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Theoretical study on twisted intramolecular charge transfer of 1-aminoanthraquinone in different solvents*

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The twisted intramolecular charge transfer and the excited state relaxation of 1-aminoanthraquinone (1-NH_2-AQ) in different solvents are investigated using quantum chemical calculations in this paper. The geometries of the ground state are optimized both in gas and solvents based on the high-level *ab initio* calculations, the lowest excited singlet state geometry is optimized only in gas for simplicity. An intramolecular charge transfer property is substantiated by the large change of dipole moments between the S_0 and S_1 states. The mechanism of twisted intramolecular charge transfer is proposed by the conformational relaxation on the potential surface of the S_1 state. Quantum chemical calculations present that internal conversion and intersystem crossing are important approaches to the ultrafast deactivation of the S_1 state via the twisting of the amino group. The smaller energy difference between the S_0 and S_1 state shows that the internal conversion process is much faster in a polar solvent than in a nonpolar solvent. Energy intersections between the T_2 and S_1 state in cyclohexane and dioxane indicate a faster intersystem crossing process in them than in ethanol. These theoretical results agree well with the previous experimental results. Energy barriers are predicted on the potential surface of the S_1 state, and they have a positive correlation to solvent viscosity, and the timescale of twisted intra-molecular charge transfer in dioxane is predicted to be longer than in cyclohexane and ethanol.

Keywords: 1-aminoanthraquinone, conformational relaxation, twisted intra-molecular charge transfer, quantum chemical calculations

PACS: 34.70.+e, 31.70.Hq, 33.15.Hp, 32.70.Cs **DOI:** 10.1088/1674-1056/27/8/083401

1. Introduction

Anthraquinones derivatives have widely been used in the dye industry, biological research, pharmacy, and medicine in the last few decades for their photosensitization and anticancer ability.[1–3] Amino-substituted anthraquinones are used to composite porphyrin-anthraquinone hybrids, which are efficient photocleavage agents of DNA.[4–7] The key to efficient photocleavage is the charge transfer efficiency.[8–13] The $-NH_2$ and $-NO_2$ groups play a role in a strong electronic donor and acceptor in intramolecular charge transfer, respectively. When an $-NH_2$ and/or $-NO_2$ group is directly bonded to a polycyclic aromatic system, the photophysics and photochemistry of the molecule are drastically changed by this substituent. Molecular systems with $-NH_2$ and/or $-NO_2$ group are of great interest and widely studied for their charge transfer character.[14–18] The intramolecular charge transfer (ICT) of compounds containing the $-NH_2$ group, 4-dimethylaminobenzonitrile (DMABN) and related molecules, are widely studied by experiments as well as quantum calculations.[19–24] The dual fluorescence of DMABN in polar solvents is observed and explained as an intramolecular charge transfer phenomenon.[19] It consists of emissions from a local excited (LE) and ICT states.[25] Several models of the reaction were proposed to reveal the influence of the molecular structure on the ICT state: ICT state with perpendicularly twisted amino and benzonitrile moieties (TICT),[26] ICT state with pyramidalized amino group (WICT),[27] ICT state with a rehybridized nonlinear C–CN group (RICT),[28] and planar ICT state (PICT).[29] However, the twisted intramolecular charge transfer (TICT) model is widely accepted.[19–22,30,31] A great majority of theoretical studies indicate that the $-NH_2$ and/or $-NO_2$ group twists as the reaction coordinates along which the ICT reaction occurs.[24,32] Köhn *et al.* pointed out that the twisting of the dimethylamino group is the dominant reaction coordinate by using correlated CC2 calculations.[24]

