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Research on Thermodynamic Properties of Polybrominated Diphenylamine by Neural Network

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Based on the location of bromine substituents and conjugation matrix, a new substituent position index ${}^0X$ not only was defined, but also molecular shape indexes K_m and electronegativity distance vectors M_m of diphenylamine and 209 kinds of polybrominated diphenylamine (PBDPA) molecules were calculated. Then the quantitative structure-property relationships (QSPR) among the thermodynamic properties of 210 organic pollutants and ${}^0X$, K_3, M_{29}, M_{36} were founded by Leaps-and-Bounds regression. Using the four structural parameters as input neurons of the artificial neural network, three satisfactory QSPR models with network structures of 4:21:1, 4:24:1, and 4:24:1 respectively, were achieved by the back-propagation algorithm. The total correlation coefficients R were 0.9999, 0.9997, and 0.9995 respectively and the standard errors S were 1.036, 1.469, and 1.510 respectively. The relative mean deviation between the predicted value and the experimental value of $S^\ominus$, $\Delta_f H^\ominus$ and $\Delta_f G^\ominus$ were 0.11%, 0.34% and 0.24% respectively, which indicated that the QSPR models had good stability and superior predictive ability. The results showed that there were good nonlinear correlations between the thermodynamic properties of PBDPAs and the four structural parameters. Thus, it was concluded that the ANN models established by the new substituent position index were fully applicable to predict properties of PBDPAs.

Key words: Polybrominated diphenylamine, Neural networks, Molecular shape index, Electronegativity distance vector, Substituent position index, Thermodynamic properties

I. INTRODUCTION

Due to good stability, diphenylamine has been widely applied to produce antioxidants, gunpowder stabilizers, intermediates of dyes and pesticide. However, its long-term exposure to the human body will damage to the nervous, cardiovascular system and blood system, also have teratogenic effect, even induce severe bladder cancer [1−5]. Polybrominated diphenylamines (PBDPAs) with typical characteristics of diphenylamine are mainly used as chemical intermediates of flame retardants, rodenticide, herbicides, fungicides, and other products [6, 7]. Because of the lack of their environmental risk assessment, the research on PBDPAs environmental toxicity is particularly important and urgent. Thermodynamic properties of PBDPAs, closely relating to their other physical and chemical properties, their formation and distribution in the environment, will be beneficial to investigate environmental toxicological effects of PBDPAs, but there are few researches reported [8].

As an easy and effective means to obtain data of the compounds properties, the quantitative structure-property relationships (QSPR) method has been widely employed in the studies of chemistry, environment, food, life, and so on [9−14]. In the work, combined with the artificial neural network (ANN) which can found models with high prediction accuracy [15−19], QSPR were used to calculate the thermodynamic properties of PBDPA. On the basis of the previous work [20, 21], a new substituent position index ${}^mX$ considering the location of bromine substituents on PBDPAs was defined, which reflected the location of bromine substituents on PBDPAs and contained characteristic information such as atomic electronegativity, molecular space structure. Then molecular shape indexes K_m and electronegativity distance vectors M_m were also calculated. Through multiple regression analysis between these indexes and thermodynamic parameters, standard entropy ($S^\ominus$), standard heat of formation ($\Delta_f H^\ominus$), and standard free energy ($\Delta_f G^\ominus$), several optimal structural parameters were selected as input neurons of ANN using the back-propagation (BP) algorithm. According to different network structures, the satisfactory prediction models for thermodynamic properties of PBDPAs were established, results were highly consistent with the values in Ref.[8].

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TABLE I The Results of ${}^0X$, K_m, M_m corresponding to $\Delta_f G^\ominus$ by Leaps-and-Bounds regression.

