China.

xgguo@henu.edu.cn \*Corresponding author. E-mail addresses:

zhangjinglai@henu.edu.cn (J. Zhang)

**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

1

## Download English Version:

## https://daneshyari.com/en/article/7670355

Download Persian Version:

https://daneshyari.com/article/7670355

<u>Daneshyari.com</u>