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

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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  $\sigma_{cc}^{ex}$  and polar substituent constant  $\sigma_p$ . 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 ( $E_T(30)$ ) 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

## 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 indepth 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  $\sigma_{\rm CC}^{\rm ex}$  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  $\sigma_{\rm CC}^{\rm ex}\,$  of substituents X and Y and the interaction between

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substituents X and Y,  $\sigma_{CC}^{ex}$  (X)  $\sigma_{CC}^{ex}$  (Y), in which the correlation result using parameter  $\sigma_{CC}^{ex}$  is better than that of using polar substituent constant  $\sigma^x$  or spin-delocalization substituent constant  $\sigma^i$  [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<sub>4</sub>. 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



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

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.

#### **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 $V_{max}$ 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  $\sigma_{CC}^{ex}$  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  $\Sigma \sigma_{CC}^{ex}$  and  $\sigma_{CC}^{ex}(XY)$ . Here  $\Sigma \sigma_{CC}^{ex}$  is the sum of  $\sigma_{CC}^{ex}(X)$  and  $\sigma_{CC}^{ex}(Y)$ , viz.  $\Sigma \sigma_{CC}^{ex} = \sigma_{CC}^{ex}(X) + \sigma_{CC}^{ex}(Y)$ .  $\sigma_{CC}^{ex}(XY)$  indicates the interaction between substituents X and Y, that is  $\sigma_{CC}^{ex}(XY) = \sigma_{CC}^{ex}(X) \times \sigma_{CC}^{ex}(Y)$ .

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

The experimental  $\nu_{\text{max}}$  measured in each solvent (cyclohexane, ether, chloroform, acetonitrile and ethanol) were correlated with parameters  $\Sigma \sigma_{\text{CC}}^{\text{ex}}$  and  $\sigma_{\text{CC}}^{\text{ex}}(XY)$  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 ( $\sigma_{\text{XY}}$ ) to the energy can be expressed with the product of their electronic effect constants (Hammett constant), viz.  $\sigma_{\text{XY}} = \sigma_{\text{p}}(X)$  $\times \sigma_{\text{p}}(Y)$ . Thus the  $\sigma_{\text{CC}}^{\text{ex}}(XY)$  in eq. (1a) is replaced by the  $\sigma_{\text{XY}}$  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  $\lambda_{max}$  (nm) and wavenumbers  $v_{max}$  (cm<sup>-1</sup>) of UV absorption maximum of XSBY in different solvents

No.	Compound (XSBY)	$\lambda_{ m max}$	$V_{\rm max}$	$\Sigma \sigma^{ m ex~a)}_{ m CC}$	$\sigma_{_{ m XY}}{}^{_{ m b)}}$	$\log P^{(c)}$	$E_{\rm T}(30)^{\rm d}$	Solvent
1	MeSBNMe <sub>2</sub>	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 <sub>2</sub>	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	HSBC1	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 <sub>2</sub>	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	FSBCI	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	CISBNMe <sub>2</sub>	358.9	27864	-2.02	-0.19	-0.34	45.6	acetonitrile
22	CISBOMe	322.7	30991	-0.71	-0.06	-0.34	45.6	acetonitrile
23	CISBEt	315.9	31657	-0.35	-0.03	-0.34	45.6	acetonitrile
24	CISBCI	315.8	31664	-0.43	0.05	-0.34	45.6	acetonitrile
25	CISBCN	322.9	30973	-0.92	0.15	-0.34	45.6	acetonitrile
26	MeSBNMe <sub>2</sub>	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	HSBNMea	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	32250	0.06	0.00	1.97	39.1	chloroform
39	HSBCI	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
40	FSBNMe	353.3	28308	-1.75	-0.05	1.97	39.1	chloroform
42	FSBOMe	320.4	31211	-0.44	-0.03	1.97	39.1	chloroform
43	FSRFt	314.6	31789	-0.08	-0.02	1.97	39.1	chloroform
43	FSBCI	315.1	31731	-0.16	0.01	1.97	30.1	chloroform
45	FSBCN	373.7	30801	0.65	0.01	1.97	30.1	chloroform
46	CISBNMe.	361.1	27602	-0.05	0.19	1.97	30.1	chloroform
40	CISBOMe	325.0	30685	-2.02	-0.19	1.97	30.1	chloroform
+/ /2	CISEFt	310.8	31260	-0.71	-0.00	1.77	30.1	chloroform
+0 40	CISDEL	319.0	31209	-0.55	-0.03	1.97	39.1	chloroform
49 50	CISPCN	217.9	31202	-0.45	0.05	1.97	39.1	chloroform
51	MASENIMA	3475	20242 28776	-0.92	0.13	2.44	37.1	cuclobayana
50	MaSBOMa	221 5	20//0	-1.98	0.14	3.44 2.44	20.9	cyclohexalle
52	MasdMa	321.3 215 F	21400	-0.6/	0.05	3.44 2.44	30.9	cyclonexane
23 54	Masdivie	313.3 215 7	21672	-0.34	0.03	3.44 2.44	30.9	cyclonexane
54 57	MESBEI	515./ 212.4	22011	-0.30	0.03	3.44 2.44	30.9	cyclonexane
22	Mesbh	512.4	32011	-0.1/	0.00	3.44	30.9	cyclonexane

								(Continued)
No.	Compound (XSBY)	$\lambda_{ m max}$	$V_{\rm max}$	$\Sigma \sigma^{ m ex~a)}_{ m CC}$	$\sigma_{_{ m XY}}{}^{^{ m b)}}$	$\log P^{(c)}$	$E_{\rm T}(30)^{\rm d}$	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 <sub>2</sub>	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	HSBC1	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 <sub>2</sub>	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	CISBNMe <sub>2</sub>	354.3	28228	-2.02	-0.19	3.44	30.9	cyclohexane
72	CISBOMe	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	CISBCI	317.9	31453	-0.43	0.05	3.44	30.9	cyclohexane
75	CISBCN	325.0	30766	-0.92	0.15	3.44	30.9	cyclohexane
76	MeSBNMe <sub>2</sub>	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 <sub>2</sub>	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 <sub>2</sub>	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	FSBCI	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	CISBNMe <sub>2</sub>	354.3	28225	-2.02	-0.19	-0.31	51.9	ethanol
97	CISBOMe	323.8	30883	-0.71	-0.06	-0.31	51.9	
98	CISBEt	316.7	31580	-0.35	-0.03	-0.31	51.9	ethanol
99	CISBCI	316.7	31576	-0.43	0.05	-0.31	51.9	ethanol
100	CISBCN	324.1	30855	-0.92	0.15	-0.31	51.9	ethanoi
101	MeSBNMe <sub>2</sub>	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
105	Masder	314.3 314.6	21700	-0.34	0.03	0.89	54.5 24 5	ether
104	Mesbel	211.0	22128	-0.30	0.03	0.89	34.3 24.5	ether
105	Mesbe	511.2 211.1	32138	-0.17	0.00	0.89	54.5 24.5	ether
100	Masdr	316.0	32139	-0.12	-0.01	0.89	54.5 24 5	ether
107	Mesbel	215.0	310 <del>4</del> 9 30720	-0.39	-0.04	0.89	54.5 24.5	ether
108	INCODUM-	523.5 248.0	30/39 20450	-0.8/	-0.11	0.89	54.5 24.5	ether
109	HSBNMe <sub>2</sub>	218.0	28038	-1.81	0.00	0.89	54.5 24.5	ether
110	пъвоме	518.0	31442	-0.50	0.00	0.89	34.3	etner

