Molecular topological index: An extension to heterosystems*

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> "... *scientists have raised statistics to the level of at least a skyscraper, if not of an institution, and in time will almost certainly succeed in calculating the specific weight of the human soul*"
>
> Pierre Daninos: "Sonia, je t'adore"
> Knopf, New York, 1959

The molecular topological index (MTI), recently introduced by Schultz, is extended to heterosystems. In order to test the utility of this formulation of the MTI, the index is used to set up the structure–property model for boiling points of alkyl alcohols. This model is comparable to related models based on the connectivity index and on the Wiener index.

1. Introduction

Recently, a novel graph-theoretical index, named the molecular topological index (MTI), has been introduced [1]. Since the term molecular topological index is not particularly precise, we call this index the Schultz index after its originator [2]. Because the MTI index is a molecular descriptor with structural significance and a number of attractive features [1–5], we decided to extend it to a form that can embrace the heterosystems. The utility of this extended version of the MTI will be tested in QSPR (quantitative structure–property relationships) modeling of boiling points of alkyl alcohols. This property of alkyl alcohols was selected because a very accurate QSPR model, based on the connectivity index [6], has already been proposed

*Dedicated to Professor Frank Harary on the occasion of his 70th birthday.
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by Kier and Hall [7,8]. The connectivity index of Randić and its variants are the most successful graph-theoretical descriptors to date to be used in the structure–property–activity correlations [9–15] and thus we will be able to investigate how the MTI descriptor performs in comparison with the connectivity index on the same sample. We will also compare the QSPR model with the MTI with the model based on the Wiener number [16]. The Wiener number is another topological index which is successfully used in the QSPR modeling of physical properties of molecules [10,13,17,18].

In order to simplify the presentation, molecules will be depicted by the corresponding graphs using the standard rules of conversion [19,20]. Hydrocarbons will be represented by simple molecular graphs, while heterosystems will be represented with weighted graphs. In both cases, the hydrogen atoms will be omitted from the consideration.

This paper is structured as follows. In section 2, we give the definition of the MTI index. Section 3 contains an extension of the MTI to heterosystems. In sections 4 and 5, expressions are given for computing the connectivity index and the Wiener number. Section 6 includes the QSPR model (property = boiling point) with the MTI index, and a comparison between this model and the structure–property models based on the connectivity index and the Wiener number. The paper ends with concluding remarks.

2. The definition of the MTI index

The molecular topological index or the Schultz index is defined as [1,21]

$$\mathrm{MTI} = \sum_{i=1}^{N} e_i, \tag{1}$$

where e_i ($i = 1, 2, \ldots, N$) are the elements of the following row matrix of order N:

$$\upsilon[\mathbf{A} + \mathbf{D}] = [e_1\ e_2 \ldots e_N]. \tag{2}$$

In (2), $\mathbf{A}$ is the adjacency ($N \times N$) matrix [22,23], $\mathbf{D}$ the distance ($N \times N$) matrix [22–24], and υ the valency ($1 \times N$) matrix of a structure G. The entries in the valency row matrix υ are the graph-theoretical valencies. An example of computing the Schultz index is given in table 1.

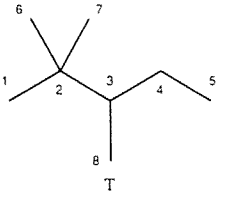
3. An extension of the Schultz index to heterosystems

The Schultz index may be extended to heterosystems by replacing the elements of the adjacency matrix and of the distance matrix corresponding to heteroatoms and heterobonds with the values incorporating the corrections due to the changes induced when a carbon atom is replaced by a heteroatom. One way of introducing

Table 1

Steps involved in the computation of the Schultz index for a tree T depicting 2,2,3-trimethylpentane.

(1) A labeled tree T



(2) The adjacency matrix of T

$$\mathbf{A}(T) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

(3) The distance matrix of T

$$\mathbf{D}(T) = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 2 & 2 & 3 \\ 1 & 0 & 1 & 2 & 3 & 1 & 1 & 2 \\ 2 & 1 & 0 & 1 & 2 & 2 & 2 & 1 \\ 3 & 2 & 1 & 0 & 1 & 3 & 3 & 2 \\ 4 & 3 & 2 & 1 & 0 & 4 & 4 & 3 \\ 2 & 1 & 2 & 3 & 4 & 0 & 2 & 3 \\ 2 & 1 & 2 & 3 & 4 & 2 & 0 & 3 \\ 3 & 2 & 1 & 2 & 3 & 3 & 3 & 0 \end{bmatrix}$$

