

## REGULAR ARTICLE

# Theoretical Investigation on ESIPT Process of 3-(1,3-benzothiazol-2-yl)-2-hydroxynaphthalene-1-carbaldehyde Chemosensor Between Polar and Non-polar Solvent

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**Abstract:** The comparisons of excited state intramolecular proton transfer (ESIPT) process of a new chemosensor 3-(1,3-benzothiazol-2-yl)-2-hydroxynaphthalene-1-carbaldehyde (Spectrochimica Acta Part A, 127 (2014) 16-24) have been studied based on the time-dependent density functional theory (TDDFT) method. The reproduced experimental absorption and fluorescence spectrum based on calculation indicates the reasonability of the DFT and TDDFT we adopted. The primary bond lengths, bond angles and infrared (IR) vibrational spectra demonstrated that the intramolecular hydrogen bond was strengthened in both polar solvent dimethylformamide (DMF) and non-polar solvent toluene. Two kinds of ESIPT mechanisms for these different solvents have proved that there exists a low potential barrier in the ESIPT process in the DMF solvent, but there exists no potential barrier in the ESIPT process in the toluene solvent. Hence, based on our calculated results, upon the photoexcitation, the ESIPT process of A2 chemosensor is much easier in toluene non-polar solvent.

**AMS subject classifications:** 65D18, 74M40, 78M50

**Key words:** ESIPT, intramolecular hydrogen bond, TDDFT, potential energy curves.

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## 1. Introduction

Proton transfer (PT), a fundamental kind of photochemistry, is ubiquitous as an elementary process [1, 2]. A photo-induced PT process can be considered to be a series of elementary steps, which has been described by the Eigen-Weller mechanism [3, 4]. That is to say, electronic redistribution upon photo-excitation, hydrogen bond rearrangement, proton transfer, ionpair formation, diffusion processes and so on. Excited state intra- as well as inter- molecular proton transfer (ESIPT) reaction has attracted considerable interest due to its relevance in electronic properties and photoinduced function of materials and biological systems such as luminescent down converters (LDCs), luminescent solar concentrators (LSCs), laser dyes, molecular switches fluorescence sensors, UV-light polymer stabilizers and so forth [5-20]. Naturally, the attention focused on this phenomenon is both cognitive and applied, through which it crops up as a demanding subject of research even today.

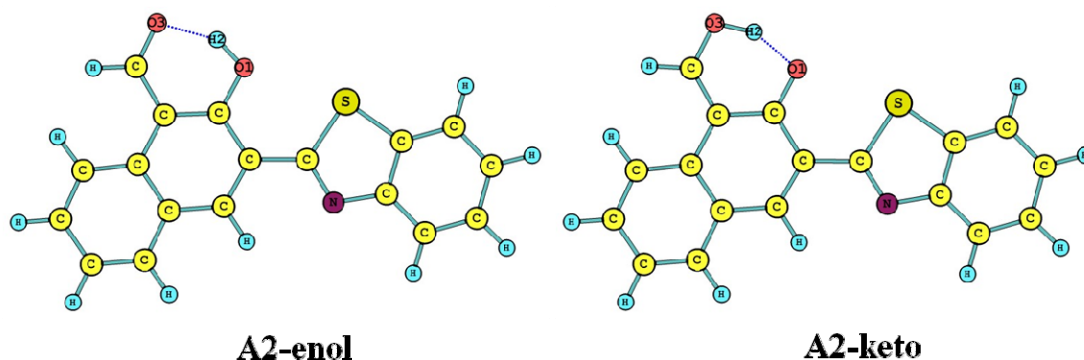


Figure 1: The structures of A2-enol and A2-keto.

Recently, 3-(1,3-benzothiazol-2-yl)-2-hydroxynaphthalene-1-carbaldehyde was investigated on the effect of solvent polarity and PH [21], the ESIPT phenomenon was reported. As one possible conformer of this sensor 3-(1,3-benzothiazol-2-yl)-2-hydroxynaphthalene-1-carbaldehyde **A2** (seen in **Figure 1**), it was studied about ESIPT reaction experimentally and theoretically [21]. However, the expression of influence of solvent polarity on the ESIPT process and mechanism is ambiguous. Particularly, the primary potential barrier of ESIPT process and potential energy curves were not provided [21]. In addition, just the indirect information about photochemical and photophysical properties can be provided based on experiment. Therefore, in order to elaborate detailed ESIPT mechanism and the effect of solvation, in the present work, a theoretical investigation with DMF polar solvent and toluene non-polar solvent has been