No.         Compound (SSBY) $A_{vac}$ $\nu_{vac}$ $2\sigma_{c}^{c}$ <sup>-0</sup> $\tau_{c}$ $t_{c}$ $\theta_{c}$ $\theta_{c$									(Continued)
111         HSBH         311.5         32101         -0.13         0.00         0.89         34.5         ether           112         HSBF         307.3         32540         0.00         0.00         0.89         34.5         ether           113         HSBF         307.3         32570         0.06         0.00         0.89         34.5         ether           115         HSBCN         310.2         31326         -0.70         0.00         0.89         34.5         ether           116         ISBNMe:         347.3         28777         -1.75         -0.02         0.09         34.5         ether           117         ISBUMe         311.8         32072         -0.08         -0.01         0.89         34.5         ether           119         ISBUL         312.0         32248         -0.02         -0.19         0.89         34.5         ether           121         CISBIMs:         3316.4         31649         -0.35         -0.03         0.89         34.5         ether           123         CISBIN*         316.4         31649         -0.87         -0.11         -0.46         55.4         mechand           124         C	No.	Compound (XSBY)	$\lambda_{ m max}$	$V_{\rm max}$	$\Sigma \sigma^{ m ex~a)}_{ m CC}$	$\sigma_{_{ m XY}}{}^{_{ m b)}}$	$\log P^{(c)}$	$E_{\rm T}(30)^{\rm d}$	Solvent
113         HSBH         307.3         32540         0.00         0.89         34.5         ether           114         HSBC         311.8         32074         -0.02         0.00         0.89         34.5         ether           115         HSBCN         311.2         312.6         -0.70         0.00         0.89         34.5         ether           116         FSBNMe         318.1         31440         -0.02         0.89         34.5         ether           117         FSBOMe         318.1         31440         -0.04         -0.02         0.89         34.5         ether           119         FSBCN         312.0         320.49         0.16         0.01         0.89         34.5         ether           121         CISBNRe;         316.4         31604         -0.03         0.03         0.89         34.5         ether           122         CISBCN         323.5         30935         -0.02         0.15         0.89         34.5         ether           123         MCSBCN         327.6         30524         -0.87         -0.11         0.40         4.9         n-methaol           124         CISBCN         328.9         3	111	HSBEt	311.5	32101	-0.13	0.00	0.89	34.5	ether
113         HSBE         307.0         2270         0.06         0.00         0.89         34.5         ether           115         HSBCN         319.2         31326         -0.70         0.00         0.89         34.5         ether           116         FSBNMc;         317.3         2877         -0.70         0.00         0.89         34.5         ether           117         FSBOMe         318.1         31440         -0.44         -0.02         0.89         34.5         ether           118         FSBRE         311.8         32072         0.06         0.01         0.89         34.5         ether           120         LSBNMe;         331.0         322.82         -2.02         -0.01         0.89         34.5         ether           121         CLSBNMe;         332.5         30912         -0.61         0.05         0.89         34.5         ether           122         CLSBNMe;         332.3         30912         -0.67         -0.11         -0.66         55.4         mechanol           124         CLSBCN         323.3         30492         -0.87         -0.11         0.48         49.7         #-batanol           125	112	HSBH	307.3	32540	0.00	0.00	0.89	34.5	ether
114         HSBCN         311.8         32074         -0.22         0.00         0.89         34.5         ether           116         HSBCN         347.3         28797         -1.75         -0.06         0.89         34.5         ether           116         FSBFR         311.8         312.0         -0.08         -0.01         0.89         34.5         ether           118         FSFBR         311.3         312.0         -0.66         0.04         0.39         34.5         ether           120         FSBCN         332.3         31320         -0.66         0.04         0.39         34.5         ether           121         CISBNMe;         334.0         282.8         -20.2         -0.19         0.49         34.5         ether           122         CISBCN         316.4         3164         0.67         -0.11         -0.66         35.4         ether           124         CISBCN         323.5         3093         -0.87         -0.11         0.48         80.7         methaol           125         MSBCN         322.9         30954         -0.87         -0.11         0.48         80.7         methaol           128	113	HSBF	307.0	32570	0.06	0.00	0.89	34.5	ether
115       HSBCN       312.0       -0.70       0.00       0.89       34.5       ether         116       FSBNMec       318.1       314.0       -0.44       -0.02       0.89       34.5       ether         118       FSRF       311.8       32072       0.08       0.01       0.89       34.5       ether         119       FSRCN       312.0       32049       -0.16       0.01       0.89       34.5       ether         121       CISBNMec       354.0       224.48       -0.20       -0.19       0.89       34.5       ether         122       CISBNMec       316.4       31609       -0.31       0.89       34.5       ether         123       CISBCN       322.5       30954       -0.87       -0.11       -0.66       35.4       mehmodi         126       MeSBCN       328.0       30452       -0.87       -0.11       0.48       49.7 <i>n</i> -butanol         127       MeSBCN       328.0       30454       -0.87       -0.11       1.44       48.5 <i>n</i> -butanol         130       MeSBCN       322.2       30373       0.87       -0.11       2.44       48.5 <i>n</i> -butanol	114	HSBCl	311.8	32074	-0.22	0.00	0.89	34.5	ether
116         FSRNe,         34.7.3         28707         -1.7.5         -0.05         0.89         34.5         ether           117         ISBOMe         318.1         31740         -0.04         -0.02         0.89         34.5         ether           118         FSRE1         312.0         320.99         -0.16         0.01         0.89         34.5         ether           120         FSBCN         312.0         -2.05         0.04         0.89         34.5         ether           121         CISBOMe         32.5.3         30912         -0.71         -0.66         0.89         34.5         ether           123         CISBCM         32.3.3         30935         -0.92         0.15         0.89         34.5         ether           124         CISBCN         32.5.9         30650         -0.87         -0.11         0.84         9.07 <i>m</i> ptunol           125         McSBCN         32.9.0         30492         0.87         -0.11         0.84         49.7 <i>m</i> ptunol           128         McSBCN         32.9.0         30344         0.87         -0.11         0.34         48.8 <i>m</i> hetanol           129         McS	115	HSBCN	319.2	31326	-0.70	0.00	0.89	34.5	ether
117       FSBCH       318.1       31440       0.44       -0.02       0.89       34.5       ether         119       FSBC1       31.0       32072       -0.06       0.01       0.89       34.5       ether         120       FISBCN       310.3       31220       -0.65       0.04       0.89       34.5       ether         121       CISBNMe:       325.3       30912       -0.71       -0.06       0.89       34.5       ether         123       CISBE2       316.4       31609       -0.32       0.05       0.89       34.5       ether         124       CISBCN       325.3       30053       -0.92       0.15       0.89       34.5       ether         125       CISBCN       325.3       30054       -0.87       -0.11       0.66       55.4       mechanol         126       McSBCN       325.0       30492       -0.87       -0.11       0.46       49.7 <i>n</i> -propanol         130       McSBCN       328.9       30498       -0.87       -0.11       2.44       48.5 <i>n</i> -pecpanol         131       McSBCN       322.2       30739       -0.87       -0.11       0.44       48.5	116	FSBNMe <sub>2</sub>	347.3	28797	-1.75	-0.05	0.89	34.5	ether
118         FSBEr         31.18         32072         -0.08         -0.01         0.89         34.5         ether           119         FSBCN         312.0         32049         -0.16         0.01         0.89         34.5         ether           121         CISBNMe;         354.0         282.48         -2.02         -0.19         0.89         34.5         ether           122         CISBCM         316.4         31604         -0.33         -0.05         0.89         34.5         ether           123         CISBCI         316.4         31604         -0.43         0.05         0.89         34.5         ether           125         MCSRCN         325.9         30680         -0.87         -0.11         0.76         55.4         ether           126         McSRCN         325.0         30394         -0.87         -0.11         0.48         49.7         mebranol           131         McSRCN         329.0         30394         -0.87         -0.11         2.04         48.8         mebranol           132         McSRCN         329.2         30379         -0.87         -0.11         0.44         48.1         m-cetanol           133 <td>117</td> <td>FSBOMe</td> <td>318.1</td> <td>31440</td> <td>-0.44</td> <td>-0.02</td> <td>0.89</td> <td>34.5</td> <td>ether</td>	117	FSBOMe	318.1	31440	-0.44	-0.02	0.89	34.5	ether
119         FSBCN         312.0         32049         -0.16         0.01         0.89         34.5         ether           120         FSBCN         319.3         31320         -0.65         0.044         0.89         34.5         ether           121         CISBIMe         323.5         30012         -0.71         -0.06         0.89         34.5         ether           123         CISBIC         316.4         31604         -0.43         0.05         0.89         34.5         ether           124         CISBCN         323.5         30035         -0.92         0.15         0.89         34.5         ether           126         CISBCN         323.3         30035         -0.92         0.11         0.44         50.7         #propanol           127         McSBCN         328.0         30492         -0.87         -0.11         0.44         49.7         #betanol           130         McSBCN         329.0         30394         -0.87         -0.11         2.03         48.8         #hetanol           131         McSBCN         329.2         3079         -0.87         -0.11         2.44         48.5         #hetanol           132	118	FSBEt	311.8	32072	-0.08	-0.01	0.89	34.5	ether
120         CSBCN         314.3         312.0         -0.65         0.04         0.89         34.5         ether           121         CUSBNMe         324.5         30912         -0.71         -0.06         0.89         34.5         ether           123         CUSBCI         316.4         31609         -0.33         -0.03         0.89         34.5         ether           124         CUSBCI         326.4         31604         -0.43         0.05         0.89         34.5         ether           125         McSDCN         327.6         30630         -0.87         -0.11         -0.46         55.4         methanol           127         McSDCN         327.6         30408         -0.87         -0.11         0.44         40.7 <i>m</i> -paranol           128         McSBCN         329.0         30394         -0.87         -0.11         2.34         48.8 <i>m</i> -hexanol           130         McSBCN         329.2         30373         -0.87         -0.11         2.34         48.5 <i>m</i> -hexanol           131         McSBCN         327.3         30534         -0.87         -0.11         0.14         48.6 <i>i</i> -propanol	119	FSBCl	312.0	32049	-0.16	0.01	0.89	34.5	ether
121         C(SBNMe)         35.40         28.248         -2.02         -0.19         0.89         34.5         erber           122         C(SBOMe         323.5         30912         -0.06         0.89         34.5         erber           124         C(SBC)         316.4         31609         -0.35         -0.03         0.89         34.5         erber           125         C(SBCN         322.3         30035         -0.92         0.15         0.85         34.5         erber           126         McSBCN         322.9         30054         -0.87         -0.11         -0.64         55.4         methanol           127         McSBCN         328.0         30492         -0.87         -0.11         0.34         50.7         n-prepation           130         McSBCN         329.0         30394         -0.87         -0.11         2.34         48.8         n-hexanol           131         McSBCN         329.0         30379         -0.87         -0.11         0.41         48.4         i-propanol           132         McSBCN         327.8         30503         -0.07         0.01         1.44         45.7         s-propanol           134	120	FSBCN	319.3	31320	-0.65	0.04	0.89	34.5	ether
122       CISBOM       32.5.3       30912       -0.71       -0.06       0.89       34.5       ether         123       CISBC1       316.4       31604       -0.43       0.05       0.89       34.5       ether         124       CISBC1       32.5.3       30033       -0.92       0.13       0.89       34.5       ether         125       McSBCN       32.5.7       30524       -0.87       -0.11       0.34       50.7 <i>n</i> -propand         128       McSBCN       328.9       30408       -0.87       -0.11       1.40       49.1 <i>n</i> -pertand         130       McSBCN       328.9       30408       -0.87       -0.11       2.34       48.8 <i>n</i> -becand         131       McSBCN       329.2       30373       -0.87       -0.11       2.34       48.5 <i>n</i> -betrand         133       McSBCN       327.8       30503       0.87       -0.11       0.14       48.4 <i>i</i> -propand         134       McSBCN       327.8       30503       0.87       -0.11       0.44       47.1       -sbutand         135       McSBCN       327.8       30649       0.87       -0.11       0.14	121	ClSBNMe <sub>2</sub>	354.0	28248	-2.02	-0.19	0.89	34.5	ether
123       CISBER       316.4       31609       -0.35       -0.03       0.89       34.5       ether         124       CISBCN       323.3       30935       -0.92       0.15       0.89       34.5       ether         126       McSBCN       322.9       30680       -0.87       -0.11       -0.66       55.4       methanol         127       McSBCN       322.0       30932       -0.87       -0.11       0.84       40.7 <i>n</i> -bruanol         129       McSBCN       328.0       30942       -0.87       -0.11       1.40       49.1 <i>n</i> -breatanol         130       McSBCN       329.0       30034       -0.87       -0.11       2.03       48.8 <i>n</i> -breatanol         131       McSBCN       329.2       30770       -0.87       -0.11       0.14       48.4 <i>n</i> -octanol         133       McSBCN       327.0       30579       -0.87       -0.11       0.14       48.4 <i>i</i> -breatanol         134       McSBCN       327.3       3054       -0.87       -0.11       0.44       45.5       2-pertanol         135       McSBCN       328.3       30449       -0.87       -0.11       0.	122	CISBOMe	323.5	30912	-0.71	-0.06	0.89	34.5	ether
124         CISBCN         3164         31004         -0.43         0.05         0.89         34.5         ether           125         CISBCN         325.9         30680         -0.87         -0.11         0.44         55.4         methanol           127         McSBCN         325.9         30680         -0.87         -0.11         0.48         50.7 <i>n</i> -ptuanol           128         McSBCN         328.9         30408         -0.87         -0.11         1.40         49.1 <i>n</i> -pertanol           130         McSBCN         329.2         30379         -0.87         -0.11         2.34         48.8 <i>n</i> -hectanol           131         McSBCN         329.2         30373         -0.87         -0.11         2.44         48.1 <i>n</i> -octanol           133         McSBCN         327.8         30503         -0.87         -0.11         0.14         48.4 <i>i</i> -propanol           134         McSBCN         327.8         3054         -0.87         -0.11         0.44         47.1         >-butanol           135         McSBCN         326.3         30449         -0.87         -0.11         1.14         46.5         2-pentanol	123	ClSBEt	316.4	31609	-0.35	-0.03	0.89	34.5	ether
125       CISBCN       323.3       30935       -0.92       0.15       0.89       34.5       ether         126       McSBCN       322.6       30580       -0.87       -0.11       0.34       50.7       n=propanol         128       McSBCN       328.0       30492       -0.87       -0.11       1.40       49.1       n=pertanol         129       McSBCN       322.0       30394       -0.87       -0.11       2.03       48.8       n=heptanol         131       McSBCN       329.0       30379       -0.87       -0.11       2.34       48.5       n=heptanol         132       McSBCN       329.2       30379       -0.87       -0.11       0.14       48.4       i=propanol         134       McSBCN       327.0       30579       -0.87       -0.11       0.14       48.6       i=propanol         135       McSBCN       326.3       30649       -0.87       -0.11       0.44       47.1       s-butanol         136       McSBCN       328.5       30445       -0.87       -0.11       1.14       45.7       3=pretanol         139       HSBCN       321.5       31106       -0.70       0.00       -0.66 <td>124</td> <td>CISBCI</td> <td>316.4</td> <td>31604</td> <td>-0.43</td> <td>0.05</td> <td>0.89</td> <td>34.5</td> <td>ether</td>	124	CISBCI	316.4	31604	-0.43	0.05	0.89	34.5	ether
126       McSBCN       325.9       30680       −0.87       −0.11       −0.66       55.4       methanol         127       McSBCN       328.0       30492       −0.87       −0.11       0.34       50.7 <i>n</i> -putanol         129       McSBCN       328.9       30408       −0.87       −0.11       2.03       48.8 <i>n</i> -hexanol         130       McSBCN       329.2       30373       −0.87       −0.11       2.44       48.5 <i>n</i> -hexanol         133       McSBCN       329.2       30373       −0.87       −0.11       0.14       48.4 <i>n</i> -petanol         134       McSBCN       327.8       30539       −0.87       −0.11       0.14       48.6 <i>i</i> -butanol         135       McSBCN       327.3       3054       −0.87       −0.11       0.44       47.1 <i>s</i> -butanol         136       McSBCN       328.5       30449       −0.87       −0.11       1.14       45.5       2-pertanol         137       McSBCN       328.5       30440       −0.87       −0.11       1.14       45.7       2-pertanol         138       McSBCN       321.5       31108       −0.70       0.00	125	CISBCN	323.3	30935	-0.92	0.15	0.89	34.5	ether
