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Effects of substituent and solvent on the UV absorption energy of 4,4'-disubstituted stilbenes

CAO ChenZhong*, CHEN GuanFan & WU YaXin

Key Laboratory of Theoretical Chemistry and Molecular Simulation of Ministry of Education; Hunan Provincial University Key Laboratory of QSAR/QSPR, School of Chemistry and Chemical Engineering, Hunan University of Science and Technology, Xiangtan 411201, China

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Twenty five samples of 4,4'-disubstituted stilbene derivatives were synthesized, and their UV absorption max wavelengths were determined in over 10 kinds of solvents including cyclohexane, ether, chloroform, acetonitrile and ethanol, in which 242 experimental data were recorded. The effects of substituents and solvents on the energy of their UV absorption max wavelengths were discussed. The research results showed: the energy of UV absorption max wavelengths of 4,4'-disubstituted stilbenes was mainly affected by their intramolecular structure (substituent effect) in a given solvent, that is, the energy is dominated by both of excited-state substituent parameter $\sigma_{\mathrm{CC}}^{\mathrm{ex}}$ and polar substituent constant σ_{p}. While their energy was dominated by the substituent effect and solvent effect in different kinds of solvents. An equation quantifying the energy of UV absorption max wavelengths of 4,4'-disubstituted stilbenes was developed. In addition, it is found that the *n*-octanol/water partition coefficient (log*P*) is more effective than the solvatochromic dye ($E_{\mathrm{T}}(30)$) in scaling the solvent effect. The equation employed the parameter log*P* has a better correlation and more specific physical meaning. Further, the energies of UV absorption max wavelengths of some reported compounds were predicted by the obtained equation, which are in agreement with their experimental values.

4,4'-disubstituted stilbene, UV absorption energy, excited-state substituent parameter, solvent effect

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1 Introduction

4,4'-Disubstituted stilbene derivatives possess important optical and liquid crystalline properties, and play an important role in the fields of photochemistry, photophysics, and material technology [1–15]. Their photoisomerization is usually used as the model compound in studies of the reaction dynamics and unimolecular isomerization reactions [1–3], has been studied for more than 60 years, and its research is still active even today [5, 6, 8–10]. In the past, the researches were mainly concentrated on the energy needed for isomerization and effects of solvent-solute interactions on the isomerization [11–15]. With regard to how the optical properties of the model compound are affected by molecular structure and solvent is still unclear for lack of in-depth and systematic study. In theory, the energy of UV absorption max wavelengths of 4,4'-disubstituted stilbene derivatives was mainly affected by two factors: one is intramolecular structure (substituent effect), and the other is the internal environment of the molecule (such as solvent effect). If the 4,4'-disubstituted stilbene derivatives is to be used as optical materials, the effects of substituent and solvent on their UV absorption energy must be known. In author's recent works [16–18], the excited-state substituent parameter $\sigma_{\mathrm{CC}}^{\mathrm{ex}}$ was proposed to scale the effect of intramolecular substituent effect. It is found that the energy of UV absorption max wavelengths of *trans*-4,4'-disubstituted stilbene derivatives (XPhCH=CHPhY) can be correlated well with two parameters in a given solvent, the sum of $\sigma_{\mathrm{CC}}^{\mathrm{ex}}$ of substituents X and Y and the interaction between

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*Corresponding author (email: czcao@hnust.cn) substituents X and Y, $\sigma_{\mathrm{CC}}^{\mathrm{ex}}$ (X) $\sigma_{\mathrm{CC}}^{\mathrm{ex}}$ (Y), in which the correlation result using parameter $\sigma_{\mathrm{CC}}^{\mathrm{ex}}$ is better than that of using polar substituent constant σ^{x} or spin-delocalization substituent constant $\sigma^{\bullet}$ [16–18]. However, the changing law of the UV absorption energy for a series of XPhCH=CHPhY in different kinds of solvents is an more complex topic. The research on this issue is helpful to understand how the UV absorption energy is affected by substituent effect and solvent effect simultaneously, and has an important theoretical significance and practical value. In this work, the effects of both factors were investigated preliminarily, and a significant result was obtained.

A great deal of research was focused on the solvent effect on the UV absorption energy [19]. The results indicated that the UV absorption max wavelength shifts of different solute molecules were different even in the same solvent (some of them produce red shifts, but others produce blue shifts). Their shift direction was related to the dipole moments between the ground and excited states of the solute molecule. It was noted that their direction and magnitude of the shifts can not be predicted accurately in theory. Up to now, lots of solvent effect parameters [19] have been proposed, and many parameters quantifying the polarity of the solvent have also been reported [20, 21]. However, whether these parameters can be used to investigate the changing law of the UV absorption energy needs further studies.

2 Experimental section

Synthesis of XSBY: Twenty-five samples of 4,4'-disubstituted stilbene derivatives were synthesized with the Wittig-Honer reaction [22] shown in Figure 1. Their structures were confirmed by nuclear magnetic resonance analysis, and the details were given in ref. [23].

Measured data of UV absorption spectra: All the solvents used in this work are dried over anhydrous $MgSO_4$. Each sample of 4,4'-disubstituted stilbene derivative is weighed, placed into a 10 mL volumetric flask, and used to prepare the solution (about 2.00 g L^{-1}) by adding the dried solvent. All solutions are prepared and measured in the dark, and the corresponding solvents are taken as their reference solutions. The UV absorption spectra were recorded on a Perkin Elmer Lambda 35 spectrometer with the scan range of 210–400 nm. The energy of UV absorption max wavelengths of those *trans*-4,4'-disubstituted stilbene derivatives were measured, and listed in Table 1.

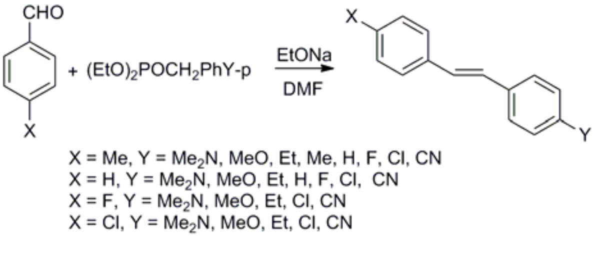

Figure 1 Synthesis of samples of *trans*-4,4'-disubstituted stilbene derivatives.

