A New Topological Index for QSPR of Alkanes

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A new topological index Xu based on the adjacency matrix **A** and the distance matrix **D** is derived in this paper. The index, which is very simple to calculate and also has good discrimination of alkane isomers, is used to correlate with the selected physicochemical properties of a wide range of alkanes. The comprehensive studies show that the proposed index correlates highly both with the normal boiling points (BP) of alkanes and with other selected physicochemical properties. Most of the investigated properties are well modeled ($r > 0.99$) by the Xu index. Moreover, the resulting regressions for all properties are discussed and also compared favorably with the results based on the well-established χ index. The proposed Xu index promises to be a useful parameter in the QSPR/QSAR studies.

1. INTRODUCTION

The use of global graph invariants (topological indices) in quantitative structure−property and structure−activity relationships (QSPR/QSAR) studies have become of major interest in recent years,[1] and especially the QSPR/QSAR models have become a powerful tool for predicting numerous physicochemical properties and/or biological activities of hypothetical compounds as well as for molecular design. Recently, several review papers on topological indices have been published.[2,3]

Topological indices are used to characterize features of chemical structures in numerical form. Most of the existing topological indices usually start either with the vertex adjacency matrix **A** or with the distance matrix **D** associated with graph. Ideally, a good topological index should show low degeneracy and high correlation ability. So far, a great number of topological indices have been proposed, including the famous Randić's index (χ),[4] Hosoya's index (Z),[5] Balaban's index (J),[6] Bonchev's index (I_D),[7] Schultz's index (MTI),[8] Wiener's index (W)[9] and its modifications,[10] and so on. However, among these indices the most successful was the Randić molecular connectivity χ[4] which was further developed and applied extensively by Randić, Kier, Hall, and their co-workers for a path of higher lengths and adapted to heteroatom-containing systems.[1,11] Despite large achievements in this field having been attained, existing topological index approaches to QSPR/QSAR need further improvement. Therefore, it is desirous to find new topological indices for modeling different properties.

In this study, a new topological index based on the adjacency matrix **A** and the distance matrix **D** is proposed. The Xu index proposed is used to correlate with a number of alkane properties: normal boiling points, heat capacities, critical temperatures, van der Waals volumes, van der Waals constants, and heats of vaporization, etc. The resulting regression equations are discussed and compared with that based on Randić's χ indices.

2. THEORETICAL SECTION

Let $G = \{V, E\}$ be a hydrogen-depleted graph, where V is the vertex set and E the edge set. The adjacency matrix $\mathbf{A} = \{a_{ij}\}_{n\times n}$ whose entries a_{ij} are 1 for adjacent vertices i, j and 0 otherwise, where n is the number of vertices. The distance matrix $\mathbf{D} = \{d_{ij}\}_{n\times n}$ whose entries d_{ij} are topological distances, i.e., the number of edges on the shortest path between the vertex i and vertex j in G, in terms of C−C bonds. The sum over row or column i of **A** yields local vertex invariants called vertex-degree v_i; the analogous sum for **D** yields distance sums s_i. The adjacency matrix **A** and a graph G are in a 1−1 correspondence, while the distance matrix **D** can be easily reduced to the corresponding adjacency matrix **A** of G by replacing all non-1 entries by 0. The topological indices derived from only **A** or **D** often result in a considerable loss of the structural information in a graph G. Consequently, it is possible that a new topological index generated by combining **A** and **D** should show high correlation ability and structural selectivity.

