

Effect of intramolecular and intermolecular hydrogen bonding on the ESIPT process in DEAHB molecule

Hui Li(李慧), Lina Ma(马丽娜), Hang Yin(尹航), Ying Shi(石英)

Citation: Chin. Phys. B . 2018, 27(9): 098201. **doi:** 10.1088/1674-1056/27/9/098201

Journal homepage: http://cpb.iphy.ac.cn; http://iopscience.iop.org/cpb

What follows is a list of articles you may be interested in

Theoretical investigation on the excited state intramolecular proton transfer in Me_2N substituted flavonoid by the time-dependent density functional theory method

Hang Yin(尹航), Ying Shi(石英)

Chin. Phys. B . 2018, 27(5): 058201. **doi:** 10.1088/1674-1056/27/5/058201

Time-dependent density functional theoretical studies on the photo-induced dynamics of an HCl molecule encapsulated in C_{60} under femtosecond laser pulses

Liu Dan-Dan, Zhang Hong

Chin. Phys. B . 2013, 22(10): 103103. **doi:** 10.1088/1674-1056/22/10/103103

Effect of intramolecular and intermolecular hydrogen bonding on the ESIPT process in DEAHB molecule*

Hui Li(李慧)[1], Lina Ma(马丽娜)[1], Hang Yin(尹航)[1,2,†], and Ying Shi(石英)[1]

[1] *Institute of Atomic and Molecular Physics, Jilin University, Changchun* 130012, *China*

[2] *State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun* 130012, *China*

(Received 19 March 2018; revised manuscript received 22 May 2018; published online 28 August 2018)

Density functional theory (DFT) and time-dependent density functional theory (TDDFT) methods are used to investigate the influences of intramolecular and intermolecular hydrogen bonding on excited-state intramolecular proton transfer (ESIPT) for the 4-N,N′-(diethylamino)-2-hydroxybenzaldehyde (DEAHB). The structures of DEAHB and its hydrogen-bonded complex in the ground-state and the excited-state are optimized. In addition, the detailed descriptions of frontier molecular orbitals of the DEAHB monomer and DEAHB-DMSO complex are presented. Moreover, the transition density matrix is worked out to gain deeper insight into the orbitals change. It is hoped that the present work not only elaborates different influence mechanisms between intramolecular and intermolecular hydrogen bonding interactions on the ESIPT process for DEAHB, but also may be helpful to design and develop new materials and applications involved DEAHB systems in the future.

Keywords: time-dependent density functional theory, excited state intramolecular proton transfer, intramolecular charge transfer

PACS: 82.39.Jn, 31.15.ee, 87.15.ht **DOI:** 10.1088/1674-1056/27/9/098201

1. Introduction

Excited-state intramolecular proton transfer (ESIPT) is a photon induced ultrafast phenomenon that the proton transfers from donor to acceptor moiety upon optical excitation.[1–6] It attracts wide attention because it may play a crucial role in fluorescent probes,[7–9] bioimaging,[10] light-emitting materials,[11] and photostabilizers.[12] ESIPT has been studied by various experimental and theoretical methods during the last several decades.[13–23] Researches have demonstrated that the ESIPT process is susceptible to both intramolecular and intermolecular interactions.[24,25] Particularly, the effect of intra- and intermolecular hydrogen bonding (H-bonding) interactions on ESIPT in many functional molecular systems has been widely investigated.[11,26–28] Because the characteristic of H-bonding is site-specific, the ESIPT process can be altered by the H-bonding interaction between solute and solvent. Specifically, dimethylsulfoxide (DMSO) is a typical solvent with great proton affinity and it has strong capability to break the intramolecular H-bonding in the solute and form the intermolecular H-bonding with the solvent.[24] Recently, Zhang has experimentally proved that due to the formation of intermolecular H-bonding between solute and solvent, which partially breaks the intramolecular H-bonding in the solute, the 2,4,6-trisbenzothiazolylphenol in DMSO shows an extra fluorescence induced by the intermolecular H-bonding besides the emission from the ESIPT state.[25] Similarly, the Zn-quinoxaline complexes with intraligand H-bonds, $[Zn(hqxc)_2(py)_2]$ and $[Zn(hqxc)_2(DMSO)_2]$, were investigated by Sakai *et al.* In the former, ESIPT emission occurs so efficiently as to show amplified spontaneous emission (ASE), whereas in the latter, normal emission coexists with ESIPT emission arising from the interaction between $Zn(hqxc)_2$ and DMSO through the intermolecular H-bonding.[24]

