Modification of Wiener Index and Its Application

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A novel topological index based on the Wiener Index is proposed as $W^* = 1/2\sum_{i,j=1}^{n} S_{ij}^*$, the element S_{ij}^* of the distance matrix is defined either as $S_{ij}^* = \alpha \cdot \sqrt{I_i I_j}/R_{ij}$ (atoms i and j are adjacent) or as $S_{ij}^* = \alpha \cdot \sqrt[j-i+1]{I_i \times \cdots \times I_j}/R_{ij}$ (atoms i and j are not adjacent), where I_i and I_j represent the electronegativity of vertices i or j, respectively, R_{ij} is the sum of the bond length between the vertices i and j in a molecular graph, and $\alpha = (Z_i/Z_j)^{0.5}$, where Z_i and Z_j are the atomic numbers of the positive valence atom i and the negative valence atom j, respectively. The properties and the interaction of the vertices in a molecule are taken into account in this definition. That is why the application of the index W^* to heteroatom-containing and multiple bond organic systems and inorganic systems is possible. Correlation coefficients above 0.97 are achieved in the prediction of the retention index of gas chromatography of the hydrocarbons, the standard formation enthalpy of methyl halides, halogen−silicon, and inorganic compounds containing transition metals.

1. INTRODUCTION

During the past 20 years, the QSPR and QSAR techniques have gained wide acceptance in physical, organic, analytical, medicinal chemistry, biochemistry, toxicology, and environmental sciences.[1−7] The molecular topological index has been widely used in QSPR/QSAR models because of its simple calculation. The Wiener number, *W*, is one of the best descriptors of molecular topology. It was defined in 1947 for saturated acyclic hydrocarbons as the sum of the bonds between all pairs of non-hydrogen atoms in the molecule.[8] Hosoya extended the original definition to cyclic compounds with the aid of the distance matrix and gave the formula for the Wiener Index as half the sum of the distance matrix.[9] In recent years a modification of the Wiener number was developed by the elements of the matrices of vertex- and edge-weighted molecular graphs. Klein and Randic introduced the Kirchhoff number based on the concepts of resistance distance and resistance matrix by analogy with the theory of electrical networks.[10,11] The idea of using reciprocal distances in computing vertex topological indices was adopted by the definition of the reciprocal distance matrix.[12,13] Hyper-Wiener Index,[14,15] Detour Index,[16] Hyper-Detour Index,[17] Harary Index,[18] Pasareti Index,[19] and Verhalom Index[19] were proposed based on the distance-related matrices, such as detour Δ,[20] detour-distance Δ-**D**,[20] and distance-valence **Dval**.[21] These distance matrices were made up of the shortest distances from vertex *i* to all other $(n-1)$ vertices in the molecular graphs, and the shortest distance of two adjacent atoms was set as "1". The Wiener number *W* and its modification are widely used to account for isomeric variations of many physicochemical properties such as boiling points, molar volumes of alkanes, alcohols, and so on; however, it could not reveal the real connection among atoms. The Wiener Index is applicable to hydrocarbons. However, to our knowledge, no application in the inorganic system has been reported. The Wiener number *W* is considered the distance between the atoms in the molecule, and this concept is still valid. We have extended the concept of Wiener, defined a novel topological index, and applied it to some unsaturated hydrocarbons, organic compounds and inorganic compounds.[22,23] In this study, we redefined the element of the distance matrix, which revealed the properties and the interaction of vertices in a molecule, and extended the applicable scope of distance matrix index *w* to the heteroatom-containing organic compounds, unsaturated organic compounds, and inorganic compounds.

2. DEFINITION

The distance matrix **S** is composed of the shortest distances from one atom to the others in a molecular graph. If a molecule contains *n* atoms, there is a symmetric matrix **S**:

$$S = \begin{pmatrix} S_{11} & S_{12} & \cdots & S_{1n} \\ S_{21} & S_{22} & \cdots & S_{2n} \\ \vdots & \vdots & & \vdots \\ S_{n1} & S_{n2} & \cdots & S_{nn} \end{pmatrix} \quad (1)$$

The Wiener number W^8 is

$$W = \frac{1}{2}\sum_{i,j=1}^{n} S_{ij} \quad (2)$$

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Table 1. α, R_{ij}, and S_{ij}^* of Some Bonds

