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An attempt of molecular design and synthesis of 3,4'/4,3'-disubstituted benzylideneanilines with specified UV–Vis absorption maximum wavelength

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Thirty-one samples of 3,4'/4,3'-disubstituted benzylideneanilines (XBAY) with specified UV–Vis absorption maximum wavelength (λ_{max}) were designed and synthesized by applying the equation (Eqn (1)) which was abstracted from the UV–Vis absorption maximum wavelength energy ($v_{max} = 1/\lambda_{max}$) of 4,4'-disubstituted benzylideneanilines. Then, the UV–Vis data (λ_{max}) of the designed compounds were measured in anhydrous ethanol. The predicted UV–Vis data of designed compounds are in agreement with the experimental ones, in which the mean absolute error is 2.9 nm. The results show that Eqn (1) is applicative for the prediction of UV–Vis absorption λ_{max} values of both 4,4'-disubstituted benzylideneanilines and 3,4'/4,3'-disubstituted benzylideneanilines. For a same pair of groups (X and Y), one can at least get four disubstituted benzylideneaniline compounds which have different λ_{max} values. It perhaps provides a convenient method to design an optical material for benzylideneaniline compounds. Copyright © 2014 John Wiley & Sons, Ltd.

Keywords: disubstituted benzylideneaniline; UV spectrum; molecular design; synthesis

INTRODUCTION

In recent years, optoelectronic materials have attracted extensive attention as a new type of function material. In the field of optoelectronic materials, the liquid crystal and nonlinear optical (NLO) material are the hot topics and have been studied deeply, which involve inorganic materials and organic materials.^[1-3] Compared with inorganic materials, organic materials have vaster application prospects because their molecules are easy to be designed and assembled. Some organic compounds containing classical π conjugate system are applied well in many fields of optical function materials due to their potential optoelectronic properties.^[4–7] The benzylideneanilines are a kind of typical compounds that have π conjugate system; their polymers and coordination compounds are important optical functional compounds and have been applied extensively in the fields of liquid crystal and NLO material.^[3,8–10] For example, Ramamurthi^[11,12] et al. have made many linear and nonlinear studies deeply about the compounds of 4-bromo-4'-chloro benzylideneaniline and 4-bromo-4'-dimethylamino benzylideneaniline, and attained meaningful results. The previous studies of benzylideneanilines mostly focus on the synthesis, photoelectric performance and guantitative molecular structure-performance relationship.^[10,13–15] As we know, luminescent materials and filters have particularly a close connection to their UV-Vis absorption maximum wavelength energy; if a designed optoelectronic material can be put into a practical application, its molecular UV-Vis absorption maximum wavelength energy (vmax) must be predicted accurately in advance. Therefore, to design and synthesize a series of target compounds with the specified UV-Vis absorption v_{max} values is a key and an important work for getting the optoelectronic materials with the desired performance.

In our previous research,^[15–20] the excited-state substituent constants have been proposed to quantify the influence of substituent on the UV–Vis absorption v_{max} values and were applied successfully in quantifying the UV–Vis absorption v_{max} values of compounds, such as XPh, XPhY, XPh(CH = CH)_nPhY (n = 0, 1, 2), XPhCH = NPhY and XPh(CH = CHPh)_nY (n = 0, 1, 2). Moreover, a general equation of quantifying the UV–Vis absorption v_{max} values of 4,4'-disubstituted benzylideneanilines (XBAY) has been proposed,^[15] which is rewritten as shown in Eqn (1).

$$v_{\text{max}} = 32119.79 - 718.51\sigma(X) + 1197.18\sigma(Y) - 1017.23\Delta\sigma^{2} + 1632.49\sum \sigma_{cc}^{ex} - 229.53\Delta\sigma_{cc}^{ex2}$$
(1)