To further explore the effect of intra- and inter-molecular H-bonding on the ESIPT process, we focus on the 4-N,N′-(diethylamino)-2-hydroxybenzaldehyde (DEAHB) molecule. It is a typical chromophore with a heterocyclic ring which consists of the intramolecular hydrogen bond between a hydroxyl group and a neighboring proton acceptor, and has a potential to exhibit the ESIPT phenomenon. It is an ideal model for investigation because the transition from intramolecular H-bonding to solute-solvent intermolecular H-bonding is possible in H-bonding acceptor solvents, which has been proved by Jana *et al.* with steady state and time-resolved spectroscopy experiments.[29] They found that the DEAHB exhibits dual emission in DMSO, whereas it shows single fluorescence in nonpolar solvents with a large Stokes shift. This interesting phenomenon is induced by the intermolecular H-bonding interaction between the hydrogen in the hydroxyl group and solvent with great proton affinity such as DMSO. Even to this day, the different influence mechanism between intramolecular and intermolecular H-bonding interactions on the ESIPT process

*Project supported by the National Basic Research Program of China (Grant No. 2013CB922204) and the National Natural Science Foundation of China (Grant Nos. 11574115 and 11704146).

†Corresponding author. E-mail: yinhang@jlu.edu.cn

© 2018 Chinese Physical Society and IOP Publishing Ltd

of DEAHB is still not clear. Therefore, it is of great significance to explore the difference between the DEAHB monomer and its hydrogen-bonded complex, which is helpful to further understand the effect of the solvent on the ESIPT process.

In the present work, we investigated the DEAHB molecule and DEAHB-DMSO complex theoretically aiming at providing the details of different influence mechanisms between intramolecular and intermolecular H-bonding interactions on ESIPT for DEAHB molecule. To be specific, we optimized the ground-state and the excited-state structures of DEAHB and its hydrogen-bonded complex using the density functional theory (DFT) and time-dependent density functional theory (TDDFT) methods, respectively. In addition, the detailed descriptions of the frontier molecular orbitals were presented to understand the ESIPT of DEAHB monomer and DEAHB-DMSO complex. Besides, the comparative analyses of infrared (IR) spectra between the ground-state and the excited-state have been carried out for both DEAHB monomer and DEAHB-DMSO complex. The potential energy curves along the proton transfer coordinate for DEAHB monomer both in the ground-state and excited-state were investigated as well.

2. Computation methods

In this work, all the geometry optimizations of DEAHB and hydrogen-bonded DEAHB-DMSO complex in the ground and the first excited states were carried out by using the DFT and the TDDFT[30–40] methods, respectively. Becke's three-parameter hybrid exchange function with the Lee–Yang–Parr gradient-corrected correlation functional (B3LYP)[41,42] and the triple-ζ valence quality with one set of polarization functions (TZVP)[43] basis set were employed for all the calculations. The method and basis set have been confirmed to be appropriate to study the electronic excited-state hydrogen bond. Moreover, the bond lengths, angles, or dihedral angles were included in the configuration optimization calculations. The potential energy curves for the DEAHB monomer in both the ground-state and the first excited-state were calculated through constrained optimizations, keeping the hydroxyl group (–OH) bond length increased by the increments of 0.1 Å based on the optimized ground- and excited-state geometries, respectively. Additionally, the infrared spectra of the ground-state and the first excited-state of the research system were computed using the TDDFT method at the B3LYP/TZVP level on the basis of the optimized ground- and excited-state structures. The vibration frequency was determined by the diagonalization of the Hessian matrix, and the intensity of the infrared depended on the gradient of the dipole. All of the local minima have been confirmed by no imaginary frequencies mode in the vibrational analysis. All the electronic structure calculations were carried out using the Gaussian 09 program package.[44]

