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Relationship between ESIPT properties and antioxidant activities of 5-hydroxyflavone derivates*

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It is of great significance to study the relationship between the excited state intramolecular proton transfer (ESIPT) properties and antioxidant activities of compounds in the field of life sciences. In this work, two novel compounds 5HF–OMe and 5HF–NH_2 are designed through introducing a methoxy- and amino-group into the structure of 5-hydroxyflavone (5HF) respectively. The relationship between the ESIPT reaction and antioxidant activities of the three compounds is studied via the density functional theory (DFT) and time-dependent DFT (TD-DFT) methods. The calculated potential energy curves suggest that the rate of ESIPT reaction will gradually slow down from 5HF to 5HF–OMe and 5HF–NH_2. In addition, the antioxidant activities of the three compounds gradually enhance from 5HF to 5HF–OMe and 5HF–NH_2, which can be seen from the calculated energy gaps and ionization potential values. Interestingly, the above results imply that the rate of ESIPT reaction has a negative relationship with the antioxidant activities of the compounds, *i.e.*, the slower rate of ESIPT reaction will reflect the higher antioxidant activity of the compound, which will provide valuable reference for detecting the antioxidant activity of compound via the photophysical method.

Keywords: 5-hydroxyflavone, excited state intramolecular proton transfer, antioxidant activity, density functional theory

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1. Introduction

The excessive free radicals can cause many diseases such as cancers, inflammation, atherosclerosis, and so on because of its high reactive activity.[1–3] Flavonoids, as polyphenols, are widely distributed in nature. Numerous studies have shown that the flavonoids exhibit the functions of antioxidant, antineoplastic, antimicrobial, antiviral, and immune regulation.[4–6] In recent years, many new antioxidants have been found in theory and experiments by modifying the structures of flavonoids.[7–9]

Pharmacal surveys show that the 5-position hydroxyl in 5-hydroxyflavone (5HF) can significantly affect its biological activity,[10] which may be related to the formation of an intramolecular hydrogen bond (IMHB) between 5-hydroxyl and the adjacent carbonyl group, resulting in greater delocalization of electrons in the molecule.[11,12] Abo Markeb and co-workers[13] found that the intermolecular hydrogen atom transfer in the excited triplet state as well as in the excited singlet state might determine the quenching process of photoexcited molecules in biological systems through investigating the quantitation of 5- and 7-hydroxyflavone antioxidants. Moreover, due to the excited state intramolecular proton transfer (ESIPT) reaction existing in 5HF, its photophysical properties have been widely studied.[12,14] Chou *et al.*[15] investigated the spectroscopy and dynamics of ESIPT in 5HF, and observed the dual fluorescence maxima at $\sim$ 420 nm and 700 nm in cyclohexane. Ash and collaborator[16] studied the potential energy curves (PECs) for the intramolecular proton transfer in the ground and excited states of 3HF and 5HF by using the density functional theory (DFT) and time-dependent DFT (TD-DFT) methods, and the characteristics of ground and excited state PECs explained the large stokes shifted and broad ESIPT band of 3HF. However, the relationship between antioxidant activity and ESIPT characteristic of 5HF has not been thoroughly studied.

In recent decades, the DFT method based on quantum chemical calculation has been widely used to study the antioxidant activity and excited state properties of molecules.[17–24] In this work, two novel compounds 5HF–OMe and 5HF–NH_2 are designed through introducing a methoxy- and amino-group into the 3-position of 5HF respectively. The properties related to the ESIPT reaction and the antioxidant activities of the three compounds were calculated in the framework of DFT and TD-DFT methods. The chemical structures of the three compounds are shown in Fig. 1. Specifically, the calculated PECs of the three compounds were used to evaluate the rate of ESIPT reaction, and the highest occupied molecular orbital (HOMO) energies, energy gaps, and global descriptive parameters containing chemical hardness (η), softness (S), potential (μ), electronegativity (χ), and electrophilicity index (ω) were obtained to estimate the chemical reactivity of the three compounds. By revealing the relationship between ESIPT be-

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havior and antioxidant activity of compounds, it can provide reference for detecting the antioxidant activity of compound via the photophysical method.

