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EFFECT OF IONIC FORM FORMATION ON SPECTRAL PROPERTIES AND PHOTOLYSIS OF BISPHENOL A

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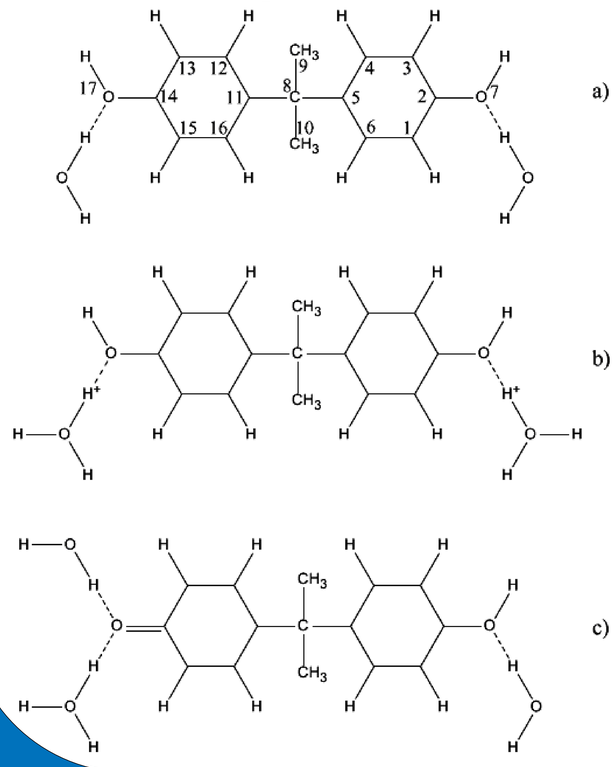
Object: Bisphenol A

Bisphenol A (4,4'-dihydroxy-2,2-diphenylpropane or BPA) is a chemical of the phenol derivatives.



Bisphenol A is an organic molecule that is produced by a condensation reaction between acetone and phenol, catalyzed by an acid or resin.

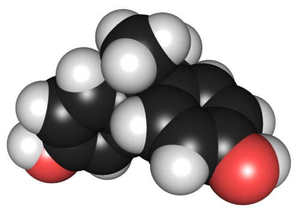


Fig 1. The structural formulas of the neutral complex BPA with water of the composition 1: 2 (a), the BPA cation (q = + 2e) (b), and the anion (q = -1e) + $2H_2O$ (c)

The aim of the work

Search for ways of effective degradation of BPA to reduce the risk of harmful effects on the environment and humans.

Applications

Bisphenol A is used in the following industries:

- ✓construction
- ✓manufacture of electrical engineering
- ✓medicine
- ✓engineering
- ✓food industry

Potential curves of the ground and excited states

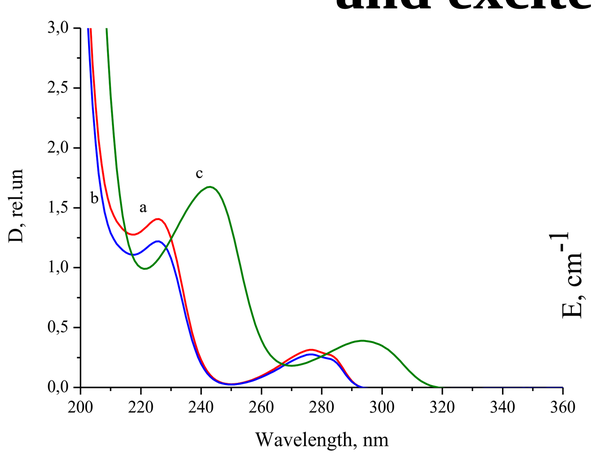


Fig 2. Absorption and fluorescence spectra of the BPA hydrogen-bonded complex (a), the BPA cation (b), and the BPA anion (c).