3 Results and discussion

In this work, 25 samples of 4,4'-disubstituted stilbene derivatives *p*-XPhCH=CHPh-*p*-Y (XSBY) were synthesized, and their UV absorption max wavelengths were determined in over 10 kinds of solvents including cyclohexane, ether, chloroform, acetonitrile and ethanol (see Table 1).

The properties of solvents employed in this paper are different from each others. Some of them are polar, and some of them are non-polar. Also some of them are proton, and some of them are non-proton. For example, cyclohexane is a non-polar and non-proton solvent, acetonitrile is a polar and non-proton solvent, and methanol is a polar and proton solvent.

3.1 The changing law of the $\nu_{\max}$ of XSBY in a given solvent

From our previous studies [18], it was known that the energy of UV absorption max wavelengths of 4,4'-disubstituted stilbenes in ethanol has a good correlation with the $\sigma_{\mathrm{CC}}^{\mathrm{ex}}$ of substituents X and Y. Thus, we also attempt to correlate the energy of UV absorption max wavelengths (wavenumbers $\nu_{\max}$) of XSBY with two parameters $\Sigma\sigma_{\mathrm{CC}}^{\mathrm{ex}}$ and $\sigma_{\mathrm{CC}}^{\mathrm{ex}}(\mathrm{XY})$. Here $\Sigma\sigma_{\mathrm{CC}}^{\mathrm{ex}}$ is the sum of $\sigma_{\mathrm{CC}}^{\mathrm{ex}}(\mathrm{X})$ and $\sigma_{\mathrm{CC}}^{\mathrm{ex}}(\mathrm{Y})$, viz. $\Sigma\sigma_{\mathrm{CC}}^{\mathrm{ex}} = \sigma_{\mathrm{CC}}^{\mathrm{ex}}(\mathrm{X}) + \sigma_{\mathrm{CC}}^{\mathrm{ex}}(\mathrm{Y})$. $\sigma_{\mathrm{CC}}^{\mathrm{ex}}(\mathrm{XY})$ indicates the interaction between substituents X and Y, that is $\sigma_{\mathrm{CC}}^{\mathrm{ex}}(\mathrm{XY}) = \sigma_{\mathrm{CC}}^{\mathrm{ex}}(\mathrm{X}) \times \sigma_{\mathrm{CC}}^{\mathrm{ex}}(\mathrm{Y})$.

$$\nu_{\max} = a + b\sum\sigma_{\mathrm{CC}}^{\mathrm{ex}} + c\sigma_{\mathrm{CC}}^{\mathrm{ex}}(\mathrm{XY}) \qquad (1a)$$

The experimental $\nu_{\max}$ measured in each solvent (cyclohexane, ether, chloroform, acetonitrile and ethanol) were correlated with parameters $\Sigma\sigma_{\mathrm{CC}}^{\mathrm{ex}}$ and $\sigma_{\mathrm{CC}}^{\mathrm{ex}}(\mathrm{XY})$ as eq. (1a), respectively. The regression results are given in Table 2. Guo *et al.* [26] has reported that the contribution of the interaction between substituents X and Y (σ_{XY}) to the energy can be expressed with the product of their electronic effect constants (Hammett constant), viz. $\sigma_{\mathrm{XY}} = \sigma_{\mathrm{p}}(\mathrm{X}) \times \sigma_{\mathrm{p}}(\mathrm{Y})$. Thus the $\sigma_{\mathrm{CC}}^{\mathrm{ex}}(\mathrm{XY})$ in eq. (1a) is replaced by the σ_{XY} as shown in eq. (1b), and a further investigation was carried out. Using the same data sets in eq. (1a), we made regression analysis with eq. (1b). The correlation results of eq. (1b) are better than that of eq. (1a) (see Table 2).

Table 1 The wavelengths λ_{max} (nm) and wavenumbers v_{max} (cm^{-1}) of UV absorption maximum of XSBY in different solvents