	C−C	C=C	C≡C	C···C	C−O	C=O	C−F	C−Cl	C−Br	C−I
α	1.0000	1.0000	1.0000	1.0000	0.8660	0.8660	0.8165	0.5941	0.4140	0.3365
R_{ij}	1.0000	0.8701	0.7792	0.9026	0.9286	0.7922	0.8961	1.1494	1.2534	1.3896
S_{ij}^*	2.5000	2.8733	3.2085	2.7698	2.7586	3.2337	2.8814	1.4155	0.8739	0.6054

Chart 1. A molecular graph of 5 linked atoms
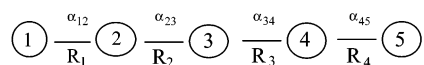
Table 2. W^* and RI^{25} of Some Compounds

compd	W^*	RI	compd	W^*	RI
propane	6.2500	300.0	pentene	16.5603	481.0
butane	10.8333	400.0	hexene	22.2818	581.8
pentane	16.0415	500.0	heptene	28.4161	681.5
hexane	21.7498	600.0	ethyne	3.2085	155.1
heptane	27.8748	700.0	butyne	11.7633	385.4
octane	34.3571	800.0	pentyne	17.0080	484.1
nonane	41.1519	900.0	hexyne	22.7393	585.5
propene	6.7100	286.7	heptyne	28.8800	686.5
butene	11.3310	384.8			

In Wiener's study,[8] W is only considered the length of edge but not the properties and interaction of the vertices. Electronegativity, which represents the ability of atoms to obtain or lose electrons, is one of the main properties of atoms. The larger the electronegativity of an atom, the stronger the ability of the atom to attract electrons. Furthermore, the interaction between atoms, which is the process in which the atomic energies are reassigned among them, involves not only their distance but also their energies. The measurement elements of the foregoing distance-related matrices only considered their distances but not their energies. We know electronegativity represents the ionization energy and the electron affinity of atoms. So electronegativity and the distance between atoms are used to represent the properties and the interaction of the vertices in a molecule. S_{ij} is redefined as S_{ij}^* as follows.

$$S_{ij}^* = \begin{cases} \dfrac{\alpha_{ij} \cdot \sqrt{I_i I_j}}{R_{ij}} = x & i,j \text{ are adjacent} \\[3mm] \dfrac{\alpha_{ik\cdots j} \cdot \sqrt[j-i+1]{I_i I_k \cdots I_j}}{R_{ij}} = x' & i,j \text{ are not adjacent} \\[3mm] 0 & i = j \end{cases}$$

(3)

In eq 3, I_i and I_j refer to Pauling's electronegativity values of the vertices i and j, respectively.[24] R_{ij} is the sum of the bond length from the vertices i to j. If the vertices i and j are adjacent, R_{ij} is the bond length. R_{ij} can be obtained in three ways: (1) the relative value of the bond length[24] (take C−C bond length 0.154 nm as 1); (2) the relative value of the sum of the covalent radius (take the sum of C−C covalent radius 0.154 nm as (1); (3) $R_{ij} = n_i + n_j$, where n_i and n_j represent the maximum principal quantum number of atoms i and j, respectively. On the other hand, if the vertices i and j are not adjacent, R_{ij} is the sum of all the bond length of adjacent atoms from vertices i to j in the molecular graph. The same is done, if the vertices i and j are adjacent, $\alpha = (Z_i/Z_j)^{0.5}$, where Z_i is the atomic number of the positive atom i and Z_j is the atomic number of the negative atom j (but hydrogen is always positive atom). Otherwise, α is the

arithmetic mean of all α values for all bonds from vertices i to j. α means the differences of interaction of the electrons in the vertices i and j. In the following example, Chart 1, where there are *five* linked atoms in a molecule, the values of S_{ij}^* were calculated as follows:

$$S_{12}^* = \frac{\alpha_{12}\sqrt{I_1 I_2}}{R_1}, \quad S_{23}^* = \frac{\alpha_{23}\sqrt{I_2 I_3}}{R_2}, \quad S_{34}^* = \frac{\alpha_{34}\sqrt{I_3 I_4}}{R_3},$$

