# Selected Properties of the Schultz Molecular Topological Index

Ivan Gutman†

Institute of Physical Chemistry, Attila József University, P.O. Box 103, H-6701 Szeged, Hungary

Received February 28, 1994®

Some properties of the Schultz molecular topological index (MTI) are established which show why, in certain series of isomers, MTIs decreases with the increasing extent of branching of the molecular carbon–atom skeleton. The relation between MTI and the Wiener index is examined, and some of its hitherto unnoticed aspects are pointed out.

## INTRODUCTION

The "molecular topological index" (MTI), put forward by Schultz only a few years ago,[1] became the topic of a large number of examinations by both Schultz, Schultz, and Schultz[2-7] and other researchers.[8-12] This quantity is defined in the following manner:[1,8]

$$\mathrm{MTI} = \mathrm{MTI}(\Gamma) = \sum_{i=1}^{N} [\mathbf{v}(\mathbf{A} + \mathbf{D})]_i$$

where $\Gamma$ is the molecular graph[13] considered, possessing $N = N(\Gamma)$ vertices. Further, $\mathbf{A}$ is the ($N \times N$ dimensional) adjacency matrix,[13] $\mathbf{D}$ is the ($N \times N$ dimensional) distance matrix,[13,14] and $\mathbf{v} = (v_1, v_2, \ldots, v_N)$ is the ($1 \times N$ dimensional) vector of the vertex valencies (degrees)[13] of the molecular graph $\Gamma$. Recall that $v_i = v_i(\Gamma)$ is the number of first neighbors of the $i$th vertex of $\Gamma$. Recall also that

$$\sum_{i=1}^{N} v_i(\Gamma) = 2M(\Gamma) \qquad (1)$$

where $M(\Gamma)$ stands for the number of edges of the graph $\Gamma$.

Bearing in mind that $\mathbf{v} = (1, 1, \ldots, 1)\mathbf{A}$, we can write MTI in the form

$$\mathrm{MTI} = \sum_{i=1}^{N} [(1,1,\ldots,1)\mathbf{A}(\mathbf{A} + \mathbf{D})]_i = \sum_{i=1}^{N}\sum_{j=1}^{N} [\mathbf{A}^2 + \mathbf{AD})]_{ij} = M + S \qquad (2)$$

where

$$M_2 = \sum_{i=1}^{N}\sum_{j=1}^{N} [\mathbf{A}^2]_{ij} = \sum_{i=1}^{N} (v_i)^2$$

$$S = S(\Gamma) = \sum_{i=1}^{N}\sum_{j=1}^{N} [\mathbf{AD}]_{ij} \qquad (3)$$

It is worth noting that

$$\sum_{i=1}^{N}\sum_{j=1}^{N} [\mathbf{AD}]_{ij} = \sum_{i=1}^{N}\sum_{j=1}^{N} [\mathbf{DA}]_{ij}$$

The sum $M_2$ of the squares of the vertex valencies is a graph invariant often occurring in chemical graph theory.[13] It found chemical applications as early as 1975.[15] Its relation to the molecular structure is, however, trivially simple.

The nontrivial part of MTI is the quantity $S$. In some earlier works[7,10] it has been denoted by MTI′. We prefer the new notation because the symbol $S$ can be associated with the name of th discoverer of the "molecular topological index".

By an easy calculation we transform the right-hand side of (3) into

$$S = {}^1/_2 \sum_{i=1}^{N}\sum_{j=1}^{N} [v_i + v_j] D_{ij} \qquad (4)$$

which should be compared with the definition of the Wiener index[13,16]

$$W = {}^1/_2 \sum_{i=1}^{N}\sum_{j=1}^{N} D_{ij} \qquad (5)$$

Hence, whereas $W$ is the sum of the distances between all pairs of vertices of the molecular graph, $S$ can be considered a vertex-valency-weighted sum of the same vertex distances.

