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REGULAR ARTICL

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.

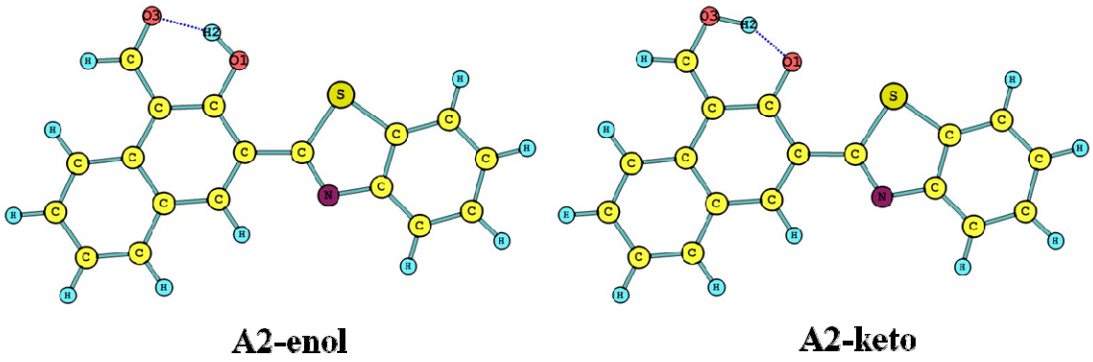

Figure 1: The strucures of **A2**-enol and **A2**-keto.

Recently, 3-(1,3-benzothiazol-2-yl)-2-hydroxynaphthalene-1-carbal-dehyde 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

adopted. The study of the S_0 and S_1 states relevant to the ESIPT was based on DFT and TDDFT method, respectively. Detailed potential energy curves and potential barriers are calculated and analyzed to provide the direct information of ESIPT process.

2. Computational Details

In the present work, all the electronic structure calculations were carried out depending on the Gaussian 09 program suite [22]. The geometric optimization of the A2 was performed in the ground state using DFT method and the electronic excited state was performed depending on TDDFT method, respectively. The TDDFT method has become a very useful tool to theoretically investigate the hydrogen bonding interaction that occurs in the excited-state of hydrogen-bonded systems [23-30]. Becke' three-parameter hybrid exchange functional with Lee-Yang-Parr gradient-corrected correlation (B3LYP functional) was used in both the DFT and TDDFT methods [31-33]. The triple-ζ valence quality with one set of polarization functions (TZVP) was chosen as basis sets throughout, which is an appropriate basis set for this system. There were no constraints to all the atoms, bonds, angles or dihedral angles during the geometric optimization.

To evaluate the solvent effect, DMF and toluene were used as solvent in the calculations depending on the model that the Polarizable Continuum Model (PCM) using the integral equation formalism formalism variant (IEFPCM). All the local minima were confirmed by the absence of an imaginary mode in vibrational analysis calculations. The S_0 and S_1 potential energy curves have been scanned by constrained optimizations in their corresponding electronic state, and keeping the O-H distances fixed at a serious of values. Fine quadrature grids 4 were also employed. The self-consistent field (SCF) convergency thresholds of the energy for both the ground state and excited state optimization were set to be 10^{-8} (default settings are 10^{-6}). Harmonic vibrational frequencies in both ground state and excited state were determined by diagonalization of the Hessian [34]. The excited state Hessian was obtained by numerical differentiation of analytical gradients using central differences and default displacements of 0.02 Bohr [35]. The infrared intensities were determined from the gradients of the dipole moment.