$$S_{45}^* = \frac{\alpha_{45}\sqrt{I_4 I_5}}{R_4}$$

$$S_{13}^* = \frac{(\alpha_{12} + \alpha_{23})/2}{R_1 + R_2} \cdot \sqrt[3]{I_1 I_2 I_3}, \ \ldots,$$

$$S_{35}^* = \frac{(\alpha_{34} + \alpha_{45})/2}{R_3 + R_4} \cdot \sqrt[3]{I_3 I_4 I_5}; \ldots$$

$$S_{15}^* = \frac{(\alpha_{12} + \alpha_{23} + \alpha_{34} + \alpha_{45})/4}{R_1 + R_2 + R_3 + R_4} \cdot \sqrt[5]{I_1 I_2 I_3 I_4 I_5}$$

The definition of S_{ij}^* infers that the longer the distance between vertices i to j, the smaller S_{ij}^*. The interaction between vertices i and j becomes weaker indeed, when the distance between the vertices i and j grows.

3. RESULTS AND DISCUSSION

For Hydrocarbons. In the hydrogen-suppressed graph of the organic compounds, hydrogen atoms were neglected. Some bonds of organic compounds, such as C−C, C=C, C ≡ C, C···C, C=O, C−O, C−F, C−Cl, C−Br, C−I, α, R_{ij}, S_{ij}^* are listed in Table 1, where R_{ij} [24] is the relative value of bond length. (Take C−C bond length 0.154 nm as 1).

According to eqs 2 and 3, a novel topological index W^* stood for the old Wiener Index W (formula 4).

$$W^* = \frac{1}{2}\sum_{i,j=1}^{n} S_{ij}^* \tag{4}$$

Listed in Table 2 are the values of W^* and the corresponding retention indices of gas chromatography RI^{25} of the hydrocarbons, where W^* is calculated by formula 4 and RI are from ref 25. The correlative result obtained by applying W^* to RI is

$$\ln RI = 4.4046 + 0.6405 \ln W^* \tag{5}$$

$$r = 0.9934, \sigma = 0.0519, F = 1124.59, n = 17$$

Here r is the correlation coefficient, σ is the standard error, F means *Fischer* value, and n is the regression number of molecules. The above-mentioned result shows that W^* has a high correlativity to hydrocarbons with multiple bonds.

For Methyl Halide. For such small molecules as methyl halides, hydrogen atoms have great influence on their

Table 3. W^* and $\Delta_f H_m^{\Phi}$ [26](kJ·mol^{-1}) of Halide Halides

compd	W^*	$\Delta_f H_m^{\Phi}$	compd	W^*	$\Delta_f H_m^{\Phi}$	compd	W^*	$\Delta_f H_m^{\Phi}$	compd	W^*	$\Delta_f H_m^{\Phi}$
CH$_2$F$_2$	3.3807	−452.9	CBr$_3$F	2.0327	−190.0	CBrClF$_2$	3.1351	−471.5	CH$_2$I$_2$	1.4267	118.4
CCl$_2$F$_2$	3.4326	−493.3	CBr$_3$Cl	1.5314	12.6	CH$_2$BrCl	1.9472	−50.2	CH$_2$FCl	2.7862	−264.4
CH$_2$Cl$_2$	2.2215	−95.4	CHI$_3$	1.1161	210.9	CHBrClF	2.5318	−295.0	CH$_2$ClI	1.8132	12.6
CHCl$_2$F	2.8182	−284.9	CF$_4$	4.6766	−933.0	CH$_2$BrI	1.5522	50.2	CH$_3$I	1.7732	13.8
CBr$_2$F$_2$	2.8455	−429.7	CCl$_4$	2.3078	−95.8	CHF$_3$	4.0198	−693.3	CH$_2$FBr	2.4965	−252.7
CBr$_2$Cl$_2$	1.7823	−29.3	CI$_4$	0.8414	262.9	CF$_3$I	3.5636	−589.9	CH$_4$	2.1556	−74.9
CH$_2$Br$_2$	1.6808	−14.8	CBr$_4$	1.2884	79.5	CCl$_3$F	2.8553	−284.9	CBrCl$_3$	2.0411	−37.2
CHBr$_2$F	2.2543	−223.4	CHBrF$_2$	3.1028	−463.6	CHF$_2$Cl	3.4041	−483.7	CH	0.3118	594.1
CHBr$_2$Cl	1.7290	−20.9	CHBrCl$_2$	1.9916	−58.6	CF$_3$Cl	4.0397	−707.9	CH$_2$	0.7750	386.4
CBr$_2$ClF	2.2990	−231.8	CBrCl$_2$F	2.5732	−269.4	CF$_3$Br	3.7268	−648.9	CH$_3$	1.3896	145.7
CHBr$_3$	1.4743	16.7	CH$_3$Br	1.9079	−37.7	CH$_3$F	2.7593	−237.7	CHCl$_3$	2.2621	−102.9