127         McSBCN         327.6         30524         -0.87         -0.11         0.34         50.7 <i>p</i> -prognol           128         McSBCN         328.9         30408         -0.87         -0.11         1.40         49.1 <i>m</i> -bratanol           130         McSBCN         329.0         30394         -0.87         -0.11         2.34         48.8 <i>m</i> -hcptanol           131         McSBCN         329.2         30373         -0.87         -0.11         2.44         48.1 <i>m</i> -canol           133         McSBCN         329.2         30579         -0.87         -0.11         0.61         48.6 <i>i</i> -propanol           134         McSBCN         327.3         30554         -0.87         -0.11         0.44         47.1 <i>s</i> -butanol           135         McSBCN         322.5         30449         -0.87         -0.11         0.14         45.7         3-pentanol           139         McSBCN         321.5         31064         -0.70         0.00         -0.66         55.4         methanol           140         HSBCN         322.8         30978         -0.70         0.00         0.48         49.7 <i>m</i> -butanol <td>126</td> <td>MeSBCN</td> <td>325.9</td> <td>30680</td> <td>-0.87</td> <td>-0.11</td> <td>-0.66</td> <td>55.4</td> <td>methanol</td>	126	MeSBCN	325.9	30680	-0.87	-0.11	-0.66	55.4	methanol
128         McSBCN         328.0         30492         -0.87         -0.11         0.48         49.7 <i>n</i> -betanol           129         McSBCN         329.0         30394         -0.87         -0.11         2.03         48.8 <i>n</i> -betanol           131         McSBCN         329.2         30379         -0.87         -0.11         2.34         48.5 <i>n</i> -betanol           132         McSBCN         329.2         30373         -0.87         -0.11         2.34         48.5 <i>n</i> -betanol           133         McSBCN         329.2         30373         -0.87         -0.11         0.14         48.4 <i>i</i> -propanol           134         McSBCN         327.8         30503         -0.87         -0.11         0.44         47.1 <i>s</i> -butanol           135         McSBCN         326.3         30649         -0.87         -0.11         0.37         43.3 <i>t</i> -butanol           138         McSBCN         319.8         31272         -0.70         0.00         -0.66         55.4         methanol           140         HSBCN         321.9         31064         -0.70         0.00         0.34         8.9.7 <i>n</i> -butanol </td <td>127</td> <td>MeSBCN</td> <td>327.6</td> <td>30524</td> <td>-0.87</td> <td>-0.11</td> <td>0.34</td> <td>50.7</td> <td>n-propanol</td>	127	MeSBCN	327.6	30524	-0.87	-0.11	0.34	50.7	n-propanol
129       McSBCN       328.9       30408       -0.87       -0.11       1.40       49.1 <i>n</i> -pertanol         130       McSBCN       329.2       30379       -0.87       -0.11       2.03       48.8 <i>n</i> -bexanol         131       McSBCN       329.2       30373       -0.87       -0.11       2.84       48.1 <i>n</i> -octanol         133       McSBCN       327.3       30579       -0.87       -0.11       0.14       48.6 <i>i</i> -butanol         135       McSBCN       327.3       30554       -0.87       -0.11       0.37       43.3 <i>i</i> -butanol         136       McSBCN       328.5       30445       -0.87       -0.11       0.14       45.7       3-pertanol         138       McSBCN       328.5       30440       -0.87       -0.11       1.14       45.5       2-pertanol         139       HSBCN       328.5       31044       -0.70       0.00       -0.66       5.4       methanol         140       HSBCN       321.5       31108       -0.70       0.00       0.34       50.7 <i>n</i> -propanol         144       HSBCN       322.9       30969       -0.70       0.00	128	MeSBCN	328.0	30492	-0.87	-0.11	0.88	49.7	n-butanol
150       McSBCN       329.0       30394       -0.87       -0.11       2.03       48.8 <i>n</i> -hexanol         131       McSBCN       329.2       30373       -0.87       -0.11       2.84       48.5 <i>n</i> -heptanol         133       McSBCN       327.0       30579       -0.87       -0.11       0.14       48.6 <i>i</i> -bropanol         134       McSBCN       327.8       30503       -0.87       -0.11       0.14       48.6 <i>i</i> -butanol         135       McSBCN       326.3       30649       -0.87       -0.11       0.44       47.1 <i>s</i> -butanol         136       McSBCN       326.3       30445       -0.87       -0.11       0.14       45.5       2-pentanol         137       McSBCN       328.5       30440       -0.87       -0.11       1.14       45.5       2-pentanol         138       McSBCN       319.8       31272       -0.70       0.00       -0.66       55.4       methanol         141       HSBCN       321.5       31004       -0.70       0.00       0.34       89.7 <i>n</i> -butanol         142       HSBCN       322.4       31013       -0.70       0.00 <t< td=""><td>129</td><td>MeSBCN</td><td>328.9</td><td>30408</td><td>-0.87</td><td>-0.11</td><td>1.40</td><td>49.1</td><td>n-pentanol</td></t<>	129	MeSBCN	328.9	30408	-0.87	-0.11	1.40	49.1	n-pentanol
131       McSBCN       329.2       30379       -0.87       -0.11       2.34       48.5       n-heptanol         132       McSBCN       329.2       30373       -0.87       -0.11       0.14       48.4       i-propanol         133       McSBCN       327.0       30579       -0.87       -0.11       0.14       48.4       i-propanol         134       McSBCN       327.3       30554       -0.87       -0.11       0.44       47.1       s-butanol         135       McSBCN       326.3       30649       -0.87       -0.11       0.14       48.5       z-butanol         136       McSBCN       328.5       30445       -0.87       -0.11       1.14       45.7       3-pentanol         138       McSBCN       328.5       30440       -0.87       -0.11       1.14       45.7       3-pentanol         140       HSBCN       321.5       31108       -0.70       0.00       -0.66       55.4       methanol         141       HSBCN       322.4       31013       -0.70       0.00       2.34       48.5       n-heptanol         144       HSBCN       322.8       30978       -0.70       0.00       2.44	130	MeSBCN	329.0	30394	-0.87	-0.11	2.03	48.8	n-hexanol
152       MeSBCN       329.2       3073       -0.87       -0.11       2.84       48.1 <i>n</i> -octanol         133       MeSBCN       327.0       30579       -0.87       -0.11       0.14       48.6 <i>i</i> -propanol         134       MeSBCN       327.3       30554       -0.87       -0.11       0.44       47.1 <i>s</i> -butanol         136       MeSBCN       326.3       30649       -0.87       -0.11       0.44       47.1 <i>s</i> -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         140       HSBCN       321.5       31108       -0.70       0.00       0.34       50.7 <i>n</i> -propanol         141       HSBCN       322.4       30078       -0.70       0.00       1.40       49.1 <i>n</i> -pentanol         144       HSBCN       322.9       30969       -0.70       0.00       2.34       48.5 <i>n</i> -heptanol         144       HSBCN       321.5       31103       -0.70       0.00 <t< td=""><td>131</td><td>MeSBCN</td><td>329.2</td><td>30379</td><td>-0.87</td><td>-0.11</td><td>2.34</td><td>48.5</td><td>n-heptanol</td></t<>	131	MeSBCN	329.2	30379	-0.87	-0.11	2.34	48.5	n-heptanol
133       McSBCN       327.0       30579       -0.87       -0.11       0.14       48.4 <i>i</i> -propanol         134       McSBCN       327.3       30554       -0.87       -0.11       0.61       48.6 <i>i</i> -butanol         135       McSBCN       326.3       30649       -0.87       -0.11       0.37       43.3 <i>i</i> -butanol         137       McSBCN       328.5       30445       -0.87       -0.11       1.14       46.5       2-pentanol         138       McSBCN       328.5       30440       -0.87       -0.11       1.14       46.7       3-pentanol         140       HSBCN       328.5       31040       -0.70       0.00       -0.66       55.4       methanol         141       HSBCN       321.5       31108       -0.70       0.00       0.88       49.7 <i>n</i> -butanol         142       HSBCN       322.4       31013       -0.70       0.00       2.03       48.8 <i>n</i> -beptanol         143       HSBCN       322.9       30968       -0.70       0.00       2.34       48.5 <i>n</i> -beptanol         144       HSBCN       321.6       31098       -0.70       0.00       0.	132	MeSBCN	329.2	30373	-0.87	-0.11	2.84	48.1	n-octanol
134       McSBCN       327.8       30533       -0.87       -0.11       0.64       48.6 <i>i</i> -butanol         135       McSBCN       326.3       3054       -0.87       -0.11       0.44       47.1 <i>s</i> -butanol         136       McSBCN       326.3       30649       -0.87       -0.11       1.14       46.5       2-pentanol         138       McSBCN       328.5       30440       -0.87       -0.11       1.14       45.7       3-pentanol         139       MSBCN       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 <i>n</i> -pentanol         144       HSBCN       321.9       31064       -0.70       0.00       2.03       48.8 <i>n</i> -betanol         144       HSBCN       322.8       30978       -0.70       0.00       2.34       48.5 <i>n</i> -betanol         144       HSBCN       321.0       31156       -0.70       0.00       2.84       48.1 <i>n</i> -octanol         144       HSBCN       321.0       31103       -0.70       0.00       0.14 <td>133</td> <td>MeSBCN</td> <td>327.0</td> <td>30579</td> <td>-0.87</td> <td>-0.11</td> <td>0.14</td> <td>48.4</td> <td><i>i</i>-propanol</td>	133	MeSBCN	327.0	30579	-0.87	-0.11	0.14	48.4	<i>i</i> -propanol
135       McSBCN       327.3       30554       -0.87       -0.11       0.44       47.1       s-butanol         136       McSBCN       326.3       30649       -0.87       -0.11       0.37       43.3       r-butanol         137       McSBCN       328.5       30445       -0.87       -0.11       1.14       45.7       3-pentanol         138       McSBCN       328.5       30440       -0.87       -0.11       1.14       45.7       3-pentanol         140       HSBCN       321.5       31108       -0.70       0.00       0.34       50.7       n-popanol         141       HSBCN       321.9       31064       -0.70       0.00       1.40       49.1       n-pentanol         142       HSBCN       322.4       31013       -0.70       0.00       2.34       48.8       n-hebranol         144       HSBCN       322.0       30958       -0.70       0.00       2.84       48.1       n-octanol         144       HSBCN       321.6       31098       -0.70       0.00       0.41       48.4       i-propanol         145       HSBCN       321.6       31098       -0.70       0.00       0.41	134	MeSBCN	327.8	30503	-0.87	-0.11	0.61	48.6	<i>i</i> -butanol
136         MeSBCN         326.3         30649         -0.87         -0.11         0.37         43.3 <i>i</i> -butanol           137         MeSBCN         328.5         30445         -0.87         -0.11         1.14         46.5         2-pentanol           138         MeSBCN         312.8         310440         -0.87         -0.11         1.14         45.7         3-pentanol           140         HSBCN         312.5         31108         -0.70         0.00         -0.66         55.4         methanol           141         HSBCN         321.9         31064         -0.70         0.00         0.88         49.7 <i>n</i> -betanol           142         HSBCN         322.4         31013         -0.70         0.00         2.34         48.8 <i>n</i> -becanol           144         HSBCN         322.0         30958         -0.70         0.00         2.84         48.1 <i>n</i> -octanol           145         HSBCN         321.6         31098         -0.70         0.00         0.61         48.6 <i>i</i> -butanol           146         HSBCN         321.6         31099         -0.70         0.00         0.14         48.6 <i>i</i> -butanol <td>135</td> <td>MeSBCN</td> <td>327.3</td> <td>30554</td> <td>-0.87</td> <td>-0.11</td> <td>0.44</td> <td>47.1</td> <td>s-butanol</td>	135	MeSBCN	327.3	30554	-0.87	-0.11	0.44	47.1	s-butanol
137       McSBCN       328.5       30445       -0.87       -0.11       1.14       46.5       2-pentanol         138       McSBCN       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 <i>n</i> -propanol         141       HSBCN       321.5       31108       -0.70       0.00       0.88       49.7 <i>n</i> -butanol         142       HSBCN       322.4       31013       -0.70       0.00       2.03       48.8 <i>n</i> -hexanol         144       HSBCN       322.8       30978       -0.70       0.00       2.34       48.5 <i>n</i> -hexanol         144       HSBCN       321.0       31156       -0.70       0.00       2.34       48.5 <i>n</i> -hexanol         145       HSBCN       321.0       31156       -0.70       0.00       0.61       48.6 <i>i</i> -butanol         144       HSBCN       321.0       31156       -0.70       0.00       0.61       48.6 <i>i</i> -butanol         144       HSBCN       321.0       31156       -0.70       0.00       0.14	136	MeSBCN	326.3	30649	-0.87	-0.11	0.37	43.3	<i>t</i> -butanol
138       McSBCN       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       0.88       49.7       n-butanol         141       HSBCN       321.5       31044       -0.70       0.00       1.40       49.1       n-pentanol         143       HSBCN       322.4       31013       -0.70       0.00       2.03       48.8       n-heptanol         144       HSBCN       322.9       30969       -0.70       0.00       2.34       48.5       n-heptanol         144       HSBCN       323.0       30958       -0.70       0.00       2.84       48.1       n-octanol         144       HSBCN       321.0       31156       -0.70       0.00       0.61       48.6       i-butanol         147       HSBCN       321.6       31098       -0.70       0.00       0.44       47.1       s-butanol         148       HSBCN       320.4       31209       -0.70       0.00       1.14       46.	137	MeSBCN	328.5	30445	-0.87	-0.11	1.14	46.5	2-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         2.03         48.8         n-bexanol           144         HSBCN         322.9         30969         -0.70         0.00         2.84         48.5         n-heptanol           145         HSBCN         323.0         30958         -0.70         0.00         0.14         48.4 <i>i</i> -propanol           146         HSBCN         321.0         31156         -0.70         0.00         0.61         48.6 <i>i</i> -butanol           148         HSBCN         321.6         31098         -0.70         0.00         0.37         43.3 <i>i</i> -butanol           149         HSBCN         321.6         31098         -0.70         0.00         0.37         43.3 <i>i</i> -butanol	138	MeSBCN	328.5	30440	-0.87	-0.11	1.14	45.7	3-pentanol
140       HSBCN       321.5       31108       -0.70       0.00       0.34       50.7 <i>n</i> -propanol         141       HSBCN       321.9       31064       -0.70       0.00       0.88       49.7 <i>n</i> -butanol         142       HSBCN       322.4       31013       -0.70       0.00       1.40       49.1 <i>n</i> -pentanol         143       HSBCN       322.8       30978       -0.70       0.00       2.03       48.8 <i>n</i> -hexanol         144       HSBCN       322.9       30969       -0.70       0.00       2.34       48.5 <i>n</i> -heptanol         145       HSBCN       321.0       31156       -0.70       0.00       0.14       48.4 <i>i</i> -propanol         147       HSBCN       321.6       31098       -0.70       0.00       0.61       48.6 <i>i</i> -butanol         148       HSBCN       321.6       31098       -0.70       0.00       0.37       43.3 <i>r</i> -butanol         149       HSBCN       322.1       31051       -0.70       0.00       1.14       46.5       2-pentanol         150       HSBCN       322.2       31032       -0.70       0.00       1.14 <td>139</td> <td>HSBCN</td> <td>319.8</td> <td>31272</td> <td>-0.70</td> <td>0.00</td> <td>-0.66</td> <td>55.4</td> <td>methanol</td>	139	HSBCN	319.8	31272	-0.70	0.00	-0.66	55.4	methanol
141       HSBCN       321.9       31064       -0.70       0.00       0.88       49.7 <i>n</i> -butanol         142       HSBCN       322.4       31013       -0.70       0.00       1.40       49.1 <i>n</i> -pentanol         143       HSBCN       322.8       30978       -0.70       0.00       2.03       48.8 <i>n</i> -heptanol         144       HSBCN       322.9       30969       -0.70       0.00       2.34       48.5 <i>n</i> -heptanol         145       HSBCN       323.0       30958       -0.70       0.00       2.84       48.1 <i>n</i> -octanol         146       HSBCN       321.0       31156       -0.70       0.00       0.14       48.4 <i>i</i> -propanol         147       HSBCN       321.6       31109       -0.70       0.00       0.44       47.1 <i>s</i> -butanol         149       HSBCN       322.1       31051       -0.70       0.00       0.37       43.3 <i>t</i> -butanol         150       HSBCN       322.2       31032       -0.70       0.00       1.14       45.7       3-pentanol         151       HSBCN       322.2       31076       -0.92       0.15       0.34 <td>140</td> <td>HSBCN</td> <td>321.5</td> <td>31108</td> <td>-0.70</td> <td>0.00</td> <td>0.34</td> <td>50.7</td> <td><i>n</i>-propanol</td>	140	HSBCN	321.5	31108	-0.70	0.00	0.34	50.7	<i>n</i> -propanol
142       HSBCN       322.4       31013       -0.70       0.00       1.40       49.1 <i>n</i> -pentanol         143       HSBCN       322.8       30978       -0.70       0.00       2.03       48.8 <i>n</i> -heptanol         144       HSBCN       322.9       30969       -0.70       0.00       2.34       48.5 <i>n</i> -heptanol         145       HSBCN       323.0       30958       -0.70       0.00       2.84       48.1 <i>n</i> -octanol         146       HSBCN       321.0       31156       -0.70       0.00       0.14       48.6 <i>i</i> -butanol         147       HSBCN       321.6       31098       -0.70       0.00       0.44       47.1 <i>s</i> -butanol         148       HSBCN       320.4       31209       -0.70       0.00       0.37       43.3 <i>i</i> -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       CISBCN       325.7       30702       -0.92       0.15       0.48	141	HSBCN	321.9	31064	-0.70	0.00	0.88	49.7	<i>n</i> -butanol
