Modified Connectivity Indices and Their Application to QSPR Study

Chunsheng Yang and Chongli Zhong*

Department of Chemical Engineering, P.O. Box 100, Beijing University of Chemical Technology, Beijing 100029, China

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A modified adjacency matrix was developed to delineate the chemical graph of a compound, in which the element a_{ii} along the diagonal of the matrix reflects the numbers of the lone-pair electrons and π bonds of the *i*th atom, and the off-diagonal element a_{ij} of the matrix characterizes whether the *j*th non-hydrogen atom is bonded to the *i*th non-hydrogen atom as well as the number of hydrogen atoms bonded to the *j*th non-hydrogen atom. The corresponding vertex-degree matrix can distinguish the non-hydrogen atoms in the compound better than that from the original adjacency matrix. Based on the newly proposed adjacency matrix, modified molecular connectivity indices (mMCIs) were proposed as structural descriptors for organic compounds, which were applied to the QSPR studies on the boiling point temperature, molar volume and molar refraction of alkanes, alkenes and alcohols. The results show that, in most cases, the mMCIs give improved correlations than the original molecular connectivity indices (MCIs), which are particularly suitable to distinguish isomers.

INTRODUCTION

Topological indices have received great attention in quantitative structure−property/activity relationship (QSPR/QSAR) studies and have become a powerful tool for predicting physical properties, biological activities, and pharmacological and toxicological properties of organic compounds. Since topological indices can be derived directly from the molecular structure without any experimental effort, they provide a simple and straightforward method for property prediction. A variety of topological indices have been proposed, such as the molecular connectivity index (χ),[1,2] Hosoya's index (Z),[3] Balaban's index (J),[4] Schultz's index (MTI),[5] Wiener index (W)[6] and electrotopological index (S),[7] and a great number of investigations have been made to extend and apply them.[8−17]

Among the existing topological indices, the molecular connectivity index (MCI) is one of the most commonly used indices and has found wide applications in both simple and complex systems.[1,2,13,16,17] However, the adjacency matrix for the calculation of the atomic connectivity index δ_i only takes into account the number of non-hydrogen atoms bonded to the *i*th non-hydrogen atom, which cannot, as will be discussed in the next section, distinguish the atoms in the compound very well. In this work, an effort is made to solve this problem, at least partly. The proposed modified molecular connectivity index (mMCI), which can distinguish the atoms in a compound better, is applied to the QSPR studies for some properties of alkanes, alkenes and alcohols to test its capability.

METHODS

A common way to describe a chemical graph is to use an adjacency matrix. An important characteristic of graphs is the degrees of their vertexes, which denote the connections of the chemical vertexes. The degree of a vertex suggests one of the chemical concepts of valence, and the degree of vertex *i* is equal to the sum of the elements of raw *i* in the adjacency matrix. The molecular connectivity indices can be calculated from the degrees of the vertexes directly.

The hydrogen-suppressed graph, the adjacency matrix, and the vertex-degree matrix for 2-methylpentane are shown in Figure 1.

The general expression for the *m*th-order molecular connectivity index is as follows

$$ {}^{m}\chi_t = \sum_{j=1}^{n_m} \prod_{i=1}^{m+1} (\delta_i)_j^{-0.5} \qquad (1) $$

where *m* is the order of the molecular connectivity index, and *t* denotes a contiguous path type of fragment, which is divided into paths (P), clusters (C), path/clusters (PC) and chains (cycles)(CH). n_m is the number of the relevant paths, and δ_i is the atomic connectivity index, equal to the number of non-hydrogen atoms to which the *i*th non-hydrogen atom is bonded, that is the degree of vertex *i*.

When Kier's approach[18] is followed, the atoms of a compound are divided into classes according to their equivalence or nonequivalence. In 2-methylpentane (Figure 1(a)), carbons 1 and 6 are equivalent and the remaining carbons are unique; therefore, there are five classes of carbon atoms in 2-methylpentane. However, the vertex-degree matrix (Figure 1(c)) shows that carbons 1, 5 and 6 are equivalent, and carbons 3 and 4 are equivalent, so there are three classes of carbon atoms. As a result, the adjacency matrix, and the corresponding vertex-degree matrix cannot distinguish the atoms in a compound very well.

To solve this problem, a modified adjacency matrix was proposed, where the element a_{ij} is defined as

* Corresponding author phone and fax: +86-10-64419862; e-mail: zhongcl@mail.buct.edu.cn.

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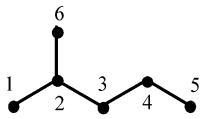


$$A=\begin{bmatrix}0&1&0&0&0&0\\1&0&1&0&0&1\\0&1&0&1&0&0\\0&0&1&0&1&0\\0&0&0&1&0&0\\0&1&0&0&0&0\end{bmatrix} \qquad \delta=\begin{bmatrix}1\\3\\2\\2\\1\\1\end{bmatrix}$$

(a) (b) (c)

Figure 1. The hydrogen-suppressed graph, the adjacency and vertex-degree matrices for 2-methylpentane: (a) hydrogen-suppressed graph; (b) adjacency matrix; and (c) vertex-degree matrix.

$$a_{ij}=\begin{cases}n+\pi & i=j,\\ 0 & i\neq j,\text{vertexes } i \text{ and } j \text{ are not connected}\\ 1+n_{H_j}/6 & i\neq j,\text{vertexes } i \text{ and } j \text{ are connected}\end{cases} \quad (2)$$

where n is the number of lone-pair electrons and π is the number of π bonds of the atom corresponding to vertex i; n_{H_j} is the number of hydrogen atoms connecting to the non-hydrogen atom j.

The modified molecular adjacency matrix and the vertex-degree matrix for 2-methylpentane are shown in Figure 2.