(4) The adjacency-plus-distance matrix of T

$$[\mathbf{A} + \mathbf{D}](T) = \begin{bmatrix} 0 & 2 & 2 & 3 & 4 & 2 & 2 & 3 \\ 2 & 0 & 2 & 2 & 3 & 2 & 2 & 2 \\ 2 & 2 & 0 & 2 & 2 & 2 & 2 & 2 \\ 3 & 2 & 2 & 0 & 2 & 3 & 3 & 2 \\ 4 & 3 & 2 & 2 & 0 & 4 & 4 & 3 \\ 2 & 2 & 2 & 3 & 4 & 0 & 2 & 3 \\ 2 & 2 & 2 & 3 & 4 & 2 & 0 & 3 \\ 3 & 2 & 2 & 2 & 3 & 3 & 3 & 0 \end{bmatrix}$$

. . . continues

Table 1 (continued)

(5) The valence row matrix υ of T

$$\upsilon(T) = [1\ 4\ 3\ 2\ 1\ 1\ 1\ 1]$$

(6) The $\upsilon[\mathbf{A}+\mathbf{D}]$ row matrix of T

$$\upsilon[\mathbf{A}+\mathbf{D}](T) = [31\ 21\ 22\ 27\ 37\ 31\ 31\ 30]$$

(7) The Schultz index of T

$$\mathrm{MTI}(T) = 230$$

these corrections is described here. The corrections due to heteroatoms and heterobonds are denoted as the atomic parameters and the bond parameters, respectively, and are based on the concept of the atomic number.

The atomic parameter and the bond parameter are defined in terms of atomic number as follows [25]:

$$\text{atomic parameter} = 1 - \frac{Z_C}{Z_i}, \tag{3}$$

$$\text{bond parameter} = \frac{1}{b_{ij}}\ \frac{Z_C^2}{Z_i Z_j}, \tag{4}$$

where Z_C is the atomic number of the carbon atom and Z_i the atomic number of an atom i. The values of bond parameter b_{ij} are 1, 1.5, 2 and 3 for a single bond, an aromatic bond, a double bond and a triple bond, respectively.

In table 2 are given the atomic parameters and in table 3 the bond parameters for the most common atoms and heterobonds in organic chemistry.

Table 2

Atomic parameters for common atoms in organic chemistry.

Atom	Atomic parameter
carbon	0
nitrogen	0.143
oxygen	0.25
sulphur	0.625
chlorine	0.647

Table 3

Bond parameters for common bonds in organic chemistry.

Bond	Bond parameter
C–C	1
C=C	0.5
C≡C	0.333
C–N	0.857
C=N	0.429
C–O	0.75
C=O	0.375
C–Cl	0.353
C–S	0.375
C=S	0.188

In the case of the adjacency matrix, the diagonal elements corresponding to heteroatoms are identical to (3), i.e.

$$(\mathbf{A})_{ii} = \text{atomic parameter for } i = \text{heteroatom};$$
$$= 0 \text{ for carbon atom.} \tag{5}$$

The non-vanishing off-diagonal elements of the adjacency matrix corresponding to heterobonds are identical to (4), i.e.

$$(\mathbf{A})_{ij} = \text{bond parameter if atoms } i \text{ and } j \text{ are bonded;}$$
$$= 0 \text{ otherwise.} \tag{6}$$

In the case of the distance matrix, the diagonal elements corresponding to heteroatoms are also identical to (3), i.e.

$$(\mathbf{D})_{ii} = \text{atomic parameter} \tag{7}$$

for i = heteroatom. Since the off-diagonal elements of the distance matrix represent the length of a shortest path between atoms i and j, eq. (4) gives a weight of an individual heterobond which contributes its weight to the path between i and j. Such a path containing a weighted edge is called a weighted path. Therefore, off-diagonal elements of the distance matrix containing heterobonds are given by

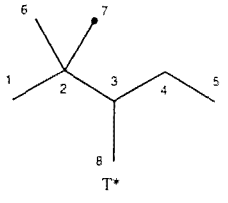
$$(\mathbf{D})_{ij} = \text{weighted path between sites } i \text{ and } j. \tag{8}$$

In table 4, we give as an illustrative example the computation of the Schultz index for 2,3-dimethyl-2-pentanol represented by a rooted tree T^* [26].