Chart 2. Molecular Graph of CHFClBr
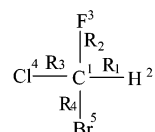
properties, so the effect of hydrogen atoms cannot be neglected. A hydrogen atom must be treated as a vertex in the molecular graph. Now we take an example to illustrate how to get W^*. For the CHFClBr molecule (the molecular graph is Chart 2), the central atom C is labeled as "1", and the others are labeled as "2", "3", "4", and "5" at random. Their bond lengths with the central atom C are successively R_1, R_2, R_3, and R_4, respectively. The distance matrix S^* and W^* of the CHFClBr molecule can be expressed as follows:

$$S^* =$$

$$\begin{vmatrix} 0 & \dfrac{\alpha_{12}\sqrt{I_1 I_2}}{R_1} & \dfrac{\alpha_{13}\sqrt{I_1 I_3}}{R_2} & \dfrac{\alpha_{14}\sqrt{I_1 I_4}}{R_3} & \dfrac{\alpha_{15}\sqrt{I_1 I_5}}{R_4} \\ \dfrac{\alpha_{21}\sqrt{I_1 I_2}}{R_1} & 0 & \dfrac{\alpha_{23}\sqrt[3]{I_1 I_2 I_3}}{R_1+R_2} & \dfrac{\alpha_{24}\sqrt[3]{I_1 I_2 I_4}}{R_1+R_3} & \dfrac{\alpha_{25}\sqrt[3]{I_1 I_2 I_5}}{R_1+R_4} \\ \dfrac{\alpha_{31}\sqrt{I_1 I_3}}{R_2} & \dfrac{\alpha_{32}\sqrt[3]{I_1 I_2 I_3}}{R_1+R_2} & 0 & \dfrac{\alpha_{34}\sqrt[3]{I_1 I_3 I_4}}{R_2+R_3} & \dfrac{\alpha_{35}\sqrt[3]{I_1 I_3 I_5}}{R_2+R_4} \\ \dfrac{\alpha_{41}\sqrt{I_1 I_4}}{R_3} & \dfrac{\alpha_{42}\sqrt[3]{I_1 I_2 I_4}}{R_1+R_3} & \dfrac{\alpha_{43}\sqrt[3]{I_1 I_3 I_4}}{R_2+R_3} & 0 & \dfrac{\alpha_{45}\sqrt[3]{I_1 I_4 I_5}}{R_3+R_4} \\ \dfrac{\alpha_{51}\sqrt{I_1 I_5}}{R_4} & \dfrac{\alpha_{52}\sqrt[3]{I_1 I_2 I_5}}{R_1+R_4} & \dfrac{\alpha_{53}\sqrt[3]{I_1 I_3 I_5}}{R_2+R_4} & \dfrac{\alpha_{54}\sqrt[3]{I_1 I_4 I_5}}{R_3+R_4} & 0 \end{vmatrix}$$

$$W^* = \frac{1}{2}\sum_{i \cdot j=1}^{5} S_{ij}^*$$

$$= \frac{\alpha_{12}\sqrt{I_1 I_2}}{R_1} + \frac{\alpha_{13}\sqrt{I_1 I_3}}{R_2} + \frac{\alpha_{14}\sqrt{I_1 I_4}}{R_3} + \frac{\alpha_{15}\sqrt{I_1 I_5}}{R_4} +$$

$$\frac{\alpha_{23}\sqrt[3]{I_1 I_2 I_3}}{R_1+R_2} + \frac{\alpha_{24}\sqrt[3]{I_1 I_2 I_4}}{R_1+R_3} + \frac{\alpha_{25}\sqrt[3]{I_1 I_2 I_5}}{R_1+R_4} + \frac{\alpha_{34}\sqrt[3]{I_1 I_3 I_4}}{R_2+R_3} +$$