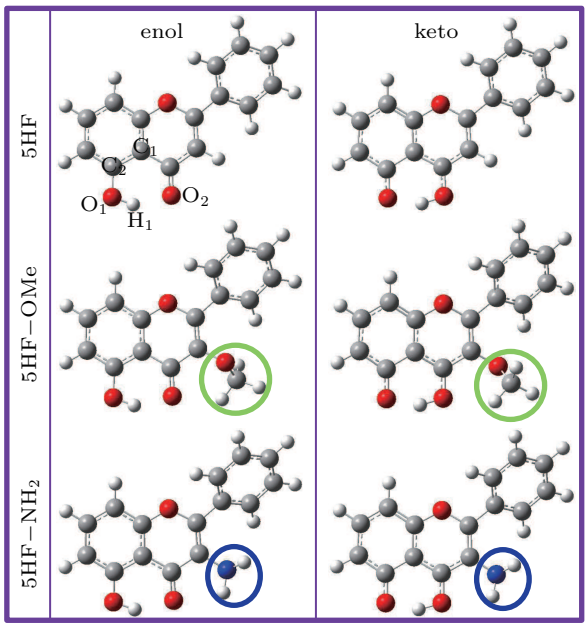


Fig. 1. Enol and keto forms of 5HF and its derivatives.

2. Methods

The ground- and excited-state structures of 5HF and its derivatives were optimized in the framework of DFT[25,26] method, with B3LYP[27,28] functional at 6–311++G(d) basis set. Based on the optimized ground state structures, the absorption peaks and oscillator strengths of the compounds were calculated via TD-DFT[29] method, with PBEPBE[30] functional at 6–311++G(d) basis set. In addition, the PECs for the S_0 and S_1 states of the three compounds were scanned along with the increasing bond length of O_1–H_1 to explore the ESIPT reactions respectively. In this work, the ethanol was used as the solvent adopting the polarizable continuum model (PCM) with the integral equation formalism variant (IEFPCM).[31,32] The Gaussian 09 software was used to complete all the calculations in this work.[33]

Moreover, in order to evaluate the activity of these three compounds, the global descriptive parameters, containing chemical hardness (η), softness (S), potential (μ), electronegativity (χ), and electrophilicity index (ω), were calculated via the following equations:[34,35]

$$\text{Chemical hardness } (\eta) \approx (\text{IP} - \text{EA})/2, \tag{1}$$

$$\text{Softness } (S) \approx 1/(2\eta), \tag{2}$$

$$\text{Electronegativity } (\chi) \approx (\text{IP} + \text{EA})/2, \tag{3}$$

$$\text{Chemical potential } (\mu) \approx -\chi, \tag{4}$$

$$\text{Electrophilicity index } (\omega) \approx \mu^2/(2\eta), \tag{5}$$

where IP and EA represent the ionization potential and electron affinity of the compound, respectively. Furthermore, the antioxidant activity to scavenge free radicals of the compound at ground- and excited-states can also be defined with the IP value.[36] According to the previous literatures,[35,37] the IP and EA values of the compound can be calculated based on the difference between the total energies of neutral molecule (E_{neutral}) and its corresponding anion (E_{anion}) and cation (E_{cation}) forms, and usually call it as "energy vertical method", which can be expressed by using the equations:

$$\text{IP} = E_{\text{cation}} - E_{\text{neutral}}, \tag{6}$$

$$\text{EA} = E_{\text{neutral}} - E_{\text{anion}}. \tag{7}$$

3. Results and discussion

3.1. Intensity of intramolecular hydrogen bond

According to the previous literatures,[16,20,38] the relative characteristic peak of hydroxyl group in the infrared (IR) spectrum can be used to estimate the strength of IMHB. In view of this, the IR spectra of the three compounds were simulated and the vibration peaks corresponding to O_1–H_1 are shown in Fig. 2(a). It can be found that compared with that of 5HF, the peaks for 5HF–OMe and 5HF–NH_2 exhibit a blue-shift of 25 cm^{-1} and 37 cm^{-1} respectively, indicating that the strength of the IMHB O_1–$H_1\cdots O_2$ gradually weakens from 5HF to 5HF–OMe and 5HF–NH_2.

