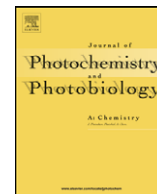




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[2 + 2]-Photocycloaddition reaction of self-assembled crown-containing 2-styrylpyridinium perchlorate in a solid state

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ABSTRACT

The dimer assembly of crown ether styrylpyridinium perchlorates (CSP) in solid state and MeCN solution were studied. The obtained data in solid state allowed us to conclude that molecules spontaneously form dimeric complexes. The dimeric complex is stable due to dipole interaction between crown ether donor substitutor of one molecule and the acceptor pyridinium residue of the other one. Irradiation of the dimer complex leads to regio- and stereoselective [2 + 2]-cycloaddition, giving only one cyclobutane isomer. The formation of dimers in solution has not been found. The irradiation of MeCN solution of CSP molecules resulted in the reversible E–Z isomerization.

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1. Introduction

Research and development of photocycloaddition reactions were originally motivated by their practical applicability as photochemically reversible photochromic transformation to photolithographic processes, novel elements of optical memory and versatile photonics applications.

Concerted [2 + 2]-photocycloaddition reactions (PCA) of alkenes involve the lowest singlet excited state of one of the two alkene partners, and are allowed processes based on molecular orbital symmetry considerations [1]. In solution, intermolecular [2 + 2]-photocycloaddition reactions require high alkene concentrations and are characterized by low quantum yields. In this case bimolecular PCA reactions compete with rapid unimolecular excited state alkene deactivation primarily along torsional coordinates leading to E–Z photoisomerization [2].

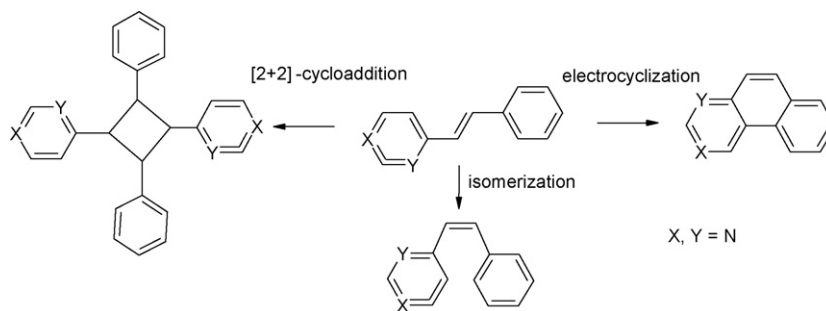
The detailed analysis of E-2-styrylpyridine (E-2-SP) and E-4-styrylpyridine (E-4-SP) photolysis have been presented in literature. Thus, the photolysis of E-2-SP in benzene solvent under nitrogen atmosphere results in E–Z isomerization, where as the irradiation in the solid state under oxygen atmosphere leads to formation of significant amounts of photooxidation products [3]. A small amount of photodimer (2.6%) is also obtained. However, when E-2-SP is irradiated as its hydrochloride or methiodide, the dimers were obtained as the major product in the solid state as well as in benzene suspension [4–6]. The species of dimer produced

is influenced by steric and charge interference factors. Irradiation of E-2-SP in cyclohexane in the presence of oxygen results in the rapid E–Z isomerization and subsequent cyclization to dihydrobenzo[f]quinoline which is oxidized to benzo[f]quinoline, in addition to the formation of a small amount of 1-phenyl-2-(2-pyridyl)ethanol [7] (Scheme 1).

The dependence of photobehavior on molecular environment is clearly demonstrated by studying the selectivity obtained in the dimerization of E-4-SP cations over organized assemblies like micelles, crystals and monolayers [8]. In contrast to homogeneous photolysis, where in 13% of the Z-isomer a 60% of the *syn-head-to-tail* dimer are formed, the irradiation of E-4-styrylpyridinium cations in reversed micelles formed from hexane–aerosol OT–water, leads to an efficient and selective formation of *syn-head-to-head* dimer [9]. 4-Styrylpyridinium cations give selectively the *syn-head-to-tail* dimers when irradiated between clay interlayers [10]. It was established that the photolysis of α - and β -cyclodextrin complexes of E-2-SP in the solid state leads to unimolecular reactions (photoisomerization and/or photocyclization) and γ -cyclodextrin complex to bimolecular reaction (photodimerization) [11]. The photochemical transformation of E-2-styrylpyridine in various cation-exchanged faujasite zeolites produced significant amounts of dimerization and cyclization products; the products distribution depended on the free volume available [12]. Some examples of the photodimerization of heterostylbene molecules containing oxazole residues have been also reported [13–15].

