Molecular Topological Index: A Relation with the Wiener Index

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It is shown analytically that the recently introduced molecular topological index and the Wiener index, known since 1947, are closely related graph-theoretical invariants for acyclic structures.

Schultz[1] has recently introduced an index for characterization of alkanes by an integer, which he named the molecular topological index (MTI). Since this is not a particularly distinctive label, the MTI was also called the Schultz index[2] after its originator. The MTI appears to be an attractive graph-theoretical index that is easy to compute and has structural significance, although it is not an especially discriminative descriptor.[3]

The Schultz index is defined as

$$\mathrm{MTI} = \sum_{j=1}^{N} e_j \tag{1}$$

where

$$e_j = \sum_{i=1}^{N} v_i (A_{ij} + D_{ij}) \tag{2}$$

In eq 2 v_i is the valence of vertex i in a molecular graph[4] **G**, A_{ij} is the element of the adjacency matrix[5,6] for **G** (which is equal to unity if vertices i and j are adjacent and otherwise is zero), D_{ij} is the element of the distance matrix[5,6] for **G** (which is equal to the length of the shortest path between vertices i and j), and N is the number of vertices in **G**.

In a recent comparative study[7] of molecular descriptors derived from the distance matrix, it has been found that the MTI and the Wiener index[8] (W) are strongly ($r = 0.999$) linearly correlated distance indices for the set of trees (depicting carbon skeletons of alkanes) with up to 10 vertices. This result suggests the existence of a formal relation between MTI and W for trees. In the present report we wish to show that there is indeed a close connection between these two distance descriptors.

The Wiener index was introduced by Wiener[8] in 1947, but its graph-theoretical definition was first given by Hosoya[9] in 1971. The Wiener index W is defined as

$$W = \frac{1}{2} \sum_{i,j=1}^{N} D_{ij} \tag{3}$$

or if

$$W_i = \sum_{j=1}^{N} D_{ij} \tag{4}$$

then

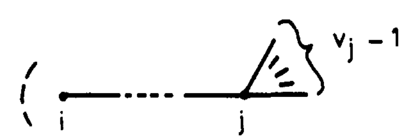
$$W = \frac{1}{2} \sum_{i=1}^{N} W_i \tag{5}$$

We now propose the following theorem: *If G is a tree, then*

$$e_i = 2W_i + (v_i + v'_i) - N + 1 \tag{6}$$

where v'_i is the number of next-nearest neighbors to i.

The proof of this theorem is as follows. For a pair of vertices i and j define the sum S_{ji} over all D_{ki} such that k is adjacent to j but more distant from i than j is. Clearly $S_{ii} = v_i$. For $j \neq i$ we have in a tree the circumstance depicted below:



That is, there is a single path of length D_{ji} from i to j, followed by single steps to $v_j - 1$ more distant neighbors of j. Thence

$$S_{ji} = (v_j - 1)(D_{ji} + 1),\ i \neq j \tag{7}$$

With the addition of the appropriate correction for $i = j$, we then have

$$S_{ji} = (v_j - 1)(D_{ji} + 1) + \delta_{ij} \tag{8}$$

Now returning to the definition of S_{ji}, one sees that summation over all j results in a sum over all D_{ki} each a single-time since each k ($\neq i$) is adjacent (in a tree) to exactly one other vertex (say j) that is closer to i than k is. That is

$$\sum_{j=1}^{N} S_{ji} = \sum_{k=1}^{N} D_{ki} = W_i \tag{9}$$

But with the substitution from eq 8, we have

$$\begin{aligned} W_i &= \sum_{j=1}^{N} [(v_j - 1)(D_{ji} + 1) + \delta_{ij}] \\ &= \sum_{j=1}^{N} v_j D_{ji} - \sum_{j=1}^{N} D_{ji} + \sum_{j=1}^{N} (v_j - 1) + \sum_{j=1}^{N} \delta_{ij} \end{aligned} \tag{10}$$

Here the last j-sum clearly is equal to 1, while the next to the last j-sum gives

$$\sum_{j=1}^{N} v_j - N = 2(N-1) - N = N - 2 \tag{11}$$

The above follows from the handshaking lemma[10]

$$\sum_{j=1}^{N} v_j = 2M \tag{12}$$

(where M is the number of edges in G) and the relationship between M and N in a tree

$$M = N - 1 \tag{13}$$

Thence, further recalling the definitions of e_i and W_i we have

$$W_i = e_i - \sum_{j=1}^{N} v_j A_{ij} - W_i + N - 1 \tag{14}$$

The j-sum in eq 14 can be given in a more convenient form

$$\sum_{j=1}^{N} v_j A_{ij} = \sum_{j=1}^{N} (v_j - 1) A_{ji} + \sum_{j=1}^{N} A_{ji} = v'_i + v_i \tag{15}$$

Combining eqs 14 and 15 we obtain

$$W_i = e_i - (v'_i + v_i) - W_i + N - 1 \tag{16}$$

and the theorem follows immediately.

We may now readily note

$$\begin{aligned} \mathrm{MTI} &= \sum_{i=1}^{N} e_i \\ &= \sum_{i=1}^{N} [2W_i + (v_i + v'_i) - N + 1] \\ &= 4W + \sum_{i=1}^{N} (v_i + v'_i) - N^2 + N \end{aligned} \tag{17}$$

Since the remnant i-sum in our last equation can be given, utilizing again the (generalized) handshaking lemma, in terms of the number of vertices and the number p_2 of paths of length two in a tree

$$\sum_{i=1}^{N} (v_i + v'_i) = 2[(N-1) + p_2] \tag{18}$$

we have the following corollary: *If G is a tree, then*

$$\mathrm{MTI} = 4W + 2p_2 - (N-1)(N-2) \tag{19}$$

Therefore, if we know the Wiener index of a tree, we immediately also know its molecular topological index, because the information on p_2-number is also contained in the distance matrix used to generate W. We note here that the p_2-number is identical to the Gordon–Scantlebury index,[11] which in turn is equal to half of the Platt index.[12,13] It is also interesting to mention that there exist several relationships among topological indices as one discussed here, or similar ones, which all belong to the so-called "quadratic index family".[14] Combinations of the Wiener and Platt indices, like the Schultz index, had been used already successfully by Platt[15] for correlations with thermodynamic properties of alkanes.

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