3. Results and discussion

3.1. Ground-state geometric structures

Figure 1 depicts the optimized ground-state (S_0) geometric conformations together with the corresponding hydrogen bond lengths of the DEAHB monomer and hydrogen-bonded DEAHB-DMSO complex by using B3LYP function with the TZVP basis set. All the conformations were shown to have no virtual frequency by vibrational analysis calculations. For the hydrogen-bonded DEAHB-DMSO complex, we calculated the open-ring and closed-ring structures in the S_0 state. We found that the energy of the open-ring structure (−1186.90737966 a.u.) is lower than that of the closed-ring structure (−1186.90481117 a.u.). Therefore, the open-ring structure is more stable in the hydrogen-bonded DEAHB-DMSO complex. The following calculations and discussions of the DEAHB-DMSO complex are all based on the open-ring structure. The numerical values of main structure parameters involved in the intramolecular and intermolecular hydrogen bonds are shown in Table 1. The corresponding atom numbers can be seen in Fig. 1. From our optimized results, one can find that the DEAHB monomer and DEAHB-DMSO complex have planar structures. At the same time, it can be clearly seen that the intramolecular H-bonding of DEAHB can be formed by the hydroxyl group (–OH) together with the carbonyl (C=O) group. There is an intramolecular H-bonding characterized by C(8)=O(11)···H(14)–O(13) with bond length of 1.737 Å in the S_0 state. For the DEAHB-DMSO complex, the closed intramolecular H-bonding chelating ring is broken by DMSO. Then the H(39) atom turns outside of the ring to form the solute-solvent intermolecular H-bonding S(30)=O(29)···H(39)–O(13) with DMSO. In addition, the length of the intermolecular H-bonding is 1.701 Å and it is shorter than the intramolecular H-bonding, which means that the solute-solvent intermolecular H-bonding interaction is more intense.

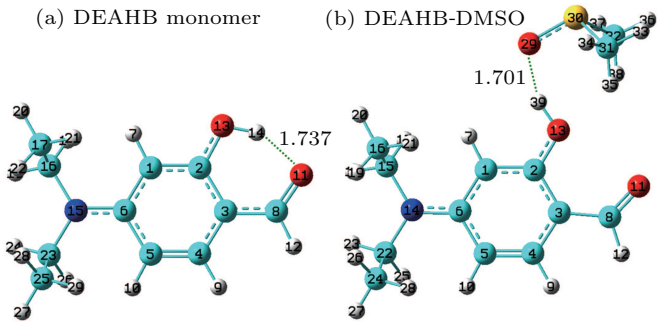


Fig. 1. (color online) Most stable geometries of (a) DEAHB and (b) DEAHB-DMSO complex in the ground state.

Table 1. Calculated bond lengths (in Å) of DEAHB monomer and DEAHB-DMSO complex in different excited states.

	DEAHB					
	O_{13}–H_{14}	C_8–O_{11}	O_{11}–H_{14}	C_2–O_{12}	O_1–H_{29}	O_{10}–H_{29}
S_0	0.989	1.234	1.737	–	–	–
S_1	0.969	1.320	1.872	–	–	–
S_1'	–	–	–	1.267	1.710	0.996
	DEAHB-DMSO					
	O_{13}–H_{39}		O_{29}–H_{39}		S_{30}–O_{29}	
S_0	0.99303		1.701		1.547	
S_1	0.99337		1.695		1.545	

3.2. Absorption spectra and frontier molecular orbitals

Table 2 shows the calculated electronic excitation energies and corresponding oscillator strengths of six low-lying excited states for the isolated DEAHB and DEAHB-DMSO complex. The absorption spectrum was calculated by vertical excitation from the ground-state to the first excited-state (S_1). The results show that the absorption peak of the hydrogen-bonded DEAHB-DMSO complex is red-shifted compared to that of the DEAHB monomer. The shift tendency is in good agreement with the experimental results from Jana's work.[29]

Table 2. Calculated electronic excitation energies (E) and corresponding oscillator strengths (OS) of DEAHB and DEAHB-DMSO complex. The orbital transitions and contributions for S_1 are also listed. H: the highest occupied molecular orbital (HOMO) L: the lowest unoccupied molecular orbital (LUMO).

	DEAHB		DEAHB-DMSO	
	E/nm	OS	E/nm	OS
S_1	341	0.1447	357	0.0002
Exp.	337		349	
	H-1→ L	54.10%	H-1→ L	70.38%
Flu.	516		408	
Exp.	531		384	
S_2	332	0.0005	320	0.2249
S_3	321	0.3112	312	0.2203
S_4	278	0.0315	295	0.0003
S_5	256	0.0003	294	0.0000
S_6	243	0.0268	292	0.0008

It is known to all that the frontier molecular orbitals (FMOs) play an important role in analyzing the charge distribution properties of molecules in their excited state transitions. Drawing the FMOs is a way to get a deeper understanding of the ESIPT process of the DEAHB molecule under the effect of both intramolecular and intermolecular H-bonding interactions. The orbital transitions and contributions for the different excited-states of the DEAHB monomer and DEAHB-DMSO complex are listed in Table 2. Through the calculation results of TDDFT, we know that the first excited state of the DEAHB monomer and DEAHB-DMSO complex corresponds mainly to a dominant transition from HOMO-1 to LUMO. Therefore, we plot the HOMO-1 and LUMO orbitals in Fig. 2.

