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Relation between the Wiener Index and the Schultz Index for Several Classes of Chemical Graphs*

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It is shown that the Wiener index and the Schultz index are highly intercorrelated topological indices. For some classes of chemical graphs such as weighted and unweighed trees and cycles, the Schultz index can be expressed exactly in terms of the Weiner index, the number of vertices, the number of paths of length two and the position of weighted vertex in a chemical graph. Consequently, the structure-property-activity relationships based on either of these two indices should be closely congruent.

INTRODUCTION

The development of the quantitative structure-property relationships (QSPR) and the quantitative structure-activity relationships (QSAR) has been a major field of research for a long time.[1–6] In the last two decades, the QSPR and QSAR modeling based on topological (graph-theoretical) indices has shown an explosive growth.[7–16] Two factors greatly influenced research in this area. The first was a rapid progress of chemical graph theory[10,14,17] and the second was an amazing advance of computer technology, especially in terms of the portability and performance of PCs.

A topological index is a single number, derived following a certain rule, which can be used to characterize the molecule.[7] More than 120 topological indices have been proposed so far.[18] This large number of topological indices indicates that a clear and

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unambiguous criterion for their selection and verification is missing. However, Randić[19] has recently proposed a set of desirable properties of topological indices which will hopefully put some constraints on the unreasonable proliferation of indices. These requirements are summarized in Table I. When a molecular descriptor[20] fulfills the requirements in Table I, only then it can be »promoted« to the status of a topological index.

TABLE I

List of requirements for topological indices as proposed by Randić[19]

1	Direct structural interpretation
2	Good correlation with at least one physical or chemical property
3	Good discrimination of isomers
4	Locally defined
5	Generalizable to higher analogues
6	Linearly independent
7	Simplicity
8	Not based on physical or chemical properties
9	Not trivially related to, or highly intercorrelated with, other indices
10	Efficiency of construction
11	Based on familiar structural concepts
12	Showing size dependence
13	Gradual change with gradual structural changes

In the present report we will consider two topological indices: the Wiener index[21] and the Schultz index.[22] These two indices obey all the requirements from Table I, but two (No. 3 and No. 9), that is, they are not particularly discriminative indices[23,24] and they are closely mutually related for several classes of chemical structures. Here we discuss the latter point, *i.e.*, relationship between these two topological indices, also called distance indices[16] because both can be derived from the distance matrix.[10,14,24]

DEFINITIONS

Both the Wiener index and the Schultz index are well presented in literature.[7,14,16,23,24] Therefore, they will be described here rather briefly.

Wiener Index

The Wiener index $W = W(G)$ of a chemical graph G was introduced in 1947 as the path number.[21] It was elegantly defined 25 years later as a half-sum of the elements of the distance matrix $\boldsymbol{D} = \boldsymbol{D}(G)$ of G:[7]

$$W = \frac{1}{2} \sum_i \sum_j \boldsymbol{D}_{ij} \tag{1}$$

Since the distance matrix is also defined for weighted graphs,[26,27] the respective Wiener index can also be computed by means of Eq. (1).

An efficient computer program for the calculation of the Weiner index for any chemical graph is available in the literature.[28]

The Weiner index has been used in various structure-property relationships with considerable success.[16,29,30]

Schultz Index

The Schultz index MTI = MTI(G) of a chemical graph G was introduced in 1989 as the molecular topological index, and hence its acronym MTI.[22] It was defined succinctly as:[24]

$$\mathrm{MTI} = \sum_i e_i \tag{2}$$

where $e_i (i = 1, \cdots, N)$ are the elements of the row (1xN) matrix:

$$\boldsymbol{v}[\boldsymbol{A} + \boldsymbol{D}] = [e_1 \cdots e_N] \tag{3}$$

where $\boldsymbol{v}$ is the valency (1xN) matrix, $\boldsymbol{A}$ the adjacency (NxN) matrix and $\boldsymbol{D}$ the distance (NxN) matrix of a chemical graph.