3. Results and discussion

The optimized structures of the A2-enol and A2-keto of S_0 and S_1 states were obtained based on the B3LYP function with the TZVP basis set and a subsequent vibrational frequency analysis to ensure the validity of the stationary points. Considering the consistent with previous experiment [21], DMF and toluene been selected as the reaction solvent in the

IEFPCM model. The homologous absorption and fluorescence spectra of A2 structure in DMF and toluene solvents have been displayed in **Figure 2**. The strong absorption peak for A2-enol is located at 374 nm in DMF solvent. After the photoexcitation, the fluorescence peak of A2-enol is calculated to be 477 nm, which is in consistent with 468 nm in the experiment [21]. The other emission peak for A2-keto form is located at 538 nm, which is also in agreement with experimental 538 nm [21]. Similarly, the consistent with experiment is also in toluene solvent. Therefore, it demonstrates that the calculated excited state of A2 chromophore in DMF and toluene solvents based on the TDDFT method can delineate the excited-states properties well.

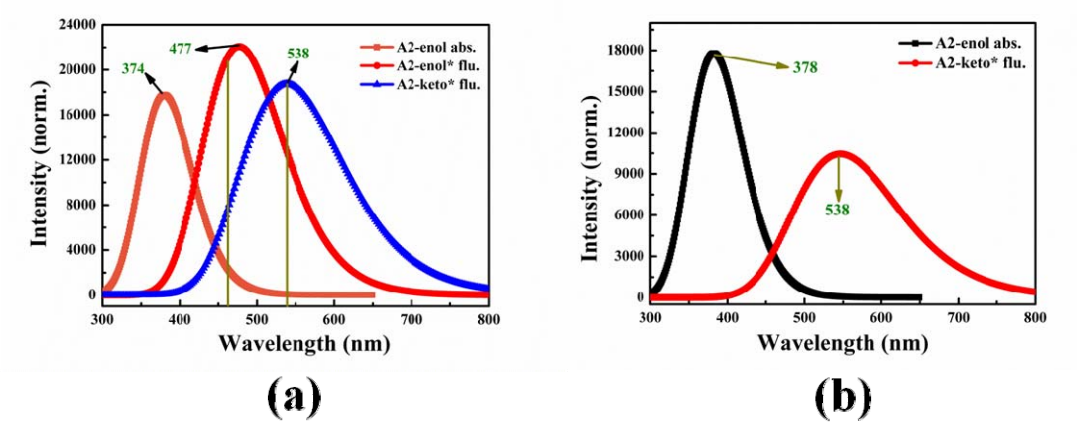

Figure 2: Electronic spectra of A2-enol and A2-keto in DMF (a) and toluene (b) solvents.

Table 1 The calculated electronic excitation energy (nm), corresponding oscillator strengths (*f*) and relative compositions in DMF and toluene solvents for A2-enol chemosensor.

	Transition	λ_{cal} **(nm)**	*f*	**CI (%)**	**Composition**
	S_0-S_1	374.32	0.3318	0.2371	H-1 → L
				0.7162	H → L
DMF	S_0-S_2	361.2	0.0992	0.6728	H-1 → L
				-0.2888	H → L
	S_0-S_3	350.8	0.0209	0.9829	H-2 → L
	S_0-S_1	378.3	0.3317	-0.1425	H-1 → L
				0.8269	H → L
	S_0-S_2	367.56	0.1062	-0.0214	H-2 → L
Toluene				0.7921	H-1 → L
				0.1458	H → L
	S_0-S_3	357.96	0.0227	0.9615	H-2 → L
				0.0293	H-1 → L

In the UV-Vis spectra, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) play important roles based on the frontier molecular orbital (MO) analys shown in **Figure 3**. In addition, the calculated electronic excitation energy (nm), corresponding oscillator strengths (*f*) and relative compositions in DMF and toluene solvents for A2-enol chemosensor are shown in **Table 1**. It can be seen that the intense S_0-S_1 transition is predicted at 374 and 378 nm in DMF and toluene with the large oscillator strength, respectively. It should be noted that the HOMO and LUMO are located on different parts. The evident can be that the atomic orbitals of the O_3 atom takes more proportion in LUMO than those in HOMO. Therefore, we may forecast that the electron density of O_3 atom increases based on the excitation to the S_1 state. Consequently, the O_3-H_2 bond length may be shortened in the S_1 state, which may cause the ESPT process.