The amino anthraquinone derivatives are used as catalytic DNA photonucleases for their special charge and structure character.[5,33–37] 1-aminoanthraquinone (1-NH_2-AQ) is the simplest anthraquinone derivative and has two chromophoric groups, namely anthraquinone and the amino groups. The amino ($-NH_2$) group in 1-NH_2-AQ is a strong electron donor and induces an ICT property after an excitation. The ICT character with the excitation to the S_1 state has been proved by using Shpol'skii matrix fluorescence and fluorescence excitation spectra.[38,39] From CCl_4 to more polar solvents, the fluorescence lifetimes of 1-NH_2-AQ were determined to be 400 ps∼

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2000 ps, and fluorescence quantum yields were measured to be 0.006∼0.0715 in different solvents by steady absorption and time-resolved spectra.[40,41] It is interesting that no dual fluorescence was observed in various solvents, but the absorption and fluorescence spectra, fluorescence quantum yields are strongly correlative to solvent polarity. The phenomenon of no dual fluorescence was also observed in other ICT molecular systems.[17,18,42] Although the ICT character has been observed in several experiments in 1-aminoanthraquinone, its theoretical description and discussion are still absent.

Quantum chemical calculations are important tools for theoretical researches.[43–45] In this paper, the electronically excited states of 1-NH_2-AQ are studied theoretically using ab initio methods with focusing on the mechanism for TICT and the following radiationless processes. Optimized geometries of the ground and excited states are calculated and discerned by several methods with different basis sets. The mechanism of TICT is proposed by dipole moments and the conformational relaxation with the twisted angle of the amino group. The energies and potential surface of the excited states involved in radiationless relaxation are described and discussed in detail. The deactivation of the S_1 state is deduced to be due to the contribution of both intersystem crossing (ISC) and internal conversion (IC) channels.

2. Computational methods

All calculations in this work were performed with the Gaussian 09 program.[46] In the gas phase, geometry optimizations at ground state are performed using B3LYP, B3PW91, and MP2 in conjunction with 6-311G and Lanl2dz basis sets, respectively. All optimized geometries were confirmed to be stationary points by vibrational frequencies analysis. The molecular orbitals of 1-NH_2-AQ were calculated using the B3LYP with the 6-311G basis set, and the optimization of the first excited singlet state was also performed using the TDDFT/B3LYP method with the 6-311G basis set. In gas and solvents, the energies, oscillator strengths, and dipole moments of the ground and excited states were calculated as the twisted angle of the $-NH_2$ group changes. Energies and oscillator strengths of the ground and excited states were obtained under the optimized S_1 structure in order to explain the radiationless relaxation. Thus, the effect of the bulk solvent dielectric on the ground-state geometry and on the excited-state vertical energy were modeled by performing self-consistent reaction field (SCRF) calculations using the polarizable continuum model (PCM) with the integral equation formalism.

3. Results and discussion

The energies and dipole moments of the ground state in the gas phase are calculated by several methods with different basis sets and listed in Table 1. However, all optimized geometries are determined to be planar structures with Cs symmetry and confirmed to be stationary points by vibrational frequencies analysis. The lowest ground state energy is given by DFT/B3LYP/6-311G.

Table 1. Values of energy (in unit a.u., the unit a.u. is short for atomic unit) and dipole moment (D) of the ground state in the gas phase, calculated by several methods with different basis sets.

Method/basis set	Energy/a.u.	Dipole moment (D)
DFT/B3LYP/6-311G	–744.1210	2.382
DFT/B3LYP/Lanl2dz	–744.0368	2.380
DFT/ B3PW91/6-311G	–743.8241	2.402
DFT/ B3PW91/Lanl2dz	–743.7548	2.401
MP2/6-311G	–741.1487	1.710
MP2/Lanl2dz	–740.9021	1.734

The vertical excitation energies, oscillator strengths, orbital transition coefficients, and the percentages of the transition orbits of the singlet excited states in a planar form in the gas phase are calculated by using several methods with different basis sets, and the results are listed in Table 2. The energy of the S_1 state 2.6756 eV at the B3LYP/6-311G level is the closest to the experimental value, which is determined to be 2.6325 eV using time-resolved fluorescence spectroscopy.[47] Since the B3LYP/6-311G level gives a minimum energy of the ground state and is the most consistent energy value of the S_1 state, the other calculations in this work are performed at the same method level. All calculations of the planar structure reveal that the lowest excited S_1 state is a bright state and mainly originates from a 59←58 transition, whereas the second excited S_2 state mainly derives from a 59←57 transition and is a dark state for its zero transition strength.