Figure 2(b) shows that carbons 1 and 6 are equivalent, and the remaining carbons are unique; so, there are five classes of carbon atoms in 2-methylpentane, which is consistent with the atom classification approach proposed by Kier.[18]

Comparing the modified and the original molecular adjacency matrices, it is clear that the information included in the matrices is different. In the original adjacency matrix, only the information on the number of non-hydrogen atoms bonded to the ith non-hydrogen atom is included, while in the modified adjacency matrix, the information on the number of hydrogen atoms bonded to the non-hydrogen atoms connected to the ith non-hydrogen atom is also included. In addition, the presence of lone-pair electrons and π bonds of the ith non-hydrogen atom is also taken into account. Therefore, the modified adjacency matrix encodes more information on the connective characteristic of the non-hydrogen atoms in a compound. As a result, the corresponding vertex-degree matrix can represent better the non-hydrogen atoms in the compound.

An example for the modified adjacency and vertex-degree matrices for heteroatom-containing compound, 2-propanol, is shown in Figure 3.

Replacing δ_i in eq 1 by δ_i^h, we can define the modified molecular connectivity index as

$${}^m\chi_t{}^h=\sum_{j=1}^{n_m}\prod_{i=1}^{m+1}(\delta_i{}^h)_j^{-0.5} \quad (3)$$

The molecular connectivity index, ${}^m\chi_t$, the valence molecular connectivity index, ${}^m\chi_t{}^v$, and the modified molecular connectivity index, ${}^m\chi_t{}^h$, up to second order are shown in Table 1 for some selected isomers, where the mth-order valence molecular connectivity index ${}^m\chi_t{}^v$ is defined as

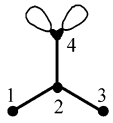
$${}^m\chi_t{}^v=\sum_{j=1}^{n_m}\prod_{i=1}^{m+1}(\delta_i{}^v)_j^{-0.5} \quad (4)$$

where $\delta_i{}^v$ is the atomic valence connectivity index.

$$A^h=\begin{bmatrix}0&7/6&0&0&0&0\\3/2&0&4/3&0&0&3/2\\0&7/6&0&4/3&0&0\\0&0&4/3&0&3/2&0\\0&0&0&4/3&0&0\\0&7/6&0&0&0&0\end{bmatrix} \qquad \delta^h=\begin{bmatrix}1.1667\\4.3333\\2.5\\2.8333\\1.3333\\1.1667\end{bmatrix}$$

(a) (b)

Figure 2. The modified adjacency and vertex-degree matrices for 2-methylpentane: (a) modified adjacency matrix and (b) vertex-degree matrix.



$$A^h=\begin{bmatrix}0&7/6&0&0\\3/2&0&3/2&7/6\\0&7/6&0&0\\0&7/6&0&4\end{bmatrix} \qquad \delta^h=\begin{bmatrix}1.1667\\4.1667\\1.1667\\5.1667\end{bmatrix}$$

(a) (b) (c)

Figure 3. The pseudograph and the modified adjacency and vertex-degree matrices for 2-propanol: (a) pseudograph; (b) modified adjacency matrix; and (c) vertex-degree matrix.

From Table 1, it can be seen that second-order MCI has to be adopted in order to distinguish the isomers when the original MCIs are used. However, if mMCIs are used, even the zeroth-order mMCI can distinguish the isomers. Previous investigations show that most physical properties correlate well with zeroth- or first-order MCI; therefore, the inability of distinguishing isomers with zeroth- and first-order MCIs may lead to a correlation requiring second- or higher-order MCI, resulting in a more complex QSPR model when isomers are involved. Therefore, it is clear that the mMCI has an advantage over the original MCI in describing isomers.

RESULTS AND DISCUSSION

To test the proposed mMCI and compare with the original MCI, the data for normal boiling point temperature (BPT), molar volume (MV) at 20 °C and molar refraction (MR) at 20 °C of alkanes, alkenes and alcohols are collected from the literature,[19−21] as shown in Table 2. The mMCIs used in this work are listed in Table 3.

For each property the following general expression is adopted to develop a QSPR model to relate the property concerned to mMCI or MCI

$$\text{property}=a_0+a_1{\cdot}\chi \quad (5)$$

where a_0 and a_1 are constants, χ can be any order of MCI or the mMCI. It should be pointed out that when original MCI is considered, both the molecular connectivity index, ${}^m\chi_t$, and the valence molecular connectivity index, ${}^m\chi_t{}^v$, are tested, and only the best results are given.

Boiling Point Temperature. As a first step to test the proposed mMCI and compare it with the original MCI, boiling point temperature data for 18 octanes and 27 heptenes, as shown in Table 2, were adopted to develop the QSPR models to compare the two indices in describing isomers.

Octanes. The boiling point temperature QSPR models for the 18 octanes shown in Table 2 are presented in Table 4, where the correlation coefficient (r^2), standard error (s) and Fischer ratio (F) are also listed. The best QSPR model

Table 1. Molecular Connectivity Indices and the Modified Molecular Connectivity Indices for Some Selected Isomers

compound	$^0\chi$	$^1\chi$	$^2\chi$	$^0\chi^v$	$^1\chi^v$	$^2\chi^v$	$^0\chi^h$	$^1\chi^h$
2-methylheptane	6.4058	3.7701	2.8896				5.6493	2.8339
3-methylheptane	6.4058	3.8081	2.6556				5.5991	2.8593
4-methylheptane	6.4058	3.8081	2.6825				5.6009	2.8537
3-methyl-1-hexene	5.6987	3.3081	2.3021	5.2760	2.9343	2.0017	4.7323	2.2998
4-methyl-1-hexene	5.6987	3.3081	2.3021	5.2760	2.9175	2.0378	4.7504	2.3013
5-methyl-1-hexene	5.6987	3.2701	2.5361	5.2760	2.8794	2.2599	4.7985	2.2784
o-xylene	5.9831	3.8045	3.2390	5.3094	2.8274	2.0843	5.1452	2.5760
m-xylene	5.9831	3.7877	3.3769	5.3094	2.8214	2.1582	5.1587	2.5617
p-xylene	5.9831	3.7877	3.3650	5.3094	2.8214	2.1547	5.1575	2.5637

obtained using the original MCI is

$$\mathrm{BPT} = 143.952 - 9.515^2\chi \quad (6)$$
$$r^2 = 0.777,\ s = 3.0,\ F = 55.8,\ N = 18$$