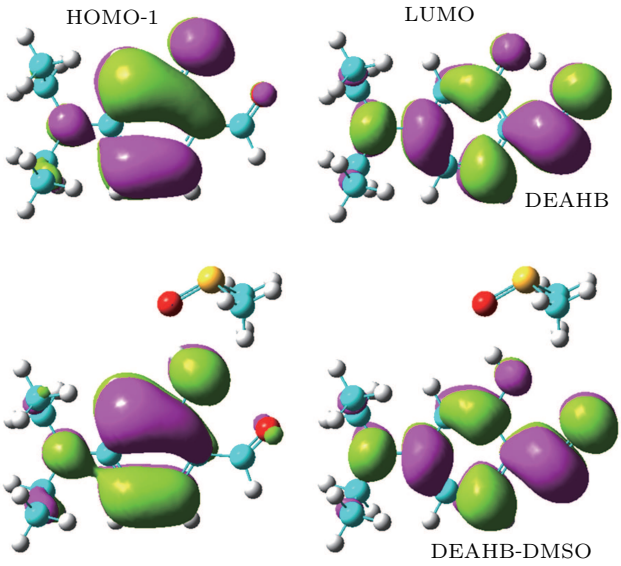


Fig. 2. (color online) Frontier molecular orbitals of DEAHB and DEAHB-DMSO complex.

From Fig. 2, we can conclude that the HOMO-1 orbital of the studied molecular is a π type orbit while the LUMO orbit has the π^* type feature for both monomer and hydrogen-bonded complex. That is to say, the S_1 state is of the $\pi\pi^*$-type transition feature which is believed to facilitate the proton transfer. We can also find that the charge densities are totally localized at the DEAHB molecular for both monomer and the complex, meanwhile the charge density in the LUMO moves to the right in comparison to the HOMO-1. For the DEAHB monomer, it can be seen clearly that the high electron density of HOMO-1 is mainly localized on the benzene ring, while most charges are transferred to the hydrogen-bonded chelating ring in the LUMO. Interestingly, upon the excitation from HOMO-1 to the LUMO, the electron density on the carbonyl group is increased, while the hydroxyl group is decreased. What needs to be mentioned is the electronegativity of the O(11) atom which is directly participated in the ESIPT process increases a lot, while the attraction between O(11) and H(14) is also greatly increased. That is the reason why the ESIPT process happens. When the intramolecular H-bonding is disconnected, the charge distribution of the C(8)=O(11) group also hugely increases upon electronic excitation for the DEAHB-DMSO complex. Therefore, the hydroxyl proton (H) is expected to be more acidic, and the carbonyl oxygen (O) is more basic compared with that in the S_0 state. There is no doubt that it is a very important positive factor for the proton transfer.

3.3. Electronic excited state geometric structures

We optimized the geometric structures of the DEAHB monomer and hydrogen-bonded DEAHB-DMSO complex in the S_1 state as shown in Fig. 3. It is worth mentioning that all the structures shown here are the lowest energy

conformers, as confirmed by their vibrational frequencies. As can be seen, DEAHB is still a planar conformation in the S_1 state, either for monomer or hydrogen-bonded complex. It should be noticed that the length of intramolecular H-bonding C(8)=O(11)···H(14)–O(13) for the DEAHB monomer is longer than that of intermolecular H-bonding S(30)=O(29)···H(39)–O(13) for the DEAHB-DMSO complex in the S_1 state. This is consistent with the change of the H-bonding length in the ground state of the two systems. Interestingly, for the DEAHB monomer, we can see that the intramolecular H-bonding C(8)=O(11)···H(14)–O(13) is lengthened (increases from 1.737 Å to 1.872 Å) in the S_1 state when compared to that in the ground state. A longer H-bonding length means that the intramolecular H-bonding is weakened in the S_1 state. It is noted in Table 1 that the bond length of C(8)=O(11) is lengthened from 1.234 Å in the S_0 state to 1.320 Å in the S_1 state, and the O(13)–H(14) bond is shortened from 0.989 Å to 0.969 Å. Furthermore, the O(13)–H(14)···O(11) angle is decreased from 147.6° to 140.4° upon the photo-excitation. The changes of the key bond lengths and bond angles are matched with the weakened intramolecular H-bonding. The equilibrium contributes to a stable configuration in the S_1 state. Simultaneously, we optimized the geometric structure of the tautomer in the S_1' state which has undergone the ESIPT process, and the corresponding structures are presented in Fig. 3(b). One can find that a new intramolecular H-bonding C(2)=O(12)···H(29)–O(10) is formed. The H-bonding length of C(2)=O(12)···H(29)–O(10), 1.711 Å, is shortened in the S_1' state compared to that of the intramolecular H-bondings we have discussed above. In the case of the DEAHB-DMSO complex, the intermolecular H-bonding S(30)=O(29)···H(39)–O(13) shortens in the S_1 state (Table 1). Upon exciting to the S_1 state, the excited state proton transfer process is destroyed due to the formation of intermolecular H-bonding between the S(30)=O(29) bond and the H(39)–O(13) bond. That is to say the hydrogen-bonded DEAHB-DMSO complex cannot exhibit the ESIPT process. It can be seen from the above data that the excited-state intramolecular proton transfer should be significantly facilitated by intramolecular H-bonding, since the proton transfer process takes place through the intramolecular H-bonding. DMSO can alter the intramolecular H-bonding and form intermolecular H-bonding, thus destroying the mechanism of ESIPT.