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       48.5       n-heptanol         146       HSBCN       321.0       31156       -0.70       0.00       0.61       48.6       i-propanol         147       HSBCN       321.6       31098       -0.70       0.00       0.44       47.1       s-butanol         148       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       30943       -0.92       0.15       0.34       50.7       n-propanol         153       CISBCN       325.0       30765       -0.92       0.15       0.34       50.7       n-petanol         155       CISBCN       326.2       30653       -0.92       0.15       2.44       48	142	HSBCN	322.4	31013	-0.70	0.00	1.40	49.1	<i>n</i> -pentanol
144       HSBCN       322.9       30969       -0.70       0.00       2.34       48.5 <i>n</i> -heptanol         145       HSBCN       321.0       31156       -0.70       0.00       2.84       48.1 <i>n</i> -octanol         146       HSBCN       321.0       31156       -0.70       0.00       0.14       48.4 <i>i</i> -propanol         147       HSBCN       321.5       31103       -0.70       0.00       0.61       48.6 <i>i</i> -butanol         148       HSBCN       321.6       31098       -0.70       0.00       0.44       47.1 <i>s</i> -butanol         149       HSBCN       320.4       31209       -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         153       CISBCN       322.2       30943       -0.92       0.15       0.34       50.7 <i>n</i> -butanol         153       CISBCN       325.7       30702       -0.92       0.15       0.34       50.7 <i>n</i> -butanol         154       CISBCN       326.2       30653       -0.92       0.15       2.34 <td>143</td> <td>HSBCN</td> <td>322.8</td> <td>30978</td> <td>-0.70</td> <td>0.00</td> <td>2.03</td> <td>48.8</td> <td><i>n</i>-hexanol</td>	143	HSBCN	322.8	30978	-0.70	0.00	2.03	48.8	<i>n</i> -hexanol
145       HSBCN       323.0       30958       -0.70       0.00       2.84       48.1 <i>n</i> -octanol         146       HSBCN       321.0       31156       -0.70       0.00       0.14       48.4 <i>i</i> -propanol         147       HSBCN       321.5       31103       -0.70       0.00       0.61       48.6 <i>i</i> -butanol         148       HSBCN       321.6       31098       -0.70       0.00       0.44       47.1 <i>s</i> -butanol         149       HSBCN       320.4       31209       -0.70       0.00       0.37       43.3 <i>r</i> -butanol         150       HSBCN       322.2       31032       -0.70       0.00       1.14       46.5       2-pentanol         151       HSBCN       322.2       30943       -0.92       0.15       -0.66       55.4       methanol         153       CISBCN       325.0       30765       -0.92       0.15       0.34       50.7 <i>n</i> -propanol         154       CISBCN       326.2       30653       -0.92       0.15       2.44       48.8 <i>n</i> -hexanol         155       CISBCN       326.6       30617       -0.92       0.15       2.34	144	HSBCN	322.9	30969	-0.70	0.00	2.34	48.5	<i>n</i> -heptanol
146       HSBCN       321.0       31156       -0.70       0.00       0.14       48.4 <i>i</i> -propanol         147       HSBCN       321.5       31103       -0.70       0.00       0.61       48.6 <i>i</i> -butanol         148       HSBCN       321.6       31098       -0.70       0.00       0.44       47.1 <i>s</i> -butanol         149       HSBCN       320.4       31209       -0.70       0.00       0.37       43.3 <i>i</i> -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       CISBCN       323.2       30943       -0.92       0.15       -0.66       55.4       methanol         153       CISBCN       326.2       30653       -0.92       0.15       0.34       50.7 <i>n</i> -porpanol         154       CISBCN       326.6       30617       -0.92       0.15       2.03       48.8 <i>n</i> -hexanol         157       CISBCN       326.9       30594       -0.92       0.15       2.34	145	HSBCN	323.0	30958	-0.70	0.00	2.84	48.1	<i>n</i> -octanol
147       HSBCN       321.5       31103       -0.70       0.00       0.61       48.6 <i>i</i> -butanol         148       HSBCN       321.6       31098       -0.70       0.00       0.44       47.1 <i>s</i> -butanol         149       HSBCN       320.4       31209       -0.70       0.00       0.37       43.3 <i>t</i> -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       CISBCN       323.2       30943       -0.92       0.15       -0.66       55.4       methanol         153       CISBCN       325.0       30765       -0.92       0.15       0.34       50.7 <i>n</i> -propanol         154       CISBCN       326.2       30653       -0.92       0.15       1.40       49.1 <i>n</i> -pentanol         155       CISBCN       326.6       30617       -0.92       0.15       2.03       48.8 <i>n</i> -hexanol         157       CISBCN       326.9       30593       -0.92       0.15       2.14 <td>146</td> <td>HSBCN</td> <td>321.0</td> <td>31156</td> <td>-0.70</td> <td>0.00</td> <td>0.14</td> <td>48.4</td> <td><i>i</i>-propanol</td>	146	HSBCN	321.0	31156	-0.70	0.00	0.14	48.4	<i>i</i> -propanol
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       CISBCN       323.2       30943       -0.92       0.15       -0.66       55.4       methanol         153       CISBCN       325.0       30765       -0.92       0.15       0.34       50.7       n-propanol         154       CISBCN       326.2       30653       -0.92       0.15       1.40       49.1       n-pentanol         155       CISBCN       326.6       30617       -0.92       0.15       2.03       48.8       n-hexanol         157       CISBCN       326.9       30594       -0.92       0.15       2.34       48.5       n-heptanol         158       CISBCN       322.4       30730       -0.92       0.15       0.14 <t< td=""><td>147</td><td>HSBCN</td><td>321.5</td><td>31103</td><td>-0.70</td><td>0.00</td><td>0.61</td><td>48.6</td><td><i>i</i>-butanol</td></t<>	147	HSBCN	321.5	31103	-0.70	0.00	0.61	48.6	<i>i</i> -butanol
149HSBCN320.431209-0.700.000.3743.37-butanol150HSBCN322.131051-0.700.001.1446.52-pentanol151HSBCN322.231032-0.700.001.1445.73-pentanol152CISBCN323.230943-0.920.15-0.6655.4methanol153CISBCN325.030765-0.920.150.3450.7n-propanol154CISBCN326.230653-0.920.151.4049.1n-pentanol155CISBCN326.630617-0.920.152.0348.8n-hexanol156CISBCN326.930594-0.920.152.3448.5n-heptanol157CISBCN326.930593-0.920.152.4448.1n-octanol158CISBCN326.430834-0.920.150.1448.4i-propanol160CISBCN325.430730-0.920.150.4447.1s-butanol161CISBCN325.530725-0.920.150.4447.1s-butanol162CISBCN323.830886-0.920.150.4447.1s-butanol163CISBCN325.930683-0.920.151.1446.52-pentanol164CISBCN325.830697-0.920.151.1445.73-pentanol	148	HSBCN	321.6	31098	-0.70	0.00	0.44	47.1	s-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       CISBCN       323.2       30943       -0.92       0.15       -0.66       55.4       methanol         153       CISBCN       325.0       30765       -0.92       0.15       0.34       50.7 <i>n</i> -propanol         154       CISBCN       325.7       30702       -0.92       0.15       0.88       49.7 <i>n</i> -butanol         155       CISBCN       326.2       30653       -0.92       0.15       1.40       49.1 <i>n</i> -pentanol         156       CISBCN       326.6       30617       -0.92       0.15       2.03       48.8 <i>n</i> -hexanol         157       CISBCN       326.9       30594       -0.92       0.15       2.34       48.5 <i>n</i> -heptanol         158       CISBCN       326.9       30593       -0.92       0.15       0.14       48.4 <i>i</i> -propanol         160       CISBCN       325.4       30730       -0.92       0.15       0.4	149	HSBCN	320.4	31209	-0.70	0.00	0.37	43.3	t-butanol
151       HSBCN       322.2       31032       -0.70       0.00       1.14       45.7       3-pentanol         152       CISBCN       323.2       30943       -0.92       0.15       -0.66       55.4       methanol         153       CISBCN       325.0       30765       -0.92       0.15       0.34       50.7 <i>n</i> -propanol         154       CISBCN       325.7       30702       -0.92       0.15       0.88       49.7 <i>n</i> -butanol         155       CISBCN       326.2       30653       -0.92       0.15       1.40       49.1 <i>n</i> -pentanol         156       CISBCN       326.6       30617       -0.92       0.15       2.03       48.8 <i>n</i> -hexanol         157       CISBCN       326.9       30594       -0.92       0.15       2.34       48.5 <i>n</i> -heptanol         158       CISBCN       326.9       30593       -0.92       0.15       0.14       48.4 <i>i</i> -propanol         160       CISBCN       325.4       30730       -0.92       0.15       0.61       48.6 <i>i</i> -butanol         161       CISBCN       325.5       30725       -0.92       0.15       0	150	HSBCN	322.1	31051	-0.70	0.00	1.14	46.5	2-pentanol
152       CISBCN       525.2       30945       -0.92       0.15       -0.66       55.4       methanol         153       CISBCN       325.0       30765       -0.92       0.15       0.34       50.7       n-propanol         154       CISBCN       325.7       30702       -0.92       0.15       0.88       49.7       n-butanol         155       CISBCN       326.2       30653       -0.92       0.15       1.40       49.1       n-pentanol         156       CISBCN       326.6       30617       -0.92       0.15       2.03       48.8       n-hexanol         157       CISBCN       326.9       30594       -0.92       0.15       2.34       48.5       n-heptanol         158       CISBCN       326.9       30593       -0.92       0.15       2.84       48.1       n-octanol         159       CISBCN       324.3       30834       -0.92       0.15       0.14       48.6       i-butanol         160       CISBCN       325.5       30725       -0.92       0.15       0.44       47.1       s-butanol         161       CISBCN       323.8       30886       -0.92       0.15       0.37	151	HSBCN	322.2	31032	-0.70	0.00	1.14	45.7	3-pentanol
153       CISBCN       325.0       30763       -0.92       0.15       0.34       50.7 <i>n</i> -propanol         154       CISBCN       325.7       30702       -0.92       0.15       0.88       49.7 <i>n</i> -butanol         155       CISBCN       326.2       30653       -0.92       0.15       1.40       49.1 <i>n</i> -pentanol         156       CISBCN       326.6       30617       -0.92       0.15       2.03       48.8 <i>n</i> -hexanol         157       CISBCN       326.9       30594       -0.92       0.15       2.34       48.5 <i>n</i> -heptanol         158       CISBCN       326.9       30593       -0.92       0.15       2.84       48.1 <i>n</i> -octanol         159       CISBCN       324.3       30834       -0.92       0.15       0.14       48.4 <i>i</i> -propanol         160       CISBCN       325.5       30725       -0.92       0.15       0.44       47.1 <i>s</i> -butanol         161       CISBCN       323.8       30886       -0.92       0.15       0.37       43.3 <i>t</i> -butanol         162       CISBCN       325.9       30683       -0.92       0.15       <	152	CISBUN	323.2	30943	-0.92	0.15	-0.66	55.4	methanol
154       CISBCN       325.7       30702       -0.92       0.15       0.88       49.7       n-butanoi         155       CISBCN       326.2       30653       -0.92       0.15       1.40       49.1       n-pentanoi         156       CISBCN       326.6       30617       -0.92       0.15       2.03       48.8       n-hexanoi         157       CISBCN       326.9       30594       -0.92       0.15       2.34       48.5       n-heptanoi         158       CISBCN       326.9       30593       -0.92       0.15       2.84       48.1       n-octanoi         159       CISBCN       324.3       30834       -0.92       0.15       0.14       48.4 <i>i</i> -propanoi         160       CISBCN       325.4       30730       -0.92       0.15       0.61       48.6 <i>i</i> -butanoi         161       CISBCN       325.5       30725       -0.92       0.15       0.44       47.1 <i>s</i> -butanoi         162       CISBCN       323.8       30886       -0.92       0.15       0.37       43.3 <i>t</i> -butanoi         163       CISBCN       325.9       30683       -0.92       0.15       1.14 <td>155</td> <td>CISBUN</td> <td>325.0</td> <td>30765</td> <td>-0.92</td> <td>0.15</td> <td>0.34</td> <td>50.7 40.7</td> <td><i>n</i>-propanol</td>	155	CISBUN	325.0	30765	-0.92	0.15	0.34	50.7 40.7	<i>n</i> -propanol
133       CISBEN       326.2       50033       -0.92       0.13       1.40       49.1 <i>n</i> -peritation         156       CISBEN       326.6       30617       -0.92       0.15       2.03       48.8 <i>n</i> -hexanol         157       CISBEN       326.9       30594       -0.92       0.15       2.34       48.5 <i>n</i> -heptanol         158       CISBEN       326.9       30593       -0.92       0.15       2.84       48.1 <i>n</i> -octanol         159       CISBEN       324.3       30834       -0.92       0.15       0.14       48.6 <i>i</i> -propanol         160       CISBEN       325.4       30730       -0.92       0.15       0.61       48.6 <i>i</i> -butanol         161       CISBEN       325.5       30725       -0.92       0.15       0.44       47.1 <i>s</i> -butanol         162       CISBEN       323.8       30886       -0.92       0.15       0.37       43.3 <i>t</i> -butanol         163       CISBEN       325.9       30683       -0.92       0.15       1.14       46.5       2-pentanol         164       CISBEN       325.8       30697       -0.92       0.15       <	154	CISBUN	325.7	30702	-0.92	0.15	0.88	49.7	<i>n</i> -butanol
136       CLSBCN       326.0       50017       -0.92       0.13       2.05       46.8 <i>n</i> -hexanol         157       CLSBCN       326.9       30594       -0.92       0.15       2.34       48.5 <i>n</i> -heptanol         158       CLSBCN       326.9       30593       -0.92       0.15       2.84       48.1 <i>n</i> -octanol         159       CLSBCN       324.3       30834       -0.92       0.15       0.14       48.6 <i>i</i> -propanol         160       CLSBCN       325.4       30730       -0.92       0.15       0.61       48.6 <i>i</i> -butanol         161       CLSBCN       325.5       30725       -0.92       0.15       0.44       47.1 <i>s</i> -butanol         162       CLSBCN       323.8       30886       -0.92       0.15       0.37       43.3 <i>t</i> -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       -0.6	155	CISDON	320.2	20617	-0.92	0.15	1.40	49.1	<i>n</i> -pentanoi
137       CLSBCN       320.9       50394       -0.92       0.13       2.54       46.5 <i>h</i> -hepfanloi         158       CISBCN       326.9       30593       -0.92       0.15       2.84       48.1 <i>n</i> -octanol         159       CISBCN       324.3       30834       -0.92       0.15       0.14       48.4 <i>i</i> -propanol         160       CISBCN       325.4       30730       -0.92       0.15       0.61       48.6 <i>i</i> -butanol         161       CISBCN       325.5       30725       -0.92       0.15       0.44       47.1 <i>s</i> -butanol         162       CISBCN       323.8       30886       -0.92       0.15       0.37       43.3 <i>t</i> -butanol         163       CISBCN       325.9       30683       -0.92       0.15       1.14       46.5       2-pentanol         164       CISBCN       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	150	CISDON	320.0	20504	-0.92	0.15	2.03	40.0	<i>n</i> -nexanol
156       CISBER       320.9       50595       -0.92       0.15       2.84       46.1 <i>h</i> -octanol         159       CISBEN       324.3       30834       -0.92       0.15       0.14       48.4 <i>i</i> -propanol         160       CISBEN       325.4       30730       -0.92       0.15       0.61       48.6 <i>i</i> -butanol         161       CISBEN       325.5       30725       -0.92       0.15       0.44       47.1 <i>s</i> -butanol         162       CISBEN       323.8       30886       -0.92       0.15       0.37       43.3 <i>t</i> -butanol         163       CISBEN       325.9       30683       -0.92       0.15       1.14       46.5       2-pentanol         164       CISBEN       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	157	CISPCN	326.0	30594	-0.92	0.15	2.34	48.J 19 1	<i>n</i> -neptanoi
157       CISBER       324.3       30634       -0.92       0.13       0.14       46.4       I-propanoi         160       CISBEN       325.4       30730       -0.92       0.15       0.61       48.6 <i>i</i> -butanoi         161       CISBEN       325.5       30725       -0.92       0.15       0.44       47.1 <i>s</i> -butanoi         162       CISBEN       323.8       30886       -0.92       0.15       0.37       43.3 <i>t</i> -butanoi         163       CISBEN       325.9       30683       -0.92       0.15       1.14       46.5       2-pentanoi         164       CISBEN       325.8       30697       -0.92       0.15       1.14       45.7       3-pentanoi         165       HSBH       307.0       32570       0.00       0.00       -0.66       55.4       methanoi	150	CISBON	320.9	20292	-0.92	0.15	2.0 <del>4</del> 0.14	40.1 19 1	<i>i</i> -propagal
160       CISBEN       323.4       50750       -0.92       0.15       0.01       48.6       Pollabol         161       CISBEN       325.5       30725       -0.92       0.15       0.44       47.1       s-butanol         162       CISBEN       323.8       30886       -0.92       0.15       0.37       43.3       t-butanol         163       CISBEN       325.9       30683       -0.92       0.15       1.14       46.5       2-pentanol         164       CISBEN       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	159	CISPCN	324.3 225 4	20720	-0.92	0.15	0.14	40.4 10 C	<i>i</i> -propanol
161       CISBER       325.5       50725       -0.92       0.15       0.44       47.1       3-butanol         162       CISBEN       323.8       30886       -0.92       0.15       0.37       43.3 <i>t</i> -butanol         163       CISBEN       325.9       30683       -0.92       0.15       1.14       46.5       2-pentanol         164       CISBEN       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	100	CISPCN	325.4 325.5	30730	-0.92	0.15	0.01	40.0 17 1	<i>i</i> -outail01
162     CISBER     325.0     30600     -0.92     0.15     0.57     45.5     7-bitanol       163     CISBEN     325.9     30683     -0.92     0.15     1.14     46.5     2-pentanol       164     CISBEN     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	101	CISBON	323.3	30723	-0.92	0.15	0.44	+/.1 /2 2	s-outanoi
165         LISBER         325.7         50065         -0.92         0.15         1.14         40.5         2-pentanol           164         CISBEN         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	162	CISBON	325.0	30683	-0.92	0.15	0.57	45.5	<i>i</i> -outail01
165 HSBH $307.0$ $32570$ $0.00$ $0.00$ $-0.66$ $55.4$ methanol	103	CISPCN	325.9	30607	-0.92	0.15	1.14	40.5	2-pentanol
	165	HSBH	307.0	32570	0.00	0.00	-0.66	55.4	methanol