The most primary structural parameters involved in hydrogen bonding have been listed in **Table 2**. It should be noted that the elongation of the O_1-H_2 bond from 1.003 Å (S_0) to 1.054 Å (S_1) and the shorting of H_2-O_3 (H_2···O_3) bond from 1.597 Å to 1.432 Å with the concomitant enlargement of O_1-H_2···O_3 angle from 149.5º to 155.3º in DMF solvent following the photo-excitation. Based on these calculated results, the intramolecular hydrogen bond O_1-H_2···O_3 is strengthened in the S_1 state [23-30]. However, in view of the toluene solvent, no stable A2-enol structure in the S_1 state can be optimized. In order words, when we optimized the A2-enol in S_1 state based on the structure of S_0 state, the result revealed the A2-keto (S_1) form. It demonstrates that the ESIPT of A2 sensor may be a process with no potential barrier, which would be discussed below in detail. In addition, in view of the A2-keto form, the length of O_1-H_2 (O_1···H_2) changes from 1.588 Å (S_1) to 1.467 Å (S_0) as well as H_2-O_3 elongates from 1.008 Å (S_1) to 1.041 Å (S_0) in DMF solvent. It demonstrates that the intramolecular hydrogen bond O_1···H_2-O_3 is more stable in the S_0 state. That is to say, the A2-keto (S_1) form is likely to undergo the radiative transition to the S_0 state. The similar description can be used to interpret A2 in toluene solvent.

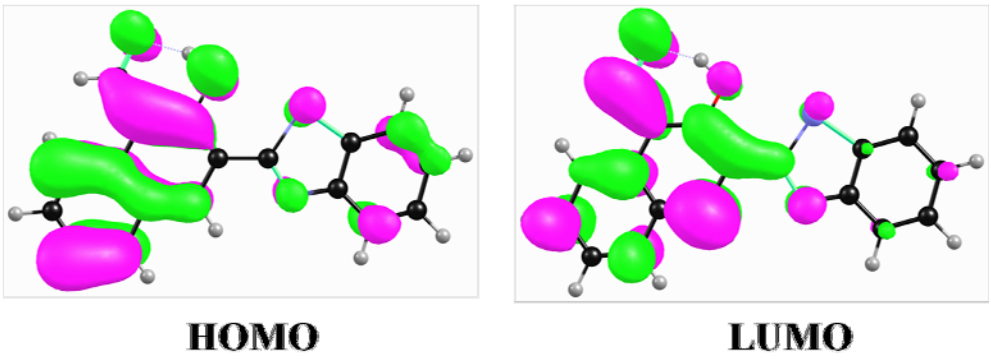

Figure 3: HOMO and LUMO oribits of A2-enol.

In fact, the phenomenon of ESIPT is percussion of the substantial adjustment of electronic charge density distribution on the heavy atoms induced by photoexcitation. The detailed investigation of the charge distribution over the atoms involved in intramolecular hydrogen bond can be used as a reasonable evidence to explore the proton transfer reaction based on the Mulliken's charge distribution analysis method. The one should be noted that the decrease of negative charge distribution about O_1 atom of the –OH moiety is from -0.287 in the S_0 state to -0.272 in the S_1 state together with the increase on the O_3 atom from -0.381 to -0.394 based on the B3LYP/TZVP theoretical level in DMF solvent. In addition, the NBO analysis method has also been used to study the charge distribution. The analogous results that the decrease of O_1 atom negative charge distribution from -0.368 to -0.329 and increase of O_3 atom negative charge distribution from -0.461 to -0.497 have also been concluded. Therefore, the ESIPT process can be predicted based on the above discussion.