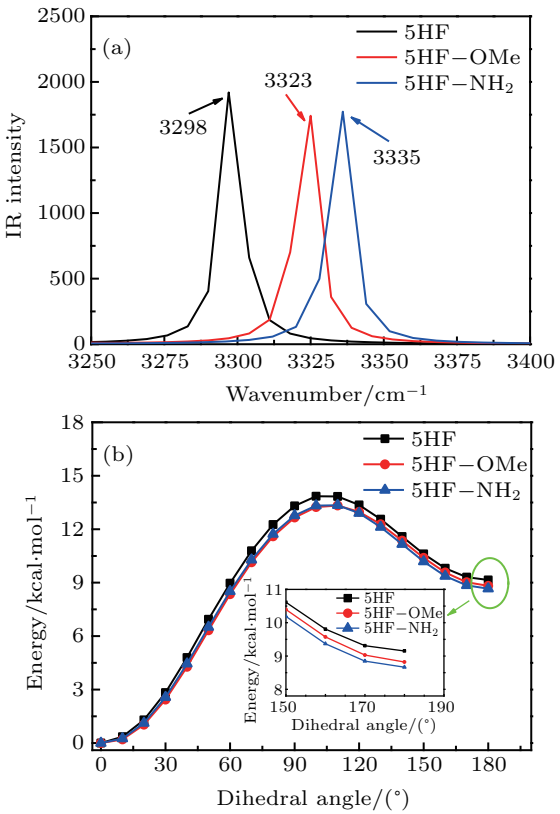
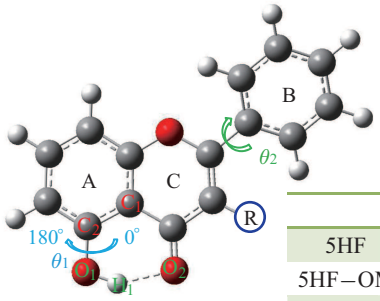


Fig. 2. Strength of the IMHBs existing in the three compounds: (a) the characteristic peaks corresponding to the stretching vibration of O_1–H_1; (b) energies of the transformation of IMHB from normal form to the non-hydrogen bonded form.

In addition, the energy difference of the transformation of IMHB from normal form to the non-hydrogen bonded form can also be used to examine the strength of IMHB,[16] and Scheme 1 shows the structures of the compounds with and without IMHB. The total energies of the three compounds through rotating the dihedral angle C_1–C_2–O_1–H_1 are presented in Fig. 2(b). As shown, the calculated total energies for 5HF, 5HF–OMe, and 5HF–NH_2 are 9.152 kcal/mol, 8.821 kcal/mo, and 8.665 kcal/mol, respectively. The above results indicate that the strength of the IMHB for the three compounds is gradually decreased from 5HF to 5HF–OMe and 5HF–NH_2.



	Dihedral angle (θ_2)
5HF	20.74°
5HF−OMe	32.41°
5HF−NH_2	36.43°

Scheme 1. Structures of the compounds with and without IMHBs (θ_1 = 0° → 180°); and the dihedral angles (θ_2) between B-ring and C-ring of the three compounds.

3.2. Absorption spectra and frontier molecular orbitals

Ultraviolet (UV) radiation is one of the factors leading to the increase of free radicals in human body, and the ability of compound to absorb UV radiation can be used as a basis for an effective antioxidant.[39] Based on this, the absorption spectra of 5HF and its derivatives are intuitively presented in Fig. 3(a), and the corresponding transition properties have been listed in Table 1. From Fig. 3(a) we can find that the absorption peak of 5HF is located at 324 nm, which agrees well with the experimental results,[40] and proves the reliability of the selected theoretical method. Relative to 5HF, the absorption peaks of 5HF–OMe and 5HF–NH_2 are red-shifted to 344 nm and 456 nm respectively. Scheme 1 presents the dihedral angles (θ_2) between B-ring and C-ring of the three compounds, from which can be found that the distortion degree between B-ring and C-ring increases gradually from 5HF to 5HF–OMe and 5HF–NH_2. The increased noncoplanarity of molecular structure induces the red shift of absorption spectra.[41] However, the stronger absorption ability on UV radiation by 5HF and 5HF–OMe makes them as the effective antioxidants.

