

ELECTRONIC SPECTRA AND PHOTOLYSIS OF BISPHENOL A IN WATER

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A quantum chemical study of the spectral and luminescent properties of the BPA + 2H₂O complex was carried out. Calculations were performed by the semi-empirical method of intermediate neglect of differential overlap using a program complex and a special parameterization. The spectral behavior of BPA in water was modeled by a complex with water molecules in the ratio 1: 2 forming the hydrogen bond. The calculated data were compared with the results of investigation of the isolated BPA molecule. The nonplanar BPA structure leads to the strong mixing of the π - and σ -type atomic wave functions. The main reason for the low quantum yield of the BPA fluorescence is the efficient process of singlet-triplet conversion in the $S_1(\pi\pi^) \gtrsim T_n(\pi\sigma^*)$ channel of the BPA molecule and its complex with water. A study of the photolysis of the isolated BPA molecule upon exposure to solar radiation, the short-wavelength boundary of which on the Earth's surface is located at ~ 290 nm (~ 34480 cm⁻¹), showed that the energy of the photodissociative state localized on the O–H bond is much higher than this value for BPA. The binding curve is characteristic of the $S_1(\pi\pi^*)$ state, while the singlet and triplet states of the $\pi\sigma^*$ type, localized on the single C–C bonds of the central fragment of the molecule, are repulsion curves with a barrier. From our point of view, the low efficiency of the BPA degradation under the influence of solar radiation is due to the presence of a significant potential barrier to the photolysis in the singlet or triplet state. The mechanisms of bond breaking in the BPA + 2H₂O complex are different for the singlet and triplet states, namely, for the $S_3(\pi\sigma^*)$ state, the break occurs by the predissociation mechanism, and for the $T_n(\pi\sigma^*)$ state, due to its population through the singlet-triplet conversion in the $S_1(\pi\pi^*) \rightarrow T_n(\pi\sigma^*)$ channel.*

Keywords: bisphenol A (BPA), photophysical processes, quantum chemical calculation, semiempirical method, photolysis.

INTRODUCTION

Nowadays more and more investigations testify to the negative influence of bisphenol A (BPA) used in manufacture of polycarbonate plastic on human health. Penetrating into the human body with water or mother's milk [1], bisphenols cause serious endocrine disorders and exhibit genotoxic properties [2] leading to gene mutations. Both *in vivo* and *in vitro* analyses showed that bisphenols can inhibit the androgen receptor [3]. In this regard, a problem of bisphenol utilization arises, one of the method of which is the photolysis of molecules. A study of the bisphenol behavior upon exposure to solar radiation showed that the effective destruction of bisphenol in water solutions occurs only in the presence of the TiO₂ catalyst which is also toxic for live organisms [1]. Thus, a search for the methods of bisphenol utilization remains still extremely relevant. A successive solution of this problem requires profound knowledge of the physical and chemical properties of the BPA molecule not only in the ground, but also in the excited states, since light can significantly affect the photoprocesses. It is well known that after excitation of a molecule, its

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physical and chemical properties change in comparison with the ground state because of changes in the distribution of the electronic density. Therefore, a study of the physical and chemical properties and their changes caused by the substitution, solvent, or external states is extremely important. The physical and chemical properties of organic compounds are studied by experimental (IRS, RS, UVS, chromatography, mass spectroscopy, etc.) and theoretical methods. The methods of quantum chemistry facilitating the interpretation and understanding of the mechanisms of photoprocesses in the molecule and of the influence of substitution and environment belong to the latter. One of the methods of studying the physical and chemical properties and their changes involves analysis of the spectra of electronic absorption and fluorescence of the examined systems. However, in most cases this problem cannot be solved only on the experimental basis, because the physical and chemical properties reflect the state of the electron shell of molecules, and the dependence of the electronic structure of the molecule on its composition can be correctly taken into account only by the methods of quantum chemistry. Therefore, at the first stage, experimental investigations of the absorption and fluorescence spectra of bisphenol in various solvents are necessary for the success, followed at the next step by quantum chemical calculations and comparison of their results with the experiment. A satisfactory agreement between the results of calculations and experiments demonstrate the correctness of the interpretation of the calculated spectra and the explanation of changes in the physical and chemical properties of molecules in the excited states. The purpose of the present work is to study the possibility of breaking of the single C–C bond combining the phenol molecules into the bisphenol A molecule and the effect of water molecules on the photolysis efficiency.