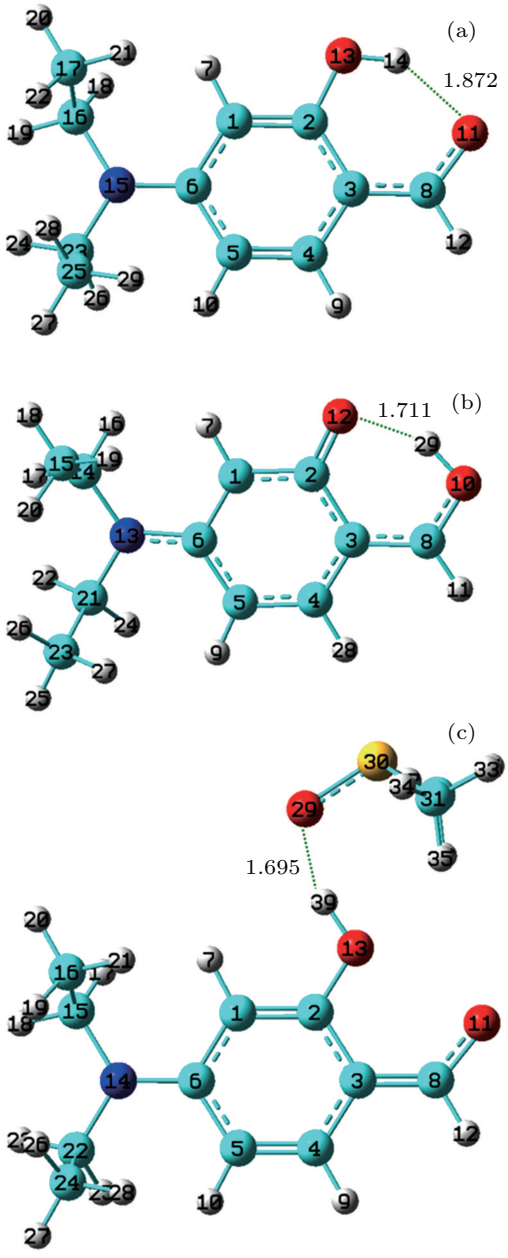


Fig. 3. (color online) Calculated excited state geometric structures of DEAHB ((a) normal form in the S_1 state, (b) tautomer form in the S_1' state), and (c) DEAHB-DMSO.

3.4. Potential energy curves

To reveal more features of the ESIPT process of the DEAHB monomer, the ground state and the first excited state potential energy curves have been scanned. We optimized the geometrical structures with only the variable parameter of the O(13)–H(14) bond length from 0.9 Å to 1.8 Å in steps of 0.1 Å, and constructed the potential energy profile on the S_0 and S_1 states. It is found that the energy of the ground state increases along with lengthening the O(13)–H(14) bond from the optimized length about 1.0 Å, which suggests that no proton transfer occurs in the ground state. While for the first excited state potential energy curve (i.e., tautomer form), it reaches the stable point when the O(13)–H(14) bond is lengthened to 1.71 Å. From the results, we can also see that the energy of the tautomer form is lower than that of the normal form in the S_1 state. Upon photo-excitation to the S_1 state of the DEAHB monomer, the S_1 state potential energy curve is almost barrierless of 0.4 kcal/mol. Therefore, this proves that transferring the proton H(14) from O(13) to O(11) in the DEAHB monomer overcomes a very low barrier (see Fig. 4), suggesting that the proton transfer process proceeds easily in the excited state. From our discussion above, it is evident that

excited-state intramolecular H-bonding plays a very important role in the ESIPT reaction.