The HOMO energy and energy gap of the compound are closely related to its antioxidant activity, *i.e.*,, the higher HOMO energy and smaller energy gap can produce the stronger antioxidant activity.[42–44] Under the specific light excitation, the studied compounds will exhibit two different forms: enol-form and keto-form. Therefore, we considered the antioxidant activity of these two molecular configurations for the three compounds in this work. The obtained HOMO energies and energy gaps of the three compounds at enol and keto forms are shown in Fig. 3(b). As it can be found, the HOMO energies of the three compounds at enol and keto forms all are in the increasing order of 5HF < 5HF–OMe < 5HF–NH_2, which means that the antioxidant activity of the three compounds at the two forms will gradually increase in the same order. Attentively, the HOMO energies of the three compounds at enol forms are lower than the corresponding compound at keto form, indicating the compounds at keto forms would show the higher antioxidant activity. In addition, the energy gaps of the three compounds at the two forms all follow the decreasing order of 5HF > 5HF–OMe > 5HF–NH_2, which again proved that the antioxidant activity of the three compounds gradually increase from 5HF to 5HF–OMe and 5HF–NH_2. Besides, the energy gaps of the compounds at keto form all are lower than that of the compounds at enol form, again illustrating the keto forms of the compounds have the higher antioxidant activity.

Table 1. Calculated absorption properties of 5HF and its derivatives via TD-DFT/PBEPBE/6-311++G(d) in ethanol.

	State	λ_{max}/(eV/nm)	Contribution MO	Strength f
5HF	S1	2.9065/427	(68.80%)H→ L	0.0247
	S2	3.3907/366	(67.01%)H-1→ L	0.0027
	S3	3.8215/324	(58.38%)H-2→ L	0.5279
5HF–OMe	S1	2.8819/430	(67.33%)H→ L	0.0722
	S2	3.2734/379	(60.44%)H-1→ L	0.0235
	S3	3.6055/344	(57.59%)H-2→ L	0.3456
5HF–NH_2	S1	2.7172/456	(68.14%)H→ L	0.1901
	S2	3.3391/371	(66.80%)H-1→ L	0.1404
	S3	3.6642/338	(62.49%)H→L+2	0.0056

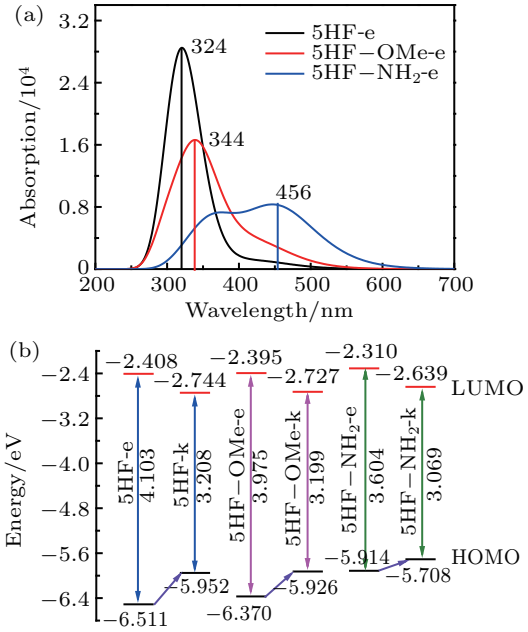


Fig. 3. (a) Absorption spectra and (b) frontier molecular orbital energies of 5HF and its derivatives at enol and keto forms.