When the mMCIs are adopted, the best results are obtained with the following equation:

$$\mathrm{BPT} = -245.113 + 127.176^1\chi^h \quad (7)$$
$$r^2 = 0.814,\ s = 2.7,\ F = 70.0,\ N = 18$$

Heptenes. The QSPR models for the BPT of 27 heptene isomers are shown in Table 5, and the best models obtained using the MCI and the mMCI are given by eqs 8 and 9, respectively.

$$\mathrm{BPT} = 120.370 - 14.984^2\chi^v \quad (8)$$
$$r^2 = 0.672,\ s = 4.0,\ F = 51.2,\ N = 27$$
$$\mathrm{BPT} = -229.715 + 136.823^1\chi^h \quad (9)$$
$$r^2 = 0.816,\ s = 3.0,\ F = 110.7,\ N = 27$$

The calculated BPT of the 18 octane and the 27 heptene isomers with eqs 7 and 9 are reported in Table 2.

From the statistical results given above, it is clear that the mMCIs work better than the original MCIs in the QSPR modeling of the normal boiling point temperature for isomers. In this work, we just presented the QSPR models for the most simple form, that is one-variable correlation because our purpose is to compare the proposed mMCI and the original MCI, and a better QSPR model for BPT can be obtained if a more complex correlation form is used.

Molar Volume. The molar volumes (MV) at 20 °C of alkanes, alkenes and alcohols are further adopted to develop QSPR models to compare the mMCI and the MCI. The statistical results of the models for 34 alkanes, 48 alkenes and 42 alcohols are presented in Tables 6−8 respectively, and the calculated results for the best models based on the mMCIs are shown in Table 2. The best models obtained are summarized as follows:

For alkanes:

$$\mathrm{MV} = 38.757 + 18.541^0\chi \quad (10)$$
$$r^2 = 0.938,\ s = 3.7,\ F = 483.8,\ N = 34$$
$$\mathrm{MV} = 51.809 + 38.532^1\chi^h \quad (11)$$
$$r^2 = 0.949,\ s = 3.4,\ F = 593.6,\ N = 34$$

For alkenes:

$$\mathrm{MV} = 25.129 + 19.842^0\chi \quad (12)$$
$$r^2 = 0.954,\ s = 3.1,\ F = 961.8,\ N = 48$$
$$\mathrm{MV} = 44.384 + 40.921^1\chi^h \quad (13)$$
$$r^2 = 0.935,\ s = 3.7,\ F = 661.3,\ N = 48$$

For alcohols:

$$\mathrm{MV} = 6.212 + 22.857^0\chi^v \quad (14)$$
$$r^2 = 0.989,\ s = 4.2,\ F = 3510.2,\ N = 42$$
$$\mathrm{MV} = 26.461 + 43.798^1\chi^h \quad (15)$$
$$r^2 = 0.994,\ s = 3.0,\ F = 6666.6,\ N = 42$$

The results given above show that the mMCI is slightly better than the MCI in QSPR modeling of molar volumes of alkanes, alkenes and alcohols, and both of them give good correlative accuracy.

Molar Refraction. Molar refraction (MR) is of interest because of its relationship to molecular polarizability. In this work, it is also used to test and compare the mMCI and MCI. The QSPR models for alkanes, alkenes and alcohols, obtained with one-variable linear equation, are shown in Tables 9−11, and the calculated results obtained by the best models based on the mMCI are listed in Table 2. The best QSPR models are given below:

For alkanes:

$$\mathrm{MR} = 1.107 + 5.751^0\chi \quad (16)$$
$$r^2 = 0.958,\ s = 0.9,\ F = 738.3,\ N = 34$$
$$\mathrm{MR} = 4.925 + 12.042^1\chi^h \quad (17)$$
$$r^2 = 0.984,\ s = 0.6,\ F = 2031.1,\ N = 34$$

For alkenes:

$$\mathrm{MR} = 2.427 + 5.479^0\chi \quad (18)$$
$$r^2 = 0.961,\ s = 0.8,\ F = 1143.5,\ N = 48$$
$$\mathrm{MR} = 7.363 + 11.482^1\chi^h \quad (19)$$
$$r^2 = 0.973,\ s = 0.7,\ F = 1632.5,\ N = 48$$

Table 2. Literature Data and Calculated Results for Normal Boiling Point Temperature (BPT, °C), Molar Volume at 20 °C (MV, cm^3/mol), Molar Refraction at 20 °C (MR, cm^3/mol)