First, here we define $L = \sum_i^n v_i s_i^2 / \sum_i^n v_i s_i$, where the term L represents the valence average topological distance in a G according the statistics theory, i.e., the valence average length of the distance sums s_i. On the other hand, consider the reason that molecular weight makes a dominant contribution to most properties of alkanes, although branching and steric factors also have smaller influences. Therefore, we must take into account the number of n vertices in G, and then we define a new topological index Xu based on matrix **A** and **D** of G

$$\mathrm{Xu} = n^{1/2} \log L = n^{1/2} \log\left(\sum_n^i v_i s_i^2 / \sum_n^i v_i s_i\right) \qquad (1)$$

where the sum is over all i vertices in the graph, and n is the number of vertices, respectively. Because the Xu index combines vertex degree v_i and distance sums s_i, there is no doubt that Xu index contains more considerable topological information in a G than other topological indices derived

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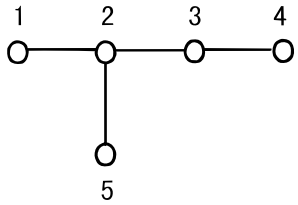

Figure 1. Labeled hydrogen-depleted graph of 2-methylbutane.

only from *A* or *D*. Moreover, it should show high correlation ability and good structural discrimination for isomers.

As an example, the labeled hydrogen-depleted graph *G* of 2-methylbutane is shown in Figure 1. The corresponding Xu index is calculated as below:

The adjacency matrix **A** and vertex-degree matrix **F** of *G*:

$$\mathbf{A} = \begin{bmatrix} 0&1&0&0&0 \\ 1&0&1&0&1 \\ 0&1&0&1&0 \\ 0&0&1&0&0 \\ 0&1&0&0&0 \end{bmatrix} \quad \mathbf{F} = \begin{bmatrix} 1 \\ 3 \\ 2 \\ 1 \\ 1 \end{bmatrix}$$

The distance matrix **D** and distance sums matrix **S** of *G*:

$$\mathbf{D} = \begin{bmatrix} 0&1&2&3&2 \\ 1&0&1&2&1 \\ 2&1&0&1&2 \\ 3&2&1&0&3 \\ 2&1&2&3&0 \end{bmatrix} \quad \mathbf{S} = \begin{bmatrix} 8 \\ 5 \\ 6 \\ 9 \\ 8 \end{bmatrix}$$

The Xu index of *G*:

$$\mathrm{Xu} = 5^{1/2} \log \left(\frac{1 \times 8^2 + 3 \times 5^2 + 2 \times 6^2 + 1 \times 9^2 + 1 \times 8^2}{1 \times 8 + 3 \times 4 + 2 \times 6 + 1 \times 9 + 1 \times 8} \right) = 1.8681$$

3. RESULTS AND DISCUSSION

Alkanes represent an especially attractive class of compounds usually as a starting point for the QSPR models. So the index Xu is calculated for C_2-C_{10} alkanes isomers according to eq 1. Xu indices of C_2-C_8 alkanes are shown in Table 1.

The normal boiling point (BP) is a physical property universally and precisely measured for low molecular compounds. Therefore, to obtain the structure−property relationships between the physicochemical properties of alkanes and Xu index proposed, firstly Xu index, along with several selected topological indices, is utilized to correlate with the BP of alkanes. The resulting regression equations and statistical parameters are shown as follows:

$$\mathrm{BP}\ (^\circ\mathrm{C}) = -80.7898 + 56.6425\mathrm{Xu} \quad (r = 0.993,\ \mathrm{sd} = 5.791,\ f = 2615,\ N = 39) \quad (2)$$

$$\mathrm{BP}(^\circ\mathrm{C}) = -130.3039 + 67.3286\chi \quad (r = 0.987,\ sd = 7.908,\ f = 1428,\ N = 39) \quad (3)$$

$$\mathrm{BP}(^\circ\mathrm{C}) = -20.616 + 0.5496\mathrm{MTI} \quad (r = 0.933,\ sd = 17.975,\ f = 248,\ N = 39) \quad (4)$$

$$\mathrm{BP}(^\circ\mathrm{C}) = -9.7483 + 4.8288Z \quad (r = 0.888,\ sd = 22.924,\ f = 138,\ N = 39) \quad (5)$$