3.3. Potential energy curves at S_0- and S_1-states

Based on the optimized structures, the constructed PECs at S_0- and S_1-states for the three compounds are shown in Fig. 4. As shown, 5HF, 5HF–OMe, and 5HF–NH_2 go through the energy barriers of 8.641 kcal/mol, 9.311 kcal/mol, and 9.761 kcal/mol at the S_0 state respectively, larger than the energy barrier of the corresponding compound at the S_1 state. This illustrates the three compounds tend to the occurrence of ESIPT reaction upon the light-excitation. Focus shifts to the S_1 state, it can be noted that 5HF and 5HF–OMe undergo the ESIPT reaction with barrierless, and an energy barrier of 3.034 kcal/mol exists in the ESIPT reaction of 5HF–NH_2. The energy differences between two stable structures in the S_1 state for 5HF and 5HF–OMe are 13.280 kcal/mol and 12.098 kcal/mol, respectively. The above results suggest that the rate of ESIPT reaction would gradually slow down from 5HF to 5HF–OMe and 5HF–NH_2,[45] which means that the transition of molecular configuration from enol form to keto form will become more and more difficult. These results also confirm that the introduction of electron-donating groups can inhibit the occurrence of ESIPT in the previous reports.[46,47] Combined with the conclusions drawn above, the degree of difficulty in molecular configuration transition would affect the antioxidant activity of compound.

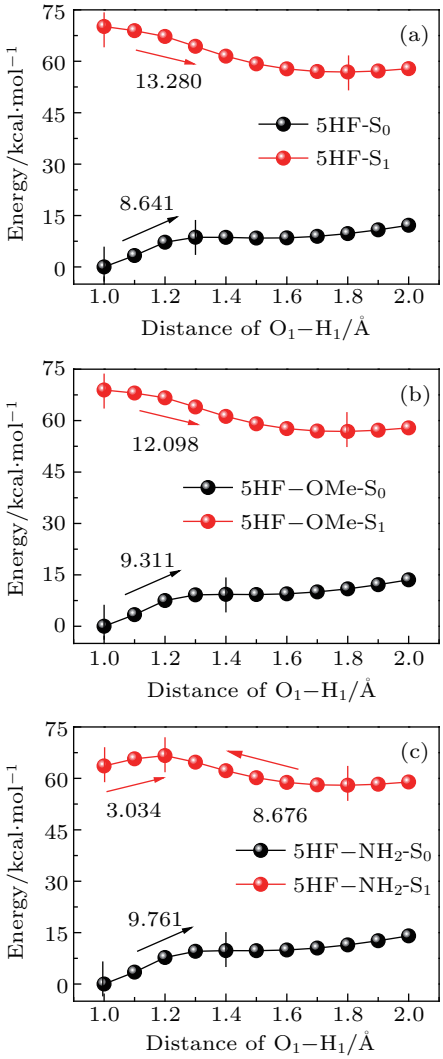


Fig. 4. PECs for the S_0- and S_1-states of (a) 5HF, (b) 5HF–OMe, and (c) 5HF–NH_2 along with the increasing bond length of O_1–H_1.

3.4. Global descriptive parameters

The global descriptive parameters including chemical hardness (η), softness (S), potential (μ), electronegativity (χ), and electrophilicity index (ω) are calculated to evaluate the chemical reactivity of the three compounds, and the detailed results are listed in Table 2. The chemical hardness represents the resistance towards the deformation or polarization of the electron cloud of the atoms, ions or compounds under the accidental tiny interference during chemical reaction process, and the lower chemical hardness means the higher reactivity of the compound.[48,49] It can be found from Table 2 that the obtained chemical hardness of the three compounds by two different calculation methods all are in the decreasing order of 5HF > 5HF–OMe > 5HF–NH_2, implying that the reactivity of the compounds is gradually enhanced from 5HF to 5HF–OMe and 5HF–NH_2. Chemical softness is used to weigh the ability of molecule to receive electrons and inversely proportional to the chemical hardness, and the higher chemical softness reflects the stronger reactivity of compound.[50] In terms of this, 5HF–NH_2 would exhibit the strongest activity among the three compounds owing to its highest chemical softness. The chemical potential judges the escaping tendency of an electron from equilibrium and is also the negative value of electronegativity, which is a scale of the tendency to attract electrons in a chemical bond.[51,52] It can be seen from Table 2 that the electronegativity of the three compounds gradually decreases from 5HF to 5HF–OMe and 5HF–NH_2, which is due to the gradual enhancement of the electron donating ability from –OMe to –NH_2 group. The electrophilicity index describes the electrophilicity strength of the compound,[53] and it can be noted from Table 2 that the order for the electrophilicity indexes of the three compounds is consistent with that for the electron affinities of the three compounds and 5HF–NH_2 shows the lower electrophilicity strength compared with that of the other two compounds.