		BPT		MV		MR				BPT		MV		MR	
no.	compound[a]	exptl	calcd	exptl	calcd	exptl	calcd	no.	compound[a]	exptl	calcd	exptl	calcd	exptl	calcd
							Alkanes								
1	5			115.2	119.5	25.27	26.08	19	2M7	117.6	115.3	163.7	161.0	39.23	39.05
2	2M4			116.4	117.9	25.29	25.57	20	3M7	118.9	118.5	161.8	162.0	39.10	39.36
3	22MM3			122.1	114.7	25.72	24.59	21	4M7	117.7	117.8	162.1	161.8	39.12	39.29
4	6			130.7	133.9	29.91	30.59	22	25MM6	109.1	109.3	164.7	159.2	39.26	38.48
5	2M5			131.9	132.1	29.95	30.02	23	3E6	118.5	121.1	160.1	162.8	38.94	39.60
6	3M5			129.7	133.3	29.80	30.38	24	24MM6	109.4	112.1	163.1	160.0	39.13	38.75
7	23MM4			130.2	131.0	29.81	29.66	25	22MM6	106.8	110.0	164.3	159.4	39.25	38.55
8	22MM4			132.7	130.9	29.93	29.63	26	23MM6	115.6	113.7	160.4	160.5	38.98	38.90
9	7			146.5	148.4	34.55	35.11	27	34MM6	117.7	117.2	158.8	161.6	38.85	39.23
10	2M6			147.7	146.6	34.59	34.54	28	33MM6	112.0	115.0	160.9	160.9	39.01	39.03
11	3M6			145.8	147.5	34.46	34.84	29	2M3E5	115.7	116.5	158.8	161.4	38.84	39.17
12	3E5			143.5	148.5	34.28	35.14	30	224MMM5	99.2	103.3	165.1	157.4	39.26	37.91
13	24MM5			148.9	144.6	34.62	33.92	31	234MMM5	113.5	109.4	158.9	159.2	38.87	38.49
14	22MM5			148.7	144.9	34.62	34.03	32	3M3E5	118.3	121.0	157.0	162.7	38.72	39.59
15	23MM5			144.2	146.3	34.32	34.45	33	223MMM5	109.8	109.8	159.5	159.3	38.92	38.53
16	33MM5			144.5	146.9	34.33	34.63	34	233MMM5	114.8	112.1	157.3	160.1	38.76	38.75
17	223MMM4			145.2	144.1	34.37	33.78	35	2233MMMM4	106.5	103.4				
18	8	125.7	121.4	162.6	162.8	39.19	39.63								
							Alkenes								
1	1-butene			94.3	93.7	22.66	21.20	25	2-M-1-hexene	92.0	87.5	139.7	139.2	34.12	33.98
2	*cis*-2-butene			90.3	95.1	20.59	21.60	26	3-M-1-hexene	84.0	85.0	142.0	138.5	34.16	33.77
3	2-M-propene			94.4	92.4	22.63	20.82	27	4-M-1-hexene	86.7	85.2	140.6	138.6	34.08	33.79
4	1-pentene			109.4	108.8	24.85	25.45	28	5-M-1-hexene	85.3	82.0	141.9	137.6	34.14	33.52
5	*cis*-2-pentene			107.0	110.7	24.95	25.97	29	2-M-2-hexene	95.4	92.8	138.7	140.9	34.40	34.43
6	2-M-1-butene			107.8	108.9	24.85	25.47	30	3-M-*cis*-2-hexene	94.0	95.6	137.2	141.7	34.18	34.66
7	3-M-1-butene			111.8	107.1	24.94	24.96	31	4-M-*cis*-2-hexene	87.4	90.8	140.4	140.3	34.22	34.26
8	2-M-2-butene			105.9	110.3	24.95	25.85	32	5-M-*cis*-2-hexene	91.0	87.2	139.9	139.2	34.20	33.96
9	1-hexene			125.0	124.2	29.49	29.76	33	2-M-*cis*-3-hexene	86.0	88.5	141.5	139.6	34.37	34.07
10	*cis*-2-hexene			122.5	125.9	29.53	30.22	34	3-M-*cis*-3-hexene	95.4	97.1	137.7	142.1	34.32	34.79
11	*cis*-3-hexnee			123.8	126.3	29.66	30.34	35	2-E-1-pentene	94.0	90.9	138.7	140.3	33.99	34.27
12	2-M-1-pentene			123.8	123.9	29.48	29.67	36	3-E-1-pentene	85.1	88.0	141.1	139.4	34.06	34.03
13	3-M-1-pentene			126.1	123.4	29.49	29.52	37	2,3-MM-1-pentene	84.3	86.0	139.2	138.8	34.00	33.86
14	4-M-1-pentene			126.8	122.2	29.55	29.19	38	2,4-MM-1-pentene	81.6	80.3	141.5	137.1	34.18	33.38
15	2-M-2-pentene			122.6	125.7	29.74	30.17	39	3,3-MM-1-pentene	77.5	81.7	140.8	137.5	34.01	33.50
16	3-M-*cis*-2-pentene			122.2	126.7	29.55	30.46	40	3,4-MM-1-pentene	81.0	80.4	140.7	137.1	34.05	33.39
17	4-M-*cis*-2-pentene			125.8	124.0	29.67	29.70	41	4,4-MM-1-pentene	72.5	75.8	143.9	135.8	34.23	33.00
18	2-E-1-butene			122.0	125.3	29.37	30.07	42	3-E-2-pentene	96.0	99.9	136.3	143.0	34.11	35.02
19	2,3-MM-1-butene			124.1	122.7	29.43	29.33	43	2,3-MM-2-pentene	97.5	97.0	134.9	142.1	34.22	34.78
20	3,3-MM-1-butene			128.9	120.6	29.58	28.75	44	2,4-MM-2-pentene	83.4	86.3	141.3	138.9	34.53	33.88
21	2,3-MM-2-butene			118.8	125.8	29.59	30.20	45	3,4-MM-*cis*-2-pentene	87.0	91.3	137.6	140.4	34.12	34.30
22	1-heptene	93.6	88.5	140.9	139.6	34.13	34.07	46	4,4-MM-*cis*-2-pentene	80.4	81.3	140.4	137.4	34.23	33.47
23	*cis*-2-heptene	98.5	94.0	138.9	141.2	34.17	34.53	47	2-E-3-M-1-butene	89.0	86.4	138.5	138.9	33.96	33.89
24	*cis*-3-heptene	95.8	94.8	139.7	141.4	34.31	34.60	48	2,3,3-MMM-1-butene	77.9	78.1	139.3	136.4	33.99	33.19
							Alcohols								
1	ethanol			58.4	61.3	12.93	13.52	22	3,3-MM-2-butanol			124.8	122.5	31.27	30.66
2	1-propanol			74.8	77.4	17.57	18.04	23	3-hexanol			124.7	126.4	31.30	31.74
3	2-propanol			76.6	75.6	17.61	17.53	24	3-M-3-pentanol			123.4	113.9	31.13	28.24
4	1-butanol			91.5	93.9	22.15	22.65	25	1-heptanol			141.3	143.2	36.02	36.44
5	2-M-1-propanol			92.3	91.6	22.18	22.01	26	2-heptanol			142.2	142.1	36.08	36.14
6	2-butanol			91.9	93.0	22.14	22.40	27	3-heptanol			141.5	142.8	35.98	36.35
7	2-M-2-propanol			94.2	89.9	22.03	21.52	28	4-heptanol			142.0	142.6	35.93	36.28
8	1-pentanol			108.2	110.3	26.80	27.25	29	2,4-MM-3-pentanol			140.1	139.2	35.79	35.32
9	3-M-1-butanol			108.6	108.2	26.77	26.67	30	1-octanol			157.5	159.6	40.68	41.04
10	2-pentanol			109.0	109.2	26.72	26.94	31	2-octanol			158.7	158.5	40.67	40.74
11	2-M-1-butanol			108.0	109.2	26.75	26.92	32	4-octanol			159.0	159.0	40.65	40.89
12	3-pentanol			107.3	110.2	26.57	27.20	33	2-E-1-hexanol			156.4	159.1	40.51	40.92
13	3-M-2-butanol			107.6	107.7	26.64	26.51	34	2,2,4-MMM-1-pentanol			155.2	154.4	40.10	39.59
14	2-M-2-butanol			109.0	108.0	26.72	26.59	35	3,5-MM-1-hexanol			157.0	156.2	40.14	40.09
15	2,2-MM-1-propanol			108.6	106.1	.		36	1-nonanol			174.4	176.0	45.27	45.64
16	1-hexanol			125.6	126.7	31.64	31.85	37	2,6-MM-4-heptanol			177.6	171.1	45.24	44.26
17	2-M-1-pentanol			123.8	125.3	31.26	31.46	38	5-nonanol			172.6	175.5	44.59	45.49
18	2-E-1-butanol			122.4	126.5	31.13	31.78	39	1-decanol			190.3	192.4	49.73	50.24
19	4-M-2-pentanol			126.8	123.4	31.50	30.92	40	1-undecanol			207.7	208.9	54.64	54.84
20	2,3-MM-2-butanol			124.1	122.9	31.24	30.77	41	2,6,8-MMM-4-nonanol			227.4	219.0	59.29	57.69
21	3,3-MM-1-butanol			124.0	122.9	31.22	30.76	42	1-tridecanol			237.0	241.7	63.38	64.04