OBJECTS AND METHODS OF RESEARCH

The object of our research was 4,4'-dihydroxy-2,2-diphenylpropane (bisphenol A or BPA) synthesized by Sigma-Aldrich. BPA conventionally exists in the form of white granules (1–2 mm) with density of 1037.6 kg/m³ at a temperature of 20°C and pressure of 760 mm Hg. The absorption and fluorescence spectra of BPA solutions in hexane and distilled water with concentration of 0.22 mmol/L were registered using a CM2203 spectrofluorimeter (SOLAR, Belarus) at room temperature in the range of 200–400 nm. Measurements were performed in a quartz cell with optical path length of 10 mm. The examined compound is moderately soluble in water (6 g of substance is dissolved in 100 g of water).

In the present research, the quantum mechanical calculations were carried out by the semi-empirical method of intermediate neglect of differential overlap (INDO) using a complex of programs and special parameterization [4] developed at Tomsk State University especially for solving problems of photonics of polyatomic organic molecules. This quantum chemical method is used to calculate the energy and the oscillator force of an electronic transition, distribution of electronic density over the atoms of a molecule, its bonds and fragments, and also its change upon electronic excitation from the ground state. The geometry of the ground state of the examined compounds was determined by the *AM1* method [5]. The geometry of the excited state was determined from changes of the electronic density on chemical bonds under electronic excitation according to Mulliken [6] using the known dependence between the bond length and its population given by the formula

$$\Delta R_{AB}^* = -k\Delta P_{AB}^*,$$

where ΔP_{AB}^* is the change of the bond population during molecule transition from the ground to the excited state, and the coefficient $k = 0.46$ was obtained from the change of the C–C bond length of benzene in the $S_0 \rightarrow S_1$ transition [7].

The rate constants of the radiative decay (k_r) and nonradiative transitions (internal (k_{ic}) and intercombination (k_{ST}) conversion) were calculated by the method described in [8] and were evaluative in character. They determine the theoretical quantum fluorescence yield of molecules ($\gamma = k_r / (k_r + k_{ic} + k_{ST})$) and allow tendencies of the change in the quantum fluorescence yield to be established for a series of compounds with analogous structures.

The approach to the study of the photo-braking of a chemical bond in an electronically excited state we proposed earlier in [9] was successfully employed to study the braking of chemical bonds in phenol and its substitutes, the possibility of opening of the naphthyl ring in the coumarin molecule, and the influence of the solvent on these processes. The essence of the employed approach consists in the following. The chemical bond breaks in the states of