It was noted in some recent publications that in the photocycloaddition in a single crystal the dimeric styrene pair would not hinder substantial atomic displacements of the central fragments [16]. At the same time, this environment can level the

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Scheme 1.

changes in the exterior shape of the stacking dimer associated with a decrease in its volume in the central region as a result of the transformation into cyclobutane derivative. Hence, topochemical photocycloaddition can presumably occur in a single crystal without its destruction what has attracted attention and has been investigated [17–19].

Thus, according to the literature data successful photocycloaddition process of styrylpyridine molecules exists preferably in organized medium (micelles, zeolites, cyclodextrin complexes and monolayers). The cited papers [5,6] described the formation of photodimer products do not contain the information concerning regioselectivity and configuration of the products and what is the structure of the obtained products.

Herein we report the photochemical behavior of isomeric crown-containing 2- and 4-styrylpyridinium perchlorates (2-CSP and 4-CSP) in solid state and acetonitrile solution. In comparison with 2- and 4-SP molecules the 2-CSP and 4-CSP contain the donor crown ether substituent in the benzene ring which increases the dipole moment of molecule CSP and assists in dimer aggregation of CSP molecules by donor–acceptor interaction in solution and solid state. Otherwise, the large size of crown ether moiety substantially influences on the possibility to dimer formation.

2. Experimental

2.1. Methods

Melting points were measured on a Mel-Temp II instrument.

Elemental analyses were carried out at the Laboratory of Microanalysis of the A.N. Nesmeyanov Institute of Organoelement Compounds (Russian Academy of Sciences, Moscow).

2.1.1. NMR study

¹H NMR spectra were recorded on a Bruker DRX500 instrument (500.13 MHz) by means of a 5 mm direct QNP 1H/X probe with gradient capabilities. The COSY and NOESY 2D spectra were recorded using the standard Bruker pulse sequences (cosy45, cosygs, noesytp, roesyprtp) and processed using the Bruker XWIN-NMR program.

2.1.2. UV–vis spectra

The electronic absorption spectra were recorded on a Specord-M40 spectrometer. Solutions of CSP were irradiated with a light of the mercury lamp (DRK120, 120 W). Individual mercury lines of the spectrum of this lamp (313 and 365 nm) were isolated with the use of glass filters.

To calculate the spectrum of Z-isomers of 2-CSP and 4-CSP by Fischer's method [17], a solutions of E-isomers of 2-CSP and 4-CSP were irradiated with light at $\lambda = 313$ and 365 nm until corresponding photostationary states were established [18].

2.1.3. ESI-MS spectrometry method

Investigation of CSP molecules in acetonitrile was performed using Agilent 1100 Series LC/MSD trap ESI interface operated in positive-ion mode. Direct infusion of analyzed solution was used. Optimum flow rate was 400 $\mu\text{l/h}$. The capillary and the capillary exit were maintained at potentials of 3.5 kV and 10 V respectively. Drying gas temperature was 120 °C. Isotope patterns calculation was performed using Molecular Weight Calculator, Version 6.37 [Matthew Monroe, Molecular Weight Calculator, Version 6.37].

2.2. Materials

A synthesis and the structures of the 2-CSD and 4-CSD were described in [16].

Synthesis of Z-2-CSP or Z-4-CSP: A solution of E-2-CSP or E-4-CSP in CD₃CN (0.5 mL, $C_L = 1 \times 10^{-3}$ mol/l) was irradiated at $\lambda = 365$ nm.