For acyclic graphs (trees) Klein et al.[11] obtained a remarkable result, namely, the relation

$$\mathrm{MTI} = 4W + 2P_2 - (N-1)(N-2) \qquad (6)$$

where $P_2$ is the number of paths of length 2. Because

$$P_2 = \sum_{i=1}^{N} \binom{v_i}{2}$$

and because an $N$-vertex tree has $N - 1$ edges, from (1), (2), and (6) we immediately arrive at a simple formula:

$$S = 4W - N(N-1) \qquad (7)$$

The close (linear) correlation between MTI and $W$ (which is a straightforward consequence of eqs 6 and 7) was recently numerically verified for alkane trees with up to 10 vertices.[12]

## DECREASE OF SCHULTZ INDEX WITH BRANCHING

After comparing formulas 4 and 5, it is no surprise whatsoever that the Schultz index (MTI = $S + M_2$) has a dependence on molecular structure similar to the Wiener index ($W$). This especially applies for acyclic systems, for which eq 7 is obeyed.

We now offer a somewhat more rigorous justification of the above statement by showing that the graph transformation $G \rightarrow H$ necessarily increases both the Schultz and the Wiener

† On leave from the Faculty of Science, University of Kragujevac, Yugoslavia.

® Abstract published in *Advance ACS Abstracts*, May 15, 1994.

0095-2338/94/1634-1087$04.50/0 

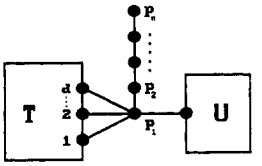
indexes. In particular, we demonstrate that

$$\mathrm{MTI}(H) - \mathrm{MTI}(G) = 2(n-1)\{N(U)[M(T)+d] + N(T)[M(U)+1]\} - 2d \quad (8)$$

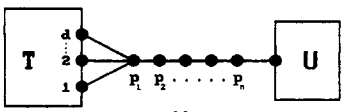
$$S(H) - S(G) = 2(n-1)\{N(U)[M(T)+d] + N(T)[M(U)+1]\} \quad (9)$$

$$W(H) - W(G) = (n-1)N(T)\,N(U) \quad (10)$$

where $N(T)$,$N(U)$ and $M(T)$,$M(U)$ denote the number of vertices and edges of the subgraphs $T$ and $U$, respectively, and where the meaning of the parameters $n$ and $d$ is evident from the following diagrams. The structure of the graphs $G$ and $H$ is given as follows:




G




H

Note that both $G$ and $H$ possess $N(T) + N(U) + n$ vertices and $M(T) + M(U) + n + d$ edges. The graphs $G$ and $H$ may be, but need not be, acyclic.

The right-hand sides of (8)–(10) are evidently positive-valued, and, consequently, $\mathrm{MTI}(H) > \mathrm{MTI}(G)$, $S(H) > S(G)$, and $W(H) > W(G)$. On the other hand, it is clear that graph $G$ is more branched than graph $H$. Namely, the only structural difference between $G$ and $H$ is at their vertices $p_1$ and $p_n$. Now, in $G$ the vertex $p_1$ is a $(d+2)$-fold branching point, whereas in $H$ it is a $(d+1)$-fold branching point, and $d \geq 1$.

To prove eqs 8–10, we first observe that

$$M_2(H) - M_2(G) = [v_{p_1}(H)^2 + v_{p_n}(H)^2] - [v_{p_1}(G)^2 + v_{p_n}(G)^2]$$

$$= [(d+1)^2 + 2^2] - [(d+2)^2 + 1] = -2d$$

Hence, (8) is an immediate consequence of (9).

Further, the only distances that are changed in the transformation $G \rightarrow H$ are those between the vertices of $T$ and $U$. Each such distance is increased by $n-1$. Since the number of vertex pairs, such that one vertex belongs to $T$ and the other to $U$, is $N(T)\,N(U)$, we immediately obtain (10).

It thus remains to prove formula 9.