Table 2. Values of vertical excitation energy (in unit eV), oscillator strength (f), orbital transition coefficient (k), and the percentage of the transition orbits (%) of 1-NH_2-AQ for optimized geometry of the S_0 state in the gas phase, calculated using the TDDFT method with different basis sets.

State	Transition	Value	B3LYP/6-311G	B3LYP/Lanl2dz	B3PW91/6-311G	B3PW91/Lanl2dz
S_1	58–59	eV	2.6757	2.6849	2.6825	2.6970
		f	0.1239	0.1260	0.1249	0.1278
		k	0.70155	0.70139	0.70167	0.70154
		%	98.43	98.38	98.47	98.43
S_2	57–59	eV	2.8895	2.8350	2.8732	2.8169
		f	0	0	0	0
		k	0.68609	0.68521	0.68727	0.68646
		%	94.14	93.90	94.47	94.25

Optimized structures of the ground and first excited singlet states of 1-NH_2-AQ in the gas phase are shown in Figs. 1(a) and 1(b), respectively. The lowest excited singlet state geometry is only optimized in gas for simplicity and the energy gap between the S_0 and S_1 state is only 0.6049 eV for the optimized geometry. The optimized geometry of the S_1 state is no longer planar, but twisted. The amino group is almost perpendicular to the anthraquinone plane. The dihedral angle between the $–NH_2$ group and anthraquinone for the optimized structure of the S_1 state becomes about 90°. The vector of the dipole moment and the charge of the nitrogen atom are also displayed in Fig. 1. The dipole moment of the optimized S_1 state is more than three times to the dipole moment of the optimized S_0 state. Such a large change of the transition dipole moment manifests a charge transfer process in the molecule upon an excitation. The charge quantity of the nitrogen atom at the optimized S_0 and S_1 states are 0.906 e^- and 0.650 e^-, respectively. This also supports the charge transfer process. The molecular orbits of the highest occupied molecular orbital (HOMO)-1, HOMO and the lowest unoccupied molecular orbital (LUMO) at optimized S_0 and S_1 structures were discussed in detail in the literature.[48] The calculations show that the excitation to the S_1 state is strongly allowed with the main contribution of the transition from the HOMO to the LUMO. For the optimized geometry of the S_0 state, the HOMO is largely localized in the amino group, whereas the LUMO is largely localized in the whole anthraquinone group. The difference in electron cloud distribution between HOMO and LUMO also shows the ICT process. The significant change of C=O and C–N bond from the S_0 state geometry to the S_1 state geometry originates from the strong donating nature of the amino group, which induces large charge localization in the amino group. The electron density distribution also suggests that the S_1 state is a strong ICT state, and such an ICT state induces a strong absorption in the visible spectrum.[40]

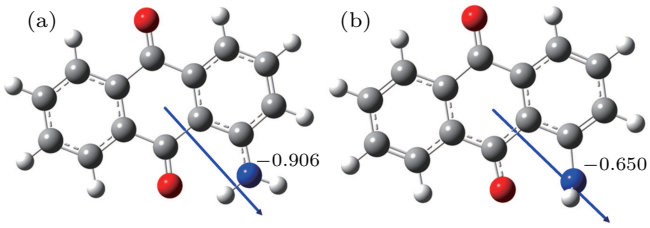


Fig. 1. (color online) Optimized conformations of 1-NH_2-AQ in (a) ground state and (b) the first excited singlet state in the gas phase. Vectors of dipole moments are displayed by the arrows: (a) ×2 and (b) ×0.7, respectively. Charge quantities of nitrogen atom in S_0 and S_1 states are 0.906 e^- and 0.650 e^-, respectively.