No.	Compound (XSBY)	λ_{max}	v_{max}	$\Sigma\sigma_{CC}^{ex}$ a)	σ_{XY} b)	log$P$ c)	$E_T(30)$ d)	Solvent
1	MeSBNMe$_2$	351.0	28489	–1.98	0.14	–0.34	45.6	acetonitrile
2	MeSBOMe	320.7	31185	–0.67	0.05	–0.34	45.6	acetonitrile
3	MeSBMe	315.2	31729	–0.34	0.03	–0.34	45.6	acetonitrile
4	MeSBEt	315.0	31749	–0.30	0.03	–0.34	45.6	acetonitrile
5	MeSBH	311.3	32127	–0.17	0.00	–0.34	45.6	acetonitrile
6	MeSBF	311.1	32146	–0.12	–0.01	–0.34	45.6	acetonitrile
7	MeSBCl	315.4	31710	–0.39	–0.04	–0.34	45.6	acetonitrile
8	MeSBCN	325.1	30757	–0.87	–0.11	–0.34	45.6	acetonitrile
9	HSBNMe$_2$	351.8	28423	–1.81	0.00	–0.34	45.6	acetonitrile
10	HSBOMe	317.4	31504	–0.50	0.00	–0.34	45.6	acetonitrile
11	HSBEt	311.5	32103	–0.13	0.00	–0.34	45.6	acetonitrile
12	HSBH	307.1	32558	0.00	0.00	–0.34	45.6	acetonitrile
13	HSBF	306.9	32581	0.06	0.00	–0.34	45.6	acetonitrile
14	HSBCl	311.6	32090	–0.22	0.00	–0.34	45.6	acetonitrile
15	HSBCN	319.0	31346	–0.70	0.00	–0.34	45.6	acetonitrile
16	FSBNMe$_2$	350.5	28528	–1.75	–0.05	–0.34	45.6	acetonitrile
17	FSBOMe	317.9	31457	–0.44	–0.02	–0.34	45.6	acetonitrile
18	FSBEt	311.3	32121	–0.08	–0.01	–0.34	45.6	acetonitrile
19	FSBCl	311.7	32081	–0.16	0.01	–0.34	45.6	acetonitrile
20	FSBCN	319.3	31319	–0.65	0.04	–0.34	45.6	acetonitrile
21	ClSBNMe$_2$	358.9	27864	–2.02	–0.19	–0.34	45.6	acetonitrile
22	ClSBOMe	322.7	30991	–0.71	–0.06	–0.34	45.6	acetonitrile
23	ClSBEt	315.9	31657	–0.35	–0.03	–0.34	45.6	acetonitrile
24	ClSBCl	315.8	31664	–0.43	0.05	–0.34	45.6	acetonitrile
25	ClSBCN	322.9	30973	–0.92	0.15	–0.34	45.6	acetonitrile
26	MeSBNMe$_2$	353.5	28289	–1.98	0.14	1.97	39.1	chloroform
27	MeSBOMe	323.8	30888	–0.67	0.05	1.97	39.1	chloroform
28	MeSBMe	317.9	31458	–0.34	0.03	1.97	39.1	chloroform
29	MeSBEt	318.1	31435	–0.30	0.03	1.97	39.1	chloroform
30	MeSBH	314.4	31805	–0.17	0.00	1.97	39.1	chloroform
31	MeSBF	314.0	31844	–0.12	–0.01	1.97	39.1	chloroform
32	MeSBCl	319.2	31329	–0.39	–0.04	1.97	39.1	chloroform
33	MeSBCN	330.1	30294	–0.87	–0.11	1.97	39.1	chloroform
34	HSBNMe$_2$	353.9	28253	–1.81	0.00	1.97	39.1	chloroform
35	HSBOMe	320.6	31189	–0.50	0.00	1.97	39.1	chloroform
36	HSBEt	314.7	31780	–0.13	0.00	1.97	39.1	chloroform
37	HSBH	310.3	32230	0.00	0.00	1.97	39.1	chloroform
38	HSBF	310.1	32251	0.06	0.00	1.97	39.1	chloroform
39	HSBCl	315.2	31721	–0.22	0.00	1.97	39.1	chloroform
40	HSBCN	323.7	30894	–0.70	0.00	1.97	39.1	chloroform
41	FSBNMe$_2$	353.3	28308	–1.75	–0.05	1.97	39.1	chloroform
42	FSBOMe	320.4	31211	–0.44	–0.02	1.97	39.1	chloroform
43	FSBEt	314.6	31789	–0.08	–0.01	1.97	39.1	chloroform
44	FSBCl	315.1	31731	–0.16	0.01	1.97	39.1	chloroform
45	FSBCN	323.7	30891	–0.65	0.04	1.97	39.1	chloroform
46	ClSBNMe$_2$	361.1	27692	–2.02	–0.19	1.97	39.1	chloroform
47	ClSBOMe	325.9	30685	–0.71	–0.06	1.97	39.1	chloroform
48	ClSBEt	319.8	31269	–0.35	–0.03	1.97	39.1	chloroform
49	ClSBCl	319.9	31262	–0.43	0.05	1.97	39.1	chloroform
50	ClSBCN	327.4	30543	–0.92	0.15	1.97	39.1	chloroform
51	MeSBNMe$_2$	347.5	28776	–1.98	0.14	3.44	30.9	cyclohexane
52	MeSBOMe	321.5	31108	–0.67	0.05	3.44	30.9	cyclohexane
53	MeSBMe	315.5	31699	–0.34	0.03	3.44	30.9	cyclohexane
54	MeSBEt	315.7	31672	–0.30	0.03	3.44	30.9	cyclohexane
55	MeSBH	312.4	32011	–0.17	0.00	3.44	30.9	cyclohexane

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No.	Compound (XSBY)	λ_{max}	ν_{max}	$\Sigma\sigma_{CC}^{ex}$ a)	σ_{XY} b)	log$P$ c)	$E_T(30)$ d)	Solvent
56	MeSBF	312.3	32019	–0.12	–0.01	3.44	30.9	cyclohexane
57	MeSBCl	317.4	31504	–0.39	–0.04	3.44	30.9	cyclohexane
58	MeSBCN	328.0	30486	–0.87	–0.11	3.44	30.9	cyclohexane
59	HSBNMe$_2$	349.6	28607	–1.81	0.00	3.44	30.9	cyclohexane
60	HSBOMe	319.4	31311	–0.50	0.00	3.44	30.9	cyclohexane
61	HSBEt	312.7	31983	–0.13	0.00	3.44	30.9	cyclohexane
62	HSBH	308.4	32421	0.00	0.00	3.44	30.9	cyclohexane
63	HSBF	307.9	32477	0.06	0.00	3.44	30.9	cyclohexane
64	HSBCl	313.3	31914	–0.22	0.00	3.44	30.9	cyclohexane
65	HSBCN	321.1	31139	–0.70	0.00	3.44	30.9	cyclohexane
66	FSBNMe$_2$	346.7	28843	–1.75	–0.05	3.44	30.9	cyclohexane
67	FSBOMe	319.4	31307	–0.44	–0.02	3.44	30.9	cyclohexane
68	FSBEt	312.4	32013	–0.08	–0.01	3.44	30.9	cyclohexane
69	FSBCl	313.1	31940	–0.16	0.01	3.44	30.9	cyclohexane
70	FSBCN	321.3	31125	–0.65	0.04	3.44	30.9	cyclohexane
71	ClSBNMe$_2$	354.3	28228	–2.02	–0.19	3.44	30.9	cyclohexane
72	ClSBOMe	324.8	30790	–0.71	–0.06	3.44	30.9	cyclohexane
73	ClSBEt	317.5	31495	–0.35	–0.03	3.44	30.9	cyclohexane
74	ClSBCl	317.9	31453	–0.43	0.05	3.44	30.9	cyclohexane
75	ClSBCN	325.0	30766	–0.92	0.15	3.44	30.9	cyclohexane
76	MeSBNMe$_2$	347.9	28741	–1.98	0.14	–0.31	51.9	ethanol
77	MeSBOMe	321.2	31129	–0.67	0.05	–0.31	51.9	ethanol
78	MeSBMe	314.9	31755	–0.34	0.03	–0.31	51.9	ethanol
79	MeSBEt	315.2	31724	–0.30	0.03	–0.31	51.9	ethanol
80	MeSBH	311.2	32133	–0.17	0.00	–0.31	51.9	ethanol
81	MeSBF	311.3	32121	–0.12	–0.01	–0.31	51.9	ethanol
82	MeSBCl	316.3	31611	–0.39	–0.04	–0.31	51.9	ethanol
83	MeSBCN	326.6	30621	–0.87	–0.11	–0.31	51.9	ethanol
84	HSBNMe$_2$	350.1	28563	–1.81	0.00	–0.31	51.9	ethanol
85	HSBOMe	318.2	31427	–0.50	0.00	–0.31	51.9	ethanol
86	HSBEt	312.0	32055	–0.13	0.00	–0.31	51.9	ethanol
87	HSBH	307.8	32485	0.00	0.00	–0.31	51.9	ethanol
88	HSBF	307.4	32536	0.06	0.00	–0.31	51.9	ethanol
89	HSBCl	312.1	32044	–0.22	0.00	–0.31	51.9	ethanol
90	HSBCN	320.5	31204	–0.70	0.00	–0.31	51.9	ethanol
91	FSBNMe$_2$	349.3	28627	–1.75	–0.05	–0.31	51.9	ethanol
92	FSBOMe	318.4	31403	–0.44	–0.02	–0.31	51.9	ethanol
93	FSBEt	311.5	32102	–0.08	–0.01	–0.31	51.9	ethanol
94	FSBCl	312.3	32018	–0.16	0.01	–0.31	51.9	ethanol
95	FSBCN	320.8	31175	–0.65	0.04	–0.31	51.9	ethanol
96	ClSBNMe$_2$	354.3	28225	–2.02	–0.19	–0.31	51.9	ethanol
97	ClSBOMe	323.8	30883	–0.71	–0.06	–0.31	51.9	ethanol
98	ClSBEt	316.7	31580	–0.35	–0.03	–0.31	51.9	ethanol
99	ClSBCl	316.7	31576	–0.43	0.05	–0.31	51.9	ethanol
100	ClSBCN	324.1	30855	–0.92	0.15	–0.31	51.9	ethanol
101	MeSBNMe$_2$	348.4	28705	–1.98	0.14	0.89	34.5	ether
102	MeSBOMe	320.6	31191	–0.67	0.05	0.89	34.5	ether
103	MeSBMe	314.5	31801	–0.34	0.03	0.89	34.5	ether
104	MeSBEt	314.6	31788	–0.30	0.03	0.89	34.5	ether
105	MeSBH	311.2	32138	–0.17	0.00	0.89	34.5	ether
106	MeSBF	311.1	32139	–0.12	–0.01	0.89	34.5	ether
107	MeSBCl	316.0	31649	–0.39	–0.04	0.89	34.5	ether
108	MeSBCN	325.3	30739	–0.87	–0.11	0.89	34.5	ether
109	HSBNMe$_2$	348.9	28658	–1.81	0.00	0.89	34.5	ether
110	HSBOMe	318.0	31442	–0.50	0.00	0.89	34.5	ether