$$\frac{\alpha_{35}\sqrt[3]{I_1 I_3 I_5}}{R_2+R_4} + \frac{\alpha_{45}\sqrt[3]{I_1 I_4 I_5}}{R_3+R_4}$$

$$= 2.5318$$

where I_1, I_2, I_3, I_4, and I_5 are 2.5, 2.1, 4, 3, 2.8 in order,[24] and $R_1 = 2 + 1 = 3$, $R_2 = 2 + 2 = 4$, $R_3 = 2 + 3 = 5$, $r_4 = 2 + 4 = 6$ ($R_{ij} = n_i + n_j$).

Listed in Table 3 are the values of W^* and the standard formation enthalpy $\Delta_f H_m^{\Phi}$(kJ·mol^{-1})[26] of the corresponding molecules, where W^* is calculated using formula 3 and formula 4, and $\Delta_f H_m^{\Phi}$ is from ref 26. The correlation result is

$$\Delta_f H_m^{\Phi} = 564.5998 - 318.0492\ W^* \tag{6}$$

$$r = 0.9851,\ \sigma = 58.8223,\ F = 1379.00,\ n = 44$$

The above-mentioned result indicates that there is a perfect correlativity between W^* and $\Delta_f H_m^{\Phi}$ for methyl halides, that is, W^* can be applied to heteroatom- containing organic systems.

For SiX$_m$ (X = F, Cl, Br, I, H, m = 1−4) Molecules. For molecules of type AB$_m$, W^*, and S_{ij}^* can be simplified.

$$\text{For AB: } W^* = x$$

$$\text{For AB}_2\text{: } W^* = 2\left(x + \frac{1}{2}x'\right)$$

$$\text{For AB}_3\text{: } W^* = 3(x + x')$$

$$\text{For AB}_4\text{: } W^* = 4\left(x + \frac{3}{2}x'\right)$$

$$\text{For AB}_m\text{: } W^* = m\left(x + \frac{m-1}{2}x'\right) \tag{7}$$

Here $x = (\alpha_{12}\sqrt{I_1 I_2})/R$, $x' = (\alpha_{22}\sqrt[3]{I_1 I_2 I_2})/2R$, and $R = n_1 + n_2$, $\alpha_{22} = (\alpha_{12} + \alpha_{12})/2 = \alpha_{12} = \alpha$.

Therefore,

$$W^* = \frac{m\alpha}{n_1+n_2}\left(\sqrt{I_1 I_2} + \frac{m-1}{4}\cdot\sqrt[3]{I_1 I_2 I_2}\right) \tag{8}$$

"1" means the central atom A, and "2" means the atom B.

Listed in Table 4 are the values of W^* and the standard formation enthalpy $\Delta_f H_m^{\Phi}$(kJ·mol^{-1})[26] of the corresponding molecules, where W^* is calculated by formula 8, and $\Delta_f H_m^{\Phi}$ is from ref 26. The correlation result shows formula 9.

$$\Delta_f H_m = 282.0955 - 398.5121 W^* \tag{9}$$

$$r = 0.9798,\ \sigma = 100.7453,\ F = 432.37,\ n = 20$$

W^* has perfect correlation with $\Delta_f H_m^{\Phi}$(kJ·mol^{-1})[26] for SiX$_m$(X = F, Cl, Br, I, H, m = 1−4) inorganic compounds, too.

For AB$_m$ Inorganic Compounds Containing Transition Metals. To assess the application of W^* in various systems,

Table 4. W^* and $\Delta_f H_m^{\Phi}$ [26](kJ·mol^{-1}) of SiX_m (X = F, Cl, Br, I, H, $m = 1-4$)

compd	W^*	$\Delta_f H_m^{\Phi}$	compd	W^*	$\Delta_f H_m^{\Phi}$
SiF	0.6693	−20.92	SiBr$_3$	0.8787	−158.99
SiF$_2$	1.7209	−589.94	SiBr$_4$	1.3741	−415.47
SiF$_3$	3.1548	−999.98	SiI	0.1363	259.41
SiF$_4$	4.9710	−1625.9	SiI$_2$	0.3446	92.05
SiCl	0.3515	154.81	SiI$_3$	0.6248	58.58
SiCl$_2$	0.8943	−167.78	SiI$_4$	0.9771	−110.46
SiCl$_3$	1.6285	−334.72	SiH	0.1299	377.4
SiCl$_4$	2.5540	−662.75	SiH$_2$	0.3265	271.96
SiBr	0.1917	196.65	SiH$_3$	0.5897	194.97
SiBr$_2$	0.4846	−46.02	SiH$_4$	0.9196	34.31