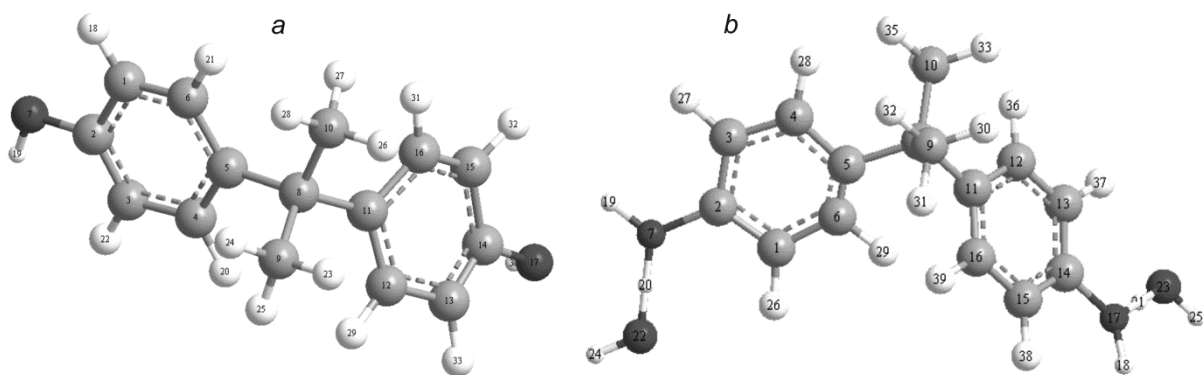


Fig. 1. Optimized structures of the isolated BPA molecule (a) and of the BPA + 2H₂O complex (b).

$\pi\sigma^*$, $\sigma\pi^*$, and $\sigma\sigma^*$ type, because only in the states of these types, the σ - σ bonds forming the structural skeleton of the molecule can be broken. The decrease of the examined bond strength demonstrates the possibility of bond breaking in the electronic state. The decrease of the population of the given bond upon excitation to this state testifies to its possible breaking. The potential curve of the ground state of the molecule was modeled using the Morse potential [10]

$$(R) = D(e^{-2\alpha x} - 2e^{\alpha x}),$$

where $\alpha = \nu R_0 \sqrt{M / 2D}$. The bond dissociation energy D , the equilibrium length of the examined bond R_0 , the oscillator frequency ω , and the reduced oscillator mass M were determined experimentally. The length of the breaking bond was varied, and at each step, the energy of the excited state localized on the examined bond was calculated, and then the potential curve of the examined excited state was constructed. We judged about the bond breaking or, on the contrary, stability by the form of the potential curve.

RESULTS AND DISCUSSION

BPA electronic absorption spectra

In [11] the mechanism of breaking of the single C-C bond of the isolated BPA molecule was investigated by the quantum chemical calculation method. The potential curves of the $S_1(\pi\pi^*)$, $S_n(\pi\sigma^*)$, and $T_n(\pi\sigma^*)$ states were calculated. When the C₈-C₁₁ bond length in the BPA molecule increases from 1.501 to 1.801 Å, it is broken. For this study, the geometry of the isolated BPA molecule was optimized. Figure 1 shows the structure and the serial numbers of atoms in the BPA molecule and its complex with water molecules optimized by the AM1 method [5].

The isolated BPA molecule is nonplanar (Fig. 1a). The geometry of the molecule comprises two identical phenol fragments, the planes of the benzene rings of which are located at an angle to each other and are linked with the C(CH₃)₂ group. Moreover, the average fragment of the C(CH₃)₂ molecule prevents the occurrence of the π -conjugation between the phenyl rings, thereby leading to the existence of two isolated π -systems in the BPA molecule. The nonplanar BPA structure caused strong *mixing* of the atomic wave functions of the π - and σ -types. Therefore, reference of the electronic state to the orbital type ($\pi\pi^*$, $\pi\sigma^*$, or $\sigma\sigma^*$) will be conditional, depending on the relative contribution of the corresponding molecular orbitals (MOs) in the configuration forming this or that electronic state.

The molecule in the solution of a nonpolar solvent is influenced by universal intermolecular interactions; therefore, it is possible to consider that the BPA spectrum in hexane (Fig. 2) is quite close to the spectrum of the isolated molecule. The fluorescence excitation spectrum of BPA in hexane coincides with the absorption spectrum of the luminescent substance. This provides important information that the electronic BPA levels participate in the electronic excitation energy transfer (Fig. 2a). When the fluorescent state of the isolated BPA molecule is formed, the

