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An investigation of excited-state intramolecular proton transfer mechanism of new chromophore

Yanling Cui[a,c†], Pengyu Li[a,c†], Jing Wang[b], Peng Song[a*] and Lixin Xia[b*]

[a] *Department of Physics, Liaoning University, Shenyang 110036, P. R. China*
[b] *Department of Chemistry, Liaoning University, Shenyang 110036, P. R. China*
[c] *State Key Lab of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, P. R. China*

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Abstract. Based on the time-dependent density functional theory (TDDFT), the excited state intramolecular proton transfer (ESIPT) mechanism of a new compound 1 chromophore synthesized and designed by Liu *et al.* [Journal of Photochemistry and Photobiology B: Biology., 138 (2014), 75-79] has been investigated theoretically. The calculations of primary bond lengths, angles and the IR vibrational spectra verified the intramolecular hydrogen bond was strengthened. The fact that reproducing the experimental absorbance and fluorescence emission spectra well theoretically demonstrates that the TDDFT theory we adopted is reasonable and effective. In addition, intramolecular charge transfer based on the frontier molecular orbitals demonstrated the indication of the ESIPT reaction. The constructed potential energy curves of ground state and the first excited state based on keeping the O-H distance fixed at a serious of values have been used to illustrate the ESIPT process. A little barrier of 2.45 kcal/mol in the first excited state potential energy curve provided the transfer mechanism. Further, the phenomenon of fluorescence quenching has been explained reasonably based on the ESIPT mechanism.

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Key words: Hydrogen bond; ESIPT; TDDFT; Potential energy curve.

1 Introduction

The hydrogen bonding interaction has formed the nucleus of intensive research for years due to its pivotal roles in physics, chemistry, and biology [1-14]. Proton transfer (PT), as

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[†] These authors contributed equally.

[*] Corresponding author. *Email address:* `songpeng@lnu.edu.cn` (P. Song), `lixinxia@lnu.edu.cn` (L.X. Xia)

one fundamental class of photochemistry, has attracted more and more attentions along hydrogen bonding in recent years [15-30]. In fact, in the middle of the last century, the investigation of the excited-state intramolecular proton transfer (ESIPT) reaction has been a new arena of research in the field of photochemistry since the experimental observation of the phenomenon reported by Weller *et al.* firstly [31, 32]. PT occurs containing both acidic and basic groups in close proximity, which could rearrange structures in the electronic excited state via a proton or hydrogen atom transfer. After photo-excitation, the molecules could be projected on a potential energy surface, which could make the position of a proton unstable. The driving force for the transformation could be provided based on the energy difference between the locally excited state and the relaxed excited state. In turn, the slope of the surface connecting these two points determines the relative kinetics. The stationary fluorescence spectroscopy provides important indications of the occurrence of proton transfer in the excited state. The observation of a nearly mirror symmetry between absorption and fluorescence spectra demonstrates that the nuclear configuration of the molecule and its surrounding medium remains close to that of the ground state over the timescale of the excited state lifetime. And the effect of the proton transfer on the Frank-Condon factors is enough to result in the break-up of the mirror symmetry. The light emission originating from the proton-transferred state occurs at longer wavelength with a red shift with respect to absorption ranging. It is hence possible to interpret the normal, shorter wavelength emission as originating from the locally excited state, and to associate the red shifted long wavelength emission with the product of the proton transfer.

Recently, a new compound 1 chromophore has been synthesized and designed by Liu *et al.* [33], which shows high selectivity for some biologically ions. Based on the absorption spectra, fluorescence spectra, ^{1}HNMR and more experiment measures, Liu *et al.* offered the important spectrum properties of 1 chromophore and inferred the ESIPT mechanism. However, only the indirect information about photo-physical properties could be provided based on spectroscopic techniques. Therefore, in order to give a clear and detailed picture of this proton transfer mechanism, in the present work, a theoretical investigation based on the density functional theory (DFT) and the time-dependent density functional theory (TDDFT) method have been applied to study both the ground and the excited state of molecular relevant to the transfer mechanism, respectively. We mainly forced our attention on the configurations of ground state and the first excited state, and further calculated and analyzed the vertical excitation energies, the frontier molecular orbitals and homologous ground state and the first excited state potential energy curves to elaborate the proton transfer mechanism.

2 Computational details

In the present work, the DFT and TDDFT methods have been adopted to optimize the ground state and the first excited state structures, respectively [34-38]. Becke's three-

Table 1: The calculated primary bond lengths (Å) and angles (°) in the S_0 state and the S_1 state based on the DFT and TDDFT methods, respectively.