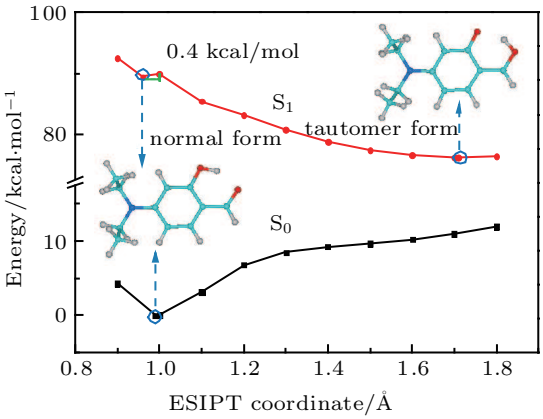


Fig. 4. (color online) The calculated potential energy curves of S_0 and S_1 states for DEAHB monomer by the TDDFT/B3LYP/TZVP method.

3.5. IR spectra

The intramolecular H-bonding plays a significant role in the excited state proton transfer process. Thus, the study of H-bonding dynamics in different electronic states is the key to understanding ESIPT. As we know, the electronic excited-state H-bonding dynamics can be detected by spectral shift with special vibrational modes. Figure 5 shows the calculated infrared spectra (B3LYP/TZVP, scaling factor 0.9630[45]) of the DEAHB monomer in the S_0 state and S_1 state. Here, the stretching modes of both the C=O and O–H groups in the DEAHB monomer are shown. As clearly shown in Fig. 5, two sharp peaks appear in the IR spectrum of the DEAHB monomer in the S_0 state. It should be noted that the calculated O(13)–H(14) stretching vibrational frequency is located at 3193 cm^{-1}, whereas another stronger peak centered at 1620 cm^{-1} is assigned to the C(8)=O(11) stretch mode. In the S_1 state (normal form), the O(13)–H(14) stretching band is blue shifted to 3520 cm^{-1}. Meanwhile, the C(8)=O(11) stretching band has a red shift of 1570 cm^{-1} in the S_1 state relative to that in the S_0 state. Based on the conclusions presented by Zhao mentioned above,[33] the IR spectra show obviously that, after being excited to the S_1 state, the intramolecular H-bonding of the DEAHB monomer is weakened. Additionally, the observed IR spectrum of the tautomer in the excited state S_1' is different from that of the normal cluster in the ground state and excited state. One can clearly see that the characteristic peaks of S_0 and S_1 disappear, and a new characteristic band appears around 3047 cm^{-1}, which is assigned as the formation of O(10)–H(29). Thus, the O–H stretching vibrational frequency shift indicates that the bond of O(13)–H(14) breaks up and the new bond should be O(10)–H(29) forms.