Table 5. W^* and $\Delta_f H_m^{\Phi}$ [26](kJ·mol^{-1}) of AB_m Inorganic Compounds Containing Transition Metals

compd	W^*	$\Delta_f H_m^{\Phi}$	compd	W^*	$\Delta_f H_m^{\Phi}$
CdF$_2$	2.2167	690	FeI$_2$	0.4174	125
CdCl$_2$	1.2094	389	MnI$_2$	0.3760	248
CdBr$_2$	0.7220	314	HgBr$_2$	0.8834	170
CdI$_2$	0.4970	201	HgI$_2$	0.6143	105
CrCl$_2$	0.9503	396	NiF$_2$	2.0281	667
CrCl$_3$	1.7351	563	NiCl$_2$	1.0841	316
CoF$_2$	1.9917	665	NiBr$_2$	0.6371	227
CoCl$_2$	1.0645	326	NiI$_2$	0.4331	85.5
CoBr$_2$	0.6256	232	AgF	0.9000	203
CoI$_2$	0.4253	102	AgCl	0.4962	127
CuF$_2$	2.1165	531	AgBr	0.2970	99.5
CuCl	0.4455	135	AgI	0.2064	62.4
CuCl$_2$	1.1313	206	UF$_4$	7.8358	1850
CuBr	0.2625	105	VCl$_3$	1.6986	573
CuBr$_2$	0.6649	141	ZnCl$_2$	1.0624	416
CuI	0.1791	67.8	ZnI$_2$	0.4244	209
FeCl$_2$	1.0446	341	PbI$_2$	0.6065	175
FeCl$_3$	1.9022	405	FeBr$_2$	0.6139	251

the following is set forth about AB_m inorganic compounds containing transition metals.

Listed in Table 5 are W^* and the standard formation enthalpy $\Delta_f H_m^{\Phi}$(kJ·mol^{-1})[25] of the corresponding molecules, where W^* is calculated by formula 8, and $\Delta_f H_m^{\Phi}$ is from ref 26. The correlation result shows formula 10.

$$\Delta_f H_m^{\Phi} = 61.5428 + 238.7929 W^* \qquad (10)$$

$$r = 0.9712, \sigma = 75.4473, F = 584.65, n = 36$$

For these inorganic compounds containing transition metals, the correlation result is favorable.

The foregoing study proved that W^* can be applied not only to heteroatom-containing and multiple bond-containing organic compounds but also to inorganic compounds containing transition metals. Especially, W^* is the index D[27] for saturated hydrocarbons. According to eqs 1−4, if $1/R$ stands for R, W^* is Wiener number W.[8]

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REFERENCES AND NOTES

(1) Kier, L.; Hall, L. H. *Molecular Connectivity in Chemistry and Drug Research*; Academic Press: New York, 1976.

(2) Kier, L.; Hall, L. H. *Molecular Connectivity in Structure−Activity Analysis*; Research Studies Press: Letchworth, U.K., 1986.

(3) Xu, L.; Zhong, f. Method of Topological Indices in Quantitative Study of Structure Property/Activity Relationships. *Chin. J. Applied Chem.* (*in Chinese*) **1997**, *14*(6), 26−29.

(4) Weida, D. R.; Rerkins, R. Y.; Welsh, W. J.; shechan, D. Evaluation of Quantitative Structure−Activity Relationship Methods for Lange-Scale Prediction of Chemicals Binding to Estrogen Receptor. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 669−677.

(5) Henk, J. M. V.; Cees, J. V. L.; Joop, L. M. Classifing Environmental Pollutants. 1: Structure−Activity Relationships for Prediction of Aquatic Toxicity. *Chemosphere* **1992**, *24*, 471−491.