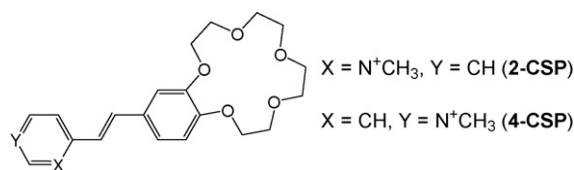
1-Methyl-2-[(Z)-2-(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)vinyl]pyridinium perchlorate (Z-2-CSP), ¹H NMR: (CD₃CN), 30 °C, $\delta = 3.59$ (s, 8 H, H-5, H-6, H-8, H-9); 3.72 (m, 4H, H-3, H-11); 3.94 (t, 2H, H-12, $J = 4.1$); 4.04 (t, 2H, H-2, $J = 4.1$); 4.25 (s, 3H, NCH₃); 6.50 (d, 1H, H-a, $J = 12.2$); 6.68 (d, 1H, H-14, $J = 1.5$); 6.77 (dd, 1H, H-16, $^3J = 8.3$, $J = 1.5$); 6.79 (d, 1H, H-17, $J = 8.3$); 7.25 (d, 1H, H-b, $J = 12.2$); 7.62 (d, 1H, H-3', $J = 7.8$); 7.71 (tr, 1H, H-5', $J = 6.3$); 8.21 (tr, 1H, H-4', $J = 7.8$), 8.62 (d, 1H, H-6', $J = 6.3$).

1-Methyl-4-[(Z)-2-(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)vinyl]pyridinium perchlorate (Z-4-CSP), ¹H NMR: (CD₃CN), 30 °C, $\delta = 3.61$ (s, 8H, H-5, H-6, H-8, H-9); 3.73 (m, 4H, H-3, H-11); 3.92 (t, 2H, H-12, $J = 4.5$); 4.04 (t, 2H, H-2, $J = 4.5$); 4.22 (s, 3H, NCH₃); 6.65 (d, 1H, H-a, $J = 12.1$); 6.85 (dd, 1H, H-16, $^3J = 8.3$, $J = 1.5$); 6.88 (d, 1H, H-14, $J = 1.5$); 6.90 (d, 1H, H-17, $J = 8.3$); 7.12 (d, 1 H, H-b, $J = 12.1$); 7.83 (d, 2 H, H-3', H-5', $J = 6.7$); 8.69 (d, 2 H, H-2', H-6', $J = 6.7$).

Synthesis of the cyclobutane derivative CB: A 15 mg of dye E-2-CSP or E-4-CSP was dissolved in 3 ml MeCN and placed on quartz plate. The slow evaporation resulted in the formation of thin film of solid dye which was irradiated with light from a DRK-120 mercury lamp at 365 nm for 3 h.

When the dye was wholly consumed (monitoring by UV–vis spectroscopy), the product was applied for optical, NMR investigations and analysis by ESI-MASS and elemental analysis.

Perchlorate of 2,2'-(3,4-bis-2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclo-pentadecyn-15-yl)cyclobutane-1,2-diyl)-bis(1-methylpyridinium), 91%, m.p. 135–137 °C. Anal. calcd. for C₄₄H₅₆Cl₂N₂O₁₈ × H₂O: C, 53.39; H, 5.91; N, 2.83; found: C, 53.20; H, 6.02; N, 2.74. MS (ESI-MS): m/z [386.2]⁺. ¹H NMR: (CD₃CN), 30 °C, $\delta = 3.59$ (m, 16 H, H-5, H-5'', H-6, H-6'', H-8, H-8'', H-9, H-9''), 3.74 (m, 8 H, H-3, H-3'', H-11, H-11''); 3.83 (m, 4 H, H-12, H-12''); 3.96 (m, 4 H, H-2, H-2''); 4.07 (s, 6 H, NCH₃); 4.81 (dd, 2 H, H-a, H-a'', $J = 8.1$, $J = 8.9$); 5.10 (dd, 2 H, H-b, H-b'', $J = 8.1$, $J = 8.9$); 6.75 (d, 2 H, H-17, H-17'', $J = 8.4$); 6.85 (d, 2 H, H-14, H-14'', $J = 1.9$); 6.95 (dd, 1 H, H-16, H-16'', $^3J = 8.4$, $J = 1.9$); 7.77 (tr, 2 H, H-5', H-5''',



Scheme 2.

$J=6.8$); 8.31 (d, 2 H, H-3', H-3''', $J=8.0$); 8.43 (d, 2 H, H-6', H-6''', $J=6.8$), 8.45 (t, 2 H, H-4', H-4''', $J=8.0$).

3. Results and discussion

According to the vicinal coupling constants for the ethylen bond protons, $^3J_{H(a),H(b)} = 16.0$ and 15.7 Hz, both compounds were obtained as *E*-isomers [20]. The compound *E*-2-CSP could exist as 4 conformers presented in Scheme 2. The NOESY spectrum of compound *E*-2-CSP exhibits cross signals between the protons in conformers C and D. The NOESY observation proved the existence of *E*-4-CSP as mixture of two possible isomers A and C (Scheme 3).