[a] 5 = pentane, 6 = hexane, etc.; M = methyl, E = ethyl; e.g., 2M3E5 = 2-methyl-3-ethylpentane.

Table 3. Modified Molecular Connectivity Indices of Organic Compounds Used

no.	compound	$^0\chi^h$	$^1\chi^h$	$^2\chi^h$	$^3\chi_p{}^h$	$^3\chi_c{}^h$	no.	compound	$^0\chi^h$	$^1\chi^h$	$^2\chi^h$	$^3\chi_p{}^h$	$^3\chi_c{}^h$
						Alkanes							
1	5	3.5326	1.7566	0.8463	0.3744	0.0000	19	2M7	5.6493	2.8339	1.9354	0.7923	0.2604
2	2M4	3.8104	1.7140	1.2112	0.4717	0.2521	20	3M7	5.5991	2.8593	1.7490	1.0087	0.1757
3	22MM3	4.4082	1.6330	2.4495	0.0000	1.6330	21	4M7	5.6009	2.8537	1.7886	0.8925	0.1814
4	6	4.1450	2.1316	1.0757	0.5182	0.0000	22	25MM6	5.9290	2.7866	2.3330	0.8039	0.5208
5	2M5	4.4246	2.0836	1.4802	0.4905	0.2604	23	3E6	5.5494	2.8795	1.6184	1.0530	0.1186
6	3M5	4.3725	2.1142	1.2588	0.7993	0.1701	24	24MM6	5.8808	2.8086	2.1790	0.9329	0.4514
7	23MM4	4.6831	2.0542	1.7286	0.8229	0.4114	25	22MM6	6.1412	2.7924	2.7745	0.8028	1.2272
8	22MM4	4.9125	2.0517	2.2545	0.6803	1.1996	26	23MM6	5.8599	2.8214	2.0612	1.1354	0.3534
9	7	4.7573	2.5066	1.3053	0.6587	0.0000	27	34MM6	5.8084	2.8489	1.8664	1.3477	0.2835
10	2M6	5.0370	2.4589	1.7055	0.6543	0.2604	28	33MM6	6.0333	2.8320	2.4057	1.1824	0.8886
11	3M6	4.9867	2.4840	1.5236	0.8474	0.1757	29	2M3E5	5.8091	2.8435	1.9229	1.1646	0.3083
12	3E5	4.9352	2.5095	1.3580	0.9743	0.1148	30	224MMM5	6.4254	2.7393	3.2371	0.6556	1.5376
13	24MM5	5.3187	2.4080	2.1392	0.5595	0.5391	31	234MMM5	6.1197	2.7875	2.3523	1.3118	0.5424
14	22MM5	5.5288	2.4166	2.5531	0.6225	1.2272	32	3M3E5	5.9218	2.8786	2.0214	1.5869	0.6196
15	23MM5	5.2458	2.4515	1.7989	1.0731	0.3488	33	223MMM5	6.3351	2.7908	2.7944	1.3851	1.1854
16	33MM5	5.4170	2.4670	2.1110	1.2114	0.8674	34	233MMM5	6.2765	2.8092	2.5839	1.6231	0.9353
17	223MMM4	5.7717	2.3961	2.7079	1.1668	1.2302	35	2233MMMM4	6.8528	2.7402	3.6493	1.6364	1.9437
18	8	5.3697	2.8816	1.5350	0.7993	0.0000							
						Alkenes							
1	1-butene	2.6800	1.2049	0.4942	0.1882	0.0000	25	2-M-1-hexene	4.8742	2.3182	1.5323	0.6121	0.2037
2	*cis*-2-butene	2.8961	1.2397	0.5050	0.2338	0.0000	26	3-M-1-hexene	4.7323	2.2998	1.4041	0.7200	0.1565
3	2-M-propene	3.1401	1.1722	1.0454	0.0000	0.3062	27	4-M-1-hexene	4.7504	2.3013	1.4306	0.7820	0.1818
4	1-pentene	3.2942	1.5753	0.7460	0.3032	0.0000	28	5-M-1-hexene	4.7985	2.2784	1.5998	0.5981	0.2604
5	*cis*-2-pentene	3.4610	1.6203	0.7129	0.3063	0.0000	29	2-M-2-hexene	5.0802	2.3575	1.6055	0.5736	0.2410
6	2-M-1-butene	3.6455	1.5770	1.0270	0.4114	0.1967	30	3-M-*cis*-2-hexene	5.0223	2.3773	1.4204	0.7837	0.1565
7	3-M-1-butene	3.5554	1.5321	1.0827	0.3294	0.2245	31	4-M-*cis*-2-hexene	4.9000	2.3428	1.3777	0.7431	0.1553
8	2-M-2-butene	3.9003	1.6099	1.1280	0.4354	0.2352	32	5-M-*cis*-2-hexene	4.9693	2.3166	1.6034	0.5682	0.2696
9	1-hexene	3.9065	1.9507	0.9718	0.4568	0.0000	33	2-M-*cis*-3-hexene	4.9022	2.3259	1.5229	0.5087	0.2300
10	*cis*-2-hexene	4.0751	1.9909	0.9612	0.4423	0.0000	34	3-M-*cis*-3-hexene	4.9718	2.3885	1.3681	0.7539	0.1549
11	*cis*-3-hexene	4.0258	2.0010	0.9169	0.4102	0.0000	35	2-E-1-pentene	4.7676	2.3430	1.3479	0.7172	0.1309
12	2-M-1-pentene	4.2618	1.9425	1.3107	0.4403	0.2037	36	3-E-1-pentene	4.6814	2.3223	1.2531	0.8485	0.1024
13	3-M-1-pentene	4.1181	1.9298	1.1413	0.6665	0.1515	37	2,3-MM-1-pentene	5.0693	2.3078	1.6179	0.9717	0.2910
14	4-M-1-pentene	4.1883	1.9007	1.3906	0.4157	0.2696	38	2,4-MM-1-pentene	5.1584	2.2658	1.9809	0.5110	0.4911