	1-enol		1-keto	
Electronic state	S0	S1	S0	S1
O_1-H_2	1.000	1.026	1.754	1.848
H_2-N_3	1.699	1.625	1.038	1.031
$\delta(O_1\text{-}H_2\text{-}N_3)$	149.6°	150.3°	140.7°	139.3°

parameter hybrid exchange functions with the Lee-Yang-Parr gradient-corrected correlation functional (B3LYP) and the 6-31+G (d) basis set have been selected throughout. No constraints to all the atoms, bonds, angles or dihedral angles have been ensured during the geometric optimization. In order to ensure the consistency with the experiment [33], acetonitrile has been used as solvent in the calculations based on the model that the Polarizable Continuum Model (PCM) based on the integral equation formalism variant (IEFPCM). All the local minima were confirmed by the absence of an imaginary mode in the vibrational analysis. The S_0 and S_1 potential energy curves have been scanned by constrained optimizations in their corresponding electronic state with keeping the O-H distance fixed at a serious of values. Fine quadrature grids of size 4 were employed.

Harmonic vibrational frequencies in the ground state and the first excited state were determined by diagonalization of the Hessian. The excited-state Hessian was obtained by numerical differentiation of analytical gradients using central differences and default displacements of 0.02 Bohr. The infrared intensities were determined from the gradients of the dipole moment. All the electronic calculations were carried out depending on the Gaussian 09 program suite [39].

3 Results and discussion

3.1 Optimized structures

The ground state and the first excited stated structures of the 1 chromophore were obtained using the B3LYP function with 6-31+G (d) basis set level of theory, with a subsequent vibrational frequency analysis to ensure the validity of the stationary points. The acetonitrile solvent was selected in the IEFPCM model insuring consistency with the experiment [33]. And the most primary structure parameters have been shown in Table 1. We labeled a serial numbers from 1 to 3 on the atoms connected to the hydrogen bonds for describing clearly (see Fig. 1). It should be noted that the calculated lengths of O_1-H_2 and $H_2 \cdots N_3$ are 1.000 and 1.699 Å in the ground state. However, upon the photo excitation, the O_1-H_2 was lengthened to be 1.026 Å and $H_2 \cdots N_3$ was shortened to be 1.625 Å. The variable-length O_1-H_2 band as well as variable-short $H_2 \cdots N_3$ bond indicates that the intramolecular hydrogen bond was strengthened in the first excited state.

In effect, the hydrogen bond strengthening or weakening could also be revealed by

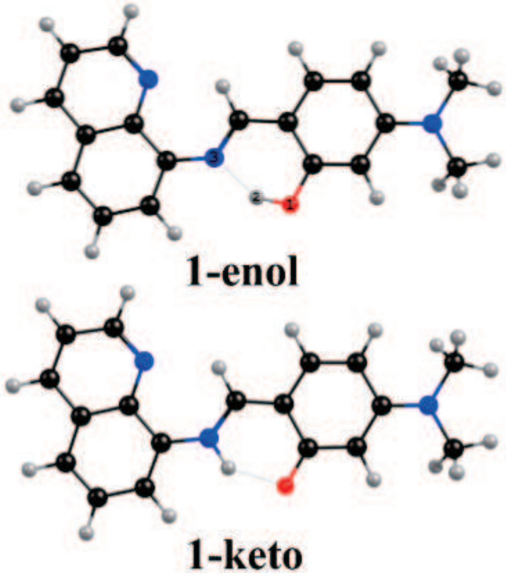

Figure 1: The optimized structures of 1-enol and its corresponding 1- keto tautomer at B3LYP/ 6-31+G (d) calculation level.

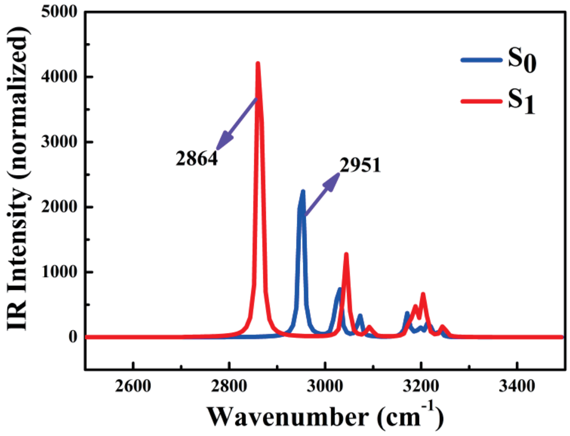

Figure 2: The calculated IR spectra of 1-enol and 1-enol* structure in acetonitrile solvent at the spectral region of O-H stretching band.