Subsets of variables	R	${R_{adj}}^2$	F	S	FIT
${}^0X$	0.976	0.953	4239.791	10.660	19.988
${}^0X$, K_3	0.991	0.981	5492.342	6.720	49.943
${}^0X$, K_3, M_{29}	0.992	0.984	4251.683	6.245	57.850
${}^0X$, K_3, M_{29}, M_{36}	0.994	0.989	4495.525	5.272	225.863
${}^0X$, K_3, M_{29}, M_{36}, K_1	0.994	0.988	3578.929	5.285	71.472

II. METHODOLOGY

A. Data of PBDPAs' thermodynamic properties

Based on the position and number of bromine substituents on the benzene ring, there exist maybe 209 kinds of isomers of PBDPA. The numbering system for C atoms in diphenylamine is shown in Fig.1.

The experimental data of three thermodynamic parameters, $S^\ominus$, $\Delta_f H^\ominus$ and $\Delta_f G^\ominus$ were obtained from Ref.[8].

B. New substituent position index ${}^mX$

Through studying the relationships between molecular structures of 209 kinds of PBDPAs or diphenylamine and their thermodynamic properties which were listed in Ref.[8], it can be concluded that the thermodynamic properties were closely related to the position and number of bromine substituents on the benzene ring. Taking the nitrogen atom as the starting point denoted by 0, the atomic characteristic value of atom i was defined as δ_i:

$$\delta_{i,1-6} = \frac{\chi_i - 2.5}{\chi_{\rm C} - 2.5} P^{(\chi_{\rm C}-2.3)/(\chi_i-2.3)} \tag{1}$$

where χ_i was the electronegativity of atom i, $\chi_{\rm C}$ denoted the electronegativity of the carbon atom and P represented the serial number of bromine substituents on the benzene ring of PBDPA. When there were two or more substituents locating at position $1'-6'$, their contribution to the molecule was different from the same substituents locating at position 1−6. After optimization, the matrices δ_i of atoms locating at position $1'-6'$ was modified as follows:

$$\delta_{i,1'-6'} = 1.04\delta_{i,1-6} \tag{2}$$

Therefore, matrices δ_i of diphenylamine are also presented in Fig.1.

Using Eqs.(1) and (2), $\delta_{\rm Br}$ of Br atoms locating at position 2−6 and $2'-6'$ were calculated and their results are: $\delta_{\rm Br2}$=11.962, $\delta_{\rm Br3}$=13.948, $\delta_{\rm Br4}$=15.554, $\delta_{\rm Br5}$=16.926, $\delta_{\rm Br6}$=18.136, $\delta_{\rm Br2'}$=12.440, $\delta_{\rm Br3'}$=14.506, $\delta_{\rm Br4'}$=16.176, $\delta_{\rm Br5'}$=17.603, $\delta_{\rm Br6'}$=18.861. Based on the above results, the substituent position index ${}^mX$ was defined:

$${}^mX = \sum(\delta_i\delta_j\delta_k\cdots)^{0.5} \tag{3}$$

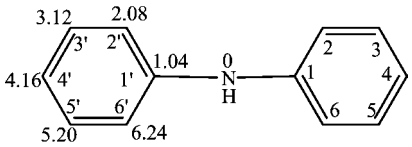

FIG. 1 Numbering system for C atoms and matrices in diphenylamine.

where j represents the non-hydrogen atom directly attached to atom i, k indicates the non-hydrogen atom directly attached to atom j, and so forth. In this work, only the 0-order index was calculated as ${}^0X$:

$${}^0X = \sum(\delta_i)^{0.5} \tag{4}$$

C. Establishing indices and selecting variables

On the basis of molecular conjugation matrix [22], molecular shape index K_m was defined by Kier and it was used to characterize molecular shape [23, 24]. The electronegativity distance vector M_m obtained by a certain formula [25] was employed to simulate molecular interactions among different non-hydrogen atoms. In this work, K_m, M_m and ${}^mX$ were applied as independent variables. Meanwhile three thermodynamic parameters of PBDPAs, $S^\ominus$, $\Delta_f H^\ominus$ and $\Delta_f G^\ominus$, were used as dependent variables. By Leaps-and-Bounds regression (LBR), the variables were extracted to carry out statistical regression analysis, such as the regression analysis of $\Delta_f G^\ominus$ presented in Table I.