When solution of *E*-2-CSP or *E*-4-CSP in acetonitrile are irradiated with light at $\lambda = 365$ nm absorption in the region of the long wavelength band decreases with the simultaneous increase in the absorption in the short wavelength spectral region until the photostationary state is achieved. The subsequent irradiation of the resulting solution with the light $\lambda = 313$ nm results in inverse changes in the absorption spectra up to the transition of *E*-2-CSP or *E*-4-CSP to the new photostationary state. In all cases, a distinct isosbestic point and a linear relation between the absorbance at

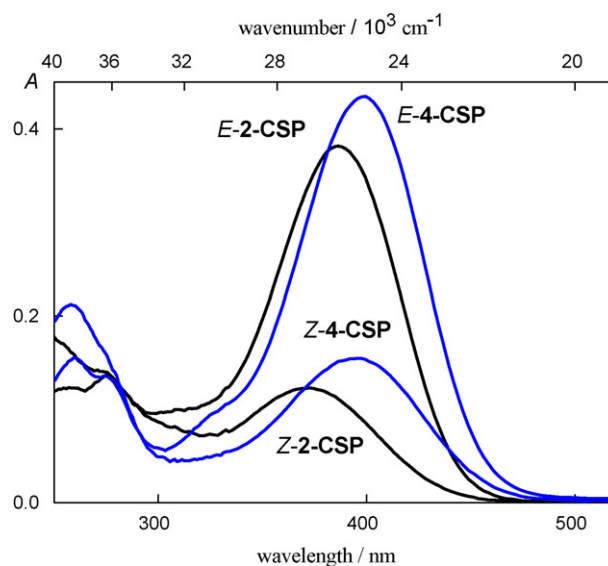
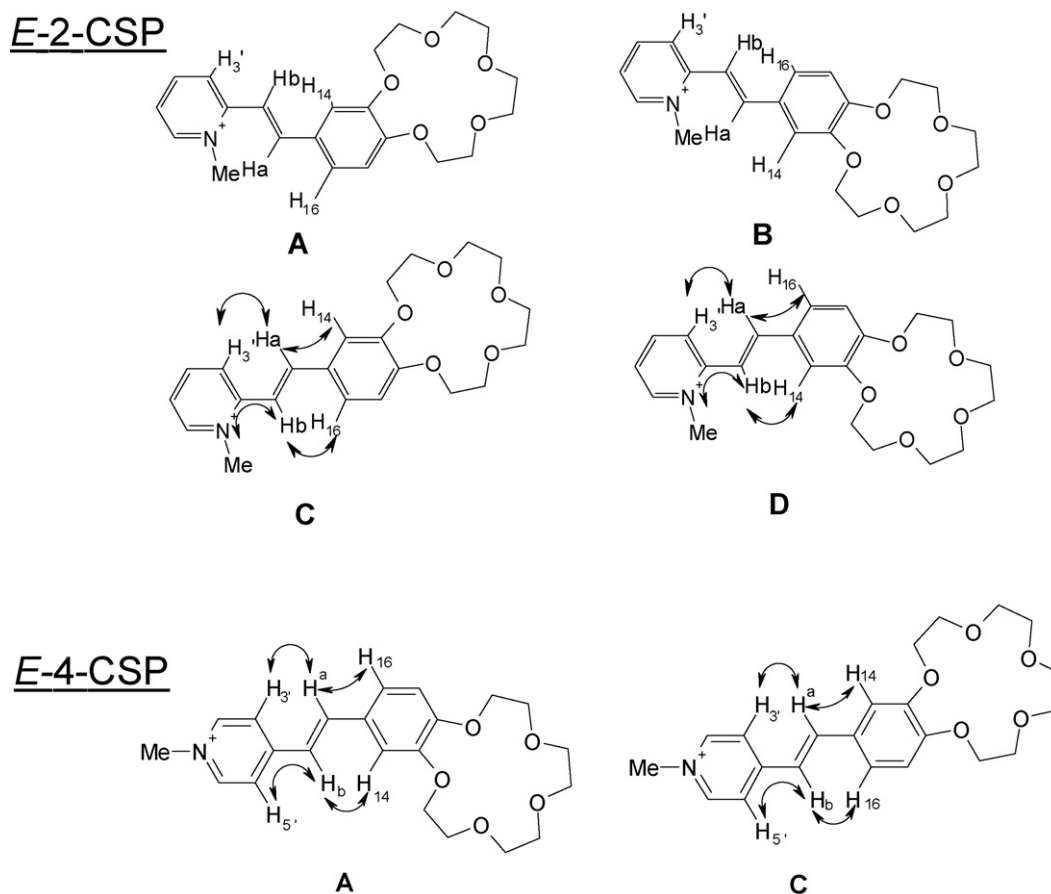
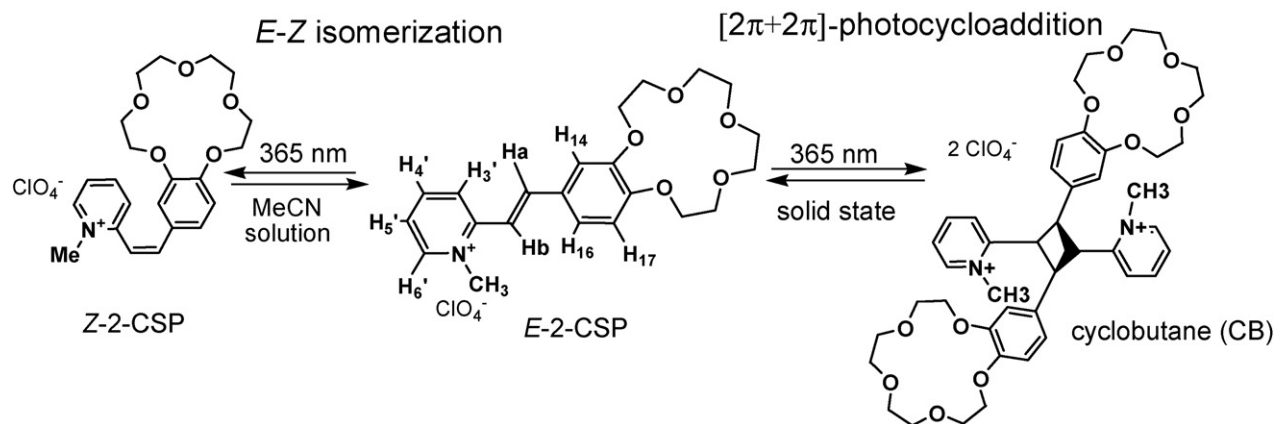