Where *r*, *s*, *f*, and *N* represent the correlation coefficient, standard deviation of linear regression, Fischer criterion, and sample numbers, respectively. In general, the quality of the QSPR models can be conveniently measured by the correlation coefficient *r* and the standard deviation *s*. As suggested by Mihalić and Trinajstić,[13] a good QSPR model must have $r > 0.99$, while *s* depends on the property under study. The correlation coefficient *r* and the standard deviation *s* are 0.993 and 5.791 for eq 2, respectively, and the absolute average deviation is 4.08 °C between experimental values of BP and calculated values. Furthermore, the use of the Kolmogoroy−Smirnov test also proves that residuals are normally distributed, whereas eq 3 gives a correlation coefficient of 0.987 and standard deviation of 7.908 for the same alkanes. Therefore, it is apparent that eq 2 represents a better model than eq 3 for modeling BP of alkanes. In addition, similar results were also obtained by other authors;[14,15] for example,

Table 1. Normal Boiling Points (BP) of Alkanes and Predicted Values Fitted with the Model of Eq 2[a]

		BP/°C				BP/°C	
alkanes	Xu	exptl	calcd	alkanes	Xu	exptl	calcd
2	0.0000	−88.630	−80.790	223MMM4	2.7652	80.882	75.838
3	0.7188	−42.070	−40.075	8	3.7280	125.655	130.373
4	1.3728	−0.500	−3.031	2M7	3.6805	117.647	127.683
2M3	1.2568	−11.730	−9.602	3M7	3.5852	118.925	122.285
5	1.9948	36.074	32.201	4M7	3.5699	117.709	121.418
2M4	1.8681	27.852	25.024	25MM6	3.5321	109.103	119.277
22MM3	1.7252	9.503	16.930	3E6	3.5098	118.534	118.014
6	2.5923	68.740	66.045	24MM6	3.4783	109.429	116.230
2M5	2.4753	60.271	59.417	22MM6	3.4859	106.840	116.660
3M5	2.4381	63.282	57.310	23MM6	3.4643	115.607	115.437
23MM4	2.3429	57.988	51.918	34MM6	3.4227	117.725	113.080
22MM4	2.3052	49.741	49.782	33MM6	3.4289	111.969	113.432
7	3.1691	98.427	98.716	2M3E5	3.3992	115.650	111.749
2M6	3.0645	90.052	92.791	224MMM5	3.3668	99.238	109.914
3M6	3.0167	91.850	90.084	234MMM5	3.3464	113.467	108.759
3E5	2.9613	93.475	86.946	3M3E5	3.3613	118.259	109.603
24MM5	2.9472	80.500	86.147	223MMM5	3.3071	109.840	106.533
22MM5	2.9015	79.197	83.558	233MMM5	3.2849	114.760	105.275
23MM5	2.8963	89.784	83.264	2233MMMM4	3.1762	106.470	99.118
33MM5	2.8423	86.064	80.205				

[a] M: methyl; E: ethyl.

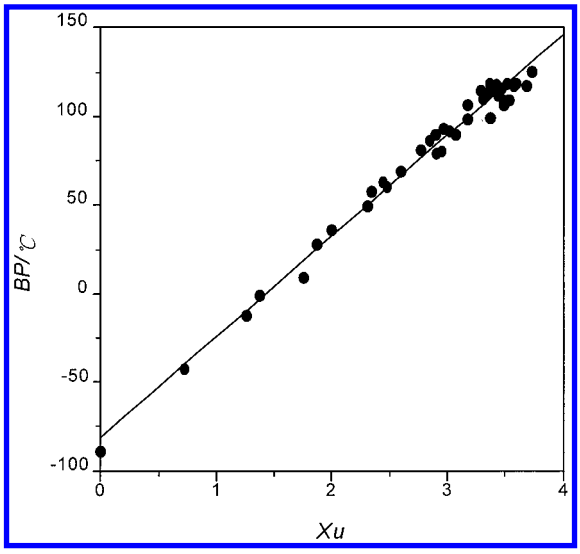

Figure 2. Plot of BP versus Xu indices of C_2-C_8 alkanes.