In Table I, R, ${R_{adj}}^2$, F and S were correlation coefficient, the coefficient of determination, Fischer test value and the standard error, respectively. To be noted, the value of FIT (Kubinyi function) [26], was introduced and calculated as follows:

$$\text{FIT} = \frac{R^2(y-b-1)}{(y+b^2)(1-R^2)} \tag{5}$$

where y represents the sample size of compounds and b is the number of variables. The bigger the value of FIT was, the more stable the model would be, as well as the higher the predictive ability of the model would be. From the results in Table I, the best regression results with PBDPAs' thermodynamic properties were achieved by selecting substituent position index

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^0X, molecular shape index K_3, electronegativity distance vectors M_{29} and M_{36}.

III. RESULTS AND DISCUSSION

A. Multiple regression model

According to the thermodynamic properties of PBDPAs reported in Ref.[8], the correlations between thermodynamic properties and four kinds of variables including ^0X, K_3, M_{29}, M_{36} have been analyzed. Multiple regression equations are shown as follows:

$$S^\ominus = 9.431\,^0X + 6.504K_3 - 1.446M_{29} + 0.0517M_{36} + 210.269 \quad (6)$$

$$\Delta_f H^\ominus = 7.225\,^0X - 16.877K_3 - 1.960M_{29} + 2.383M_{36} + 49.181 \quad (7)$$

$$\Delta_f G^\ominus = 5.402\,^0X - 19.902K_3 - 1.683M_{29} + 2.351M_{36} + 231.401 \quad (8)$$

The correlation coefficient R, represented standard error S, and the Fischer test value F for Eqs.(6)−(8) are shown in Table II.

From Table II, all the correlation coefficients of the multiple regression equations are bigger than 0.99, which indicates that the QSPR models were satisfactory.

B. Neural network model

The four parameters ^{0}X, K_3, M_{29} and M_{36} were selected as input neurons while the thermodynamic properties of PBDPAs were used as output neurons. The optimal number of hidden layer unit H, was calculated according to the rules proposed by Xu *et al.* [27]: $2.2>\rho(=N/M)\geq 1.4$, where N was the sample size and M denoted the total weight of the network which was obtained by the following equation:

$$M = (I+1)H + (H+1)Q \quad (9)$$

where I, H and Q were the numbers of variables in the input layer, the hidden layer, and the output layer, respectively. In this work, N=210 and I=4 so that the value of H was an integer arranging from 16 to 24. After repeated testing, the optimal results of $S^\ominus$ were achieved when H=21, while H=24 to obtain those of $\Delta_f H^\ominus$ and $\Delta_f G^\ominus$. In order to test the stability and predictive ability of the model, the sample data of each property have been divided into three groups, *viz.* training set, test set and validation set, to establish various neural network models as shown in Table III.

The correlation coefficients of the three sets were almost equal to the corresponding total correlation coefficients, which indicated that the models were quite stable and there was no overfitting or overtraining phenomenon. The predictive results of thermodynamic properties by the neural network model are presented in Table IV. Comparing the results in Table II with those in Table III, it showed that the standard errors of the neural network model were significantly less than those obtained by the multiple regression method. In the meantime, the correlation coefficients of the neural network model were all close to 1. Our predictive results highly agreed with those reported in Ref.[8]. Moreover, our neural network model with four variables had better correlation coefficients and smaller standard errors than the model in the literature [8]. Hence, our model had stronger predictive ability.

TABLE II QSPR between characteristic parameters and $S^\ominus$, $\Delta_f H^\ominus$, $\Delta_f G^\ominus$ of PBDPAs.