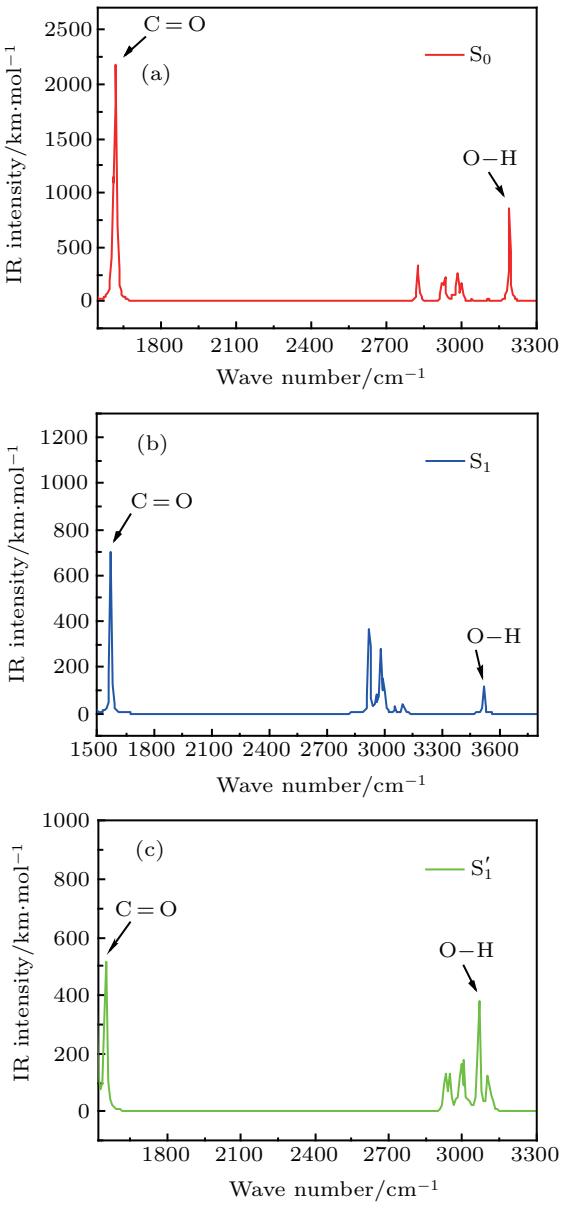


Fig. 5. (color online) The calculated IR spectra of DEAHB monomer in the (a) S_0, (b) S_1, and (c) S_1' states.

3.6. Dual mechanism in DEAHB-DMSO

In order to get further insight into the effect of the intermolecular hydrogen bond on the ESIPT process, the fluorescence peaks of the DEAHB monomer and the DEAHB-DMSO complex were further calculated. As shown in Table 2, it can be noted that fluorescence from the ESIPT state of the DEAHB monomer is 516 nm, which agrees with the experimental result in the report of Jana *et al.*[29] This means the fluorescence peak of DEAHB in the non-polar solvent comes from the ESIPT state of the DEAHB monomer. In the experiment, we found that the intensity of the fluorescence peak from the ESIPT state is weakened, a new fluorescence at 384 nm was observed. Our result reveals that fluorescence from the DEAHB-DMSO complex is 408 nm, which is in good agreement with the measured new fluorescence peak. We confirmed that, when the DEAHB molecule is dissolved in the DMSO

solvent, both the DEAHB monomer and the hydrogen bond complex DEAHB-DMSO exist. As the intramolecular hydrogen bond of DEAHB is partially destroyed by DMSO, the ESIPT process is thereby inhibited. Additionally, the new fluorescence peak should be derived from the intermolecular hydrogen-bonded complex DEAHB-DMSO.

4. Conclusion

In summary, the properties of intramolecular and intermolecular H-bonding of the DEAHB monomer and the hydrogen-bonded DEAHB-DMSO complex have been investigated using the DFT and TDDFT methods. We found that DMSO can partly disconnect the intramolecular H-bonding and form the intermolecular H-bonding with DEAHB. Our results indicated that the intramolecular H-bonding interaction is weakened while the intermolecular H-bonding interaction is strengthened after being photo-excited to the S_1 state. Combined with the experimental results, we demonstrated that the fluorescence of the DEAHB monomer comes from the ESIPT state, while the formation of intermolecular H-bonding between DEAHB and DMSO hinders the fluorescence from the ESIPT state for DEAHB, and then induces new fluorescence from the DEAHB-DMSO complex. The result is helpful in developing the high performance sensor based on DEAHB.

Acknowledgment

We express heartfelt thanks to members of our discussion group for their valuable comments.