Yoshihara *et al.* pointed out that the absorption and fluorescence spectra are dependent on strong solvent polarity.[40,41] The calculated steady absorption spectra of 1-NH_2-AQ in three solvents with different polarities at the B3LYP/6-311G level are depicted in Fig. 2. The results show that the calculated absorption spectra are well consistent with the experimental absorptions in the visible region,[48] and are dependent on the solvent polarity. The strong solvent polarity dependence leads to the charge transfer character of the S_1 state.

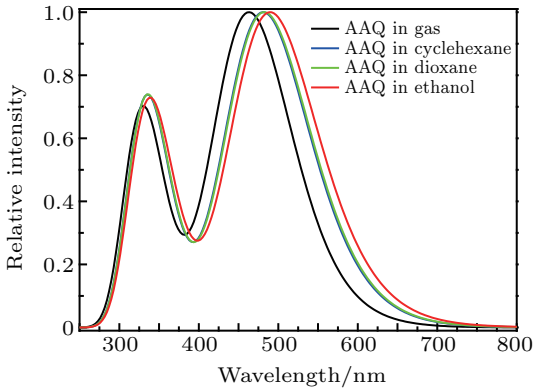


Fig. 2. (color online) Absorption spectra of 1-NH_2-AQ, calculated at the B3LYP/6-311G level in gas, cyclohexane, dioxane, and ethanol.

Table 3. Values of dipole moment μ (D) of the S_0 and S_1 states, oscillator strength f of S_1 state of 1-NH_2-AQ for different values of twisted angle (°) in gas, cyclohexane, dioxane, and ethanol using (TD)DFT/B3LYP/6-311G.

	Angle		10	20	30	40	50	60	70	80	90
Gas	$\mu(S_0)$	2.382	2.371	2.338	2.171	2.156	1.983	1.751	1.485	1.246	1.143
	$\mu(S_1)$	6.757	6.560	6.214	6.004	5.947	5.997	6.183	6.613	7.333	7.808
	$f(S_1)$	0.124	0.113	0.089	0.065	0.047	0.033	0.021	0.012	0.004	0.00
Cyclo- hexane	$\mu(S_0)$	2.802	2.788	2.742	2.654	2.506	2.287	2.000	1.671	1.377	1.251
	$\mu(S_1)$	7.865	7.792	7.600	7.393	7.270	7.266	7.430	7.884	8.687	9.223
	$f(S_1)$	0.169	0.160	0.136	0.104	0.075	0.052	0.034	0.018	0.005	0.000
Dioxane	$\mu(S_0)$	2.861	2.846	2.799	2.708	2.555	2.331	2.035	1.698	1.396	1.266
	$\mu(S_1)$	8.015	7.950	7.774	7.574	7.447	7.437	7.597	8.053	8.865	9.410
	$f(S_1)$	0.171	0.162	0.138	0.106	0.076	0.053	0.034	0.019	0.006	0.000
Ethanol	$\mu(S_0)$	3.382	3.362	3.300	3.182	2.990	2.711	2.347	1.932	1.561	1.401
	$\mu(S_1)$	9.337	9.317	9.246	9.117	8.990	8.947	9.083	9.556	10.45	11.05
	$f(S_1)$	0.167	0.160	0.138	0.109	0.080	0.057	0.037	0.020	0.006	0.000