								(Continued)
No.	Compound (XSBY)	$\lambda_{ m max}$	$V_{\rm max}$	$\Sigma\sigma^{ m ex~a)}_{ m CC}$	$\sigma_{_{ m XY}}{}^{_{ m b)}}$	$\log P^{c}$	$E_{\rm T}(30)^{\rm d}$	Solvent
166	HSBH	308.1	32459	0.00	0.00	0.34	50.7	<i>n</i> -propanol
167	HSBH	308.4	32423	0.00	0.00	0.88	49.7	<i>n</i> -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>i</i> -propanol
173	HSBH	307.9	32480	0.00	0.00	0.61	48.6	<i>i</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	<i>n</i> -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>i</i> -propanol
186	MeSBOMe	321.0	31157	-0.67	0.05	0.61	48.6	<i>i</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	<i>n</i> -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	<i>n</i> -octanol
198	MeSBH	311.4	32108	-0.17	0.00	0.14	48.4	<i>i</i> -propanol
199	MeSBH	311.8	32073	-0.17	0.00	0.61	48.6	<i>i</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	<i>t</i> -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	<i>n</i> -propanol
206	HSBOMe	319.3	31316	-0.50	0.00	0.88	49.7	<i>n</i> -butanol
207	HSBOMe	319.7	31281	-0.50	0.00	1.40	49.1	<i>n</i> -pentanol
208	HSBOMe	320.2	31230	-0.50	0.00	2.03	48.8	<i>n</i> -hexanol
209	HSBOMe	320.5	31203	-0.50	0.00	2.34	48.5	<i>n</i> -heptanol
210	HSBOMe	320.8	311/6	-0.50	0.00	2.84	48.1	<i>n</i> -octanol
211	HSBOMe	318.3	31416	-0.50	0.00	0.14	48.4	<i>i</i> -propanol
212	HSBOMe	318.2	31430	-0.50	0.00	0.61	48.6	<i>i</i> -butanol
213	HSBOMe	318.5	31393	-0.50	0.00	0.44	47.1	s-butanol
214	навоме	210.0	313/3	-0.50	0.00	0.3/	43.3	
215	HSBOME	319.U 219.5	31350	-0.50	0.00	1.14	40.5	2-pentanoi
216	HSBOMe	318.5	31396	-0.50	0.00	1.14	45./	5-pentanol
217	CISBOME	322.5	31025	-0.71	-0.06	-0.66	50.4	methanoi
218	CISBOME	524.U	30802	-0./1	-0.06	0.34	50.7 40.7	<i>n</i> -propanol
219	CISBOME	324.4 224.9	20702	-0./1	-0.06	0.88	49./	<i>n</i> -putanol
220	CISBOME	324.8	30792	-0./1	-0.06	1.40	49.1	<i>n</i> -pentanol