In order to achieve this goal we denote the vertex set of the graph $\Gamma$ by $\mathrm{V}(\Gamma)$ and rewrite (3) or (4) as

$$S(\Gamma) = \sum_{i \in \mathrm{V}(\Gamma)} v_i(\Gamma)\, d(i|\Gamma) \quad (11)$$

where $d(i|\Gamma)$ is the distance number[16] of the vertex $i$ of the graph $\Gamma$, namely, the sum of all distances between $i$ and the vertices of $\Gamma$:

$$d(i|\Gamma) = \sum_{j \in \mathrm{V}(\Gamma)} D_{ij}$$

Applying $k$ to the graphs $G$ and $H$, we obtain

$$S(G) = \sum_{i \in \mathrm{V}(T)} v_i(G)\, d(i|G) + \sum_{i \in \mathrm{V}(U)} v_i(G)\, d(i|G) + \sum_{i=1}^{n} v_{p_i}(G)\, d(p_i|G) \quad (12)$$

$$S(H) = \sum_{i \in \mathrm{V}(T)} v_i(H)\, d(i|H) + \sum_{i \in \mathrm{V}(U)} v_i(H)\, d(i|H) + \sum_{i=1}^{n} v_{p_i}(H)\, d(p_i|H) \quad (13)$$

For reasons explained above

$$d(i|H) = d(i|G) + (n-1)N(U) \qquad \text{for } i \in \mathrm{V}(T)$$

$$d(i|H) = d(i|G) + (n-1)N(T) \qquad \text{for } i \in \mathrm{V}(U)$$

In addition to this, for $i = 1, 2, \ldots, n$,

$$d(p_i|H) = d(p_i|G) + (n-1)[N(T) + N(U)]$$

$$d(p_n|G) = d(p_1|G) + (n-2i+1)N(U)$$

From the structure of the graphs $G$ and $H$ it is immediately seen that, for $i \in \mathrm{V}(T)$ and $i \in \mathrm{V}(U)$, $v_i(H) = v_i(G)$. Furthermore, $v_{p_1}(G) = d+2$, $v_{p_1}(H) = d+1$, $v_{p_n}(G) = 1$, and $v_{p_n}(H) = 2$, whereas, for $i = 2, \ldots, n-1$, $v_{p_i}(H) = v_{p_i}(G) = 2$.

Combining all these relations with eqs 12 and 13, we arrive after a lengthy calculation at

$$S(H) = S(G) + (n-1)N(U) \sum_{i \in \mathrm{V}(T)} v_i(G) + (n-1)N(T) \sum_{i \in \mathrm{V}(U)} v_i(G) + (n-1)[dN(U) + N(T)] \quad (14)$$

Now, utilizing relation 1,

$$\sum_{i \in \mathrm{V}(T)} v_i(G) = \sum_{i \in \mathrm{V}(T)} v_i(T) + d = 2M(T) + d$$

$$\sum_{i \in \mathrm{V}(U)} v_i(G) = \sum_{i \in \mathrm{V}(U)} v_i(U) + 1 = 2M(U) + 1$$

which substituted back into (14) results in (9).

If the graphs $G$ and $H$ are acyclic, then the right-hand side of (9) is significantly simplified. Then, namely, $U$ is a tree with $M(U) + 1$ vertices, whereas $T$ is a $d$-component forest with $M(T) + d$ vertices. Consequently, for acyclic $G$ and $H$,

$$S(H) - S(G) = 4(n-1)N(T)\,N(U)$$

This latter result could, of course, be obtained from (10), by taking into account the fact that relation 7 is now applicable.