Table 4

The computation of the Schultz index for a rooted tree T^* representing 2,3-dimethyl-2-pentanol.

(1) A labeled rooted tree T^* (a root-vertex denoting the oxygen atom is given as a black dot)



(2) The adjacency matrix of T^*

$$\mathbf{A}(T^*) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0.75 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.75 & 0 & 0 & 0 & 0 & 0.25 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

(3) The distance matrix of T^*

$$\mathbf{D}(T^*) = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 2 & 1.75 & 3 \\ 1 & 0 & 1 & 2 & 3 & 1 & 0.75 & 2 \\ 2 & 1 & 0 & 1 & 2 & 2 & 1.75 & 1 \\ 3 & 2 & 1 & 0 & 1 & 3 & 2.75 & 2 \\ 4 & 3 & 2 & 1 & 0 & 4 & 3.75 & 3 \\ 2 & 1 & 2 & 3 & 4 & 0 & 1.75 & 3 \\ 1.75 & 0.75 & 1.75 & 2.75 & 3.75 & 1.75 & 0.25 & 2.75 \\ 3 & 2 & 1 & 2 & 3 & 3 & 2.75 & 0 \end{bmatrix}$$

(4) The adjacency-plus-distance matrix T^*

$$[\mathbf{A} + \mathbf{D}](T^*) = \begin{bmatrix} 0 & 2 & 2 & 3 & 4 & 2 & 1.75 & 3 \\ 2 & 0 & 2 & 2 & 3 & 2 & 1.50 & 2 \\ 2 & 2 & 0 & 2 & 2 & 2 & 1.75 & 2 \\ 3 & 2 & 2 & 0 & 2 & 3 & 2.75 & 2 \\ 4 & 3 & 2 & 2 & 0 & 4 & 3.75 & 3 \\ 2 & 2 & 2 & 3 & 4 & 0 & 1.75 & 3 \\ 1.75 & 1.50 & 1.75 & 2.75 & 3.75 & 1.75 & 0.50 & 2.75 \\ 3 & 2 & 2 & 2 & 3 & 3 & 2.75 & 0 \end{bmatrix}$$

. . . continues

Table 4 (continued)

(5) The valence row matrix of υ of T

$$\upsilon(T) = [1\ 4\ 3\ 2\ 1\ 1\ 1\ 1]$$

(6) The $\upsilon[A + D]$ row matrix of T^*

$$\upsilon[A + D](T^*) = [30.75\ 20.5\ 21.75\ 26.75\ 36.75\ 30.75\ 27.25\ 29.75]$$

(7) The Schultz index of T^*

$$\mathrm{MTI}(T^*) = 224.25$$

4. The connectivity index

The connectivity index $\chi = \chi(G)$ of G is defined by Randić [6] as

$$\chi = \sum_{i,j} [d(i)d(j)]^{-1/2}, \tag{9}$$

where $d(i)$ is the valency of a vertex i in G.

In the case of heterosystems, the connectivity index is given in terms of valence delta values $\delta(i)$ and $\delta(j)$ of atoms i and j, and is denoted by χ^v. This version of the connectivity index is called the valence connectivity index and is defined as [7,8,11]

$$\chi^v = \sum_{i,j} [\delta(i)\delta(j)]^{-1/2}. \tag{10}$$

Valence delta values are given by

$$\delta(i) = \frac{Z_i^v - H_i}{Z_i - Z_i^v - 1}, \tag{11}$$

where Z_i is the atomic number of atom i, Z_i^v the number of valence electrons of atom i, and H_i is the number of hydrogen atoms attached to atom i. The δ-values are available in the books by Kier and Hall [8,11] or by us [2,27]. Note that for carbon atoms, $\delta(i) = d(i)$. The edge-weights corresponding to various edge-types in weighted trees depicting alkyl alcohols are given in table 5. An example of computing the valence connectivity index for an alkyl alcohol is given in table 6.

Table 5

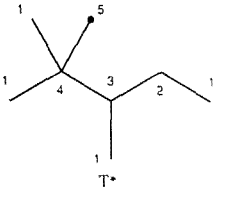
The edge-weights for edge-types in weighted trees representing alkyl alcohols.