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Key Laboratory of Theoretical Organic Chemistry and Function Molecule (Hunan University of Science and Technology), Ministry of Education, Hunan Provincial University Key Laboratory of QSAR/QSPR, Hunan University of Science and Technology, Xiangtan 411201, China In Eqn (1): σ is the Hammett constant;

 σ_{CC}^{ex} is the excited-state substituent constant;

$$\Delta \sigma^{2} = [\sigma(X) - \sigma(Y)]^{2};$$

$$\sum \sigma_{CC}^{ex} = \sigma_{CC}^{ex}(X) + \sigma_{CC}^{ex}(Y);$$

$$\Delta \sigma_{CC}^{ex}{}^{2} = [\sigma_{CC}^{ex}(X) - \sigma_{CC}^{ex}(Y)]^{2}$$

It can be seen that the UV–Vis absorption v_{max} values of compounds XBAY can be calculated only known of the σ and σ_{CC}^{ex} constants.^[17,18,21] Therefore, we try to employ Eqn (1) to design benzylideneanilines with the given UV–Vis absorption v_{max} values. First, to calculate the UV–Vis absorption v_{max} values of titled compounds, then to synthesis these compounds and determine their UV–Vis absorption λ_{max} values ($\lambda_{max} = 1/v_{max}$). In this work, a meaningful result was attained by comparing the predicted values and the experimental ones.

MOLECULAR DESIGN

Equation (1) was extracted from the UV–Vis absorption v_{max} values of 72 samples of 4,4'-disubstituted benzylideneanilines, together with the corresponding σ and σ_{CC}^{ex} constants of parasubstituents.^[15] Also, its accuracy of predicting UV–Vis absorption v_{max} values of 4,4'-disubstitued benzylideneanilines has been

$$X$$
 - CHO + H₂N - X - Solvent-free X - = N - X

$$\begin{split} & X = m \text{-} F, \quad Y = p \text{-} \text{Me}_2 \text{N}, p \text{-} \text{Me} \text{O}, p \text{-} \text{Me}, p \text{-} \text{Cl}. \\ & X = m \text{-} \text{Br}, \quad Y = p \text{-} \text{Me}_2 \text{N}, p \text{-} \text{Me} \text{O}, p \text{-} \text{Cl}, p \text{-} \text{C}, p \text{-} \text{F}. \\ & X = m \text{-} \text{Me} \text{O}, \quad Y = p \text{-} \text{Me}_2 \text{N}. \\ & Y = m \text{-} \text{Me}, \quad X = p \text{-} \text{Me}_2 \text{N}, p \text{-} \text{Me} \text{O}, p \text{-} \text{Cl}, p \text{-} \text{C} \text{N}, p \text{-} \text{NO}_2. \\ & Y = m \text{-} \text{F}, \quad X = p \text{-} \text{Me}_2 \text{N}, p \text{-} \text{Me} \text{O}, p \text{-} \text{Me}, p \text{-} \text{Cl}, p \text{-} \text{C} \text{N}, p \text{-} \text{NO}_2. \\ & Y = m \text{-} \text{Br}, \quad X = p \text{-} \text{Me}_2 \text{N}, p \text{-} \text{Me} \text{O}, p \text{-} \text{Me}, p \text{-} \text{Cl}, p \text{-} \text{CN}, p \text{-} \text{NO}_2. \\ & Y = m \text{-} \text{Me} \text{O}, \quad X = p \text{-} \text{Me}_2 \text{N}, p \text{-} \text{CN}, p \text{-} \text{NO}_2. \end{split}$$