15	2-M-2-pentene	4.4661	1.9866	1.3599	0.4229	0.2410	39	3,3-MM-1-pentene	5.1520	2.2759	1.9728	1.0127	0.7986
16	3-M-*cis*-2-pentene	4.4060	2.0117	1.1393	0.7372	0.1512	40	3,4-MM-1-pentene	4.9920	2.2663	1.6869	0.9392	0.3383
17	4-M-*cis*-2-pentene	4.3373	1.9450	1.3217	0.3892	0.2300	41	4,4-MM-1-pentene	5.2950	2.2330	2.4739	0.5405	1.2579
18	2-E-1-butene	4.1513	1.9774	1.0688	0.6562	0.1265	42	3-E-2-pentene	4.9122	2.4088	1.3773	0.8662	0.0973
19	2,3-MM-1-butene	4.5060	1.9129	1.5406	0.7068	0.3498	43	2,3-MM-2-pentene	5.4006	2.3881	1.7229	1.0247	0.3321
20	3,3-MM-1-butene	4.6472	1.8624	2.1068	0.4689	1.1104	44	2,4-MM-2-pentene	5.3434	2.3095	1.9852	0.4665	0.4832
21	2,3-MM-2-butene	4.8944	1.9889	1.6944	0.8000	0.4000	45	3,4-MM-*cis*-2-pentene	5.2668	2.3461	1.6669	0.9839	0.3165
22	1-heptene	4.5189	2.3257	1.2017	0.5951	0.0000	46	4,4-MM-*cis*-2-pentene	5.4301	2.2733	2.3634	0.4840	1.1283
23	*cis*-2-heptnee	4.6875	2.3663	1.1872	0.5938	0.0000	47	2-E-3-M-1-butene	5.0121	2.3103	1.6069	0.8648	0.2966
24	*cis*-3-heptene	4.6400	2.3717	1.1654	0.5435	0.0000	48	2,3,3-MMM-1-butene	5.5884	2.2496	2.5138	0.9933	1.1454
						Alcohols							
1	ethanol	1.9114	0.7955	0.2296	0.0000	0.0000	22	3,3-MM-2-butanol	5.3081	2.1929	2.4307	0.8989	1.1676
2	1-propanol	2.5256	1.1641	0.4881	0.1409	0.0000	23	3-hexanol	4.5217	2.2811	1.2657	0.6586	0.0870
3	2-propanol	2.7815	1.1226	0.8190	0.0000	0.1847	24	3-M-3-pentanol	4.8772	1.9960	1.6339	0.9865	0.4956
4	1-butanol	3.1380	1.5395	0.7129	0.2989	0.0000	25	1-heptanol	4.9751	2.6645	1.4020	0.7179	0.0000
5	2-M-1-propanol	3.4197	1.4875	1.1302	0.2521	0.2696	26	2-heptanol	5.1831	2.6397	1.6042	0.7169	0.1288
6	2-butanol	3.3442	1.5194	0.8870	0.3622	0.1247	27	3-heptanol	5.1340	2.6564	1.4914	0.8154	0.0870
7	2-M-2-propanol	3.8673	1.4481	1.8239	0.0000	0.9837	28	4-heptanol	5.1358	2.6512	1.5231	0.7440	0.0899
8	1-pentanol	3.7503	1.9145	0.9427	0.4365	0.0000	29	2,4-MM-3-pentanol	5.6575	2.5731	2.1683	0.9017	0.5053
9	3-M-1-butanol	4.0299	1.8672	1.3397	0.4390	0.2604	30	1-octanol	5.5874	3.0395	1.6316	0.8585	0.0000
10	2-pentanol	3.9583	1.8893	1.1488	0.4193	0.1288	31	2-octanol	5.7954	3.0147	1.8339	0.8577	0.1288
11	2-M-1-butanol	3.9818	1.8881	1.1697	0.6242	0.1818	32	4-octanol	5.7482	3.0266	1.7488	0.9009	0.0899
12	3-pentanol	3.9075	1.9109	1.0085	0.5701	0.0843	33	2-E-1-hexanol	5.7710	3.0291	1.7468	1.0774	0.1268
13	3-M-2-butanol	4.2181	1.8549	1.4330	0.6328	0.3164	34	2,2,4-MMM-1-pentanol	6.5439	2.9210	3.0323	0.9523	1.2383
14	2-M-2-butanol	4.3721	1.8609	1.7013	0.5715	0.7016	35	3,5-MM-1-hexanol	6.1003	2.9620	2.3039	0.9199	0.4573
15	2,2-MM-1-propanol	4.5264	1.8176	2.2078	0.3654	1.2579	36	1-nonanol	6.1998	3.4145	1.8613	0.9992	0.0000
16	1-hexanol	4.3627	2.2895	1.1724	0.5773	0.0000	37	2,6-MM-4-heptanol	6.9241	3.3014	2.8225	0.9465	0.6354
17	2-M-1-pentanol	4.5960	2.2578	1.4350	0.6667	0.1878	38	5-nonanol	6.3606	3.4020	1.9745	1.0578	0.0899
18	2-E-1-butanol	4.5445	2.2838	1.2605	0.8455	0.1227	39	1-decanol	6.8122	3.7895	2.0909	1.1398	0.0000
19	4-M-2-pentanol	4.8524	2.2142	1.8020	0.5059	0.4029	40	1-undecanol	7.4246	4.1645	2.3206	1.2804	0.0000
20	2,3-MM-2-butanol	5.2319	2.2020	2.1796	0.9811	0.7894	41	2,6,8-MMM-4-nonanol	8.9944	4.3964	3.7835	1.4402	0.8298
21	3,3-MM-1-butanol	5.1342	2.2011	2.4060	0.5885	1.2272	42	1-tridecanol	8.6493	4.9145	2.7798	1.5617	0.0000