recently Xu et al.[14] reported that the simple linear model only gave $r = 0.987$ and $s = 7.981$ for C_2-C_8 alkanes by the use of Y_x index also based on the matrixes **A** and **D**. Although the BPs of alkanes have been predicted by many QSPR models on the base of different indices,[8,9,11−15] and most of these models are very accurate ($r > 0.998$, $s < 2$ °C), we must keep in mind the shortcomings.[13] Firstly, in most cases ethane and propane were often excluded from studies; secondly, most models usually fitted in with a limited class of C_2-C_7 alkanes; thirdly, in some cases models were very complex. Here, we should emphasize that the selection of the values of properties has an important influence on the quality of the QSPR models, and it is also of importance that available data should be selected before the design of the QSPR models. As we know, there are usually a lot of estimated values for higher molecular weight alkane such as C_9 and especially C_{10} isomers; in addition, in some cases, the data taken from different courses are not exactly the same. Consequently, the QSPR models established on the basis of these data are not particularly available and meaningful and especially on the basis of the estimated values, although in some cases the models maybe are very accurate.

It is particularly noteworthy that attempts to establish a simple linear model by correlating BP with the indices MTI and Z are unsuccessful (see eq 3−4), just as mentioned above, more complex models are usually necessary to correlate BP with MTI and Z (also see refs 12 and 13). Table 1 lists the calculated values of BP fitted with the simple model (see eq 2) for C_2-C_8 alkanes. The plot of BP versus the index Xu for C_2-C_8 alkanes is shown in Figure 2.

In addition, it is necessary that a comprehensive study should be carried out so as to obtain extensive structure−property relationships; therefore, Xu index is further tested by the following selected properties of a wide range of alkanes: Heat capacity, C_p ($J{\cdot}mol^{-1}{\cdot}K^{-1}$) of liquid and gas ($C_5-C_{16}$)[16] at 25 °C, critical temperature, T_c(C_2-C_{10}),[16] van der Waals volume, V_i(C_2-C_8),[17] van der Waals constant, a_o ($L{\cdot}atm{\cdot}mol^{-2}$) *and* b_o ($L{\cdot}mol^{-1}$) (C_2-C_{10}),[16] and heat of vaporization at BP, H_v ($KJ{\cdot}mol^{-1}$)[16] (C_2-C_{16}), respectively. The regression results are shown in Table 2.

From Table 2 we see that most properties are fairly correlated with Xu indices ($r > 0.99$) except T_c (also $r > 0.98$). So far as T_c is concerned, where the value of r is smaller than 0.99, the reason for this perhaps results from slightly low availability or accuracy of T_c because of difficulty in experimental measurement as compared with other properties. Anyway, Xu indices produce better regressions than χ indices for all properties except a_o. These results mean that the Xu index reflects satisfactorily the dependence of the above different physicochemical parameters on the internal structures of alkanes. As we can see from Table 1 that Xu index increases with the number n of graph vertices and decreases with the extent of branching for the same n, i.e., it follows closely the molecular size and branching patterns in alkanes. The investigated physicochemical properties or parameters change nearly in the same way as Xu index. As we know, alkanes are nonpolar compounds, and a number of complexities due to polarity, polarizability, and /or hydrogen bonding are avoided, so the physicochemical properties are dominated by the inherent structural factors of a molecule, such as molecular dimension or shape. As mentioned above, the molecular size has an important influence on most properties, although other factors, such as branching and steric factors, also have smaller influences. The good correlation between the Xu index and van der Waals V_i and/or related properties allows us to interpret it as a good measurement of molecular dimension and as a suitable topological index for the properties that are bond additive compared with the well-established bond-additive χ index. As we expect, the combination of distance matrix **A** and adjacency matrix **D** does significantly improve the correlation ability of Xu index and leads to fair regressions for most properties of alkanes, as seen in Table 2 and Figure 2.