Scheme 1. The synthesis of samples of XBAYs

Table 1. compour	The predicted U nds	V–Vis absorption	maximum wavele	ngth energy (v _{max}	_x) and substitue	nt constants va	lues for the designed
No.	Х	Y	$\sigma_{\rm CC}^{\rm ex}({\rm X})~^{\rm a}$	$\sigma_{CC}^{e\!x}(Y)~^{\rm a}$	$\sigma(X)^{b}$	$\sigma(Y)^{b}$	$\nu_{max.pred.}(cm^{-1})^{c}$
1	<i>m</i> -F	<i>p</i> -Me ₂ N	0.02	-1.81	0.34	-0.83	25 799
2	<i>m</i> -F	<i>p</i> -MeO	0.02	-0.50	0.34	-0.27	30 328
3	<i>m</i> -F	<i>p</i> -Me	0.02	-0.17	0.34	-0.17	31 154
4	<i>m</i> -F	<i>p</i> -Cl	0.02	-0.22	0.34	0.23	31 799
5	<i>m</i> -Br	<i>p</i> -Me ₂ N	-0.03	-1.81	0.39	-0.83	25 601
6	<i>m</i> -Br	<i>p</i> -MeO	-0.03	-0.50	0.39	-0.27	30 157
7	<i>m</i> -Br	<i>p</i> -Me	-0.03	-0.17	0.39	-0.17	30 986
8	<i>m</i> -Br	<i>p</i> -F	-0.03	0.06	0.39	0.06	31 848
9	<i>m</i> -Br	p-Cl	-0.03	-0.22	0.39	0.23	31 672
10	<i>m</i> -MeO	<i>p</i> -Me ₂ N	0.10	-1.81	0.12	-0.83	26 493
11	<i>p</i> -Me ₂ N	<i>m</i> -Me	-1.81	-0.03	-0.83	-0.07	28 3 1 4
12	<i>p</i> -MeO	<i>m</i> -Me	-0.50	-0.03	-0.27	-0.07	31 273
13	p-Cl	<i>m</i> -Me	-0.22	-0.03	0.23	-0.07	31 363
14	p-CF₃	<i>m</i> -Me	-0.12	-0.03	0.54	-0.07	31 023
15	<i>p</i> -CN	<i>m</i> -Me	-0.70	-0.03	0.66	-0.07	29 725
16	$p-NO_2$	<i>m</i> -Me	-1.17	-0.03	0.78	-0.07	28 483
17	<i>p</i> -Me ₂ N	<i>m</i> -F	-1.81	0.02	-0.83	0.34	28 040
18	<i>p</i> -MeO	<i>m</i> -F	-0.50	0.02	-0.27	0.34	31 497
19	<i>p</i> -Me	<i>m</i> -F	-0.17	0.02	-0.17	0.34	32 131
20	p-Cl	<i>m</i> -F	-0.22	0.02	0.23	0.34	32 010
21	<i>p</i> -CN	<i>m</i> -F	-0.70	0.02	0.66	0.34	30 7 1 9
22	p-NO ₂	<i>m</i> -F	-1.17	0.02	0.78	0.34	29 567
23	<i>p</i> -Me ₂ N	<i>m</i> -Br	-1.81	-0.03	-0.83	0.39	27 938
24	<i>p</i> -MeO	<i>m</i> -Br	-0.50	-0.03	-0.27	0.39	31 422
25	<i>p</i> -Me	<i>m</i> -Br	-0.17	-0.03	-0.17	0.39	32 059
26	p-Cl	<i>m</i> -Br	-0.22	-0.03	0.23	0.39	31 979
27	<i>p</i> -CN	<i>m</i> -Br	-0.70	-0.03	0.66	0.39	30 744
28	$p-NO_2$	<i>m</i> -Br	-1.17	-0.03	0.78	0.39	29614
29	<i>p</i> -Me ₂ N	<i>m</i> -MeO	-1.81	0.10	-0.83	0.12	28 313
30	p-CN	<i>m</i> -MeO	-0.70	0.10	0.66	0.12	30 366
31	p-NO ₂	<i>m</i> -MeO	-1.17	0.10	0.78	0.12	29 1 4 3

^aFor *p*- or *m*-substituent, the σ_{CC}^{ex} is the $\sigma_{CC}^{ex}(p)$ or $\sigma_{CC}^{ex}(m)$, respectively.