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No.	Compound (XSBY)	λ_{max}	ν_{max}	$\Sigma\sigma_{\text{CC}}^{\text{ex}}$ a)	σ_{XY} b)	log$P$ c)	$E_{\text{T}}(30)$ d)	Solvent
111	HSBEt	311.5	32101	–0.13	0.00	0.89	34.5	ether
112	HSBH	307.3	32540	0.00	0.00	0.89	34.5	ether
113	HSBF	307.0	32570	0.06	0.00	0.89	34.5	ether
114	HSBCl	311.8	32074	–0.22	0.00	0.89	34.5	ether
115	HSBCN	319.2	31326	–0.70	0.00	0.89	34.5	ether
116	FSBNMe$_2$	347.3	28797	–1.75	–0.05	0.89	34.5	ether
117	FSBOMe	318.1	31440	–0.44	–0.02	0.89	34.5	ether
118	FSBEt	311.8	32072	–0.08	–0.01	0.89	34.5	ether
119	FSBCl	312.0	32049	–0.16	0.01	0.89	34.5	ether
120	FSBCN	319.3	31320	–0.65	0.04	0.89	34.5	ether
121	ClSBNMe$_2$	354.0	28248	–2.02	–0.19	0.89	34.5	ether
122	ClSBOMe	323.5	30912	–0.71	–0.06	0.89	34.5	ether
123	ClSBEt	316.4	31609	–0.35	–0.03	0.89	34.5	ether
124	ClSBCl	316.4	31604	–0.43	0.05	0.89	34.5	ether
125	ClSBCN	323.3	30935	–0.92	0.15	0.89	34.5	ether
126	MeSBCN	325.9	30680	–0.87	–0.11	–0.66	55.4	methanol
127	MeSBCN	327.6	30524	–0.87	–0.11	0.34	50.7	*n*-propanol
128	MeSBCN	328.0	30492	–0.87	–0.11	0.88	49.7	*n*-butanol
129	MeSBCN	328.9	30408	–0.87	–0.11	1.40	49.1	*n*-pentanol
130	MeSBCN	329.0	30394	–0.87	–0.11	2.03	48.8	*n*-hexanol
131	MeSBCN	329.2	30379	–0.87	–0.11	2.34	48.5	*n*-heptanol
132	MeSBCN	329.2	30373	–0.87	–0.11	2.84	48.1	*n*-octanol
133	MeSBCN	327.0	30579	–0.87	–0.11	0.14	48.4	*i*-propanol
134	MeSBCN	327.8	30503	–0.87	–0.11	0.61	48.6	*i*-butanol
135	MeSBCN	327.3	30554	–0.87	–0.11	0.44	47.1	*s*-butanol
136	MeSBCN	326.3	30649	–0.87	–0.11	0.37	43.3	*t*-butanol
137	MeSBCN	328.5	30445	–0.87	–0.11	1.14	46.5	2-pentanol
138	MeSBCN	328.5	30440	–0.87	–0.11	1.14	45.7	3-pentanol
139	HSBCN	319.8	31272	–0.70	0.00	–0.66	55.4	methanol
140	HSBCN	321.5	31108	–0.70	0.00	0.34	50.7	*n*-propanol
141	HSBCN	321.9	31064	–0.70	0.00	0.88	49.7	*n*-butanol
142	HSBCN	322.4	31013	–0.70	0.00	1.40	49.1	*n*-pentanol
143	HSBCN	322.8	30978	–0.70	0.00	2.03	48.8	*n*-hexanol
144	HSBCN	322.9	30969	–0.70	0.00	2.34	48.5	*n*-heptanol
145	HSBCN	323.0	30958	–0.70	0.00	2.84	48.1	*n*-octanol
146	HSBCN	321.0	31156	–0.70	0.00	0.14	48.4	*i*-propanol
147	HSBCN	321.5	31103	–0.70	0.00	0.61	48.6	*i*-butanol
148	HSBCN	321.6	31098	–0.70	0.00	0.44	47.1	*s*-butanol
149	HSBCN	320.4	31209	–0.70	0.00	0.37	43.3	*t*-butanol
150	HSBCN	322.1	31051	–0.70	0.00	1.14	46.5	2-pentanol
151	HSBCN	322.2	31032	–0.70	0.00	1.14	45.7	3-pentanol
152	ClSBCN	323.2	30943	–0.92	0.15	–0.66	55.4	methanol
153	ClSBCN	325.0	30765	–0.92	0.15	0.34	50.7	*n*-propanol
154	ClSBCN	325.7	30702	–0.92	0.15	0.88	49.7	*n*-butanol
155	ClSBCN	326.2	30653	–0.92	0.15	1.40	49.1	*n*-pentanol
156	ClSBCN	326.6	30617	–0.92	0.15	2.03	48.8	*n*-hexanol
157	ClSBCN	326.9	30594	–0.92	0.15	2.34	48.5	*n*-heptanol
158	ClSBCN	326.9	30593	–0.92	0.15	2.84	48.1	*n*-octanol
159	ClSBCN	324.3	30834	–0.92	0.15	0.14	48.4	*i*-propanol
160	ClSBCN	325.4	30730	–0.92	0.15	0.61	48.6	*i*-butanol
161	ClSBCN	325.5	30725	–0.92	0.15	0.44	47.1	*s*-butanol
162	ClSBCN	323.8	30886	–0.92	0.15	0.37	43.3	*t*-butanol
163	ClSBCN	325.9	30683	–0.92	0.15	1.14	46.5	2-pentanol
164	ClSBCN	325.8	30697	–0.92	0.15	1.14	45.7	3-pentanol
165	HSBH	307.0	32570	0.00	0.00	–0.66	55.4	methanol