								(Continued)
No.	Compound (XSBY)	$\lambda_{ m max}$	$V_{\rm max}$	$\Sigma \sigma^{ m ex~a)}_{ m CC}$	$\sigma_{_{ m XY}}{}^{^{ m b)}}$	$\log P^{(c)}$	$E_{\rm T}(30)^{\rm d}$	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>i</i> -propanol
225	ClSBOMe	323.7	30891	-0.71	-0.06	0.61	48.6	<i>i</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	CISBH	311.7	32079	-0.22	0.00	-0.66	55.4	methanol
231	CISBH	312.8	31966	-0.22	0.00	0.34	50.7	n-propanol
232	CISBH	313.5	31900	-0.22	0.00	0.88	49.7	n-butanol
233	CISBH	313.9	31858	-0.22	0.00	1.40	49.1	n-pentanol
234	CISBH	313.9	31854	-0.22	0.00	2.03	48.8	n-hexanol
235	CISBH	314.2	31823	-0.22	0.00	2.34	48.5	n-heptanol
236	CISBH	314.4	31809	-0.22	0.00	2.84	48.1	n-octanol
237	CISBH	312.3	32024	-0.22	0.00	0.14	48.4	<i>i</i> -propanol
238	CISBH	312.7	31983	-0.22	0.00	0.61	48.6	<i>i</i> -butanol
239	CISBH	312.5	31998	-0.22	0.00	0.44	47.1	s-butanol
240	CISBH	311.8	32075	-0.22	0.00	0.37	43.3	t-butanol
241	CISBH	312.9	31957	-0.22	0.00	1.14	46.5	2-pentanol
242	CISBH	313.1	31943	-0.22	0.00	1.14	45.7	3-pentanol