TABLE 1. Absorption Spectra of the Isolated BPA Molecule

State	Calculation ^{a)}			Experiment	
	E_i , cm^{-1}	λ , nm	f	E_i , cm^{-1}	λ , nm
$S_1(\pi\pi^*)$	35140	284	0.063	36360	275
$S_2(\pi\pi^*)$	35610	281	0.055		
$S_3(\pi\sigma^*)$	36150	277	0.012		
$S_5(\pi\pi^*)$	38510	260	0.402	41670	240
$S_6(\pi\pi^*)$	40340	248	0.233		
$S_9(\pi\pi^* + \pi\sigma^*)$	44890	223	0.135	45450	220
$S_{10}(\pi\pi^* + \pi\sigma^*)$	45320	221	0.151		
$S_{11}(\pi\pi^* + \pi\sigma^*)$	46730	214	0.109		
$S_{16}(\pi\pi^*)$	48560	206	0.291		
$S_{17}(\pi\pi^*)$	48820	204	0.163		

Note. ^{a)}Here E_i , λ , and f are the energy, wavelength, and oscillator force of the electronic transition, respectively. The experimental results were taken from the data on the second derivative of the absorption spectrum of BPA in hexane.

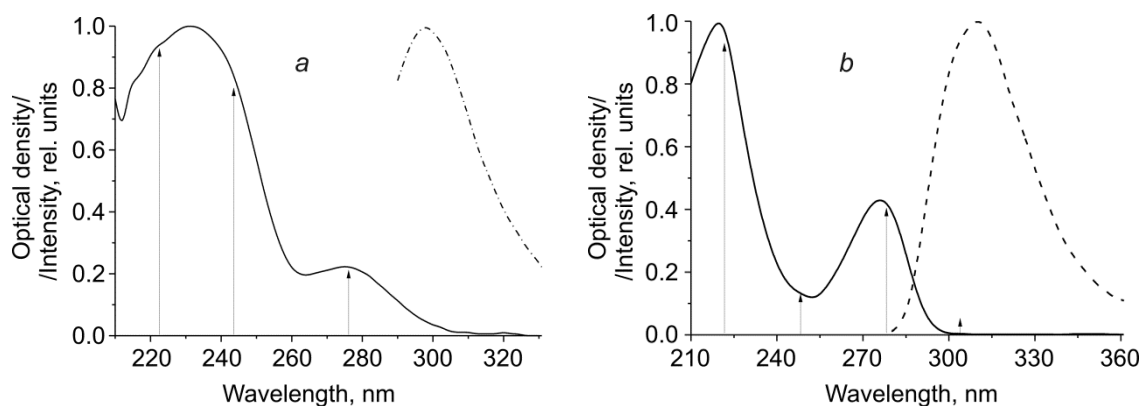


Fig. 2. Normalized absorption and fluorescence spectra of BPA in hexane (a) and water (b).

excitation energy is transferred from the energy levels at ~ 45000 , 41000 , and 36000 cm^{-1} (Table 1). According to the results of calculations of the molecular electrostatic potential [12, 13], the BPA molecule has two most electronegative centers – oxygen atoms of the hydroxyl groups. The spectral behavior of BPA in water was modeled by the complex with water molecules in the ratio 1:2 forming the hydrogen bond. The distance between the oxygen atoms of the molecules in the complex was set equal to 2.7 \AA , like the average distance in complexes with hydrogen bond of the $-\text{O}\dots\text{H}-\text{O}-\text{H}$ type [14].

Figure 2 shows the BPA absorption and fluorescence spectra. The vertical arrows indicate the electronic transitions forming the experimental band in the spectra of BPA and its complex with water obtained with the use of the second derivative. The absorption spectrum of bisphenol in hexane in the range of 200–300 nm comprised two absorption bands the maxima of which are at 36360 and 43480 cm^{-1} (Fig. 1a). The second derivative of the absorption spectrum of the BPA solution in hexane gives one transition for the long-wavelength band and two electronic transitions (41670 and 45450 cm^{-1}) for the short-wavelength band. A comparison of the data of experiment and calculation shows their satisfactory agreement and demonstrates that the long-wavelength absorption band intensity is formed by the $S_0 \rightarrow S_1(\pi\pi^*)$ and $S_0 \rightarrow S_2(\pi\pi^*)$ transitions with insignificant contribution of the $S_0 \rightarrow S_3(\pi\sigma^*)$ transition localized on the C_5-C_8 and C_8-C_{11} bonds of the average fragment of the molecule. The $S_0 \rightarrow S_5(\pi\pi^*)$ and $S_0 \rightarrow S_6(\pi\pi^*)$ electronic transitions localized on different phenyl fragments of the molecule correspond to the calculated electronic transition in