Fig. 1. Absorption spectra of *E*-2-CSP and *E*-4-CSP ($C = 1.5 \times 10^{-5}$ M) in MeCN, and spectra of *Z*-2-CSP and *Z*-4-CSP calculated by Fischer's method.

two different wavelengths are observed. These spectral changes can be explained by reversible photochemical *E*-*Z* isomerization around the central C=C double bond (Scheme 4). The spectra of *Z*-2-CSP and *Z*-4-CSP were calculated from the irradiation data using the method described in Experimental part [21]. The absorption spectra of the *Z*-2-CSP and *Z*-4-CSP are presented in Fig. 1.



Scheme 3.



Scheme 4.

Substantial changes are observed in ^1H NMR spectrum of *E*-2-CSP (as well as for *E*-4-CSP) when a solution is exposed to visible light (Fig. 2). In the novel photoproduct, the spin–spin coupling constants for the olefinic proton signals at 6.50 and 7.25 ppm are $J = 12.2$ Hz, which implies the formation of *Z*-2-CSP. In the *Z*-isomer, the signals of the aromatic protons of the benzocrown ether moiety, pyridine residue and of the olefinic protons shift upfield relative to those of *E*-isomer (Fig. 2).

The irradiation of *E*-2-CSP in solid state with light $\lambda = 365$ nm leads to consumption of the dye, which occurs in parallel with the formation of the *Z*-isomer (Fig. 3a and b). The fast changes of optical density in Fig. 3b are corresponded to the process of *E*–*Z* isomerization, more slow process is photocycloaddition. The occurrence

of two simultaneous processes does not allow the calculation of the quantum yield of photocycloaddition.

Virtually complete consumption of *E*-2-CSP was reached over reasonable time periods (1–3 h) upon photolysis with 365 nm light. Fig. 4a shows the absorption spectrum of the photolyzate resulting from [2 + 2]-photocycloaddition (PCA), Fig. 4b demonstrates the luminescence of initial solid dye *E*-2-CSP (1b) and its photocyclobutane product (1a) obtained by photolysis of *E*-2-CSP.