Parameter	R	S	F	FIT
$S^\ominus$	0.998	4.386	11720.34	81.555
$\Delta_f H^\ominus$	0.997	5.134	7668.301	128.676
$\Delta_f G^\ominus$	0.994	5.272	4495.525	225.863

For isomers of the same group, the smaller $\Delta_f G^\ominus$ was, the more stable the molecule was, and vice versa [28]. $\Delta_f G^\ominus$ of the molecule with bromine substituents located in the same benzene ring and at the adjacent position of nitrogen atom, would be bigger due to the larger interactions between bromine atom and nitrogen atom which would increase molecular instability. However, when bromine substituents located in the different benzene ring and at the meta-position of nitrogen atom or at the meta-position of each other, $\Delta_f G^\ominus$ would be smaller because of the smaller interactions between heteroatoms with large spacing which would enhance molecular stability. Furthermore, molecular volume of PBDPA as well as the values of $S^\ominus$, $\Delta_f H^\ominus$ and $\Delta_f G^\ominus$, increased with the number of bromine substituents. As shown in Table III, it was confirmed that ^0X combined with K_3, M_{29}, and M_{36} revealed essential influence factors of PBDPA's thermodynamic properties. The mean relative errors between predictive results obtained by neural network models and the data reported in the literature were only between 0.1%−0.3%, which indicated the predictive ability of neural network model was better than that of the multiple regression model.

IV. CONCLUSION

Substituent position index ^mX can reflect molecular stability. As shown in Table IV, $\Delta_f G^\ominus$ of the molecule with bromine substituents located at position 2 and 6 would be bigger, however it would be smaller when bromine substituents located at position 3(3′) and 5(5′). Thus, ^mX had good correlation with $\Delta_f G^\ominus$.

^mX contained molecular spatial structure information. The molecular volume of PBDPAs would be bigger when the number of bromine substituents increased, meanwhile those thermodynamic data would also increase. These change rules can be fully reflected by ^0X.

The neural network method was superior to the mul-

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TABLE III BP neural network model of PBDPA.

Parameter	Network structure	Correlation coefficient				S	Relative error[a]/%
		Total	Training set	Test set	Validation set		
$S^{\ominus}$	4:21:1	0.9999	0.9999	0.9999	0.9999	1.036	0.11
$\Delta_f H^{\ominus}$	4:24:1	0.9997	0.9997	0.9997	0.9998	1.469	0.34
$\Delta_f G^{\ominus}$	4:24:1	0.9995	0.9996	0.9993	0.9997	1.510	0.24

[a] Relative errors between predictive results obtained by neural network models and the data reported in Ref.[8].

TABLE IV The predicted values of the thermodynamic properties of PBDPA including $S^{\ominus}$ (in J/(mol·K)), $\Delta_f H^{\ominus}$ (in kJ/mol), and $\Delta_f G^{\ominus}$ (in kJ/mol).