TABLE 2. Calculated and Experimental Spectra of the BPA + 2H₂O Complex

State	Calculation			Experiment	
	E_i, cm^{-1}	λ, nm	F	E_i, cm^{-1}	λ, nm
$S_1(\pi\pi^*)$	34040	294	0.054	35970	278
$S_2(\pi\pi^*)$	34990	286	0.048		
$S_3(\pi\sigma^*)$	36890	271	0.012		
$S_4(\pi\pi^*)$	38090	262	0.244		
$S_5(\pi\sigma^*)$	39010	256	0.047	40320	248
$S_6(\pi\pi^*)$	40170	249	0.032		
$S_9(\pi\pi^*)$	44700	224	0.071	45040	222
$S_{11}(\pi\pi^* + \pi\sigma^*)$	45340	220	0.509		
$S_{12}(\pi\pi^* + \pi\sigma^*)$	45805	218	0.552		

the spectrum of the second derivative with maximum at 41670 cm^{-1} (Table 1). The short-wavelength absorption in the spectrum of the BPA molecule at 45450 cm^{-1} was formed by three one-electronic transitions into the S_9 – S_{11} states of mixed orbital nature. The configurations of these excited states involve not only π atomic orbitals, but also σ orbitals of the phenyl rings. Note that in the 200–300 nm region of the spectrum, the molecular orbitals of the hydroxyl groups do not participate in the formation of the electronically excited states at all.

The calculated and experimental absorption spectra of the BPA + 2H₂O complex are compared in Table 2. The absorption spectrum of BPA in water has two bands (Fig. 2b) with maxima at 36230 and 45450 cm^{-1} . The assignment of the absorption spectrum by the method of the second derivative gives three electronic transitions (Table 2 and Fig. 2b). The electronic transition at $40\,000 \text{ cm}^{-1}$ is closer to the long-wavelength absorption band of the BPA + 2H₂O complex than to the short-wavelength band of the isolated BPA molecule. A comparison of the position and intensity of the bands in the absorption spectra of BPA and its complex with water (Fig. 2) allows us to assert that the formation of the complex increases the long-wavelength absorption band intensity and shifts the maximum of the short-wavelength band toward lower energies. The increase in the intensity of the long-wavelength band occurs due to the presence in it of the $S_0 \rightarrow S_4(\pi\pi^*)$ electronic transition that forms the intensity of this band. From the spectrum of the second derivative it follows that the formation of the complex shifts toward longer wavelengths one of the transitions of the short-wavelength band of the spectrum (from 41670 cm^{-1} for BPA to 40320 cm^{-1} for the complex); therefore, the long-wavelength band intensity of the complex increased in comparison with the analogous BPA band (Tables 1 and 2).

Fluorescence spectra of BPA

BPA exhibits weak fluorescence both in hexane and water. Since the absorption spectra of BPA and solar radiation are weakly overlapped, the fluorescence of the BPA solution in water was excited at the edge of the long-wavelength absorption band of the molecule. The fluorescence band maximum of the isolated molecule (solution in hexane) in the experiment was observed approximately at 300 nm (33330 cm^{-1}). The maximum of the fluorescence band of the BPA solution in water (the BPA + 2H₂O complex) is located approximately at 310 nm (32258 cm^{-1}) (Fig. 2c). The calculated fluorescence characteristics of the solutions in hexane and water in comparison with the experiment are given in Table 3. From the table it follows that the calculated and experimental positions of the fluorescence bands and the values of the quantum fluorescence yield agree satisfactory [15]. The main reason for the low quantum fluorescence yield is the effective singlet-triplet conversion in the $S_1(\pi\pi^*) \approx T_7(\pi\sigma^*)$ channel of the BPA molecule and of the complex (Table 3). The decay products released from the water solution under solar irradiation do not change the value of the quantum yield, because one of the products (*para*-hydroxy-benzaldehyde) does not radiate at all, and the other decay product (3-(2-hydroxy-2-propyl)phenol) has the calculated quantum yield equal to 0.002.