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No.	Compound (XSBY)	$\lambda_{\max}$	$\nu_{\max}$	$\Sigma\sigma_{CC}^{ex}$ [a]	σ_{XY} [b]	log$P$ [c]	$E_T(30)$ [d]	Solvent
166	HSBH	308.1	32459	0.00	0.00	0.34	50.7	*n*-propanol
167	HSBH	308.4	32423	0.00	0.00	0.88	49.7	*n*-butanol
168	HSBH	308.7	32397	0.00	0.00	1.40	49.1	*n*-pentanol
169	HSBH	309.1	32350	0.00	0.00	2.03	48.8	*n*-hexanol
170	HSBH	309.1	32349	0.00	0.00	2.34	48.5	*n*-heptanol
171	HSBH	309.4	32317	0.00	0.00	2.84	48.1	*n*-octanol
172	HSBH	307.7	32501	0.00	0.00	0.14	48.4	*i*-propanol
173	HSBH	307.9	32480	0.00	0.00	0.61	48.6	*i*-butanol
174	HSBH	307.7	32496	0.00	0.00	0.44	47.1	*s*-butanol
175	HSBH	306.8	32592	0.00	0.00	0.37	43.3	*t*-butanol
176	HSBH	308.3	32433	0.00	0.00	1.14	46.5	2-pentanol
177	HSBH	308.3	32436	0.00	0.00	1.14	45.7	3-pentanol
178	MeSBOMe	320.3	31224	–0.67	0.05	–0.66	55.4	methanol
179	MeSBOMe	321.3	31125	–0.67	0.05	0.34	50.7	*n*-propanol
180	MeSBOMe	321.5	31106	–0.67	0.05	0.88	49.7	*n*-butanol
181	MeSBOMe	321.9	31068	–0.67	0.05	1.40	49.1	*n*-pentanol
182	MeSBOMe	322.2	31034	–0.67	0.05	2.03	48.8	*n*-hexanol
183	MeSBOMe	322.6	31002	–0.67	0.05	2.34	48.5	*n*-heptanol
184	MeSBOMe	323.0	30960	–0.67	0.05	2.84	48.1	*n*-octanol
185	MeSBOMe	320.4	31212	–0.67	0.05	0.14	48.4	*i*-propanol
186	MeSBOMe	321.0	31157	–0.67	0.05	0.61	48.6	*i*-butanol
187	MeSBOMe	321.0	31156	–0.67	0.05	0.44	47.1	*s*-butanol
188	MeSBOMe	319.8	31270	–0.67	0.05	0.37	43.3	*t*-butanol
189	MeSBOMe	321.6	31095	–0.67	0.05	1.14	46.5	2-pentanol
190	MeSBOMe	321.1	31140	–0.67	0.05	1.14	45.7	3-pentanol
191	MeSBH	311.1	32144	–0.17	0.00	–0.66	55.4	methanol
192	MeSBH	312.0	32051	–0.17	0.00	0.34	50.7	*n*-propanol
193	MeSBH	312.3	32020	–0.17	0.00	0.88	49.7	*n*-butanol
194	MeSBH	312.7	31976	–0.17	0.00	1.40	49.1	*n*-pentanol
195	MeSBH	312.9	31964	–0.17	0.00	2.03	48.8	*n*-hexanol
196	MeSBH	313.1	31936	–0.17	0.00	2.34	48.5	*n*-heptanol
197	MeSBH	313.3	31920	–0.17	0.00	2.84	48.1	*n*-octanol
198	MeSBH	311.4	32108	–0.17	0.00	0.14	48.4	*i*-propanol
199	MeSBH	311.8	32073	–0.17	0.00	0.61	48.6	*i*-butanol
200	MeSBH	311.8	32068	–0.17	0.00	0.44	47.1	*s*-butanol
201	MeSBH	310.9	32168	–0.17	0.00	0.37	43.3	*t*-butanol
202	MeSBH	312.1	32036	–0.17	0.00	1.14	46.5	2-pentanol
203	MeSBH	312.1	32037	–0.17	0.00	1.14	45.7	3-pentanol
204	HSBOMe	317.7	31481	–0.50	0.00	–0.66	55.4	methanol
205	HSBOMe	319.0	31349	–0.50	0.00	0.34	50.7	*n*-propanol
206	HSBOMe	319.3	31316	–0.50	0.00	0.88	49.7	*n*-butanol
207	HSBOMe	319.7	31281	–0.50	0.00	1.40	49.1	*n*-pentanol
208	HSBOMe	320.2	31230	–0.50	0.00	2.03	48.8	*n*-hexanol
209	HSBOMe	320.5	31203	–0.50	0.00	2.34	48.5	*n*-heptanol
210	HSBOMe	320.8	31176	–0.50	0.00	2.84	48.1	*n*-octanol
211	HSBOMe	318.3	31416	–0.50	0.00	0.14	48.4	*i*-propanol
212	HSBOMe	318.2	31430	–0.50	0.00	0.61	48.6	*i*-butanol
213	HSBOMe	318.5	31393	–0.50	0.00	0.44	47.1	*s*-butanol
214	HSBOMe	316.7	31573	–0.50	0.00	0.37	43.3	*t*-butanol
215	HSBOMe	319.0	31350	–0.50	0.00	1.14	46.5	2-pentanol
216	HSBOMe	318.5	31396	–0.50	0.00	1.14	45.7	3-pentanol
217	ClSBOMe	322.3	31025	–0.71	–0.06	–0.66	55.4	methanol
218	ClSBOMe	324.0	30862	–0.71	–0.06	0.34	50.7	*n*-propanol
219	ClSBOMe	324.4	30829	–0.71	–0.06	0.88	49.7	*n*-butanol
220	ClSBOMe	324.8	30792	–0.71	–0.06	1.40	49.1	*n*-pentanol