Detailed analysis of the structure of the photoadduct was done using COSY and NOESY 2D techniques and by comparison with available ^1H NMR spectral data for the crown-containing cyclobutanes of the quinolinium and benzothiazolium series prepared upon the exposure with light of metal ionic complexes in acetonitrile.

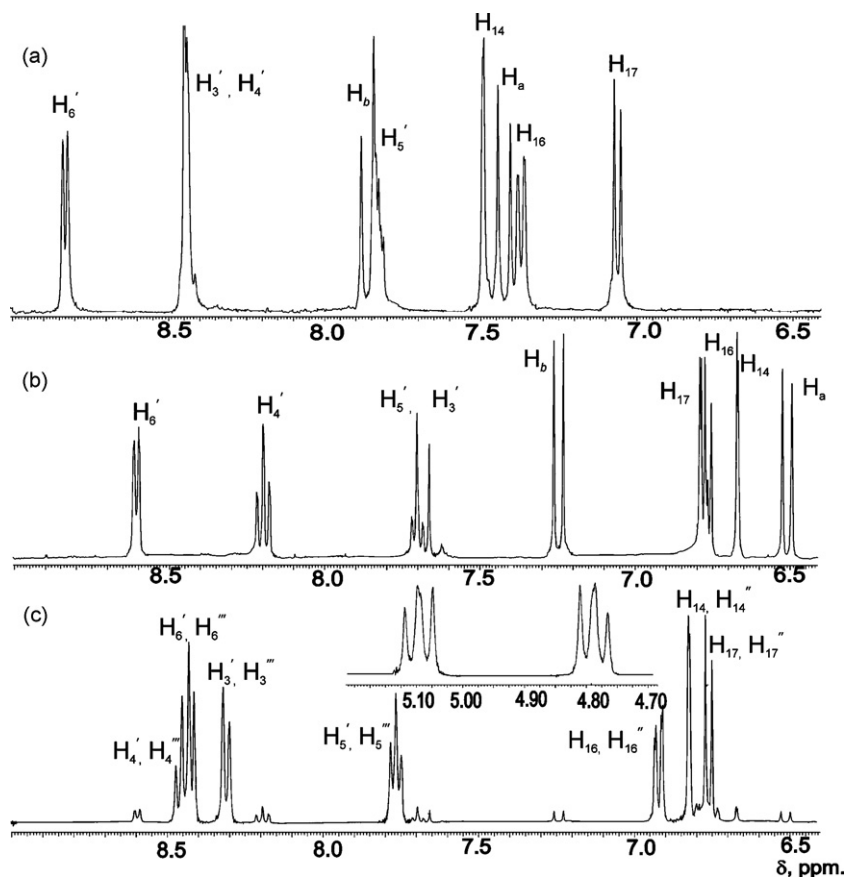


Fig. 2. ^1H NMR spectra (aromatic part) (a) *E*-2-CSP, (b) *Z*-2-CSP and (c) cyclobutane CB in CD_3CN at 303 K; in all cases $C = 1 \times 10^{-3}$ M.

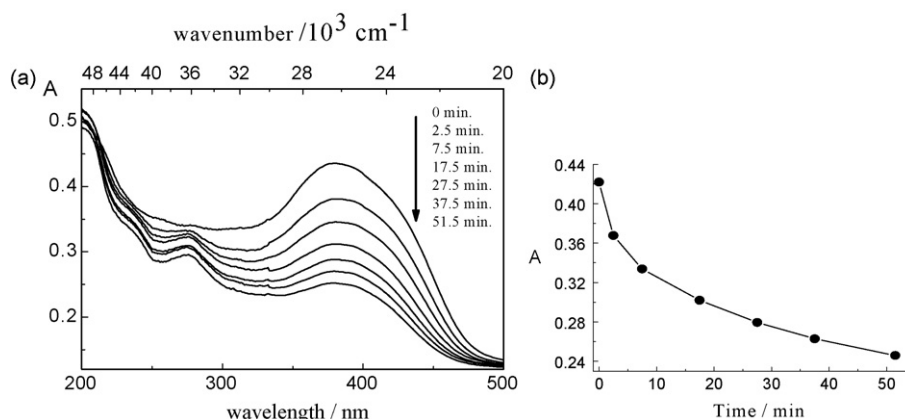


Fig. 3. (a) Dependence of the absorption spectra of *E*-2-CSP (0.15 mg/cm²) placed on a quartz plate upon the irradiation time with light at $\lambda = 365$ nm; (b) dependence of the absorption density at $\lambda = 380$ nm of *E*-2-CSP (0.15 mg/cm²) placed on a quartz plate upon the irradiation time with light at $\lambda = 365$ nm.