Edge-type $\delta(i), \delta(j)$	Edge-weight $[\delta(i)\delta(j)]^{-1/2}$	Edge-type $\delta(i), \delta(j)$	Edge-weight $[\delta(i)\delta(j)]^{-1/2}$
1, 1	1	3, 3	0.3333
1, 2	0.7071	3, 4	0.2887
1, 3	0.5774	4, 4	0.25
1, 4	0.5	2, 5	0.3162
2, 2	0.5	3, 5	0.2582
2, 3	0.4082	4, 5	0.2236
2, 4	0.3536		

Table 6

The computation of the valence connectivity index for a rooted tree T^* depicting 2,3-dimethyl-2-pentanol.

(1) A rooted tree T^* with valence delta values



(2) The count of the edge-weights in T^*

$$(1 \cdot 2)^{-1/2} = 0.7071$$
$$(1 \cdot 3)^{-1/2} = 0.5774$$
$$2(1 \cdot 4)^{-1/2} = 1.0000$$
$$(2 \cdot 3)^{-1/2} = 0.4082$$
$$(3 \cdot 4)^{-1/2} = 0.2887$$
$$(4 \cdot 5)^{-1/2} = 0.2236$$

(3) The connectivity index of T^*

$$(T^*) = 3.2050$$

5. The Wiener number

The Wiener number $W = W(G)$ of G is defined as [28]

$$W = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(\mathbf{D})_{ij}, \tag{12}$$

where $(\mathbf{D})_{ij}$ is the i,jth element of the distance matrix which denotes the shortest graph-theoretical distance between sites i and j in G.

The distance matrix of a heterosystem is constructed in the way discussed earlier in the text. Thus, the Wiener number for a heterosystem is simply the half-sum of the elements of the distance matrix for a heterosystem. From the distance matrix of a rooted tree T^* depicting 2,3-dimethyl-2-propanol as already set up in table 4, the corresponding Wiener number is found to be 61.375.

6. The structure–property models for boiling points of alkyl alcohols

The MTI indices, the valence connectivity indices and the Wiener numbers for fifty-eight alkyl alcohols together with their boiling points [13,29] are given in table 7.

The following modest structure–property model with the MTI index is obtained:

$$\mathrm{bp}(^\circ\mathrm{C}) = (6.249 \pm 0.225)\mathrm{MTI}^{1/2} + (53.43 \pm 3.47), \tag{13}$$

$$n = 58,\ R = 0.9656,\ s = 9.35,\ F = 772.$$

A plot of bp versus $\mathrm{MTI}^{1/2}$ is given in fig. 1.

The above model compares well with the corresponding models based on the valence connectivity index and the Wiener number,

$$\mathrm{bp}(^\circ\mathrm{C}) = (2.672 \pm 1.029)(\chi^{\mathrm{v}})^2 + (20.89 \pm 6.23)\chi^{\mathrm{v}} + (54.83 \pm 9.19), \tag{14}$$

$$n = 58,\ R = 0.9639,\ s = 9.66,\ F = 361;$$

$$\mathrm{bp}(^\circ\mathrm{C}) = (11.851 \pm 0.420)W^{1/2} + (54.38 \pm 3.38), \tag{15}$$

$$n = 58,\ R = 0.9666,\ s = 9.22,\ F = 796.$$

Plots of bp versus χ^{v} and bp versus $W^{1/2}$ are given in figs. 2 and 3, respectively.

These models could be improved by the multiple regression analysis, as shown by Kier and Hall [7] and by Seybold et al. [13,14].

The models based on the MTI and Wiener number are almost identical. This is so probably because these two topological indices are strongly linearly intercorrelated ($R = 0.9999$). A plot of MTI versus W is given in fig. 4.

Table 7

The Schultz indices (MTI), the valence connectivity indices (χ^v), the Wiener indices (W) of alkyl alcohols and their boiling points (bp in °C).