monitoring the spectral shifts of some characteristic vibrational modes involved in the formation of hydrogen bonds [40-48]. The vibrational spectra of 1 chromophore in the conjunct vibrational regions of the O-H stretching modes were shown in Fig. 2. It should be noted that the calculated O-H stretching vibrational frequency is located at 2951 cm^{-1} in the ground state, whereas it is located at 2864 cm^{-1} in the first excited state. It demonstrates that the intramolecular hydrogen bonds O_1-$H_2\cdots N_3$ induces about 87 cm^{-1} red-shift of O-H stretching frequency in the first excited state, which could be concluded due to the effect of the excited-state intramolecular hydrogen bond O_1-$H_2\cdots N_3$. Therefore,

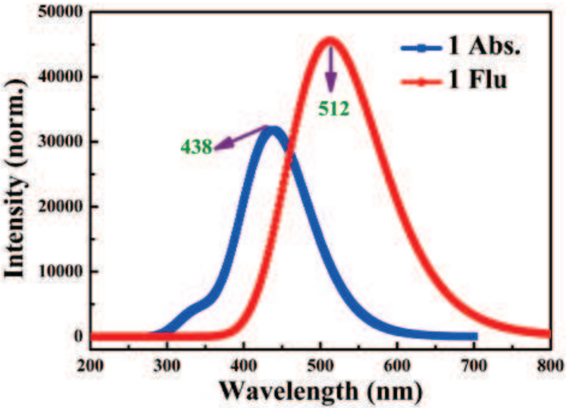

Figure 3: The calculated absorption and fluorescence spectra of 1 chromophore in acetonitrile solvent.

it further indicates that the intramolecular hydrogen bond was strengthened in excited state, which is an indication of the ESIPT reaction.

3.2 Electronic spectra and frontier molecular orbitals (MOs)

Based on the TDDFT/B3LYP/6-31+G (d) calculated level, the corresponding absorption and fluorescence spectra of 1-enol structure were displayed in Fig. 3. Although the steady-state spectral characters of 1 chromophore have been reported in the experiment [33], the investigations of the theoretical calculations and proton transfer mechanism are very limited. In order to show the shape of the spectra clearly, the calculated absorption and fluorescence spectra from 200 to 800 nm have been selected. It could be noted that the strong absorption peak for 1-enol was located at 438 nm, which is in consistent with the experiment [33]. The first excited state of 1 chromophore was fully optimized based on the ground state optimized geometric conformations as the initial conformations with the TDDFT method. In effect, the first excited state has two fates. The one is 1-enol*, and the other is 1-keto*. The results of theoretical calculations of 1-enol* shown in Fig. 3 reveal a normal Stokes shifted emission maximum at 512 nm in acetonitrile, which is also in good agreement with the experiment [33]. In addition, in the case of geometry-relaxed keto form 1-keto, a Stokes shift upon emissive relaxation was calculated at 533 nm. All the agreements with experiment demonstrate that the calculated excited state of 1 chromophore in acetonitrile solvent based on the TDDFT method can delineate the excited-states property well.

In order to discuss qualitatively on the nature of the excited state, it is necessary to understand charge distribution in electronic excited state. The frontier molecular orbitals (MOs) of the 1-enol in acetonitrile were shown in Fig. 4. Herein, we only show the highest occupied molecular oribital (HOMO), the lowest unoccupied molecular oribital (LUMO), because the first excited state is only associated with these two orbitals. The π character for the HOMO as well as the π^* character for LUMO can be seen clearly. Therefore, it

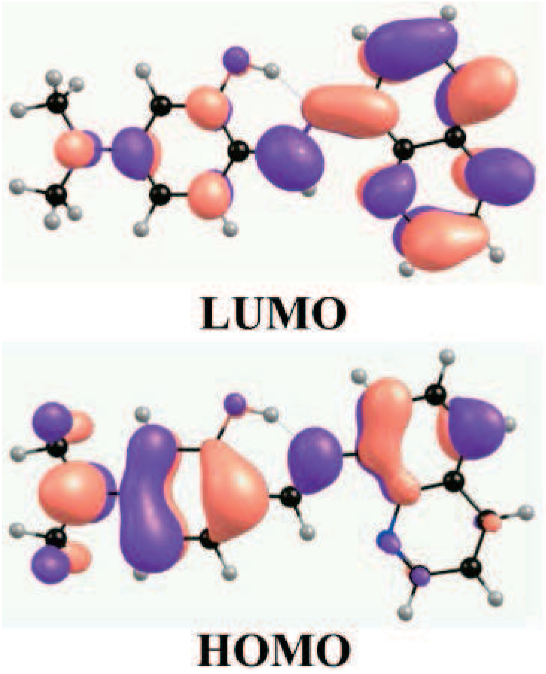

Figure 4: Frontier molecular orbitals (HOMO and LUMO) of 1 chromophore.