## RELATION BETWEEN THE SCHULTZ INDEX AND THE WIENER INDEX

In Wiener's first paper[17] on the topological index $W$ it was observed that, in the case of acyclic systems, instead of summing the distances between all pairs of vertices, it is more expedient to count the number of times an edge lies between pairs of vertices and then to sum these counts over all edges. Such a reasoning leads to the formula[16,17]

$$W(\Gamma) = \sum_{e} N_{\mathrm{L}}(e)\, N_{\mathrm{R}}(e) \quad (15)$$

where $N_L(e)$ and $N_R(e)$ are the numbers of vertices lying to the left and to the right of edge $e$ and the summation goes over all edges of the (acyclic) graph $\Gamma$. Notice that the choice of what is "left" and "right" is fully arbitrary. For all edges $e$,

$$N_L(e) + N_R(e) = N(\Gamma) \tag{16}$$

More details on the Wiener formula (15) can be found elsewhere.[16,18,19]

Bearing in mind the analogy between $W(\Gamma)$ and $S(\Gamma)$, eqs 4 and 5, it is not difficult to deduce the Wiener formula analogue for the index $S$:

$$S(\Gamma) = \sum_e \left[ N_L(e) \sum_L v_i(\Gamma) + N_R(e) \sum_R v_i(\Gamma) \right] \tag{17}$$

where $\sum_L$ and $\sum_R$ imply summation over the vertices lying to the left and to the right of edge $e$.

Now, the subgraph lying to the left of any edge $e$ of $\Gamma$ is itself a tree, possessing $N_L(e)$ vertices and $N_L(e) - 1$ edges. The same is, of course, true for the subgraph lying to the right of $e$. Taking these facts into account and applying (1), we get

$$\sum_L v_i(\Gamma) = 2[N_L(e) - 1] + 1; \quad \sum_D v_i(\Gamma) = 2[N_D(e) - 1] + 1 \tag{18}$$

which substituted back into (17) yields

$$S(\Gamma) = 4 \sum_e N_L(e)\, N_R(e) - \sum_e [N_L(e) + N_R(e)]$$

Bearing in mind (15) and (16), we see that the above result is precisely formula 7 of Klein et al.[11]

## ANOTHER SCHULTZ-TYPE MOLECULAR TOPOLOGICAL INDEX

We wish to point out another quantity, similar to $S$, which can be conceived by combining the adjacency and the distance matrices. In analogy to (3), we may define another Schultz-type topological index, namely,

$$S^* = S^*(\Gamma) = \sum_{i=1}^{N} \sum_{j=1}^{N} [\mathbf{ADA}]_{ij} \tag{19}$$

The right-hand side of (19) looks similar to, but is somewhat more symmetrical than, the right-hand side of (3). An expression having the same form as (4) and (5) is now readily obtained:

$$S^* = \sum_{i=1}^{N} \sum_{j=1}^{N} v_i v_j D_{ij}$$

Hence, $S^*$ is also a kind of a vertex-valency-weighted sum of the distances between all pairs of vertices in a graph. The difference between $S$ and $S^*$ is that in $S$ the weighting is additive, whereas in $S^*$ the weighting is multiplicative. If the graph $\Gamma$ is acyclic, then the following edge-summation formula holds for $S^*$

$$S^*(\Gamma) = 2 \sum_e \left[ \sum_L v_i(\Gamma) \right] \left[ \sum_R v_i(\Gamma) \right]$$

which should be compared with (15) and (17). Because of (18),

$$S^*(\Gamma) = 2 \sum_e [4N_L(e)\, N_R(e) - 2N_L(e) - 2N_R(e) + 1]$$

and because of (15) and (16),

$$S^* = 8W - 2(2N - 1)(N - 1) \tag{20}$$

This is a result of the same type as formula 7. It reveals the fact that in the case of acyclic structures the quantity $S^*$ is (in the same way as $S$) closely related to the Wiener index and reflects precisely the same structural features of a molecular as the Wiener index does.[19] Neither (7) nor (20) are valid for cyclic molecules. Consequently, the search for possible chemical applications of $S$, $S^*$, and similar quantities, as well as their theoretical investigations, should focus on the (much more difficult) case of polycyclic molecules.

## REFERENCES AND NOTES


(1) Schultz, H. P. Topological Organic Chemistry. 1. Graph Theory and Topological Indices of Alkanes. *J. Chem. Inf. Comput. Sci.* **1989**, *29*, 227–228.