a) The  $\sigma_{CC}^{ex}$  values of substituents NMe<sub>2</sub>, 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  $\sigma_p$  values of substituents NMe<sub>2</sub>, 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 solv-atochromic dye of the solvent, taken from ref. [19].

	$V_{\rm max}$	$= a + b \sum \sigma_{\rm CC}^{\rm ex} + c \sigma_{\rm CC}^{\rm ex}$	(XY)					
Solvents <sup>a)</sup>	$V_{\rm max}$	$a' = a' + b' \sum \sigma_{\rm CC}^{\rm ex} + c'$	$\sigma_{_{ m XY}}$	r	S	F	п	
	a a'	b b'	с с'					
CIL	32299.71	1967.774	326.388	0.9945	132.12	993.00	25	
$C_6H_{12}$	32284.33	1917.317	1414.417	0.9973	92.20	2050.57	25	
E4 0	32450.05	2034.115	360.9054	0.9939	143.65	985.57	25	
$El_2O$	32434.96	1987.815	1292.186	0.9960	116.19	1374.67	25	
CUCI	32153.18	2121.298	342.5192	0.9947	139.61	1034.48	25	
CHCl <sub>3</sub>	32137.20	2068.629	1461.726	0.9973	99.77	2035.87	25	
CH CN	32522.04	2195.636	388.6807	0.9917	180.94	657.75	25	
CH <sub>3</sub> CN	32504.47	2136.914	1578.166	0.9945	147.45	995.99	25	
	32418.29	2087.889	697.1173	0.9951	130.41	1111.00	25	
$C_2H_5OH$	32397.20	2001.540	1354.227	0.9965	109.46	1581.48	25	