is determined that the first excited state is due to a distinct $\pi\pi^*$ feature. The one should be noted that the HOMO and LUMO are localized on different parts. Especially, the part involved in the intramolecular hydrogen bond O-H$\cdots$N, the electron density of the hydroxide radical moiety changes after the transition from HOMO to LUMO. That is to say, the first excited state involves the intramolecular charge transfer, and the change of electron density in the hydroxide radical moiety can directly influence the intramolecular hydrogen bonding O-H$\cdots$N. As a consequence, the H$\cdots$O bond length could be shorted upon excitation to the first excited state. So the ESIPT process could happen due to the intramolecular charge transfer.

3.3 The potential energy curves and the PT mechanism

In order to understand the PT mechanism clearly, the ground state and the first excited state potential energy curves have been scanned. Scan is based on constrained optimizations in their corresponding electronic states with keeping the O-H distance fixed at a serious of values. Even though the TDDFT/ B3LYP calculated level may not be expected to be accurate sufficiently to surmount the correct ordering of the closely spaced excited states, previous researches have indicated that this method may be reliable as far as the shape of hydrogen-transfer potential energy curves is concerned [49-51]. The potential energy curves with only the variable parameter of O-H bond length from 1.0 to 2.3 Å among the 1-enol form and 1-keto form geometries in steps of 0.1 Å were shown in Fig.

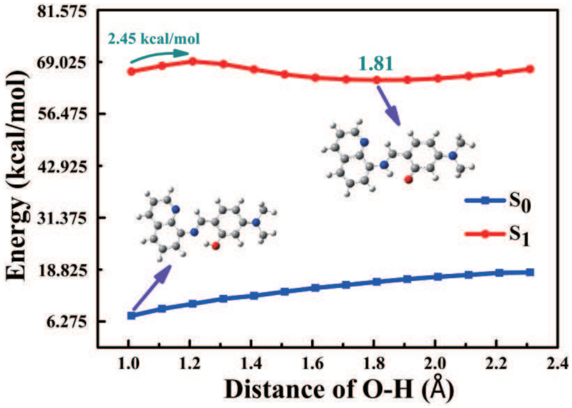

Figure 5: Potential energy curves of the ground and the first excited states for 1 chromophore along with O-H bond length. The inset shows the detailed configuration.

5, which can provide qualitative energetic pathways for the ESIPT process of 1 chromophore. It can be seen clearly that the energy of the ground state increases along with lengthening the O-H bond relaxing from the optimized length about 1.0 Å, which illustrated that no proton transfer occurs in the ground state. However, it should be noted that the first excited state potential energy curve exhibits a barrier of 2.45 kcal/mol between the reagent (from the vertical transition at the geometry of the minimum in the ground state) and the product. Therefore, it proved that transferring the proton H from O to N in 1-enol overcomes a very low barrier, thus suggesting that the ESIPT is very likely to be proceeded in the first excited state. In addition, when the O-H bond was lengthened to be 1.81 Å, there exists a stable point in the first excited state potential energy curve (i.e. 1-keto* form). Subsequently, the 1-keto* decays to the ground state 1-keto form through radiating fluorescence, which provides a possible explanation for the fluorescence quenching.

4 Conclusion

In summary, we have investigated the ESIPT mechanism of the new compound 1 chromophore reported by Liu *et al.* [33]. The hydrogen bond strengthening indicates the tendency of excited state proton transfer. The absorption and fluorescence spectra are well reappeared based on vertical transition energies calculated from the optimized geometries of ground and the first excited states. the corresponding frontier molecular orbitals have been analyzed indicating the ESIPT process could happen due to the intramolecular charge transfer. The constructed potential energy curve of the ground state demonstrated no proton transfer occurring, while a corresponding low barrier of 2.45 kcal/mol between 1-enol* and 1-keto* verified an ESIPT process. Based on ESIPT mechanism, the fluorescence peak of 533 nm could be attributed to the emission of 1-keto*, therefore, the fluorescence quenching was explained legitimately.

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