Alkyl alcohol	MTI	χ^v	W	bp (°C)	bp (°C) calc. (eq. (13))
methanol	3.50	0.4470	0.875	64.7	65.1
ethanol	14.50	1.0233	3.625	78.3	77.2
1-propanol	35.75	1.5233	9.375	97.2	90.8
2-propanol	33.50	1.4129	8.375	82.3	89.6
1-butanol	71.00	2.0233	19.125	117.7	106.1
2-butanol	64.75	1.9509	17.125	99.6	103.7
2-methyl-1-propanol	65.00	1.8792	17.125	107.9	103.8
2-methyl-2-propanol	60.50	1.7236	15.125	82.4	102.0
1-pentanol	124.25	2.5233	33.875	137.8	123.1
2-pentanol	114.00	2.4509	30.875	119.0	120.1
3-pentanol	110.00	2.4889	29.875	115.3	119.0
2-methyl-1-butanol	110.25	2.4172	29.875	128.7	119.0
3-methyl-1-butanol	114.25	2.3792	30.875	131.2	120.2
2-methyl-2-butanol	101.75	2.2843	26.875	102.0	116.5
3-methyl-2-butanol	104.00	2.3236	27.875	111.5	117.2
2,2-dimethyl-1-propanol	102.25	2.1698	26.875	113.1	116.6
1-hexanol	199.50	3.0233	54.625	157.0	141.7
2-hexanol	185.25	2.9509	50.625	139.9	138.5
3-hexanol	177.25	2.9889	48.625	135.4	136.6
2-methyl-1-pentanol	177.50	2.9172	48.625	148.0	136.7
3-methyl-1-pentanol	177.50	2.9172	48.625	152.4	136.7
4-methyl-1-pentanol	185.50	2.8792	50.625	151.8	138.5
2-methyl-2-pentanol	165.00	2.7843	44.625	121.4	133.7
3-methyl-2-pentanol	163.25	2.8616	44.625	134.2	133.3
4-methyl-2-pentanol	171.25	2.8067	46.625	131.7	135.2
2-methyl-3-pentanol	163.25	2.8616	44.625	126.5	133.3
3-methyl-3-pentanol	157.00	2.8449	42.625	122.4	131.7
2-ethyl-1-butanol	169.50	2.9552	46.625	146.5	134.8
2,2-dimethyl-1-butanol	157.50	2.7304	42.625	136.8	131.8
2,3-dimethyl-1-butanol	163.50	2.7899	44.625	149.0	133.3
3,3-dimethyl-1-butanol	165.50	2.6698	44.625	143.0	133.8
2,3-dimethyl-2-butanol	151.00	2.6670	40.625	118.6	130.2
3,3-dimethyl-2-butanol	151.25	2.6242	40.625	120.0	130.3
1-heptanol	300.75	3.5233	82.375	176.3	161.8
3-heptanol	270.50	3.4889	74.375	156.8	156.2
4-heptanol	266.50	3.4889	73.375	155.0	155.4
2-methyl-2-hexanol	254.25	3.2843	69.375	142.5	153.1
3-methyl-3-hexanol	238.25	3.3449	65.375	142.4	149.9
3-ethyl-3-pentanol	157.00	2.8449	42.625	142.5	131.7
2,3-dimethyl-2-pentanol	224.25	3.2050	61.375	139.7	147.0
2,3-dimethyl-2-pentanol	236.25	3.1401	64.375	133.0	149.5
2,2-dimethyl-3-pentanol	224.50	3.1622	61.375	136.0	147.1

. . . continues

Table 7 (continued)

Alkyl alcohol	MTI	χ^v	W	bp (°C)	bp (°C) calc. (eq. (13))
2,3-dimethyl-3-pentanol	220.25	3.2276	60.375	139.0	146.2
2,4-dimethyl-3-pentanol	230.50	3.2343	63.375	138.8	148.3
1-octanol	432.00	4.0233	118.125	195.2	183.3
2-octanol	409.75	3.9509	112.125	179.8	179.9
2-ethyl-1-hexanol	370.00	3.9552	102.125	184.6	173.6
2,2,3-trimethyl-3-pentanol	291.50	3.5343	80.125	152.2	160.1
1-nonanol	597.25	4.5233	162.875	213.1	206.1
2-nonanol	571.00	4.4509	155.875	198.5	202.7
3-nonanol	551.00	4.4889	150.875	194.7	200.1
4-nonanol	539.00	4.4889	147.875	193.0	198.5
5-nonanol	535.00	4.4889	146.875	195.1	198.0
7-methyl-1-octanol	571.25	4.3792	155.875	206.0	202.8
2,6-dimethyl-4-heptanol	483.00	4.2006	132.875	178.0	190.8
3,5-dimethyl-4-heptanol	443.00	4.3103	122.875	187.0	184.9
3,5,5-trimethyl-1-hexanol	469.25	4.0636	128.875	193.0	188.8
1-decanol	800.50	5.0233	217.625	230.2	230.2