Since the Wiener index and the Schultz index use the same distance matrix for the same structure, the MTI index can also be computed without any difficulty for weighted chemical graphs.

The Schultz index has also been used in several structure-property relationships with reasonable success.[16,23,31,32]

The Relationship Between the Wiener Index and the Schultz Index for Alkanes

The Wiener index and the Schultz index are strongly linearly intercorrelated distance indices for trees depicting the carbon skeletons of alkanes.[16] For example, the linear correlation between W and MTI for all alkane-trees with up to 10 vertices is shown in Figure 1. The high value of the correlation coefficient ($R = 0.9999$) hints that a formal relationship might exist between W and MTI for alkane-trees. In the present paper, we will show that there is indeed a close connection between the above two distance indices for alkane-trees and several other classes of chemical graphs.

RELATIONSHIPS BETWEEN W AND MTI

Alkane-trees

The relationship between the Weiner index and the Schultz index for alkane-trees is given by:

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

where N is the number of vertices and p_2 the number of paths of length two in a tree. Eq. (4) was proved by Klein *et al.*[33]

A special case of Eq. (4) is a relationship between W and MTI for chains (n-alkane-trees) which can be given only in terms of N. Since the Wiener number of chains[23] is:

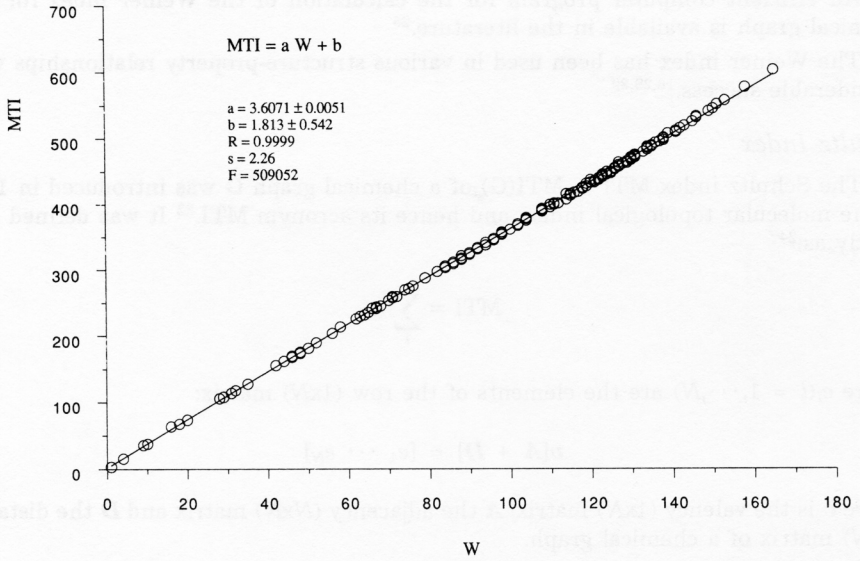

Figure 1. Plot of MTI *vs* W for the first 150 alkane-trees

$$W = N(N^2 - 1)/6 \tag{5}$$

and the number of p_2-paths of chains is given by:

$$p_2 = N - 2 \tag{6}$$

Eq. (4) reduces for chains to:

$$\text{MTI} = 2N(N^2 - 1)/3 - (N - 2)\ (N - 3) \tag{7}$$

Weighted Trees

Various acyclic molecules that contain heteroatoms can be represented graph-theoretically by weighted tress.[10,14] The Wiener index for weighted chains with, for example, a single weighted vertex is given by:

$$W = (N/6)\ (N^2 - 1) - [2(N - n)(n - 1) + (N - 1)]\ (1 - \beta) + (1/2)\alpha \tag{8}$$

where $n\ \varepsilon\ [1, N/2]$ for N = even and $n\varepsilon[1, (N + 1)/2]$ for N = odd; n being the position of weighted vertex. α is the vertex-weight and β the edge-weight.