trile solution [22–28]. The ¹H NMR spectrum of the photoproduct CB in MeCN-*d*₃ solution (Fig. 2) exhibits two triplets at 4.80 and 5.10 ppm due to the protons of the cyclobutane ring. The presence of only one set of signals in the NMR spectra is indicative of the formation of a single stereoisomer.

The signals for the protons of the cyclobutane fragment of the resulting photoadduct appear as a symmetric AA'BB' spin system with the vicinal coupling constants of 8.9 and 8.1 Hz. In NOESY spectrum of CB the following cross signals between protons were found: H^b ↔ H-16, H^b ↔ H-14, H^a ↔ H-16, H^a ↔ H-14, H-3' ↔ H^b, H-3' ↔ H^a, NMe ↔ H^a, NMe ↔ H^b, NMe ↔ H-16, NMe ↔ H-14, H-17 ↔ H-9, H-14 ↔ H-2 and NMe ↔ H-2. The presence of NOE cross signals between NMe and H-16, NMe and H-14 indicates the coordination of pyridinium N-Me-group of one molecule with crown ether of the other one. Thus, the cyclobutane could have been formed from dimeric complex constructed according to the “head-to-tail” pattern I or II (Scheme 5). It is worth to note that in the formation of dimers I and II in crystal state the both conformers of *E*-2-CSP determined in acetonitrile solution by NMR observation (Scheme 3) participated. Probably, the relative stability of conformers is similar in solid state and solution. The cycloadduct resulting from dimer I should be produced as the *anti*-conformer, while photocycloaddition with the participation of dimer II should lead to the *syn*-conformer (Scheme 5).

The quantity, position, multiplicity, and spin–spin coupling constants of the cyclobutane ring protons in cycloadduct are similar to those obtained for cyclobutanes of the quinolinium and benzothiazole series [22–28]. From the data presented in the cited papers, the

dimer I leads to the formation of cyclobutane of AA'BB'-type spectrum with one ³J = 9.8 Hz, whereas, the dimer II is able to produce the cyclobutane of AA'BB'-type spectrum with $J_{ab} = J_{a''b''} = 9.1$ and $J_{ab''} = J_{a''b} = 7.61$ Hz. Obviously, that the cyclobutane CB is produced from dimer II. This observation confirmed that the pairs of *E*-2-CSP exist in the crystals as dimers organized by dipole interaction between the donor crown ether part of one molecule with acceptor pyridinium residue of the other one. The structure of CSP plays important role in the proper arrangement of molecules in dimer assembly allowing the occurrence of photocycloaddition reaction. We found that irradiation of *E*-4-CSP in crystal state does not result in the formation of cyclobutane product.

Thus, the spontaneous formation of dimers comprising two dye molecules with a fixed mutual arrangement of the double bonds provides a pre-organization of the reactants favorable for regio- and stereoselective [2 + 2]-photocycloaddition. The realization of the pre-organization has got the strong requirements to dye structure. The photocycloaddition was also possible due to a rather loose environment of the dimeric pairs in the crystal, which does not hinder their considerable structural rearrangement during transformation into a cyclobutane derivative. This fundamental investigation has established that supramolecular assistance to the [2 + 2]-photodimerization can be carried out in the solid state, and that the photoreaction occurring with high stereospecificity in the solid state presents rare examples of such transformation. This observation is also important in designing of supramolecular photochromic systems in solid state which can be considered as a step forward in the field of photochromic materials.