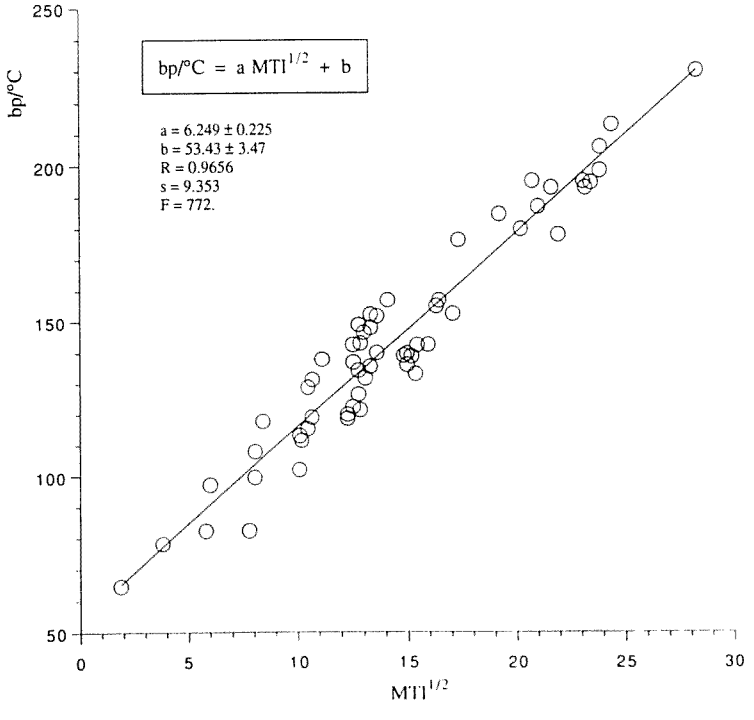


Fig. 1. Plot of bp versus $MTI^{1/2}$ for fifty-eight alkyl alcohols.

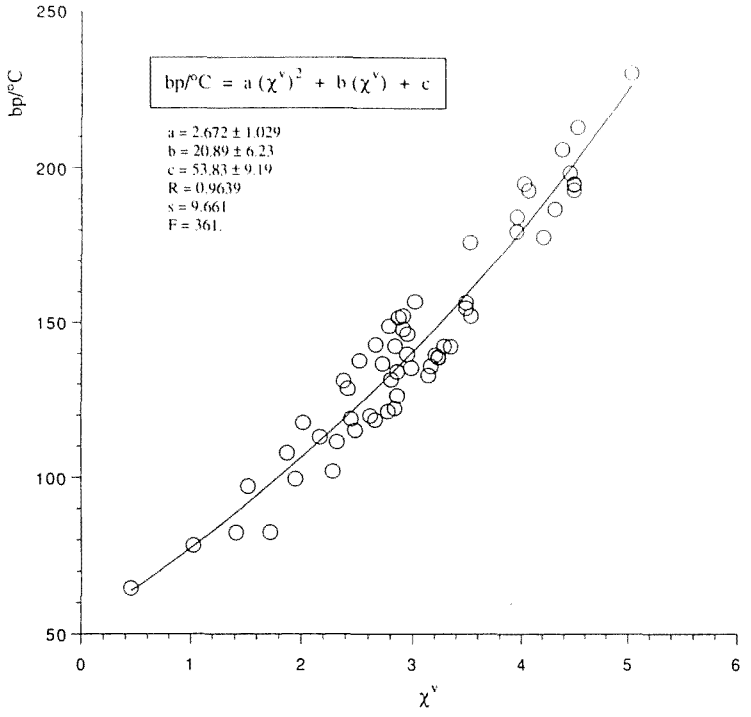


Fig. 2. Plot of bp versus χ^v for fifty-eight alkyl alcohols.