Substituent	$S^{\ominus}$	$\Delta_f H^{\ominus}$	$\Delta_f G^{\ominus}$	Substituent	$S^{\ominus}$	$\Delta_f H^{\ominus}$	$\Delta_f G^{\ominus}$
DPA	424.14	163.44	300.22	2,3,3′,4,4′	614.13	319.29	420.34
2	457.88	196.96	326.86	2,3,3′,4,5	618.37	308.42	405.56
3	465.04	185.15	312.97	2,3,3′,4′,5	621.32	300.10	392.85
4	465.59	185.77	313.86	2,3,3′,4,5′	620.04	310.17	411.02
2,2′	497.13	214.11	335.70	2,3,3′,4,6	615.60	319.54	411.00
2,3	495.57	230.57	352.49	2,3,3′,4′,6	614.82	309.57	403.91
2,3′	499.77	217.91	338.79	2,3,3′,5,5′	623.06	291.24	386.27
2,4	501.34	222.66	344.29	2,3,3′,5,6	614.95	311.57	411.86
2,4′	500.44	218.71	339.99	2,3,3′,5′,6	618.31	303.80	399.65
2,5	500.87	204.59	325.23	2,3,4,4′,5	620.40	311.65	403.83
2,6	495.58	219.59	342.08	2,3,4,4′,6	615.44	317.10	415.62
3,3′	507.73	207.06	327.12	2,3,4,5,6	609.31	341.04	439.83
3,4	504.37	216.96	336.87	2,3,4′,5,6	615.08	316.83	411.60
3,4′	507.09	208.39	327.37	2,3′,4,4′,5	620.47	297.60	393.27
3,5	506.26	208.98	326.83	2,3′,4,4′,6	618.00	301.70	401.27
4,4′	506.92	210.46	329.10	2,3′,4,5,5′	620.93	305.37	401.12
2,2′,3	535.00	246.36	361.45	2,3′,4,5′,6	619.58	297.96	394.09
2,2′,4	538.70	240.76	355.20	2,3,3′,4′,5′	616.31	320.13	416.84
2,2′,5	537.81	238.21	352.29	2,3′,4,4′,5′	622.25	301.05	393.98
2,2′,6	534.98	239.34	354.57	2,3′,4′,5,5′	621.54	298.58	395.30
2,3,3′	538.66	251.79	364.45	2,3′,4′,5′,6	617.29	308.86	407.54
2,3,4	535.38	265.95	380.55	3,3′,4,4′,5	621.79	310.16	404.81
2,3,4′	540.63	238.33	353.49	3,3′,4,5,5′	624.50	303.22	398.02
2,3,5	540.18	239.61	351.31	2,2′,3,3′,4,4′	651.96	340.92	429.50
2,3,6	534.11	255.91	369.43	2,2′,3,3′,4,5	652.01	351.51	444.21
2,3′,4	541.96	245.86	357.68	2,2′,3,3′,4,5′	654.92	343.91	428.26
2,3′,5	542.51	231.43	340.72	2,2′,3,3′,4,6	650.38	345.81	436.71
2,3′,6	538.49	243.35	354.50	2,2′,3,3′,4,6	659.38	359.28	443.58
2,4,4′	542.50	246.69	357.78	2,2′,3,3′,5,5′	657.65	335.37	425.65
2,4,5	539.59	257.36	368.42	2,2′,3,3′,5,6	650.61	344.39	432.61
2,4,6	539.68	249.39	361.00	2,2′,3,3′,5,6′	654.47	337.88	424.25
2,4′,5	541.47	244.93	356.98	2,2′,3,3′,6,6′	650.08	347.80	440.04
2,4′,6	536.86	242.68	356.77	2,2′,3,4,4′,5	654.35	345.62	432.86
2,3′,4′	538.65	248.21	361.52	2,2′,3,4,4′,5′	655.35	346.22	432.03
2,3′,5′	542.62	240.48	354.56	2,2′,3,4,4′,6	654.20	341.34	426.77
3,3′,4	545.32	240.76	352.37	2,2′,3,4,4′,6′	655.34	337.82	428.74
3,3′,5	547.65	234.44	344.38	2,2′,3,4,5,5′	654.39	336.70	430.27
3,4,4′	546.68	242.19	352.03	2,2′,3,4,5,6	647.78	361.62	452.66
3,4,5	544.09	251.98	363.52	2,2′,3,4,5,6′	652.08	362.30	452.85
3,4′,5	549.99	233.70	344.48	2,2′,3,4,5′,6	653.80	338.12	427.74

To be continued.

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Table IV continued.