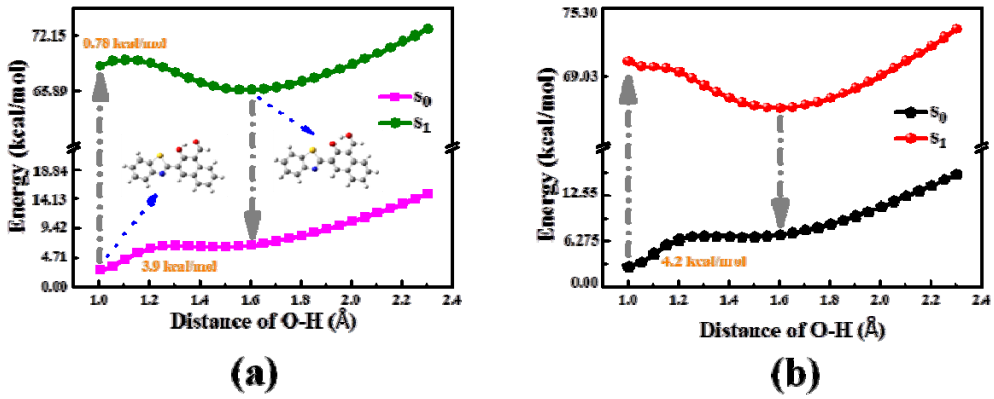

Figure 4: Potential curves of S_0 and S_1 states for **A2** chromophore along with O-H bond; (a) DFM solvent; (b) toluene solvent.

For further understanding the ESIPT process, the potential energy curves of S_0 and S_1 states have been scanned. The scan was based on the constrained optimizations in their corresponding electronic states and kept the O-H bond distance fixed at a series of values. Although the TDDFT/B3LYP method may not be expected to be sufficiently accurate to surmount the correct ordering of the closely spaced excited-states, previous research has indicated that this method is reliable as far as the shape of the hydrogen-transfer potential energy curves are concerned [36-40]. The potential energy curves of A2-enol chemosensor are shown in **Figure 4** with the variable parameter of O-H bond length limited in step of 0.05 Å. The energy of the corresponding S_0 state increases along with the O-H bond length across a barrier about 3.9 kcal/mol from the optimized length of ~0.99 Å in DMF solvent, whereas the energy of the S_1 state decreases after a low potential barrier 0.78 kcal/mol following the O-H bond length increases until it reaches a stable point (A2-keto) at ~1.588 Å, which corresponds to the stable optimized geometry of the S_1 state. However, for the toluene

solvent, it should be noted that a no barrier process of ESIPT in the S_1 state. That is to say, the so-called A2-enol* can be easily isomerized into the A2-keto* (minimum energy point) by crossing no potential barrier instantaneously. However, in the S_0 state, the A2-enol form can barely convert into A2-keto form due to the potential barrier of 4.2 kcal/mol and endothermic process. Therefore, it can be concluded that upon photoexcitation, A2 chemosensor is more likely to occur the ESIPT process in non-polar toluene than polar DMF solvent.

Table 2 The calculated bond lengthes (Å) and angles (º) for A2-enol and A2-keto forms in S0 and S1 states based on the DFT/TDDFT methods with IEFPCM (DMF and toluene), respectively.

	DMF				Toluene			
	A2-enol		**A2-keto**		**A2-enol**		**A2-keto**	
	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1
O_1-H_2	1.003	1.054	1.467	1.588	1.003	---	1.461	1.592
H_2-O_3	1.597	1.432	1.041	1.008	1.600	---	1.044	1.008
δ(O_1-H_2-O_3)	149.5°	155.3°	151.7°	149.6°	149.2°	---	152.6°	149.9°

4. Conclusion

In summary, in our present work, we compare the excited state intramolecular proton transfer process of **A2** chemosensor in both DMF polar solvent and toluene non-polar solvent 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 and bond angles involved in hydrogen bonding (O-H···O) demonstrated that the intramolecular hydrogen bond was strengthened in both DMF and toluene solvents. Two kinds of ESIPT mechanisms for these different solvents have been provided that a low potential barrier of 0.78 kcal/mol needs to cross occuring ESIPT process in DMF solvent, whereas no potential barrier exists to ESIPT reactive in toluene solvent. Therefore, upon the photoexcitation, the ESIPT process of **A2** chemosensor occurs much more easily in non-polar solvent than polar solvent.

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