^bFor *p*- or *m*-substituent, the σ is the σ_p or σ_m , respectively.

 $^{c}v_{max} = 1/\lambda_{max}$.

Table 2.	The predicted	The predicted UV–Vis data and experimental ones of the designed compounds					
No.	Х	Y	$\lambda_{max.pred.}(nm)^a$	$\nu_{max.pred.}(cm^{-1})^a$	$\lambda_{max.expt.}(nm)^b$	$\nu_{max.expt.}(cm^{-1})^b$	
1	<i>m</i> -F	<i>p</i> -Me ₂ N	387.6	25 799	385.4	25 946	
2	<i>m</i> -F	<i>p</i> -MeO	329.7	30 328	337.0	29676	
3	<i>m</i> -F	<i>p</i> -Me	321.0	31 154	321.3	31 128	
4	<i>m</i> -F	p-Cl	314.5	31 799	314.4	31 809	
5	<i>m</i> -Br	<i>p</i> -Me ₂ N	390.6	25 601	388.5	25739	
6	<i>m</i> -Br	<i>p</i> -MeO	331.6	30 157	338.6	29 531	
7	<i>m</i> -Br	<i>p</i> -Me	322.7	30 986	323.4	30 921	
8	<i>m</i> -Br	<i>p</i> -F	314.0	31 848	312.2	32 0 33	
9	<i>m</i> -Br	p-Cl	315.7	31 672	317.2	31 528	
10	<i>m</i> -MeO	<i>p</i> -Me ₂ N	377.5	26 493	379.5	26 350	
11	<i>p</i> -Me ₂ N	<i>m</i> -Me	353.2	28 314	356.9	28 0 20	
12	<i>p</i> -MeO	<i>m</i> -Me	319.8	31 273	314.8	31 765	
13	p-Cl	<i>m</i> -Me	318.9	31 363	316.2	31 631	
14	p-CF ₃	<i>m</i> -Me	322.3	31 023	321.2	31 135	
15	<i>p</i> -CN	<i>m</i> -Me	336.4	29725	330.5	30 254	
16	$p-NO_2$	<i>m</i> -Me	351.1	28 483	349.5	28 609	
17	<i>p</i> -Me ₂ N	<i>m</i> -F	356.6	28 040	349.9	28 582	
18	<i>p</i> -MeO	<i>m</i> -F	317.5	31 497	318.4	31 410	
19	<i>p</i> -Me	<i>m</i> -F	311.2	32 131	313.4	31 906	
20	p-Cl	<i>m</i> -F	312.4	32 010	310.5	32 205	
21	<i>p</i> -CN	<i>m</i> -F	325.5	30 719	323.6	30 907	
22	$p-NO_2$	<i>m</i> -F	338.2	29 567	340.3	29 388	
23	<i>p</i> -Me ₂ N	<i>m</i> -Br	357.9	27 938	360.5	27 738	
24	<i>p</i> -MeO	<i>m</i> -Br	318.3	31 422	315.2	31 722	
25	<i>p</i> -Me	<i>m</i> -Br	311.9	32 059	312.3	32017	
26	p-Cl	<i>m</i> -Br	312.7	31 979	321.5	31 103	
27	<i>p</i> -CN	<i>m</i> -Br	325.3	30 744	327.5	30 532	
28	$p-NO_2$	<i>m</i> -Br	337.7	29614	339.4	29 465	
29	<i>p</i> -Me ₂ N	<i>m</i> -MeO	353.2	28 313	353.3	28 301	
30	<i>p</i> -CN	<i>m</i> -MeO	329.3	30 366	335.2	29830	
31	p-NO ₂	<i>m</i> -MeO	343.1	29 143	348.4	28 702	