Substituent	$S^{\ominus}$	$\Delta_f H^{\ominus}$	$\Delta_f G^{\ominus}$	Substituent	$S^{\ominus}$	$\Delta_f H^{\ominus}$	$\Delta_f G^{\ominus}$
2,2′,3,3′	575.01	278.64	384.25	2,2′,3,4,6,6′	650.54	354.50	442.67
2,2′,3,4	574.92	283.16	392.43	2,2′,3,4′,5,5′	659.07	333.12	423.30
2,2′,3,4′	577.51	273.37	378.88	2,2′,3,4′,5,6	631.60	337.81	426.00
2,2′,3,5	578.30	274.57	382.28	2,2′,3,4′,5,6′	654.84	342.28	432.30
2,2′,3,5′	578.24	272.43	376.78	2,2′,3,4′,5′,6	653.71	332.71	424.44
2,2′,3,6	573.47	275.58	380.64	2,2′,3,4′,6,6′	653.32	343.31	432.89
2,2′,3,6′	574.11	271.84	379.70	2,2′,3,5,5′,6	654.76	338.61	429.75
2,2′,4,4′	580.63	264.51	372.05	2,2′,3,5,6,6′	649.63	355.53	442.41
2,2′,4,5	576.11	274.61	381.47	2,2′,4,4′,5,5′	656.78	336.35	422.21
2,2′,4,5′	579.75	263.80	369.60	2,2′,4,4′,5,6′	655.52	330.14	417.88
2,2′,4,6	574.53	267.72	372.97	2,2′,4,4′,6,6′	654.54	340.59	427.59
2,2′,4,6′	575.21	264.88	370.47	2,3,3′,4,4′,5	657.39	343.23	431.78
2,2′,5,5′	580.73	263.46	367.71	2,3,3′,4,4′,5′	655.83	355.88	444.92
2,2′,5,6′	575.45	265.58	371.89	2,3,3′,4,4′,6	655.00	348.01	438.61
2,2′,6,6′	572.09	279.10	384.48	2,3,3′,4,5,5′	659.00	337.70	423.82
2,3,3′,4	581.32	272.83	378.11	2,3,3′,4,5,6	652.89	363.91	455.02
2,3,3′,4′	575.88	283.99	387.47	2,3,3′,4,5′,6	657.38	342.92	430.26
2,3,3′,5	581.60	265.82	368.45	2,3,3′,4,5,5′	657.99	347.73	438.89
2,3,3′,5′	580.88	273.66	379.46	2,3,3′,4′,5,6	654.06	349.14	437.33
2,3,3′,6	577.74	278.87	380.43	2,3,3′,4′,5′,6	654.53	345.96	434.16
2,3,4,4′	578.62	288.99	390.71	2,3,3′,5,5′,6	656.42	342.24	431.03
2,3,4,5	578.03	284.36	388.79	2,3,4,4′,5,6	651.47	364.95	454.58
2,3,4,6	573.70	293.30	398.34	2,3′,4,4′,5,5′	633.36	345.65	440.33
2,3,4′,5	580.47	280.04	384.37	2,3′,4,4′,5′,6	658.07	340.02	428.53
2,3,4′,6	575.23	278.01	382.53	3,3′,4,4′,5,5′	661.30	345.67	432.92
2,3,5,6	572.44	292.04	396.49	2,2′,3,3′,4,4′,5	690.56	393.00	470.64
2,3′,4,4′	581.39	276.58	382.59	2,2′,3,3′,4,4′,6	690.93	381.35	466.19
2,3′,4,5	580.80	281.73	385.10	2,2′,3,3′,4,5,5′	694.40	381.33	463.31
2,3′,4,5′	582.94	270.83	373.70	2,2′,3,3′,4,5,6	687.08	394.50	475.08
2,3′,4,6	580.04	275.74	375.33	2,2′,3,3′,4,5,6′	690.94	379.04	463.81
2,3′,4′,5	580.90	276.90	380.77	2,2′,3,3′,4,5′,6	692.89	374.29	453.37
2,3′,4′,6	577.45	274.92	379.29	2,2′,3,3′,4,6,6′	687.89	386.18	471.87
2,3′,5,5′	583.35	270.18	373.43	2,2′,3,3′,4,5′,6′	692.47	380.84	458.52
2,3′,5′,6	579.35	267.73	371.94	2,2′,3,3′,5,5′,6	692.14	377.58	459.61
2,4,4′,5	581.87	264.96	368.39	2,2′,3,3′,5,6,6′	689.40	384.38	467.95
2,4,4′,6	577.97	274.47	378.20	2,2′,3,4,4′,5,5′	694.22	380.25	462.55
2,3′,4′,5′	579.12	272.34	379.03	2,2′,3,4,4′,5,6	691.27	390.02	471.13
3,3′,4,4′	584.35	272.56	377.61	2,2′,3,4,4′,5,6′	692.23	377.18	455.60
3,3′,4,5	583.77	275.42	379.78	2,2′,3,4,4′,5′,6	692.72	374.19	454.48
3,3′,4,5′	586.10	268.50	370.00	2,2′,3,4,4′,6,6′	672.44	383.46	465.12
3,3′,5,5′	586.99	261.13	363.24	2,2′,3,4,5,5′,6	690.46	383.91	464.93
3,4,4′,5	583.52	279.19	379.68	2,2′,3,4,5,6,6′	687.25	398.73	484.57
2,2′,3,3′,4	613.94	315.42	413.70	2,2′,3,4′,5,5′,6	690.89	372.81	455.83
2,2′,3,3′,5	614.65	309.22	406.46	2,2′,3,4′,5,6,6′	690.30	383.17	462.76
2,2′,3,3′,6	613.09	305.98	406.37	2,3,3′,4,4′,5,5′	693.28	394.72	476.00
2,2′,3,4,4′	616.39	313.39	406.55	2,3,3′,4,4′,5,6	693.12	395.89	478.85
2,2′,3,4,5	613.94	320.95	420.73	2,3,3′,4,4′,5′,6	694.65	385.80	466.20
2,2′,3,4,5′	616.08	308.48	404.53	2,3,3′,4,5,5′,6	692.79	390.09	471.49
2,2′,3,4,6	611.11	313.88	411.63	2,3,3′,4′,5,5′,6	692.66	383.59	463.53