As mentioned above, the conformation of 1-NH_2-AQ maintains a coplanar structure in the Franck–Condon region after excitation and relaxes to a twisted structure on the potential surface of the S_1 state. The parameters including the dipole moments of the S_0 and S_1 states and the oscillator strengths of the S_1 state as a function of twisted angle between the amino and anthraquinone group for the gas and three solvents are calculated using the B3LYP method with the 6-311G basis set, and the results are listed in Table 3. There is similarity that the oscillator strengths all decrease to zero as the twisted angle increases to 90°. This obviously suggests that the fluorescence just radiates from an initial LE state, and no fluorescence radiates from a relaxed excited state. This fits the experimental phenomenon of no dual fluorescence.[38,39,47] The dipole moments of the S_0 state decrease as the twisted angle increases, whereas the dipole moments of the S_1 state have the opposite trend. The dipole difference between the S_0 state and the S_1 state increases as the twisted angle increases. These results suggest that the TICT character, and the conformational relaxation on the potential surface of the S_1 state in the gas phase were manifested in detail by the dipole and charge change.[48] The TICT character is also easily shown by the dipole change trend in solvents.

Table 4. Energies (in unit eV) of S_0 state, and vertical excitation energies (in unit eV) of T_2 and S_1 states of 1-NH_2-AQ for different values of twisted angle (in unit degree) in different solvents using B3LYP/6-311G.

Angle	Cyclohexane			Dioxane			Ethanol		
	S_0	T_2	S_1	S_0	T_2	S_1	S_0	T_2	S_1
0	0	2.5066	2.5766	0	2.5126	2.5699	0	2.5600	2.5311
10	0.0340	2.5044	2.5661	0.0503	2.5104	2.5596	0.0336	2.5557	2.521
20	0.1301	2.497	2.5299	0.1462	2.5023	2.5239	0.1284	2.5412	2.4863
30	0.2733	2.4836	2.4611	0.2893	2.4876	2.4558	0.2706	2.5148	2.4202
40	0.4454	2.4718	2.3604	0.4615	2.474	2.3557	0.4435	2.4862	2.3219
50	0.6285	2.4788	2.2333	0.6448	2.4789	2.2291	0.6292	2.4755	2.1961
60	0.8065	2.5144	2.0837	0.8232	2.5127	2.0797	0.8118	2.4949	2.0457
70	0.9612	2.5696	1.9155	0.9785	2.5679	1.9114	0.9718	2.5437	1.874
80	1.0706	2.5715	1.7546	1.0884	2.5737	1.7500	1.0857	2.5751	1.7071
90	1.1108	2.5729	1.6802	1.1288	2.5737	1.6752	1.1277	2.5747	1.6296

In the gas phase, the energies of the S_0 and T_2 states increase as the twisted angle increases, whereas the energies of the S_1 and T_1 states decrease. At the B3LYP/6-311G level, the energy gap between the S_1 and S_0 states in the Franck-Condon region is 2.6757 eV, and the energy gap between both states is only 0.6049 eV for the optimized geometry of the S_1 state. It shows that the energy gap decreases from 2.6757 eV to 0.6049 eV along the twisting conformation relaxation coordinate. The obviously decreasing trend of the energy gap is benefitial to an ultrafast IC process from the S_1 state to the S_0 state. Srivatsavoy *et al.* also pointed out that the S_1 state is mainly deactivated through IC to the ground state experimentally.[40] The ISC process was presented by the energy inversion between the S_1 and T_2 states nearby the twisted angle of 40° along the twisting relaxation.[48] For different twisted angles, the energies of the S_0 state, and vertical excitation energies of the T_2 and S_1 states of 1-NH_2-AQ are listed in Table 4 at the B3LYP/6-311G level in three solvents. Here, the energies are calculated just by changing the twisted angle but not for partial optimization for simplicity. In solvents, the vertical excitation energies of the S_1 state also decrease as the twisted angle increases as in gas. The results show that the energy gap between the S_0 and S_1 states decreases with increasing solvent polarity. This provides further evidence for the experimental result that the rate constant of IC increases considerably in a polar solvent, and the fluorescence yield decreases gradually as cyclohexane changes into a more-polar solvent.[40,47]