Table 2. Statistical and Regression Results of Seven Selected Properties of Alkanes using Xu Indices

properties	TIs	a	b	r	s	f	N
Cp^L	Xu	52.2063	56.4471	0.9982	5.8215	6648	26
	χ	31.9612	58.8118	0.9957	8.8681	2773	26
Cp^G	Xu	40.9939	41.757	0.9963	7.1792	2150	18
	χ	23.5281	43.5842	0.9908	11.2598	858	18
T_c	Xu	57.8248	65.5171	0.9854	13.2902	672	22
	χ	3.7297	76.5295	0.9708	18.7401	328	22
V_i/100	Xu	0.2533	0.1571	0.9976	0.01363	2076	12
	χ	0.07759	0.2005	0.9952	0.01918	1034	12
a_o	Xu	2.0381	9.2770	0.9933	1.5655	739	12
	χ	−6.9979	11.265	0.9981	0.8331	2583	12
$b_o \times 10$	Xu	5.4010	4.8525	0.9977	0.4773	2138	12
	χ	0.7553	5.8623	0.9975	0.4978	1993	12
H_v	Xu	15.5324	6.2587	0.9968	1.1325	2799	20
	χ	11.5514	6.7822	0.9951	1.3890	1823	20

Another approach to the QSPR studies is usually carried out only for a selected set of alkanes, such as C_8, C_9, or C_{10} isomers, to avoid the size effect. Therefore, as an extension of the above series of studies, a comparative study on the selected properties of C_8 isomers is also tested by the Xu index. Eight selected properties are below (Table 3): i.e., entropy (S), heat of vaporization (H_v), heat of formation (H_f), quadratic mean radius (R^2), density (D), and critical volume (V_c) (taken from ref 18); Pitzer eccentric factors (ω),[19,20] and octane numbers (MON).[21] The results of linear regression are listed in Table 4.

From Table 4 we see that Xu indices give a better correlation for ω ($r = 0.9735$) and MON ($r = -0.9615$) than χ indices ($r = 0.9040$ and 0.7774, respectively). For

Table 3. Eight Selected Properties of Octane Isomers and Xu Indices[a]

alkanes	Xu	S	R^2	D	H_v	H_f	ω	V_c	MON
8	3.7280	111.67	2.0449	0.7025	73.19	−49.82	0.398	0.492	
2M	3.6805	109.84	1.8913	0.6980	70.30	−51.50	0.378	0.488	23.1
3M	3.5852	111.26	1.7984	0.7058	71.30	−50.82	0.370	0.464	35.0
4M	3.5699	109.23	1.7673	0.7046	70.91	−50.69	0.371	0.476	39.0
3E	3.5098	109.43	1.7673	0.7136	71.70	−50.40	0.361	0.455	52.4
22MM	3.4859	103.42	1.6744	0.6953	67.70	−53.71	0.338	0.478	77.4
23MM	3.4643	108.02	1.6464	0.7121	70.20	−51.13	0.346	0.468	78.9
24MM	3.4783	106.98	1.6142	0.7004	68.50	−52.44	0.343	0.472	69.9
25MM	3.5321	105.72	1.6449	0.6935	68.60	−53.21	0.352	0.482	55.7
33MM	3.4289	104.74	1.7377	0.7100	68.50	−52.61	0.320	0.443	83.4
34MM	3.4227	106.59	1.523	0.7200	70.20	−50.91	0.338	0.466	81.7
2M3E	3.3992	106.06	1.5525	0.7193	69.70	−50.48	0.329	0.443	88.1
3M3E	3.3613	101.48	1.5214	0.7274	69.30	−51.38	0.304	0.455	88.7
223MMM	3.3071	101.31	1.4306	0.7161	67.30	−52.61	0.297	0.436	99.9
224MMM	3.3668	104.09	1.401	0.6919	64.87	−53.57	0.303	0.468	100.0
233MMM	3.2849	102.06	1.4931	0.7262	68.10	−51.73	0.290	0.455	99.4
234MMM	3.3464	102.39	1.3698	0.7191	68.37	−51.97	0.315	0.461	95.9
2233MMMM	3.1762	93.06	1.4612	0.8242	66.20	−53.99	0.251	0.461	

[a] M: methyl; E: ethyl.