One way of choosing the value of the α-parameter is the use of the following relationship:[26]

$$\alpha_x = 1 - Z_c/Z_x \tag{9}$$

where Z_x is the atomic number of the element X and $Z_c = 6$. In the case of weighted trees representing, for example, alkyl-alcohols,[31] the value of the α-parameter for oxygen is obtained as follows:

$$\alpha_o = 1 - 6/8 = 0.25 \tag{10}$$

Similarly, the edge-weight β may be chosen as:[26]

$$\beta_{cx} = (Z_c^2/Z_c Z_x) / b_{cx} \tag{11}$$

where b_{cx} is the bond multiplicity parameter with values 1, 1.5, 2 and 3 for a single bond, an aromatic bond, a double bond and a triple bond, respectively. In the case of weighted trees representing, for example, alkyl-alcohols[31] the value of the β-parameters for the C–O bond is given by:

$$\beta_{C-O} = 36/(6 \cdot 8) = 0.75 \tag{12}$$

The formula for computing the MTI for weighted chains with a single weighed terminal vertex is given by:

$$\text{MTI} = (2N/3)\,(N^2 - 1) - (N - 2)\,(N - 3) - (3N - 1 - k)\,(1 - \beta) + 2\alpha \tag{13}$$

where $k = 1$ for $N = 2$ and $k = 0$ for $N > 2$.

If the weighted vertex is placed at the location n ($n \geq 2$) in the chain then the above formula changes to:

$$\text{MTI} = (2N/3)\,(N^2 - 1) - (N - 2)\,(N - 3) - 2[4Nn - 3N - 4n^2 + 4n + 2 - k/2]\,(1 - \beta) + 4\alpha \tag{14}$$

where $n \varepsilon [2, N/2]$ for N = even and $n \varepsilon [2, (N + 1)/2]$ for N = odd. The parameter k takes the following values:

$$k = \begin{cases} 2 & n=2 \text{ and } N=3 \\ 1 & n=2 \text{ and } N>3 \\ 0 & n \geq 3 \end{cases} \tag{15}$$

The relationship between W and MTI for weighted chains with a single terminal weighted vertex is given by:

$$\text{MTI} = 4W - (N - 2)(N - 3) + (N - 3 + k)(1 - \beta) \tag{16}$$

where $k=1$ for $N=2$ and $k=0$ for $N>2$. This relationship slightly changes when the weighted vertex is placed at the nonterminal location n ($n \geq 2$) in the chain:

$$\text{MTI} = 4W - (N - 2)(N - 3) + (2N - 8 + k)(1 - \beta) + 2\alpha \tag{17}$$

where:

$$k = \begin{cases} 2 & n=2 \text{ and } N=3 \\ 1 & n=2 \text{ and } N>3 \\ 0 & n \geq 3 \end{cases} \quad (18)$$

Cycles

[*N*]cycles ($N \geq 3$) can be used to depict the carbon skeletons of cycloalkanes or [*N*]annulenes. The expression for computing their Wiener indices are known:[23,24]

$$W = \begin{cases} (N/2)^3 & N = \text{even} \\ (N/8)(N^2 - 1) & N = \text{odd} \end{cases} \quad (19)$$

The explicit formulae for computing the Schultz index for cycles are given by:

$$\text{MTI} = \begin{cases} (N/2)(N^2 + 8) & N = \text{even} \\ (N/2)(N^2 + 7) & N = \text{odd} \end{cases} \quad (20)$$

The relationship between W and MTI for cycles is rather simple:

$$\text{MTI} = 4\,(W + N) \quad (21)$$

Weighted Cycles

There are possible three formulae for Wiener indices of weighted cycles with a single weighted vertex. They depend on the parity of cycles and the β-values. We will consider all three cases here.