Table 2. Calculated global descriptive parameters of 5HF and its derivatives (in unit eV).

	IP	EA	η	S	μ	χ	ω
5HF	6.32	2.76	1.78	0.28	−4.54	4.54	5.78
5HF–OMe	5.96	2.77	1.59	0.31	−4.36	4.36	5.97
5HF–NH_2	5.55	2.65	1.45	0.35	−4.10	4.10	5.81

3.5. Antioxidant activity at S_0- and S_1-states

The antioxidant activity of compound can be estimated theoretically by the ionization potential (IP), in which the compound with lower IP value would show the higher antioxidant

activity.[54] The calculated IP values of the three compounds in the enol and keto forms at S_0 and S_1 states are summarized in Fig. 5. Due to the S_1 state configurations of 5HF and 5HF–OMe in enol forms do not exist, the corresponded IP values are not available. It can be seen from the data available at present that the IP values of the three compounds in enol and keto forms are in the decreasing order of 5HF > 5HF–OMe > 5HF–NH_2, indicating that their antioxidant activities follow the order of 5HF < 5HF–OMe < 5HF–NH_2. This is consistent with the conclusion from the obtained HOMOs and the work of Sutradhar *et al.*[55] In addition, compared with that at the S_0 state, the IPs of the compounds at the S_1 state exhibit the smaller values, which means the antioxidant activity of the compound will be enhanced under the light excitation. Furthermore, the compounds in the keto form have the smaller IP values by comparison with that in the enol form, which shows that the configuration of the compounds after ESIPT reaction will exhibit the stronger antioxidant activity. In terms of the previous literatures,[19,21] the intramolecular charge transfer under photo-excitation facilitates the ESIPT reaction of the compound, so there is a certain relationship between the antioxidant activity and intramolecular charge transfer of the compound. Taken the ESIPT reaction rates of the three compounds into account, the antioxidant activities of compounds can be regulated by ESIPT reaction.

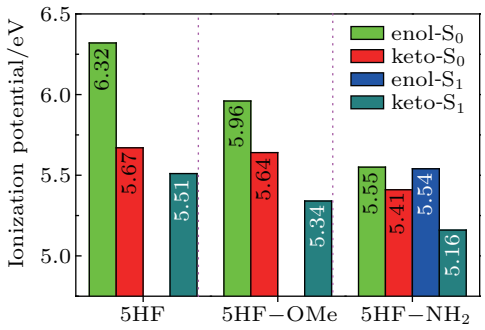


Fig. 5. Calculated ionization potentials (IPs) for the enol and keto forms of 5HF and its derivatives at S_0 and S_1 states.

4. Conclusions

In this work, the relationship between the ESIPT processes and antioxidant activities of 5HF and its two derivatives 5HF–OMe and 5HF–NH_2 were studied by using DFT and TD–DFT methods. The IR spectra and energy difference of the transformation from normal form to the non-hydrogen bonded form indicate that the strength of the IMHB for the three compounds is gradually decreased from 5HF to 5HF–OMe and 5HF–NH_2, which would affect the proton transfer in the process of antioxidant reaction. In addition, the obtained PECs imply that the ESIPT process would gradually slow down from 5HF to 5HF–OMe and 5HF–NH_2. Furthermore, the calculated HOMO energies, energy gaps, global descriptive parameters, BDE and IP values all show that the antioxidant activity of the compounds gradually enhance from 5HF to 5HF–OMe and 5HF–NH_2. The above results suggest that the ESIPT rate has a negative relationship with the antioxidant activity of the compound, which will give an interesting guidance for detecting the antioxidant activity of compound via the photophysical method.

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