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No.	Compound (XSBY)	λ_{max}	ν_{max}	$\Sigma\sigma_{CC}^{ex}$ a)	σ_{XY} b)	log$P$ c)	$E_T(30)$ d)	Solvent
221	ClSBOMe	325.2	30752	−0.71	−0.06	2.03	48.8	*n*-hexanol
222	ClSBOMe	325.6	30716	−0.71	−0.06	2.34	48.5	*n*-heptanol
223	ClSBOMe	325.9	30685	−0.71	−0.06	2.84	48.1	*n*-octanol
224	ClSBOMe	323.6	30899	−0.71	−0.06	0.14	48.4	*i*-propanol
225	ClSBOMe	323.7	30891	−0.71	−0.06	0.61	48.6	*i*-butanol
226	ClSBOMe	323.9	30875	−0.71	−0.06	0.44	47.1	*s*-butanol
227	ClSBOMe	322.7	30990	−0.71	−0.06	0.37	43.3	*t*-butanol
228	ClSBOMe	324.3	30833	−0.71	−0.06	1.14	46.5	2-pentanol
229	ClSBOMe	324.4	30828	−0.71	−0.06	1.14	45.7	3-pentanol
230	ClSBH	311.7	32079	−0.22	0.00	−0.66	55.4	methanol
231	ClSBH	312.8	31966	−0.22	0.00	0.34	50.7	*n*-propanol
232	ClSBH	313.5	31900	−0.22	0.00	0.88	49.7	*n*-butanol
233	ClSBH	313.9	31858	−0.22	0.00	1.40	49.1	*n*-pentanol
234	ClSBH	313.9	31854	−0.22	0.00	2.03	48.8	*n*-hexanol
235	ClSBH	314.2	31823	−0.22	0.00	2.34	48.5	*n*-heptanol
236	ClSBH	314.4	31809	−0.22	0.00	2.84	48.1	*n*-octanol
237	ClSBH	312.3	32024	−0.22	0.00	0.14	48.4	*i*-propanol
238	ClSBH	312.7	31983	−0.22	0.00	0.61	48.6	*i*-butanol
239	ClSBH	312.5	31998	−0.22	0.00	0.44	47.1	*s*-butanol
240	ClSBH	311.8	32075	−0.22	0.00	0.37	43.3	*t*-butanol
241	ClSBH	312.9	31957	−0.22	0.00	1.14	46.5	2-pentanol
242	ClSBH	313.1	31943	−0.22	0.00	1.14	45.7	3-pentanol

a) The σ_{CC}^{ex} values of substituents NMe_2, OMe, Me, Et, H, F, Cl, and CN are −1.81, −0.50, −0.17, −0.13, 0.00, 0.06, −0.22, and −0.70, respectively, and taken from ref. [16]; b) the σ_p values of substituents NMe_2, OMe, Me, Et, H, F, Cl, and CN are −0.83, −0.27, −0.17, −0.15, 0.00 , 0.06, 0.23, and 0.66, respectively, and taken from ref. [24]; c) the *n*-octanol/water partition coefficient of the solvent, the experimental values are taken from ref. [25]; d) the solvatochromic dye of the solvent, taken from ref. [19].

Table 2 The correlation results of ν_{max} with parameters $\Sigma\sigma_{CC}^{ex}$, $\sigma_{CC}^{ex}(XY)$ and σ_{XY} for XSBY in each solvent

Solvents a)	$\nu_{max}=a+b\sum\sigma_{CC}^{ex}+c\sigma_{CC}^{ex}(XY)$ $\nu_{max}=a'+b'\sum\sigma_{CC}^{ex}+c'\sigma_{XY}$			r	s	F	n
	a a'	b b'	c c'				
C_6H_{12}	32299.71	1967.774	326.388	0.9945	132.12	993.00	25
	32284.33	1917.317	1414.417	0.9973	92.20	2050.57	
Et_2O	32450.05	2034.115	360.9054	0.9939	143.65	985.57	25
	32434.96	1987.815	1292.186	0.9960	116.19	1374.67	
$CHCl_3$	32153.18	2121.298	342.5192	0.9947	139.61	1034.48	25
	32137.20	2068.629	1461.726	0.9973	99.77	2035.87	
CH_3CN	32522.04	2195.636	388.6807	0.9917	180.94	657.75	25
	32504.47	2136.914	1578.166	0.9945	147.45	995.99	
C_2H_5OH	32418.29	2087.889	697.1173	0.9951	130.41	1111.00	25
	32397.20	2001.540	1354.227	0.9965	109.46	1581.48	

a) Fourteen kinds of alcohols are involved in this work, the ethanol is appointed as a representative for regression analysis.

$$\nu_{max}=a'+b'\sum\sigma_{CC}^{ex}+c'\sigma_{XY} \quad (1b)$$

As can be seen from Table 2, although the properties of solvents are different from each other, all the ν_{max} of XSBY in each solvent have good correlations with the parameters $\Sigma\sigma_{CC}^{ex}$ and σ_{XY}. It indicates that the energy of UV absorption max wavelengths of XSBY is mainly affected by their intramolecular structure in a given solvent, that is to say, the ν_{max} is dominated by the excited-state substituent parameter σ_{CC}^{ex} and the ground state polar substituent constant σ_p together.