To be continued.

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Table IV continued.

Substituent	$S^{\ominus}$	$\Delta_f H^{\ominus}$	$\Delta_f G^{\ominus}$	Substituent	$S^{\ominus}$	$\Delta_f H^{\ominus}$	$\Delta_f G^{\ominus}$
2,2′,3,4,6′	616.27	307.93	405.09	2,2′,3,3′,4,4′,5,5′	728.42	426.93	501.39
2,2′,3,4′,5	618.01	304.40	398.30	2,2′,3,3′,4,4′,5,6	726.61	429.99	505.18
2,2′,3,4′,6	615.58	300.36	397.81	2,2′,3,3′,4,4′,5,6′	726.65	419.46	491.37
2,2′,3,5,5′	618.24	300.07	398.28	2,2′,3,3′,4,4′,6,6′	725.81	426.20	502.01
2,2′,3,5,6	610.21	324.16	422.71	2,2′,3,3′,4,5,5′,6	729.20	423.01	496.77
2,2′,3,5,6′	613.87	300.76	396.99	2,2′,3,3′,4,5,5′,6′	727.43	417.06	490.71
2,2′,3,5′,6	614.91	298.71	397.73	2,2′,3,3′,4,5,6,6′	725.25	438.51	511.12
2,2′,3,6,6′	611.37	315.24	413.77	2,2′,3,3′,4,5′,6,6′	728.02	427.41	499.25
2,2′,3,4′,5′	616.32	303.59	408.23	2,2′,3,3′,5,5′,6,6′	728.44	425.40	498.82
2,2′,3,4′,6′	615.08	301.46	400.15	2,2′,3,4,4′,5,5′,6	730.98	422.80	498.53
2,2′,4,4′,5	617.57	302.93	397.52	2,2′,3,4,4′,5,6,6′	728.24	428.37	502.88
2,2′,4,4′,6	616.26	295.55	395.35	2,3,3′,4,4′,5,5′,6	729.31	433.37	506.35
2,2′,4,5,5′	617.01	302.31	395.06	2,2′,3,3′,4,4′,5,5′,6	763.23	467.81	534.39
2,2′,4,5,6′	615.60	298.50	396.26	2,2′,3,3′,4,4′,5,6,6′	764.33	472.99	540.97
2,2′,4,5′,6	596.00	295.67	396.96	2,2′,3,3′,4,5,5′,6,6′	765.31	474.74	540.87
2,2′,4,6,6′	612.68	308.87	405.30	2,2′,3,3′,4,4′,5,5′,6,6′	800.97	523.49	583.02

tiple regression method. Using the former method, there were good nonlinear correlations rather than simple linear relationships between those indices and thermodynamic properties, which showed the predictive ability of neural network model was better than that of the multiple regression model. Moreover, the former also had fine stability which was reflected by FIT values.

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