There are energy intersections between the T_2 and S_1 states in cyclohexane and dioxane solvents but in the ethanol solvent, which is easily shown in Fig. 3(a). It is clear that the potential energy surfaces of the S_1 and T_2 states become isoenergetic near the twisted angle of 20°–30° in cyclohexane and dioxane solvents. This could explain the experimental result that the rate constant of ISC decreases in polar solvents. The rate constant of ISC was determined to be only 3.0×10^7 s^{-1} in methanol by picosecond fluorescence spectra.[40] The rate constant of IC is about 8 times larger than that of ISC, and the rate constant of ISC is about 3 times larger than that of the radiation.[40,47] Our calculations well support the reported large radiationless rate constant.[40,41,47]

The energies of the S_1 state at different twisted angles in three solvents are shown in Fig. 3(b). The energy barriers of 1-NH_2-AQ are 0.3330, 0.3264, and 0.3136 eV in dioxane, ethanol, and cyclohexane respectively. These barriers appear nearby the twisted angle of 50°, which is similar to the experimental result that the –NH_2 plane is tilted 38° to the ring.[49] The N–H stretching frequencies in 1-NH_2-AQ[50] are very close to those in the typical free amino groups.[51] It suggests a very weak hydrogen bond, which opposes C–N bond rotation. So the –NH_2 twisting happens easily once the excitation energy exceeds the barriers. The energy barrier decreases with solvent viscosity decreasing, and is higher than 0.2595 eV in the gas phase. The timescale of TICT was

usually measured to be a few hundred femtoseconds in some barrierless systems.[17,18] The time of TICT of 1-NH_2-AQ is demonstrated to be about 5 ps in ethanol by using ultrafast transient absorption spectroscopy. The longer time of 5 ps is attributed to the energy barrier existing on the amino twisting potential surface.[48] From these results, we can infer that the timescales of TICT of 1-NH_2-AQ in cyclohexane and ethanol are shorter than that in dioxane because of the smaller energy barrier.

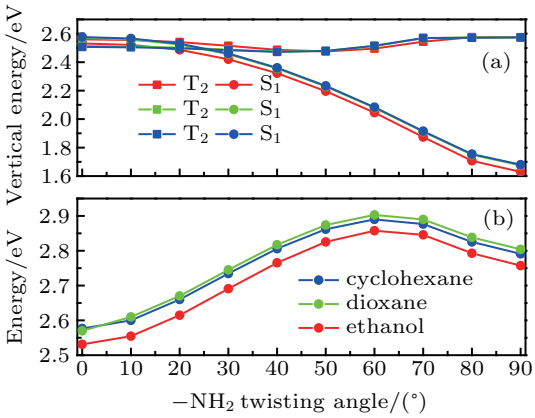


Fig. 3. (color online) Energies of the T_2 and S_1 states of 1-NH_2-AQ varying with twisted angle in cyclohexane (blue), dioxane (green), and ethanol (red) using B3LYP/6-311G, showing (a) vertical excitation energies of the excited states and (b) energies of the S_1 state.

4. Conclusions

The twisted intramolecular charge transfer and following radiationless dynamics of the excited states of 1-NH_2-AQ in different solvents have been investigated using ab initio calculations. The optimized structure of the ground state is confirmed to be a planar conformation, whereas the structure of the S_1 state is a twisted conformation with perpendicular amino group to the anthraquinone plane. The difference in dipole moment between the S_0 and S_1 states manifests a charge transfer process in the molecule upon excitation. Furthermore, it is elucidated that the dipole moment in the S_1 state increases with the twisted angle of –NH_2 increasing, i.e., the TICT is associated with the conformational relaxation on the potential surface of the S_1 state. Quantum chemical calculations indicate that the IC and ISC process via the twisting of the amino group, and the two relaxation processes, have been established and are responsible for the ultrafast deactivation of the S_1 state. The rate constants of IC and ISC processes relate to the solvent polarity, and the TICT time is predicted to be positively dependent on solvent viscosity.

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