3.2 The solvent effect on the ν_{max} of XSBY

Actually, the XSBY molecules in a solvent will interact with solvent molecules, and the solute-solvent interactions are different in different kinds of solvents for a given solute. The experimental test results showed that even if the same solute molecule, the UV absorption energy also changes in different solvents. For example, the difference of absorption wavenumbers of $\mathrm{ClSBNMe_2}$ is 536 $\mathrm{cm^{-1}}$ (about 6.9 nm) in the two solvents C_6H_{12} and $CHCl_3$. This means that the solvent effect is very obvious, and can not be neglected. Thus, if we investigate the changing law of the UV absorption energy of XSBY in different kinds of solvents, the solvent effect must be taken into account for. At present, many solvent effect parameters have been proposed, in which the solvatochromic dye $E_T(30)$ [19] attracted the most attention. In this paper, we use the $E_T(30)$ to correlate the 242 experimental $\nu_{\max}$ in Table 1 combining with parameters $\Sigma\sigma_{CC}^{ex}$ and σ_{XY}. See from Table 3, eq. (2) has a good correlation.

What we want to know is that whether the regression results can be improved, if the $E_T(30)$ in eq. (2) was replaced by other parameters. The authors [27] have proposed that the aqueous solubility of non-proton compounds is related to their molecular volume *V*, HOMO energy and LUMO energy, and the HOMO energy and LUMO energy of the water molecule. Because the HOMO energy and LUMO energy of the water molecule are invariable, the aqueous solubility of the solute molecule can be quantified with its *V*, HOMO energy and LUMO energy. Basing on the results of ref. [27], we speculate that the interaction between XSBY molecule and solvent molecule is similar to the interaction between solute molecule and water molecule. That is to say, the interaction of solute molecule and solvent molecule may be related with their HOMO and LUMO. If this hypothesis is correct, and because the HOMO energy and LUMO energy are constants for a given XSBY molecule, the $E_T(30)$ in eq. (2) can be substituted by the aqueous solubility parameters log*P* (*n*-octanol/water partition coefficient). Consequently, the eq. (2) is replaced by eq. (3) (see Table 3). Compared with eq. (2), the correlation of eq. (3) is much better, and its standard error decreases about 15 $\mathrm{cm^{-1}}$. The average absolute error between the experimental $\lambda_{\max}$ and the calculated values of eq. (2) is 1.1 nm, and that of eq. (3) is only 1.0 nm. Seen from Table 4, the numbers of absolute errors of eq. (2) and eq. (3) within 2.0 nm are 199 and 212, and account for 82.24% and 87.61% of the total samples, respectively. The plots of the calculated wavenumbers of eq. (3) against the experimental values are shown in Figure 2.

The variation of $\nu_{\max}$ values in Table 1 is in a wide range. The maximum is 32592 $\mathrm{cm^{-1}}$ (the $\nu_{\max}$ of HSBH in *t*-BuOH), and the minimum is 27692 $\mathrm{cm^{-1}}$ (the $\nu_{\max}$ of $\mathrm{ClSBNMe_2}$ in $CHCl_3$). Their variation is 4900 $\mathrm{cm^{-1}}$ (54.3 nm). In such wide range of wavenumbers, eq. (3) has an excellent correlation. It indicated that the solvent effect on the UV absorption energy of XSBY can be scaled by log*P*. This result may be explained as follows, the authors [25] have proposed the log*P* of the solute can be expressed as eq. (4),

$$\log P = aV + bE_{\mathrm{HOMO}} + cE_{\mathrm{LUMO}} + d \qquad (4)$$

In eq. (4), *a*, *b*, *c*, and *d* are coefficients, *V*, E_{HOMO}, and E_{LUMO} are the volume *V*, the HOMO energy and LUMO energy of the solute molecule. We suspect that the XSBY molecules in a solvent interact with the solvent molecules, that is the HOMO of the XSBY molecule interact with the LUMO of the solvent molecule, and the LUMO of the XSBY molecule interact with the HOMO of the solvent molecule. Thus eq. (5) can be employed to express this solvent effect (S_{solvent}),

$$\begin{aligned} S_{\mathrm{solvent}} &= a(V_{\mathrm{solvent}} - V_{\mathrm{solute}}) + b(E_{\mathrm{HOMO,\ solvent}} - E_{\mathrm{LUMO,\ solute}}) \\ &\quad + c(E_{\mathrm{LUMO,\ solvent}} - E_{\mathrm{HOMO,\ solute}}) \\ &= aV_{\mathrm{solvent}} + bE_{\mathrm{HOMO,\ solvent}} + cE_{\mathrm{LUMO,\ solvent}} \\ &\quad -[aV_{\mathrm{solute}} + bE_{\mathrm{LUMO,\ solute}} + cE_{\mathrm{HOMO,\ solute}}] \end{aligned} \qquad (5)$$

As respect to a given XSBY molecule, its V_{solute}, $E_{\mathrm{HOMO,solute}}$, and $E_{\mathrm{LUMO,solute}}$ are constants. Therefore, the last item of eq. (5) can be replaced by a coefficient *d*. So eq. (5) can be modified as eq. (4). In addition, it is generally believed that the molecular volume is related to its polarizability. Therefore, the bigger the molecular volume is, the larger the polarizability effect is, and the larger the stabilization effect on the charge is. The log*P* can be used to scale the solvent effect on the UV absorption energy of XSBY, because it expressed the electronic effect between XSBY molecules and solvent molecules. This electronic effect includes the interaction of their frontier orbitals, and the polarizability effect of solvent molecule on the solute molecule. If the solute molecule is variable, the last item of eq. (5) (the contents in the square brackets is no longer a constant. Thus, the molecular properties (such as substituent effect) of XSBY must be considered.