TABLE 3. Calculated and Experimental Characteristics of Fluorescence of Bisphenol and Its Complex with Water

Calculation					Experiment	
E_{fl} , cm ⁻¹ (nm)	k_r , s ⁻¹	k_{ic} , s ⁻¹	k_{ST} , s ⁻¹	γ	E_{fl} , cm ⁻¹ (nm)	γ
Bisphenol A						
33020 (303)	6·10 ⁷	5·10 ³	2·10 ¹⁰	0.003	33330 (300)	0.001 [15]
Bisphenol A + 2H ₂ O						
32790 (305)	1·10 ⁸	5·10 ³	2·10 ¹¹	0.0005	32260 (310)	0.0005

Note. Here E_{fl} is the energy of the $S_0 \rightarrow S_1(\pi\pi^*)$ electronic transition; k_r is the rate constant of radiative decay; k_{ic} and k_{ST} are the rate constants of nonradiative and singlet-triplet conversion, respectively; and γ is the quantum fluorescence yield.

TABLE 4. Populations of Chemical Bonds of the BPA Molecule and its BPA + 2H₂O Complex in the Electronically Excited States

State	Population of the C–C bond, e			Population of the O–H bond, e		
	C ₅ –C ₈	C ₈ –C ₁₁	C ₈ –C ₉	C ₈ –C ₁₀	O ₇ –H ₁₉	O ₁₇ –H ₁₈
Isolated molecule						
S_0	0.780	0.792	0.693	0.692	0.580	0.583
$S_1(\pi\pi^*)$	0.767	0.771	0.682	0.683	0.580	0.583
$S_3(\pi\sigma^*)$	0.165	0.152	0.380	0.399	0.580	0.583
$T_7(\pi\sigma^*)$	0.198	0.170	0.389	0.412	0.580	0.583
BPA + 2H ₂ O Complex						
S_0	0.781	0.796	0.685	0.716	0.578	0.580
$S_1(\pi\pi^*)$	0.754	0.792	0.677	0.705	0.578	0.580
$S_3(\pi\sigma^*)$	0.242	0.232	0.389	0.409	0.578	0.580
$T_7(\pi\sigma^*)$	0.160	0.137	0.327	0.348	0.578	0.580

Photolysis of BPA excited by solar radiation

Let us consider the possibility of photodissociation of BPA excited by solar radiation. Table 4 presents the populations of the single C–C bonds and the O–H bond of the BPA molecule and its complex with water in the ground and some electronically excited states. In the quantum chemical calculations, the electronic density was distributed between the atoms of the molecule and the bonds between them. The value of the electronic density on a chemical bond corresponds to its strength. An increase in the electronic density on the bond testifies to bond hardening (energy increase), and its decrease indicates the chemical bond weakening. A comparison of populations of the single C–C bonds (Table 4) suggests that the weakest bonds among the examined bonds are the O–H and C–CH₃ bonds. Indeed, the phenol photolysis examined earlier in [9] demonstrated that in the excited molecule, the photo-induced breaking of this weakest O–H bond of the molecule occurred. For BPA, the situation is different. When studying the BPA photolysis, we consider the process of molecule degradation under the influence of only solar radiation, the short-wavelength boundary of which on the Earth surface is at ~290 nm (~34480 cm⁻¹). The energy of the photodissociation state localized on the O–H bond is significantly higher than this value and was not taken into consideration when studying the BPA photolysis. Analogous situation is characteristic for the single bonds of the C–(CH₃)₂ group. As to the energy of the states localized on the single C₅–C₈ or C₈–C₁₁ bonds of BPA (Tables 1 and 2), it was much closer to ~34480 cm⁻¹, namely, the energy of the states localized on these bonds was equal to ~36000 cm⁻¹.