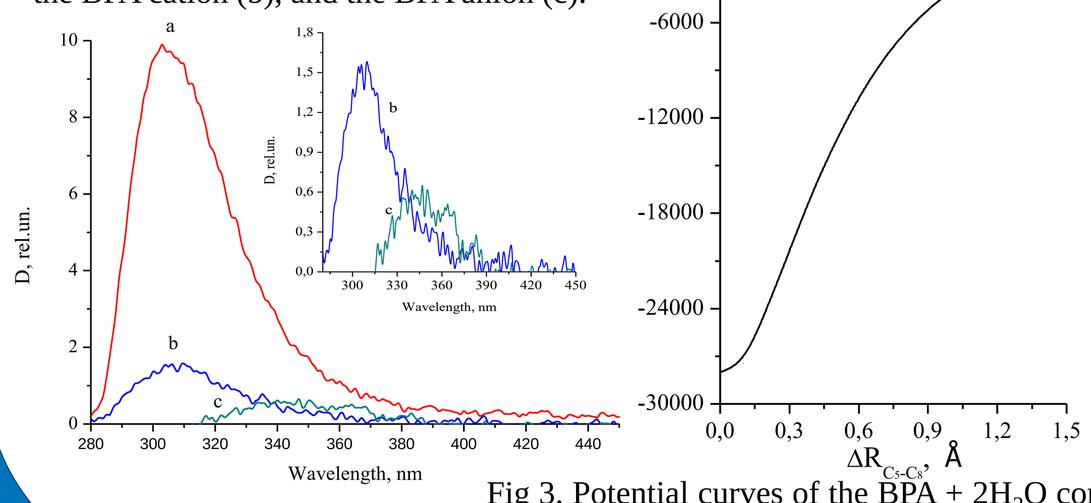


Fig 3. Potential curves of the BPA + $2H_2O$ complex (a), (b) cation and (c) BPA + $2H_2O$ anion.

Experimental and theoretical characteristics of absorption spectra

Table 1. Experimental and theoretical characteristics of absorption spectra of a complex with water and charged forms of bisphenol A in water

Calculation				Experiment		
State	*Ei*, cm^{-1}	λ_i, nm	*f*	*Ei*, cm^{-1}	λ_i, nm	ε, l/mol×cm
BPA + $2H_2O$ complex (neutral form)						
$S_1(\pi\pi^*)$	34040	294	0.054	35100	285	2000
$S_2(\pi\pi^*)$	34990	286	0.048	36230	276	3000
$S_3(\pi\sigma^*_{5\text{-}8\text{-}11})$	36890	271	0.012			
$S_4(\pi\pi^*)$	38090	262	0.244			
$S_9(\pi\pi^*)$	44700	224	0.071	44440	225	15000
$S_{11}(\pi\pi^*)$	45340	220	0.509			
$S_{12}(\pi\pi^*)$	45805	218	0.552			
BPA (BPA + $2H^+H_2O$, q = +2*e*)						
$S_1(\pi\pi^*)$	34640	289	0.040	35210	284	2000
$S_2(\pi\pi^*)$	35720	280	0.048	36230	276	3000
$S_3(\pi\sigma^*_{5\text{-}8\text{-}11})$	38510	242	0.035			
$S_4(\pi\pi^*)$	39680	252	0.256			
$S_5(\pi\pi^*+\pi\sigma^*)$	44660	224	0.140	44440	225	11000
$S_6(\pi\pi^*)$	45540	220	0.854			
BPA (BPA + $2H_2O$, q = –1*e*)						
$S_1(\pi\pi^*+\pi\sigma^*_{5\text{-}8})$	33200	301	0.020	33110	302	4000
$S_2(\pi\pi^*)$	33530	298	0.106			
$S_3(\pi\pi^*)$	35460	282	0.065	34250	292	5000
$S_6(\pi\pi^*+\pi\sigma^*_{5\text{-}8})$	39250	255	0.211	40480	247	20000
$S_8(\pi\pi^*)$	41190	243	0.086			
$S_{13}(\pi\pi^*)$	43680	244	0.244			

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Results

- the absorption spectra of charged forms do not contain new absorption bands in the region of 200-600 nm, in comparison with an isolated molecule.
- the low quantum yield of fluorescence of BPA and its charged forms is due to the significant prevalence of the efficiency of the singlet-triplet conversion channel over the efficiency of the radiation channel of decay of the fluorescent state.
- the efficiency of photolysis of the BPA cation under the influence of solar radiation is lower than in the case of the BPA + $2H_2O$ complex, as a consequence of an increase in the potential barrier.

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