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

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

$$v_{\rm max} = a' + b' \sum \sigma_{\rm CC}^{\rm ex} + c' \sigma_{\rm XY} \tag{1b}$$

As can be seen from Table 2, although the properties of solvents are different from each other, all the  $v_{\rm max}$  of XSBY in each solvent have good correlations with the parameters  $\Sigma \sigma_{\rm CC}^{\rm ex}$  and  $\sigma_{\rm XY}$ . 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  $v_{max}$  is dominated by the excited-state substituent parameter  $\sigma_{CC}^{ex}$  and the ground state polar substituent constant  $\sigma_{p}$  together.

## 3.2 The solvent effect on the $v_{\text{max}}$ 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 CISBNMe<sub>2</sub> is 536 cm<sup>-1</sup> (about 6.9 nm) in the two solvents C<sub>6</sub>H<sub>12</sub> and CHCl<sub>3</sub>. 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 parameters have been proposed, in which the solvatochromic dye  $E_{\rm T}(30)$  [19] attracted the most attention. In this paper, we use the  $E_{\rm T}(30)$  to correlate the 242 experimental  $\nu_{\rm max}$  in Table 1 combining with parameters  $\Sigma \sigma_{\rm CC}^{\rm ex}$  and  $\sigma_{\rm XY}$ . 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  $E_{\rm T}(30)$  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  $E_{\rm T}(30)$  in eq. (2) can be substituted by the aqueous solubility parameters logP (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  $15 \text{ cm}^{-1}$ . 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  $v_{max}$  values in Table 1 is in a wide range. The maximum is 32592 cm<sup>-1</sup> (the  $v_{max}$  of HSBH in *t*-BuOH), and the minimum is 27692 cm<sup>-1</sup> (the  $v_{max}$  of ClSBNMe<sub>2</sub> in CHCl<sub>3</sub>). Their variation is 4900 cm<sup>-1</sup> (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),

$$\log P = aV + bE_{\text{HOMO}} + cE_{\text{LUMO}} + d \tag{4}$$

In eq. (4), *a*, *b*, *c*, and *d* are coefficients, *V*,  $E_{\text{HOMO}}$ , and  $E_{\text{LUMO}}$  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 ( $S_{\text{solvent}}$ ),

$$S_{\text{solvent}} = a(V_{\text{solvent}} - V_{\text{solute}}) + b(E_{\text{HOMO, solvent}} - E_{\text{LUMO, solute}}) + c(E_{\text{LUMO, solvent}} - E_{\text{HOMO, solute}}) = aV_{\text{solvent}} + bE_{\text{HOMO, solvent}} + cE_{\text{LUMO, solvent}} - [aV_{\text{solute}} + bE_{\text{LUMO, solute}} + cE_{\text{HOMO, solute}}]$$
(5)

As respect to a given XSBY molecule, its  $V_{\text{solute}}$ ,  $E_{\text{HOMO, solute}}$ ,

and  $E_{\text{LUMO, solute}}$  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  $v_{max, expt}$  versus  $v_{max, calcd}$  for XSBY (cm<sup>-1</sup>).

**Table 3** The correlation results of  $v_{\text{max}}$  with parameters  $\Sigma \sigma_{cc}^{ex}$ ,  $\sigma_{xy}$  and solvent parameters for XSBY in different solvents

Correlation equations	r	S	F	п	Equation number
$22205 42 \pm 2025 201 \sum_{i=1}^{\infty} \pm 1254 (72 - 1 \pm 2.007410 E_{i}(20))$	,	142.57	2020.01	2.12	
$V_{\rm max} = 32203.42 + 2025.391 \sum \sigma_{\rm CC} + 1554.073 \sigma_{\rm XY} + 3.907419 E_{\rm T}(30)$	0.9900	143.57	3930.81	242	(2)
$v_{\rm max} = 32440.19 + 2027.815 \sum_{\rm C} \sigma_{\rm CC}^{\rm ex} + 1358.551 \sigma_{\rm XY} - 56.4827 \log P$	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<sub>2</sub>Me

Compounds <sup>a)</sup>	$\lambda_{\max, expt.}^{(b)}$	$\sigma_{ ext{cc}}^{ ext{ex}}( ext{X})$	$\sigma_{ ext{cc}}^{ ext{ex}}\left( ext{Y} ight)$	$\lambda_{ m max, pred.}^{~~c)}$	$\Delta^{d)}$
Me <sub>2</sub> NSBSO <sub>2</sub> Me	376.7	-1.81	-0.43	369.0	7.7
MeOSBSO <sub>2</sub> Me	332.0	-0.5	-0.43	329.9	2.1
MeSBSO <sub>2</sub> Me	323.1	-0.17	-0.43	321.8	1.3
HSBSO <sub>2</sub> Me	316.0	0.00	-0.43	316.6	-0.6
ClSBSO <sub>2</sub> Me	320.3	-0.22	-0.43	318.8	1.5
BrSBSO <sub>2</sub> Me	321.3	-0.33	-0.43	321.1	0.2

a) The  $\sigma_p$  values of substituents Me<sub>2</sub>N, MeO, Me, H, Cl, Br, and SO<sub>2</sub>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 excitedstate substituent parameter  $\sigma_{\rm CC}^{\rm ex}$  and the ground state polar substituent constant  $\sigma_p$  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  $E_{\rm T}(30)$  in quantifying the solvent effect. Furthermore, the regression model employed logP 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 logP can be used to scale the solvent effect on the UV absorption energy for other organic compounds requires further research.

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