References

[1] Yao H and Funada T 2014 *Chem. Commun.* **50** 2748
[2] El Nahhas A, Pascher T, Leone L, Panzella L, Napolitano A and Sundstrom V 2014 *J. Phys. Chem. Lett.* **5** 2094
[3] Tang K C, Chang M J, Lin T Y, Pan H A, Fang T C, Chen K Y, Hung W Y, Hsu Y H and Chou P T 2011 *J. Am. Chem. Soc.* **133** 17738
[4] Tang K C, Chen C L, Chuang H H, Chen J L, Chen Y J, Lin Y C, Shen J Y, Hu W P and Chou P T 2011 *J. Phys. Chem. Lett.* **2** 3063
[5] Barman S, Mukhopadhyay S K, Biswas S, Nandi S, Gangopadhyay M, Dey S, Anoop A and Singh N D P 2016 *Angew. Chem. Int. Ed.* **55** 4194
[6] Weller A 1956 *Ber. Bunsenges. Phys. Chem.* **60** 1144
[7] Zhao J Z, Ji S M, Chen Y H, Guo H M and Yang P 2012 *Phys. Chem. Chem. Phys.* **14** 8803
[8] Shiraishi Y, Matsunaga Y, Hongpitakpong P and Hirai T 2013 *Chem. Commun.* **49** 3434
[9] Liu B, Wang H, Wang T S, Bao Y Y, Du F F, Tian J, Li Q B A and Bai R K 2012 *Chem. Commun.* **48** 2867
[10] Shynkar V V, Klymchenko A S, Kunzelmann C, Duportail G, Muller C D, Demchenko A P, Freyssinet J M and Mely Y 2007 *J. Am. Chem. Soc.* **129** 2187
[11] Padalkar V S and Seki S 2016 *Chem. Soc. Rev.* **45** 169
[12] Paterson M J, Robb M A, Blancafort L and DeBellis A D 2005 *J. Phys. Chem. A* **109** 7527
[13] Demchenko A P, Tang K C and Chou P T 2013 *Chem. Soc. Rev.* **42** 1379
[14] Klymchenko A S 2017 *Acc. Chem. Res.* **50** 366
[15] Cheng X, Wang K, Huang S, Zhang H Y, Zhang H Y and Wang Y 2015 *Angew. Chem. Int. Ed.* **54** 8369
[16] Yang D P, Yang G, Zhao J F, Zheng R and Wang Y S 2017 *J. Cluster Sci.* **28** 2449
[17] Yang D P, Zheng R, Wang Y S and Lv J 2017 *J. Cluster Sci.* **28** 937
[18] Zhang M X, Zhou Q, Zhang M R, Dai Y M, Song P and Jiang Y 2017 *J. Cluster Sci.* **28** 1191
[19] Jia X L, Li C Z, Li D L and Liu Y F 2018 *Spectrochim. Acta Part A* **192** 168
[20] Zhou P W, Hoffmann M R, Han K L and He G Z 2015 *J. Phys. Chem. B* **119** 2125
[21] Han K L and Zhao G J 2011 *Hydrogen Bonding Transfer in the Excited State* (Wiley Online Library) p. 555
[22] Zheng J J, Zhang G L, Guo Y X, Li X P and Chen W J 2007 *Chin. Phys. B* **16** 1047
[23] Wu F, Lin L, Li X P, Yu Y X, Zhang G L and Chen W J 2008 *Chin. Phys. B* **17** 1461
[24] Sakai K i, Takahashi S, Kobayashi A, Akutagawa T, Nakamura T, Dosen M, Kato M and Nagashima U 2010 *Dalton T.* **39** 1989
[25] Zhang X and Liu J Y 2016 *Dyes Pigments* **125** 80
[26] Yin H, Shi Y and Wang Y 2014 *Spectrochim. Acta Part A* **129** 280
[27] Yin H, Li H, Xia G M, Ruan C Y, Shi Y, Wang H M, Jin M X and Ding D J 2016 *Sci. Rep.* **6** 19774
[28] Liang J, Tang B and Liu B 2015 *Chem. Soc. Rev.* **44** 2798
[29] Jana S, Dalapati S and Guchhait N 2013 *J. Phys. Chem. A* **117** 4367
[30] Yang D P, Yang Y G and Liu Y F 2014 *Spectrochim. Acta Part A* **117** 379
[31] Song P, Li Y Z, Ma F C, Pullerits T and Sun M T 2013 *J. Phys. Chem. C* **117** 15879
[32] Yang Y F, Zhao J F and Li Y Q 2016 *Sci. Rep.* **6** 32152
[33] Zhao G J and Han K L 2007 *J. Phys. Chem. A* **111** 2469
[34] Zhao G J and Han K L 2008 *J. Comput. Chem.* **29** 2010
[35] Zhao G J and Han K L 2012 *Acc. Chem. Res.* **45** 404
[36] Zhao X H and Chen M D 2011 *Chem. Phys. Lett.* **512** 35
[37] Huang J D, Yu K, Ma H P, Chai S and Dong B 2017 *Dyes Pigments* **141** 441
[38] Zhao J F, Liu X Y and Zheng Y J 2017 *J. Phys. Chem. A* **121** 4002
[39] Chen J S, Zhou P W, Zhao L and Chu T S 2014 *Rsc Adv.* **4** 254
[40] Zhang M Z, Ren B P, Wang Y and Zhao C X 2013 *Spectrochim. Acta Part A* **101** 191
[41] Furche F and Ahlrichs R 2002 *J. Chem. Phys.* **117** 7433
[42] Treutler O and Ahlrichs R 1995 *J. Chem. Phys.* **102** 346
[43] Feller D 1996 *J. Comput. Chem.* **17** 1571
[44] Frisch M J, Trucks G W, Schlegel H B, *et al. Gaussian* 09, *Revision B.* 01 (Gaussian, Inc., Wallingford, 2009)
[45] Lukeš V, Aquino A and Lischka H 2005 *J. Phys. Chem. A* **109** 10232