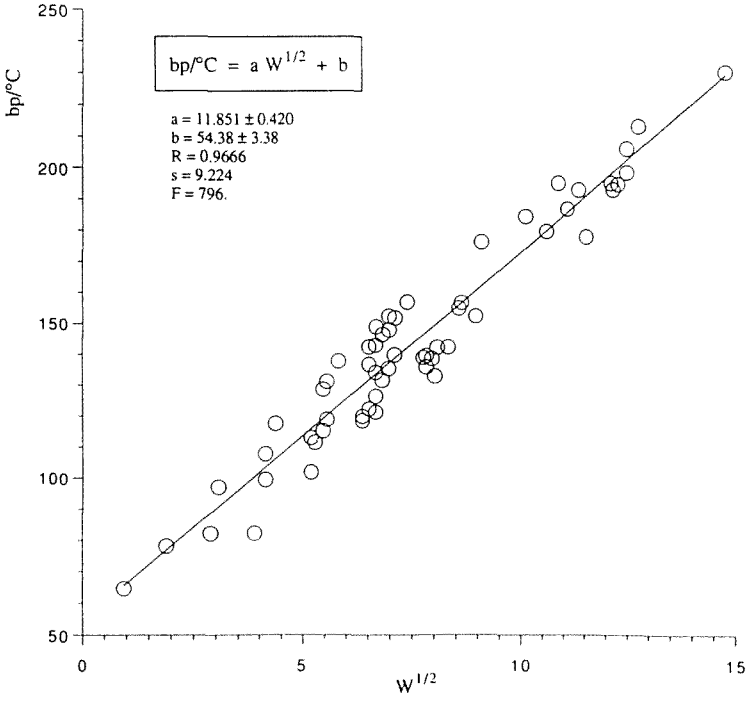


Fig. 3. Plot of bp versus $W^{1/2}$ for fifty-eight alkyl alcohols.

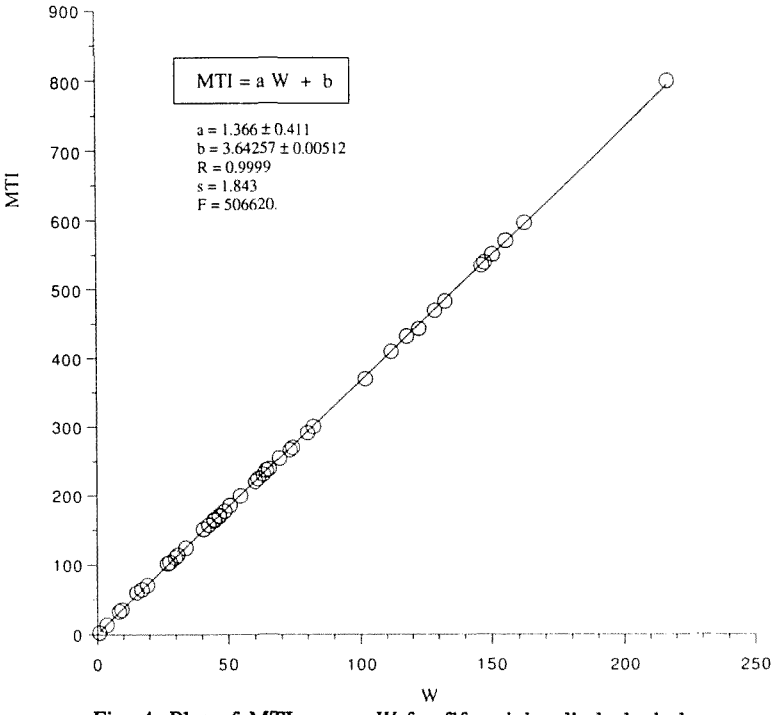


Fig. 4. Plot of MTI versus W for fifty-eight alkyl alcohols.

The result in fig. 4 suggests the existence of a formal relation between the MTI and W for weighted trees representing alkyl alcohols. We have found the following formula that connects the MTI and the Wiener number:

$$\mathrm{MTI} = 4W + 2p_2 - (N-1)(N-2) + 0.25(N-2-p_2^*), \tag{16}$$

where p_2 is the number of paths of length two in a weighted tree and p_2^* is the number of paths of length two which start at the weighted vertex. Therefore, if we know the Wiener number of a weighted tree, we immediately also know its molecular topological index. This then explains why the QSPR models with MTI and W are almost identical in their statistical characteristics.

7. Conclusions

We have proposed an extension of the molecular topological index, recently introduced by Schultz [1], to heterosystems. The extension is based on the adjustment of the adjacency matrix and distance matrix of a system for heteroatoms. The adjustment of these matrices for heterosystems is related to the changes in the atomic numbers when the carbon is replaced by a heteroatom.

The possible use of the MTI in this novel formulation in the structure–property relationships is illustrated by setting up the structure–property (property = boiling point) model for alkyl alcohol. The statistical characteristics of this model

are comparable to those for QSPR models with χ^v and W. This result indicates that the MTI is a topological index worthy of future studies about its properties and applicability in the structure–property–activity relationships.

Acknowledgement

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