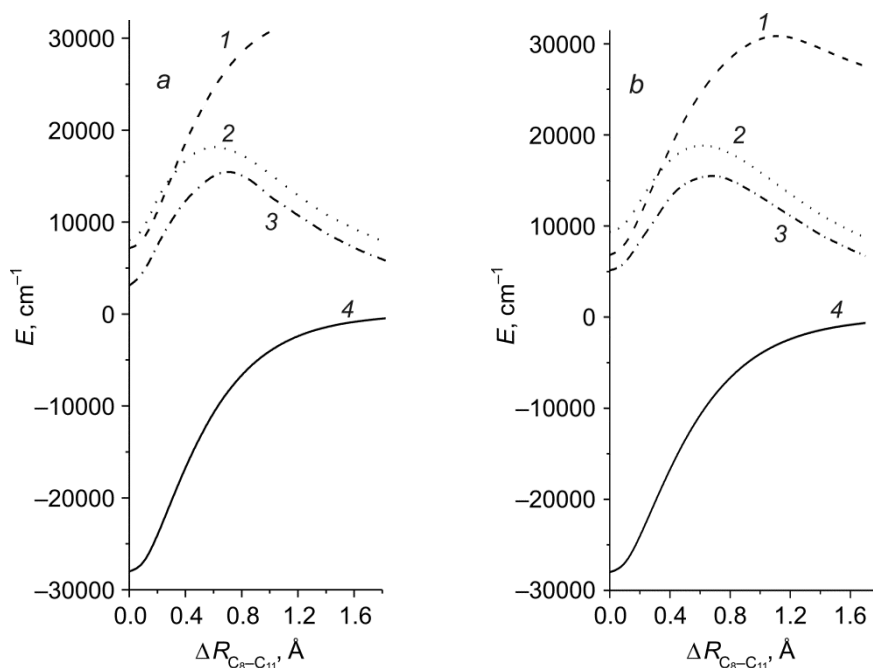


Fig. 3. Potential curves of the ground and electronically excited states of the isolated BPA molecule (a) and of BPA + 2H₂O (b). Here curve 1 is for $S_1(\pi\pi^*)$, curve 2 is for $S_n(\pi\sigma^*)$, curve 3 is for $T_n(\pi\sigma^*)$, and curve 4 is for S_0 .

Results of calculation of the bond populations in the BPA molecule showed (Table 4) that the largest decrease (by more than 4 times) in the population of the C₅–C₈ and C₈–C₁₁ bonds the energy of which is closer than the excitation energy takes place in the electronic states localized on these bonds. For example, the population of the C₈–C₁₁ bond in the state S_0 is equal to 0.792 e , and in the state $S_3(\pi\sigma_{8-11}^*)$, it decreased down to 0.152 e . In this case, the decrease of the population (strength) of these bonds in the assumed photodissociation states is characteristic for both singlet and triplet states of this orbital type. After formation of the complex with water, the tendency to the decrease in the strength of these bonds in the electronically excited states localized on them remained. The formation of the complex with hydrogen bond between the BPA and water molecules slightly affects the population of bonds in the BPA molecule. To study the photolysis, from two single bonds C₅–C₈ and C₈–C₁₁ we chose the bond C₈–C₁₁, because its strength in the excited states decreased by a greater value (Table 4).