 $^{a}\lambda_{max,pred}$ is the predicted UV–Vis absorption maximum wavelength of the target compounds, $\nu_{max,pred} = 1/\lambda_{max,pred}$. $^{b}\lambda_{max,expt}$ is the experimental UV–Vis absorption maximum wavelength of the target compounds, $\nu_{max,expt} = 1/\lambda_{max,expt}$.



of 3,4'/4,3'-disubstituted benzylideneanilines by using Eqn (1). Compared with the molecular structure of 4,4'-disubstituted benzylideneanilines, we think, the 3,4'/4,3'-disubstituted benzylideneanilines should have different UV–Vis absorption v_{max} values. Therefore, if we can design some 3,4'/4,3'-disubstituted benzylideneanilines, we will get some compounds with different UV–Vis v_{max} values from the corresponding 4,4'-disubstituted benzylideneanilines. In this work, the Hammett constants σ (para/meta-substituent) and the excited-state substituent constants σ_{ex}^{ex} (para/meta-substituent) are employed, and then we use Eqn (1) to pre-

Figure 1. The plot of the predicted UV–Vis absorption maximum wavelengths (λ_{max}) versus the experimental ones for the compounds of Table 2

verified. At that time, there were no $\sigma_{cc(m)}^{ex}$ values of metasubstituent so that the prediction of UV–Vis absorption v_{max} values of the meta-substituted benzylideneanilines couldn't be carried out. Recently, Cao^[18] et al. proposed excited-state substituent constants $\sigma_{cc(m)}^{ex}$ values for several meta-substituents, which makes it possible to calculate the UV–Vis absorption v_{max} values

Table 3. The absolute error distribution						
Range of absolute errors in nm Number of compounds	0–3.0 22	3.1–6.0 5	6.1–9.0			
from Table 2	22	5	т			



Figure 2. Plot of the predicted wavelength versus the experimental ones of 103 samples of XBAY (the symbol 'o' represents the 31 samples of this work, and the ' Δ ' represents the 72 samples of 4,4'-disubstituted benzylideneanilines in reference [15])

values are in range of 22 612 to 32 444 cm⁻¹, that is λ_{max} from 442.2 to 308.2 nm (the gap is 134 nm).

Combining the 31 samples of this work in Table 2 and the 72 samples of 4,4'-disubstitued benzylideneanilines reported by Chen^[15] into one data set (103 samples of compounds), we plot their predicted wavelength ($\lambda_{max,pred}$) versus the experimental ones ($\lambda_{max,expt}$), and got Fig. 2.

As seen from Fig. 2, the UV–Vis absorption λ_{max} values of the designed 3,4'/4,3'-disubstituted benzylideneanilines in this work fall on the trend line of the UV–Vis absorption λ_{max} values of 4,4'-disubstituted benzylideneanilines accurately. It means that Eqn (1) is feasible to

No. X Y $\lambda_{max.expt.}(nm)$ No. X	Y λ _{max.expt.} (nm)
1 p-F p-Me 317.4 3 p-F m-F p-Me 321.3 m-F p-Me p-F 311.3 p-Me p-Me m-F 313.4 p-Me p-Me m-F 313.4 p-Me 2 p-MeO p-Me_2N 370.0 4 p-F m-MeO p-Me_2N 379.5 m-F p-Me p-Me_2N p-MeO 359.7 p-Me p-Me	p-Me2N 374.6 p-Me2N 385.4 2N p-F 356.7 2N m-F 349.9 p-MeO 330.1 p-MeO 337.0 O p-F 314.9 O m-F 318.4

dict the UV–Vis absorption v_{max} values of the 3,4'/4,3'-disubstituted benzylideneanilines, including 31 samples of target compounds in all, as shown in Scheme 1. The substituents in the designed benzylideneanilines are of electron-withdrawing substituents (e.g. NO₂, CN) and electron-donating substituents (e.g. NMe₂, OMe). The predicted UV–Vis absorption v_{max} values of target compounds were listed in Table 1.