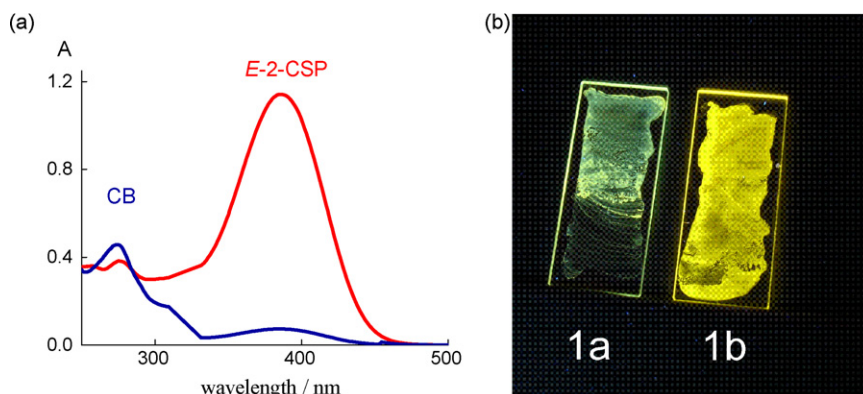
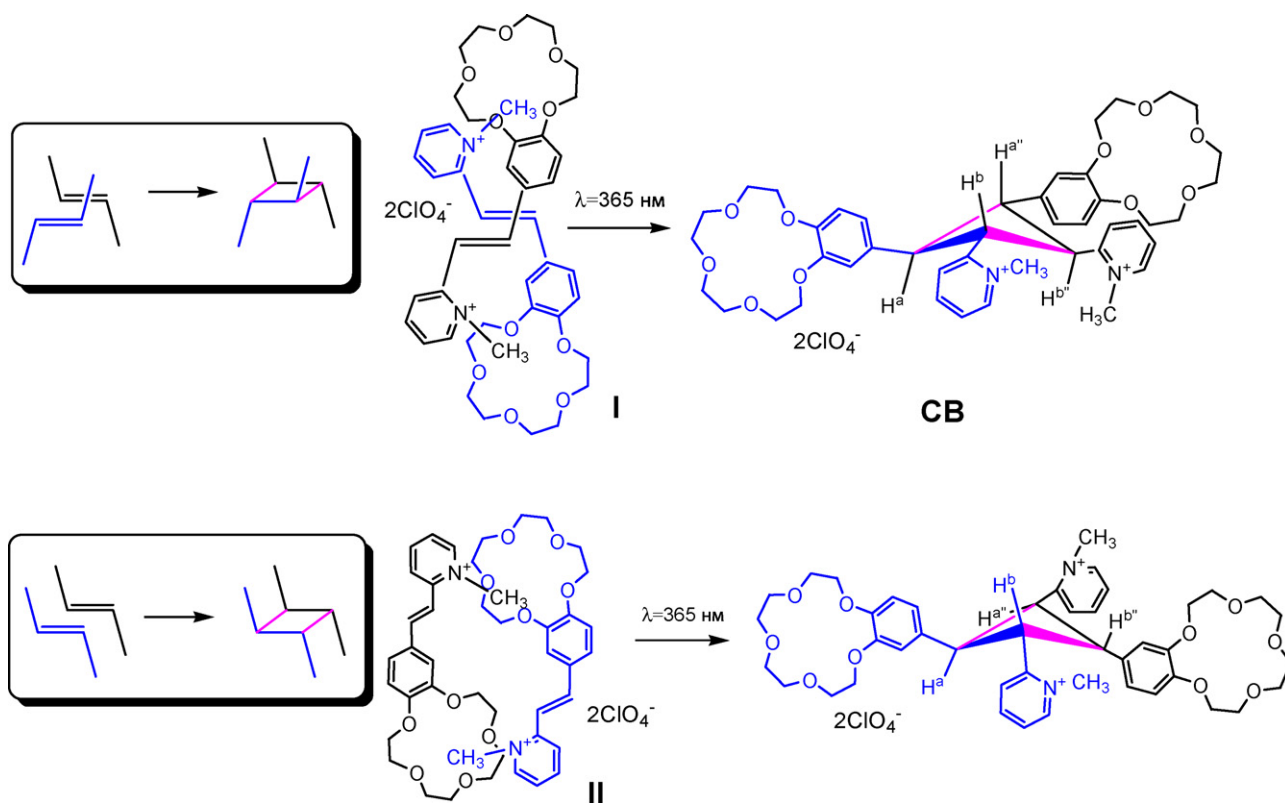


Fig. 4. (a) Absorption spectra of *E*-2-CSP and CB ($C = 1 \times 10^{-4}$ M, $l = 1$ mm), in MeCN at 293K; (b) the photo of the luminescence of CB film (1a) obtained by irradiation of *E*-2-CSP with light at 365 nm during 3 h and film of the initial solid dye *E*-2-CSP (1b).



Scheme 5.

Acknowledgements

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