Table 4. Statistical and Regression Results of Eight Selected Properties of Octane Isomers Using Xu Indices

		S	R^2	D	H_v	H_f	ω	V_c	MON
Xu	s	2.1325	0.0876	0.0231	1.3907	1.0656	0.0086	0.0116	7.0197
	r	0.8890	0.8831	−0.6434	0.7461	0.5352	0.9735	0.6870	−0.9615
	f	60.3	56.7	11.3	20.1	6.4	271.8	14.3	171.4
χ	s	1.9764	0.1192	0.0250	0.7336	0.6783	0.0161	0.0150	16.072
	r	0.9053	0.7696	−0.5576	0.9363	0.8506	0.9040	0.3344	−0.7774
	f	72.7	23.2	7.2	113.7	41.9	71.5	2.0	21.4

other properties such as S and R^2, Xu indices approach a fair regression and give correlation coefficients of $r = 0.8890$ and 0.8831, respectively. On the other hand, χ indices produce a better regression than Xu for H_v and H_f, but there remain four selected properties. Xu and χ indices do not lead to a satisfactory regression ($r < 0.800$). The reason for this might be due to the great diversity among experimental values. As Randić et al.[10,18] recently pointed out after a series of comprehensive studies on numerous properties of octane isomers by the use of a single and/or two topological indices based on the restructure of the Wiener matrix in great detail the different properties depend in a different way on the inherent structural features of molecules of the same size. In other words, some properties can be satisfactorily correlated, and other properties cannot. These results suggest that there are no simple and accurate QSPR models for C_8 isomers by the use of a single or two topological indices. However, the above results have not been well understood. So far as C_8 isomers are concerned, according to our point of view, the smaller difference in properties might mainly result from the difference in molecular branching and steric factors. But in some cases the deviation in experimental measurement might compensate or go beyond the contribution of molecular branching and steric factors to properties as compared with low molecular weight alkanes. Consequently, it is with great difficulty that the existing single topological index (only small difference among them) thoroughly reflects the difference among properties. However, it is also not surprising at all that some properties of octane isomers cannot be well modeled by a single or two topological indices. In a word, there is no simple and accurate single parameter QSPR model for C_8 isomers due to the great diversity among experimental values.

On the other hand, the Xu index has a high structural selectivity for alkane isomers as compared with other topological indices, which is another important feature required for topological indices. There is no degeneracy for C_2-C_{10} isomeric alkanes. However, even highly discriminative Balaban's J index has a couple of isomers with the same values of indices for C_2-C_{10} alkanes.

4. CONCLUSIONS

Both the vertices v_i and the distance sums s_i have been used to generate a new topological index Xu, and the proposed Xu index is used to correlate with the physicochemical properties of alkanes and compared favorably to Randić's index χ. For the normal boiling points, the Xu index gives a better regression than Randić's χ index and is also well correlated with other selected properties of alkanes ($r > 0.99$) except for T_c, such as heat capacity, critical temperature, etc. The studies indicate that the proposed Xu index with fairly high structural selectivity and correlation ability is a suitable parameter for modeling these properties of the investigated compounds. Besides, the Xu indices are tested by eight selected properties of octane isomers; however, the Xu index gives a fair regression only for four of these properties. The reason for this might be due to the great diversity among experimental values of octane isomers.

Moreover, the Xu index has better discriminatory power of alkane isomers than Balaban's J index and is very simple to calculate. It premises to be a useful parameter in the QSPR/QSAR research.

In addition, the Xu index has the advantage that it can be easily adapted for multiple bonds and/or heteroatom-containing compounds. By the way, the Xu index shows high correlation coefficients with the heat capacity of the follow-

ing compounds at 25 °C ($r > 0.99$): alkanes, olefins, aromatics, sulfur-containing, and oxygen-containing compounds, etc. The calculated data are in good agreement with experimental data, and the absolute average deviations of Cp^L for 79 compounds and Cp^G for 70 compounds are 1.61 and 2.29%, respectively. We will report on this topic in a later paper in detail.

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