Eq. (3) expressed the changing law of the energy of UV absorption max wavelengths for a series of XSBY molecule in different kinds of solvents, and can be used to calculate and predict the energy of UV absorption max wavelengths of this kind of compounds. For instance, Jiang *et al.* [28] has synthesized compounds of Table 5 and measured their energy of UV absorption max wavelengths $\lambda_{\max}$ in 95% ethanol. If the log*P* of 95% ethanol is approximated as that of pure ethanol, the $\lambda_{\max}$ of these compounds can be predicted with eq. (3). The predicated $\lambda_{\max}$ are in agreement with the experimental values (see Table 5). Here, it should be pointed out that the log*P* of pure ethanol is not equal to that of 95% ethanol, so the result listed in Table 5 is only an approximation.

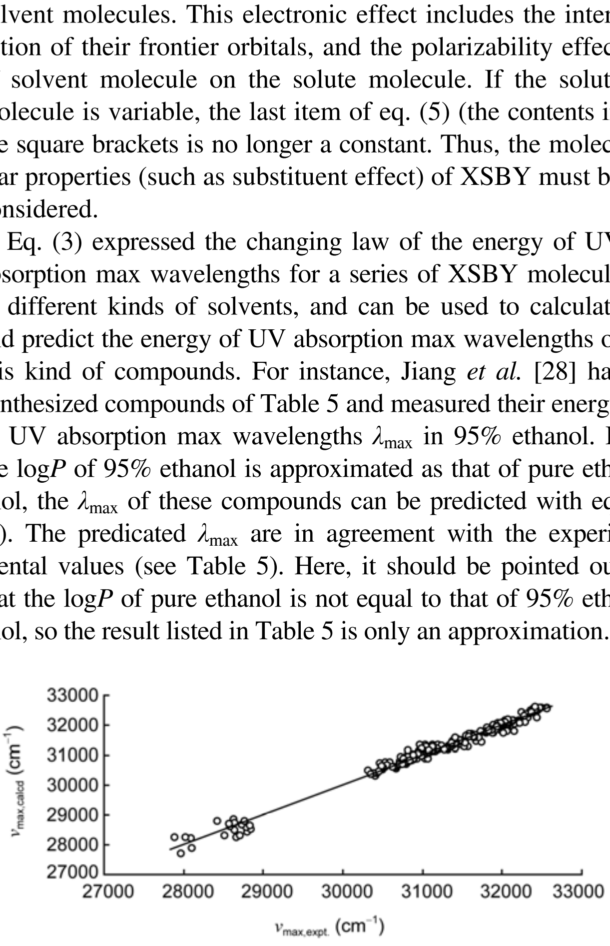

Figure 2 Plot of $\nu_{\mathrm{max,\ expt}}$ versus $\nu_{\mathrm{max,\ calcd}}$ for XSBY ($\mathrm{cm^{-1}}$).

Table 3 The correlation results of $\nu_{\max}$ with parameters $\Sigma\sigma_{CC}^{ex}$, σ_{XY} and solvent parameters for XSBY in different solvents

Correlation equations	*r*	*s*	*F*	*n*	Equation number
$\nu_{\max} = 32205.42 + 2025.391\sum\sigma_{CC}^{ex} + 1354.673\sigma_{XY} + 3.907419E_T(30)$	0.9900	143.57	3930.81	242	(2)
$\nu_{\max} = 32440.19 + 2027.815\sum\sigma_{CC}^{ex} + 1358.551\sigma_{XY} - 56.4827\log P$	0.9920	128.61	4917.70	242	(3)

Table 4 The absolute deviation ranges of the experimental and the calculated values of the wavelengths $\lambda_{\max}$ of UV absorption maximum for XSBY

Deviation ranges (nm)	0–⩽1.0	>1.0–⩽2.0	>2.0–⩽3.0	>3.0–⩽4.0	>4.0–⩽5.0	>5.0–⩽6.0
Frequency: Eq. (2)	129	70	25	12	4	2
Eq. (3)	157	55	16	9	4	1
Ratio (%): Eq. (2)	53.31	28.93	9.92	5.79	1.24	0.83
Eq. (3)	64.88	22.73	6.61	3.72	1.65	0.41

Table 5 The experimental and the predicted values of the wavelengths $\lambda_{\max}$ (nm) of UV absorption maximum for XSBSO$_2$Me

Compounds [a)]	$\lambda_{\max,expt.}$ [b)]	σ_{CC}^{ex} (X)	σ_{CC}^{ex} (Y)	$\lambda_{\max, pred.}$ [c)]	Δ [d)]
Me$_2$NSBSO$_2$Me	376.7	−1.81	−0.43	369.0	7.7
MeOSBSO$_2$Me	332.0	−0.5	−0.43	329.9	2.1
MeSBSO$_2$Me	323.1	−0.17	−0.43	321.8	1.3
HSBSO$_2$Me	316.0	0.00	−0.43	316.6	−0.6
ClSBSO$_2$Me	320.3	−0.22	−0.43	318.8	1.5
BrSBSO$_2$Me	321.3	−0.33	−0.43	321.1	0.2

a) The σ_p values of substituents Me$_2$N, MeO, Me, H, Cl, Br, and SO$_2$Me are −0.83, −0.27, −0.17, 0.00, 0.23, 0.23, and 0.72, and taken from ref. [24]; b) the experimental values are taken from ref. [28], and determined in 95% ethanol; c) predicted with eq. (3); d) $\Delta = \lambda_{\max,\ expt} - \lambda_{\max,\ pred}$.

4 Conclusion

In a given solvent, the energy of UV absorption max wavelengths of 4,4'-disubstituted stilbenes derivatives is mainly affected by the intramolecular structure, that is the excited-state substituent parameter σ_{CC}^{ex} and the ground state polar substituent constant σ_p of substituents X and Y. While in different kinds of solvents, such as cyclohexane, ether, chloroform, acetonitrile and ethanol, the solvent effect is also an important factor influencing the UV absorption energy. The statistical results of Table 4 indicated that the log*P* is a more effective parameter than the $E_T(30)$ in quantifying the solvent effect. Furthermore, the regression model employed log*P* has a more specific physical meaning. Eq. (3) shows the changing law of the UV absorption energy of 4,4'-disubstituted stilbenes derivatives are affected by substituent effect and solvent effect, and may have further applications of the optical property prediction and molecular design for this kind of compounds. Whereas, whether the parameter log*P* can be used to scale the solvent effect on the UV absorption energy for other organic compounds requires further research.

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