Case 1: N=even, $0 < \beta \leq 1$

$$W = (N/2)^3 - [(N-1) + (N^2 - 2N)/4]\,(1-\beta) + (1/2)\alpha \quad (22)$$

Case 2: N=odd, $0 < \beta \leq 1/2$

$$W = (N/8)(N^2 - 1) + (N - 1)/2 - [(N^2 + 4N - 5)/4](1 - \beta) + (1/2)\alpha \quad (23)$$

Case 3: N = odd, $1/2 \leq \beta \leq 1$

$$W = (N/8)(N^2 - 1) - [(N^2 - 1)/4](1 - \beta) + (1/2)\alpha \quad (24)$$

For the same three cases the formulae for the MTI are as follows:

Case 1: N=even, $0 < \beta \leq 1$

$$\text{MTI} = (N/2)(N^2 + 8) - (N^2 + 2\,N + 4)(1 - \beta) + 4\alpha \quad (25)$$

Case 2: N=odd, $0 < \beta \leq 1/2$

$$\text{MTI} = (N/2)(N^2 + 7) + 2(N - 1) - (N^2 + 4N + 3)(1 - \beta) + 4\alpha \quad (26)$$

Case 3: N=odd, $1/2 \leq \beta \leq 1$

$$\text{MTI} = (1/2)(N^2 + 7)(N - 2 + 2\beta) + 4\alpha \tag{27}$$

The relationship between the Wiener index and the Schultz index for weighted cycles is then given by:

$$\text{MTI} = 4(W + N) + 2(\alpha + 4\beta - 4) \tag{28}$$

for $0 < \beta \leq 1$.

Cyclic Graph With Branches

We correlated the Wiener index and the Schultz index for 102 cyclic graphs with branches with an even number of vertices. Their sizes were in a range from 4 to 32 vertices. The linear correlation between W and MTI for this case is shown in Figure 2.

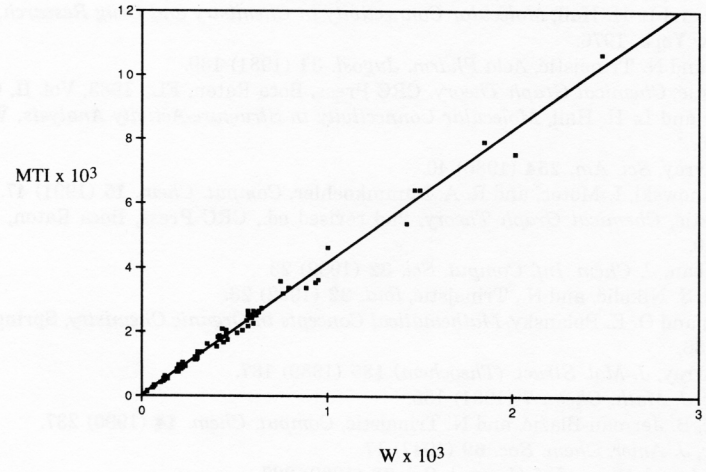

Figure 2. Plot of MTI *vs.* W for 102 cyclic graphs with branches

The linear least-squares relationship, corresponding to the line in Figure 2, possesses the following statistical characteristics: $R^2 = 0.9916$, $s = 168.314$ and $F = 11266.378$. This indicates that, for a general set of graphs, the MTI cannot be expressed in a simple way in terms of the Wiener number and some other graph-theoretical invariants.

CONCLUDING REMARKS

In this report we have shown that the MTI index can be expressed in terms of the Wiener index, the number of vertices, the number of paths of length two and the position of weighted vertex in simple classes of chemical graphs such as trees, weighted trees, cycles and weighted cycles.

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SAŽETAK

Odnos između Wienerovog indeksa i Schultzovog indeksa za neke klase kemijskih grafova

D. Plavšić, S. Nikolić, N. Trinajstić i D. J. Klein

Pokazano je da su Wienerov indeks i Schultzov indeks jako interkorelirani topologijski indeksi. Za neke klase kemijskih grafova kao što su stabla, prstenovi, utežena stabla i uteženi prstenovi, Schultzov indeks može se točno izraziti pomoću Wienerova indeksa, broja čvorova, staza duljine dva i položaja uteženog atoma. To ima za posljedicu da su odnosi strukture i svojstava (ili aktivnosti) temeljeni na jednomu od ta dva topologijska indeksa sukladni.