For alcohols:

$$\mathrm{MR} = -1.707 + 6.373\,{}^0\chi^v \qquad (20)$$

$$r^2 = 0.987,\ s = 1.3,\ F = 3022.5,\ N = 41$$

$$\mathrm{MR} = 3.762 + 12.266\,{}^1\chi^h \qquad (21)$$

$$r^2 = 0.996,\ s = 0.7,\ F = 10010.6,\ N = 41$$

The statistical results given above show that the mMCI gives a much better representation of molecular refraction

Table 4. Structural Descriptors (SD), Coefficients (a_0 and a_1), and Statistical Indices for the QSPR Models for the Normal Boiling Point Temperature (BPT) (°C) of 18 Octanes[a]

SD	a_0	a_1	r^2	s	F
		MCI			
$^0\chi$	276.817	−24.742	0.541	4.3	18.9
$^1\chi$	3.144	30.328	0.674	3.6	33.1
$^2\chi$	**143.952**	**−9.515**	**0.777**	**3.0**	**55.8**
$^3\chi_p$	106.135	4.173	0.087	6.0	1.5
$^3\chi_c$	120.478	−7.528	0.682	3.6	34.3
		mMCI			
$^0\chi^h$	193.165	−13.346	0.631	3.8	27.3
$^1\chi^h$	**−245.113**	**127.176**	**0.814**	**2.7**	**70.0**
$^2\chi^h$	134.849	−9.323	0.747	3.1	47.2
$^3\chi_p{}^h$	111.672	1.827	0.009	6.3	0.1
$^3\chi_c{}^h$	119.688	−9.325	0.673	3.6	32.9

[a] The QSPR models have the general form BPT = $a_0 + a_1$SD.

Table 5. Structural Descriptors (SD), Coefficients (a_0 and a_1), and Statistical Indices for the QSPR Models for the Normal Boiling Point Temperature (BPT) (°C) of 27 Heptenes[a]

SD	a_0	a_1	r^2	s	F
		MCI			
$^0\chi^v$	156.019	−12.520	0.076	6.8	2.1
$^1\chi^v$	−46.806	46.832	0.595	4.5	36.7
$^2\chi^v$	**120.370**	**−14.984**	**0.672**	**4.0**	**51.2**
$^3\chi_p{}^v$	87.308	0.512	0.000	7.0	0.0
$^3\chi_c{}^v$	93.829	−13.117	0.647	4.2	45.9
		mMCI			
$^0\chi^h$	148.254	−12.085	0.220	6.2	7.1
$^1\chi^h$	**−229.715**	**136.823**	**0.816**	**3.0**	**110.7**
$^2\chi^h$	110.645	−13.983	0.567	4.6	32.8
$^3\chi_p{}^h$	89.320	−2.006	0.003	7.0	0.1
$^3\chi_c{}^h$	93.145	−15.466	0.598	4.5	37.2

[a] The QSPR models have the general form BPT = $a_0 + a_1$SD.

Table 6. Structural Descriptors (SD), Coefficients (a_0 and a_1), and Statistical Indices for the QSPR Models for the Molar Volumes (MV) (cm^3/mol) at 20 °C of Alkanes[a]

SD	a_0	a_1	r^2	s	F
		MCI			
$^0\chi$	**38.757**	**18.541**	**0.938**	**3.7**	**483.8**
$^1\chi$	56.69	28.115	0.880	5.2	233.6
$^2\chi$	106.175	15.390	0.423	11.4	23.5
$^3\chi_p$	124.532	16.415	0.365	12.0	18.4
$^3\chi_c$	146.662	2.978	0.014	14.9	0.5
		mMCI			
$^0\chi^h$	51.064	18.321	0.833	6.2	159.5
$^1\chi^h$	**51.809**	**38.532**	**0.949**	**3.4**	**593.6**
$^2\chi^h$	121.461	13.001	0.271	12.8	11.9
$^3\chi_p{}^h$	126.769	24.765	0.347	12.2	17.0
$^3\chi_c{}^h$	147.399	2.818	0.008	15.0	0.3

[a] The QSPR models have the general form MV = $a_0 + a_1$SD.