To calculate the potential curves of the C₈–C₁₁ bond from the experiment data, the following values were used: the equilibrium C–C bond length $R_0 = 1.5$ Å [16], the energy of the single C–C bond $D = 346$ kJ/mol [17], and $\omega = 1000$ cm⁻¹ [18]. The calculated potential curves of the $S_1(\pi\pi^*)$, $S_3(\pi\sigma_{8-11}^*)$, and $T_n(\pi\sigma_{8-11}^*)$ BPA states are shown in Fig. 3, in which the C₈–C₁₁ bond length (Fig. 1) that increased from 1.5 to 3.0 Å was taken as the reaction coordinate. From the figure it can be seen that for the $S_1(\pi\pi^*)$ state, the binding curve is characteristic, whereas for the singlet and triplet states of the $\pi\sigma_{8-11}^*$ type, the potential curves have noticeable potential barriers presented in Table 5. From Fig. 3 it can be seen that the braking of the single C₈–C₁₁ bond is possible, but with a considerable potential barrier, which makes ineffective the photolysis of the molecule upon exposure to solar radiation. The experiment in deionized water [3] detected the bisphenol A degradation product – 3-(2-hydroxy-2-propyl)phenol which can be formed only by braking of the C₈–C₁₁ (or C₅–C₈) bond. The product was fixed only in five days. According to the results of calculations performed, the population of the singlet photodissociative states in the $S_n(\pi\pi^*) \gtrsim S_3(\pi\sigma^*)$ channel occurs with $k_{v,c} = 10^{13-12}$ s⁻¹, whereas the efficiency of population of the photodissociative triplet state is by two orders of magnitude lower ($k_{ST} = 10^{12-10}$ s⁻¹). We add only that the energy of the $S_3(\pi\sigma_{8-11}^*)$ state makes possible its direct population, whereas the photodissociative triplet is populated only through the $S_1(\pi\pi^*) \rightarrow T_7(\pi\sigma_{8-11})$ conversion. The addition of the (TiO₂) catalyst [3] accelerates the process of the photocatalytic BPA degradation. From our point of view, the low BPA

TABLE 5. Values of the Potential Barriers for the BPA Molecule and the BPA + 2H₂O Complex with Water

Compound	State	Value of the potential barrier, cm ⁻¹
BPA	$S_3(\pi\sigma^*)$	10216
	$T_n(\pi\sigma^*)$	10536
BPA + 2H ₂ O	$S_3(\pi\sigma^*)$	9579
	$T_n(\pi\sigma^*)$	10487

degradation efficiency upon exposure to solar radiation can be due to the presence of a significant potential barrier for the photolysis in the singlet or triplet state (Fig. 3 and Table 5).

Results of calculations demonstrated that the potential barriers for BPA in the singlet and triplet states are almost identical. The formation of complexes decreased the potential barrier of the singlet photodissociative state and in fact, did not change it in the triplet state. The high rate of the nonradiative transition to $S_3(\pi\sigma_{8-11}^*)$ and the decrease of the potential barrier value increased the probability of breaking of the C₈–C₁₁ bond in the singlet photodissociative state (Table 5). Note that the breaking mechanisms of the singlet and triplet states are different: in the $S_3(\pi\sigma_{8-11}^*)$ state, breaking occurs by the predissociation mechanism, and in the $T_n(\pi\sigma_{8-11})$ state, it occurs by its population due to the singlet-triplet conversion in the $S_1(\pi\pi^*) \rightarrow T_n(\pi\sigma_{8-11})$ channel. Despite a significant value of the energy of the potential barrier, the BPA degradation product experimentally detected in deionized water is possible only because of breaking of the C₈–C₁₁ (or C₅–C₈) bond and testifies to overcoming of the potential barrier. In addition, it should be taken into account that the barrier value depends on the external conditions, for example, on the temperature.

CONCLUSIONS

1. Based on the results obtained, it is possible to assert that the absorption spectra of bisphenol A and its complex with water in the 1:2 ratio are formed by the molecular orbitals of identical localizations and orbital natures. The influence of the polar solvent (water) on the BPA spectrum consists in the shift of the absorption bands toward the longer wavelengths of the spectrum and increase of their intensities.

2. The low quantum fluorescence yields of BPA and its complex with water are due to the high efficiency of the singlet-triplet conversion compared to the channel of radiative decay with negligible internal conversion into the ground state.

3. The photolysis of BPA in water solution is possible, but ineffective because of the high potential barrier and is more probable in the singlet photodissociative state localized on the broken bond.

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