RESULTS AND DISCUSSIONS

The predicted UV–Vis absorption v_{max} values of 31 samples in Table 1 are in range of 25 601 to 32 131 cm⁻¹, that is λ_{max} from 390.6 to 311.2 nm. In order to test the reliability of the predicted values, these 31 designed samples of Table 1 were synthesized, and also their UV–Vis absorption maximum wavelengths ($\lambda_{max.expt}$) in ethanol were determined, which were listed in Table 2.

Using the predicted UV–Vis absorption v_{max} values, we can calculate their corresponding UV–Vis absorption λ_{max} values ($\lambda_{max} = 1/v_{max}$). Figure 1 is the plot of $\lambda_{max,pred}$ versus $\lambda_{max,expt}$.

Table 2 and Fig. 1 show that the predicted values ($\lambda_{max,pred.}$) are in agreement with the experimental values ($\lambda_{max,expt.}$). The mean absolute error between the predicted values and the experimental ones is 2.9 nm.

Among the absolute errors, the minimum is 0.1 nm, and the maximum is 8.8 nm. The absolute error distribution can be seen in Table 3. Although the absolute errors of several compounds are somewhat large, the predicted data and the experimental data coincide well as a whole.

In our reported work,^[15] the UV–Vis absorption ν_{max} values of 72 samples of 4,4'-disubstitued benzylideneanilines were used to establish the model Eqn (1), in which the UV–Vis absorption ν_{max}

make a molecule design of 3,4'/4,3'-disubstituted benzylideneanilines with specified UV–Vis absorption λ_{max} values.

Further, comparing the designed 3,4'/4,3'-disubstituted benzylideneaniline molecules with the corresponding 4,4'-disubstitued benzylideneaniline molecules, their difference of UV–Vis maximum wavelength ($\lambda_{max.expt}$) can be observed. Some pairs of molecules were listed in Table 4. The results of Table 4 show us that one can use a pair of groups (X and Y) to design disubstituted benzylideneanilines with different λ_{max} values, for example, Me₂N and MeO, the λ_{max} values are four cases (353.3, 359.7, 370.0 and 379.5 nm) as they are in *p*- or *m*-position respectively, in which the $\Delta\lambda_{max}$ is about 26 nm. For the pair of F and Me₂N, the $\Delta\lambda_{max}$ is about 35 nm. Generally, the $\Delta\lambda_{max}$ increases as the $|\sigma(X) - \sigma(Y)|$ value increases. It provides us a convenient method to obtain the disubstituted benzylideneanilines which have different λ_{max} values in optical materials.

CONCLUSIONS

The model Eqn (1) derived from 4,4'-disubstituted benzylideneanilines is also suitable for predicting the UV–Vis absorption v_{max} values of 3,4'/4,3'-disubstituted benzylideneanilines. The predicted wavelength values accord with the experimental ones well despite the UV–Vis absorption λ_{max} values of the interested compounds distribute in a large range. Equation (1) is of great theoretical significance in guiding the design and synthesis of optoelectronic material which contains aromatic Schiff base molecules. And for the disubstituted benzylideneanilines with a same pair of groups (X and Y), we can attain the molecules with different UV–Vis absorption λ_{max} values just as the position of the substituents changes, and their $\Delta\lambda_{max}$ increases as the $|\sigma(X) - \sigma(Y)|$ value increases. Whether Eqn (1) is applicative or not for the molecular design of 3,3'-disubstituted benzylideneanilines needs to be further investigated.

DATASET

The substituted benzylideneanilines were all synthesized with the solvent-free method shown in Scheme 1.^[22,23] They were purified with anhydrous alcohol and were confirmed with ¹H-NMR and ¹³C-NMR. All UV–Vis spectra of the target compounds were measured in anhydrous ethanol, and the obtained absorption v_{max} values were listed in Table 2. The detailed data of the synthesized compounds are available in the Supporting Information.

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