(2) Schultz, H. P.; Schultz, E. B.; Schultz, T. P. Topological Organic Chemistry. 2. Graph Theory, Matrix Determinants and Eigenvalues, and Topological Indices of Alkanes. *J. Chem. Inf. Comput. Sci.* **1990**, *30*, 27–29.

(3) Schultz, H. P.; Schultz, T. P. Topological Organic Chemistry. 3. Graph Theory, Binary and Decimal Adjacency Matrices, and Topological Indices of Alkanes. *J. Chem. Inf. Comput. Sci.* **1991**, *31*, 144–147.

(4) Schultz, H. P.; Schultz, E. B.; Schultz, T. P. Topological Organic Chemistry. 4. Graph Theory, Matrix Permanents, and Topological Indices of Alkanes. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 69–72.

(5) Schultz, H. P.; Schultz, T. P. Topological Organic Chemistry. 5. Graph Theory, Matrix Hafnians and Pfaffians, and Topological Indices of Alkanes. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 364–366.

(6) Schultz, H. P.; Schultz, T. P. Topological Organic Chemistry. 6. Theory and Topological Indices of Cycloalkanes. *J. Chem. Inf. Comput. Sci.* **1993**, *33*, 240–244.

(7) Schultz, H. P.; Schultz, E. B.; Schultz, T. P. Topological Organic Chemistry. 7. Graph Theory and Molecular Topological Indices of Unsaturated and Aromatic Hydrocarbons. *J. Chem. Inf. Comput. Sci.* **1993**, *33*, 863–867.

(8) Müller, W. R.; Szymanski, K.; Knop, J. V.; Trinajstić, N. Molecular Topological Index. *J. Chem. Inf. Comput. Sci.* **1990**, *30*, 160–163.

(9) Knop, J. V.; Müller, W. R.; Szymanski, K.; Trinajstić, N. On the Determinant of the Adjacency-plus-Distance Matrix as the Topological Index for Characterizing Alkanes. *J. Chem. Inf. Comput. Sci.* **1991**, *31*, 83–84.

(10) Mihalić, Z.; Nikolić, S.; Trinajstić, N. Comparative Study of Molecular Descriptors Derived from the Distance Matrix. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 28–37.

(11) Klein, D. J.; Mihalić, Z.; Plavšić, D.; Trinajstić, N. Molecular Topological Index: A Relation with the Wiener Index. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 304–305.

(12) Plavšić, D.; Nikolić, S.; Trinajstić, N.; Klein, D. J. Relation between the Wiener Index and the Schultz Index for Several Classes of Chemical Graphs. *Croat. Chem. Acta* **1993**, *66*, 345–353.

(13) Trinajstić, N. *Chemical Graph Theory*, 2nd revised ed.; CRC Press: Boca Raton, FL, 1992.

(14) Milhalić, Z.; Veljan, D.; Amić, D.; Nikolić, S.; Plavšić, D.; Trinajstić, N. The Distance Matrix in Chemistry. *J. Math. Chem.* **1992**, *11*, 223–258.

(15) Gutman, I.; Ruščić, B.; Trinajstić, N.; Wilcox, C. F. Graph Theory and Molecular Orbitals. XII. Acyclic Polyenes. *J. Chem. Phys.* **1975**, *62*, 3399–3405.

(16) Gutman, I.; Polansky, O. E. *Mathematical Concepts in Organic Chemistry*; Springer-Verlag: Berlin, 1986.

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

(18) Gutman, I. A New Method for the Calculation of the Wiener Number of Acyclic Molecules. *J. Mol. Struct. (THEOCHEM)* **1993**, *285*, 137–142.

(19) Gutman, I.; Yeh, Y. N.; Lee, S. L.; Luo, Y. L. Some Recent Results in the Theory of the Wiener Number. *Indian J. Chem.* **1993**, *32A*, 651–661.