(6) Enaut, U. R.; Wouter, H. J. V.; Henk, J. M. V.; Joop, L. M. H. Quantitative Structure−Activity Relationships for the Aquatic Toxicity of Polar and Nonpolar Narcotic Pollutants. *J. Chem. Inf. Comput. Sci.* **1998**, *38*(8), 845−852.

(7) Cao, C. Z.; Hua, Y. Topological Indices Based on Vertex, Distance, and Ring: On the Boiling Points of Paraffins and Cycloakanes. *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 867−877.

(8) Wiener H. Structural determination of Paraffin Boiling Points. *J. Am. Chem. Soc.* **1947**, *69*, 17−20.

(9) Hosoya, H. A Newly Proposed Quantity Characterizing the Topological Nature of structural Isomers of saturated hydrocarbons. *Bull. Chem. Soc. Jpn.* **1971**, *44*, 2332−2339.

(10) Klein, D. J.; Randic, M. resistance Distance. *J. Math. Chem.* **1993**, *12*, 81−85

(11) Bonchev D.; Balaban, A. T.; Liu, X.; Klein, D. J. Molecular Cyclicity and Centricity of Polycyclic Graphs. I. Cyclicity Based on Resistance Distances or Reciprocal Distances. *Int. J. Quantum Chem.* **1994**, *50*, 1−20.

(12) Ivanciuc, O.; Balaban, T.-S.; Balaban, A. T. Design of topological Indices. Part 4. Reciprocal Distance Matrix, Related Local Vertex Invariants and topological Indices. *J. Math. Chem.* **1993**, *12*, 309−318.

(13) Diudea, M. V.; Ivanciuc, O.; Trinajstic, N. Matrices of Reciprocal Distance Matrix, Polynomials and Derived Numbers. *Comm. Math. Comput. Chem.* **1997**, *35*, 41−64.

(14) Randic, M. Novel Molecular Descriptor for structure−Property studies. *Chem. Phys. Lett.* **1993**, *211*, 478−483.

(15) Gordon, C.; Sandi, K.; Marko, P. Three Methods for Calculation of the Hyper-Wiener Index of Molecular Graphs. *J. Chem. Inf. Comput. Sci.* **2002**, *42*, 571−574.

(16) Lukovits, I. The detour Index. *Croat. Chem. Acta* **1996**, *69*, 873−882.

(17) Linert, W.; Lukovits, I. Formulas for the Hyper-Wiener and hyper-Detour Indices of Fused Bicyclic Structures. *Comm. Math. Comput. Chem.* **1997**, *35*, 65−74.

(18) Plavsic, D.; Nikolick, S.; Trinajstic, N.; Mihalic, Z. On the Harary Index for the characterization of Chemical Graphs. *J. Math. Chem.* **1993**, *12*, 235−250.

(19) Lukovits, I. An All-Path Version of the Wiener Index. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 125−129.

(20) Ivanciuc, O.; Balaban, A. T. Design of Topological Indices. Path Matrices and Derived Molecular Graph Invariants. *Comm. Math. Comput. Chem.* **1994**, *30*, 141−152.

(21) Ivanciuc, O. Design of Topological Indices. Part 11. Distance-Valence Matrices and Derived Molecular Descriptors. *Rev. Roumn. Chem.* **1999**, *44*, 619−631.

(22) Yang, F.; Wang, Z. D.; Sun, J. Study on the enlarged Topological Index of Distance Matrix and Its Application. *Acta Chimica Sinica* (*in Chinese*) **2002**, *60*, 764−768.

(23) Wang, Z. D.; Yang, F.; Zhou, P. J. Research on the features of some organic Pollutants with structure index W^*. *J. Wuhan Univ.* (*Nat. Sci. Ed.*) (*in Chinese*), **2002**, *48* (6), 79−83.

(24) Dean J. A. *Lang's Handbook of Chemistry,* 13th ed.; McGraw-Hill Book Company: 1985.

(25) Institute of Jinlin Chemical Company. *Applied Handbook Gas Chromatography*; Chemical Industry Press: Beijing, 1980 (*in Chinese*).

(26) Stark, J. G.; Wallace, H. G. *Chemistry data book*; John Murray: 50 Albemarle Street, London, 1975.

(27) MIhalic Z.; Veljian, D.; Amic D. The Distance Matrix in Chemistry. *J. Math Chem*. **1992**, *11*, 223−258.