Table 7. Structural Descriptors (SD), Coefficients (a_0 and a_1), and Statistical Indices for the QSPR Models for the Molar Volumes (cm^3/mol) at 20 °C of Alkenes[a]

SD	a_0	a_1	r^2	s	F
		MCI			
$^0\chi$	**25.129**	**19.842**	**0.954**	**3.1**	**961.8**
$^1\chi$	36.552	31.624	0.905	4.5	438.5
$^2\chi$	83.972	20.027	0.586	9.3	65.1
$^3\chi_p$	99.878	24.694	0.498	10.3	45.7
$^3\chi_c$	124.511	10.516	0.098	13.8	5.0
		mMCI			
$^0\chi^h$	43.499	18.937	0.822	6.1	212.6
$^1\chi^h$	**44.384**	**40.921**	**0.935**	**3.7**	**661.3**
$^2\chi^h$	98.421	21.905	0.469	10.6	40.6
$^3\chi_p{}^h$	104.375	41.504	0.462	10.6	39.5
$^3\chi_c{}^h$	125.318	14.230	0.095	13.8	4.8

[a] The QSPR models have the general form MV = $a_0 + a_1$SD.

Table 8. Structural Descriptors (SD), Coefficients (a_0 and a_1), and Statistical Indices for the QSPR Models for the Molar Volumes (cm^3/mol) at 20 °C of Alcohols[a]

SD	a_0	a_1	r^2	s	F
		MCI			
$^0\chi^v$	**6.212**	**22.857**	**0.989**	**4.2**	**3510.2**
$^1\chi^v$	31.460	32.425	0.981	5.4	2067.3
$^2\chi^v$	49.196	35.453	0.774	18.7	136.7
$^3\chi_p{}^v$	64.879	59.228	0.888	13.2	316.9
$^3\chi_c{}^v$	133.477	−0.151	0.000	39.4	0.0
		mMCI			
$^0\chi^h$	5.184	25.626	0.958	8.1	907.7
$^1\chi^h$	**26.461**	**43.798**	**0.994**	**3.0**	**6666.6**
$^2\chi^h$	61.106	42.925	0.607	24.7	61.8
$^3\chi_p{}^h$	63.587	98.708	0.851	15.2	228.2
$^3\chi_c{}^h$	134.273	−2.705	0.001	39.4	0.0

[a] The QSPR models have the general form MV = $a_0 + a_1$SD.

Table 9. Structural Descriptors (SD), Coefficients (a_0 and a_1), and Statistical Indices for the QSPR Models for the Molar Refraction (cm^3/mol) at 20 °C of Alkanes[a]

SD	a_0	a_1	r^2	s	F
		MCI			
$^0\chi$	**1.107**	**5.751**	**0.958**	**0.9**	**738.3**
$^1\chi$	6.393	8.804	0.916	1.3	350.1
$^2\chi$	22.883	4.461	0.378	3.6	19.4
$^3\chi_p$	26.714	5.762	0.478	3.3	29.3
$^3\chi_c$	34.818	0.601	0.006	4.6	0.2
		mMCI			
$^0\chi^h$	5.233	5.624	0.834	1.9	160.6
$^1\chi^h$	**4.925**	**12.042**	**0.984**	**0.6**	**2031.1**
$^2\chi^h$	27.497	3.965	0.231	4.0	9.6
$^3\chi_p{}^h$	27.510	8.681	0.453	3.4	26.5
$^3\chi_c{}^h$	35.043	0.426	0.002	4.6	0.1

[a] The QSPR models have the general form MR = $a_0 + a_1$SD.

than the original MCI. Since MR has a close relationship to molecular polarizability, it is a more crucial test of the capability of a topological index.

CONCLUSIONS

A modified adjacency matrix was proposed, which can incorporate more structural information of a compound than the normal adjacency matrix. The modified molecular connectivity indices developed on the basis of the modified adjacency matrix give good QSPR models for normal boiling point temperature, molar volume and molar refraction of alkanes, alkenes and alcohols. The correlative accuracy is better, in most cases, than that of the original molecular connectivity indices. An advantage of the mMCI over the original MCI is that it can distinguish isomers better, which may play an important role in the QSPR/QSAR studies. Currently, their applications to other physical properties and to more complex compounds are under investigation, and the results will be reported in a future paper.

Table 10. Structural Descriptors (SD), Coefficients (a_0 and a_1), and Statistical Indices for the QSPR Models for the Molar Refraction (cm^3/mol) at 20 °C of Alkenes[a]

SD	a_0	a_1	r^2	s	F
		MCI			
$^0\chi$	**2.427**	**5.479**	**0.961**	**0.8**	**1143.5**
$^1\chi$	5.395	8.795	0.925	1.1	567.0
$^2\chi$	18.935	5.415	0.566	2.6	60.0
$^3\chi_p$	22.834	7.014	0.531	2.7	52.1
$^3\chi_c$	30.020	2.569	0.078	3.8	3.9
		mMCI			
$^0\chi^h$	7.107	5.315	0.856	1.5	273.0
$^1\chi^h$	**7.363**	**11.482**	**0.973**	**0.7**	**1632.5**
$^2\chi^h$	22.925	5.864	0.444	3.0	36.7
$^3\chi_p{}^h$	23.987	11.995	0.510	2.8	47.9
$^3\chi_c{}^h$	30.239	3.398	0.072	3.8	3.5

[a] The QSPR models have the general form MR = $a_0 + a_1$SD.

Table 11. Structural Descriptors (SD), Coefficients (a_0 and a_1), and Statistical Indices for the QSPR Models for the Molar Refraction (cm^3/mol) at 20 °C of Alcohols[a]

SD	a_0	a_1	r^2	s	F
		MCI			
$^0\chi^v$	**−1.707**	**6.373**	**0.987**	**1.3**	**3022.5**
$^1\chi^v$	5.043	9.109	0.985	1.4	2537.9
$^2\chi^v$	10.363	9.944	0.785	5.1	142.3
$^3\chi_p{}^v$	14.121	16.852	0.902	3.5	357.8
$^3\chi_c{}^v$	33.654	0.605	0.001	11.1	0.0
		mMCI			
$^0\chi^h$	−1.851	7.128	0.956	2.3	854.2
$^1\chi^h$	**3.762**	**12.266**	**0.996**	**0.7**	**10010.6**
$^2\chi^h$	13.437	12.241	0.630	6.7	66.4
$^3\chi_p{}^h$	13.934	27.898	0.860	4.2	239.3
$^3\chi_c{}^h$	33.875	−0.088	0.000	11.1	0.0

[a] The QSPR models have the general form MR = $a_0 + a_1$SD.

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