Algebraic Connections between Topological Indices

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A relation has been recently established between the Wiener number *W* and an immanant of the Laplacian matrix of the molecular graph [Chan, O.; Lam, T. K.; Merris, R. *J. Chem. Inf. Comput. Sci*. **1997**, *37*, 762−765]. On the basis of this result we now show that there exist algebraic connections between *W* and certain molecular-graph-based structure descriptors which, until now, were believed not to be related to *W*, namely the Hosoya index and quantities derived from it and the simple topological index of Narumi.

INTRODUCTION

In the last 5−10 years, we witnessed a rapid, almost explosive proliferation of various molecular-graph-based structure descriptors, so-called "topological indices" (see, for instance, refs 1−6). In view of this, the finding of mathematical relations between topological indices, resulting in the reduction of their numbers, should be considered as something particularly desirable. Only a limited number of such relations have been established so far (see, for instance, refs 1 and 7−9), and in a single case, two independently introduced topological indices have been found to be identical.[10,11]

In this paper we point out certain algebraic relations between the Wiener number (*W*), the Hosoya indices (*Z*, Z_1, Z_2), and Narumi's simple topological index (*S*). For this we first repeat the respective definitions.

Let *G* be a molecular graph and v_1, v_2, ..., v_n be its vertices. The distance $d(v_i,v_j|G)$ between the vertices v_i and v_j of *G* is the length (number of edges) of a shortest path connecting v_i with v_j,. Then the Wiener number of *G* is given by[12]

$$W = W(G) = \sum_{i<j} d(v_i,v_j|G) \tag{1}$$

More details on the Wiener number can be found in reviews[13−15] and elsewhere.[16,17]

The number of first neighbors of a vertex v_j (of the graph *G*) is the degree of this vertex and will be denoted by $\deg(v_j)$. The product

$$S = S(G) = \prod_{j=1}^{n} \deg(v_j) \tag{2}$$

has been first studied by Narumi[18] and named the simple topological index. Some basic properties of this structure descriptor were determined.[19,20]

The connectivity index was conceived by Randić[21] and eventually became the structure descriptor with the greatest number of chemical applications.[22,23] It is defined as

$$\chi = \chi(G) = \sum_{(i,j)} \left(\frac{1}{\deg(v_i)\,\deg(v_j)} \right)^{1/2} \tag{3}$$

where the summation goes over all pairs of adjacent vertices of *G*.

Two edges of the graph *G* are said to be independent if they possess no vertex in common. The number of ways in which *k* pairwise independent edges are selected in *G*, $k \geq 2$, is denoted by $m(G,k)$. In addition, $m(G,0) = 1$ and $m(G,1)$ = number of edges of the graph *G*. Recall that $m(G,k)$ is just the number of *k* matchings of *G*.[16,24]

Note that if $m(G,k) = 0$ then necessarily $m(G,k+1) = 0$. Besides, $m(G,k) = 0$ whenever $k > n/2$. Therefore the summations on the right-hand sides of eqs 4, 5, etc., go over a finite number of terms.

Next, the Hosoya index is given by[25]

$$Z = Z(G) = \sum_{k\geq 0} m(G,k) \tag{4}$$

Another way toward the Hosoya index is via the so-called Z-counting polynomial[25]

$$Q(G,x) = \sum_{k\geq 0} m(G,k)x^k \tag{5}$$

Clearly, $Z(G) = Q(G,1)$.

By means of the *Z*-counting polynomial we can define other Hosoya-index-type quantities, viz.

$$Z_1 = Z_1(G) = Q'(G,1) \quad \text{where} \quad Q'(G,x) = \frac{\mathrm{d}Q(G,x)}{\mathrm{d}x} \tag{6}$$

and

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$$Z_2 = Z_2(G) = Q''(G,1) \quad \text{where} \quad Q''(G,x) = \frac{d^2Q(G,x)}{dx^2} \tag{7}$$

Hence

$$Z_1 = \sum_{k\geq 1} km(G,k); \quad Z_2 = \sum_{k\geq 2} k(k-1)\, m(G,k) \tag{8}$$

More details on the Hosoya index, Z-counting polynomial, and related matter can be found in a book[24] and review.[26]

Let us denote the edges of the graph G by e_1, e_2, ..., e_m. Then by G_w we denote the edge-weighted graph[27] obtained from G by associating a weight w_i to its edge e_i, $i = 1, 2, ..., m$. (Recall that, if $w_1 = w_2 = ... = w_m = 1$, then $G_w \equiv G$.)

If M is a k matching of G_w, that is, a selection of k independent edges of G_w, say e_1, e_2, ..., e_k, then the weight of M is equal to[27−29]

$$w(M) = \prod_{i=1}^{k} w_i \tag{9}$$

and the weighted-matching number[16] $m(G_w,k)$ is equal to the sum of weights of all k matchings of G_w. In particular

$$m(G_w,0) = 1 \tag{10}$$

and

$$m(G_w,1) = w_1 + w_2 + ... + w_m \tag{11}$$

For edge-weighted graphs the Z-counting polynomial and the indices Z, Z_1, and Z_2 are defined in the same manner as explained above, except that in eqs 4, 5, and 8 one writes $m(G_w,k)$ instead of $m(G,k)$.

There are evident relations between the quantities Q, Z, Z_1, and Z_2, cf. eqs 4−8. On the other hand, the topological indices W, S, and χ, as defined via eqs 1−3, appear not to be related, either mutually or with the Hosoya-type indices. In what follows we show that, nevertheless, there exist some concealed algebraic connections between them.

THE IMMANANT FORMULA FOR THE WIENER NUMBER

In our previous paper[16] the Wiener number of an acyclic molecule, whose molecular graph is the tree T, was expressed in terms of a special immanant d_3 of the Laplacian matrix, resulting in the formula

$$W(T) = {}^1/_4\left(\sum_{k\geq 0} \chi_3(k)\, m_T(k) + 2n(n-1)\right) \tag{12}$$

where χ_3 denotes the character function for the symmetric group irreducible representation associated with the partition $(3,1^{n-3})$ and $\chi_3(k)$ is the value this character takes for the product of k disjoint transpositions (for details see ref 16). The dependence of $\chi_3(k)$ on the number n of vertices of the molecular graph T and on the parameter k is given by[16]

$$\chi_3(k) = (-1)k[{}^1/_2(n-2k-1)(n-2k-2) - k] \tag{13}$$

The quantity $m_T(k)$ in (12) is related to the k matchings of T in the following manner:

If M is a k matching of T, then it embraces k independent edges of T. Let, as before, these be the edges e_1, e_2, ..., e_k. We say that the two end vertices of each of these k independent edges are contained in M. Let the end vertices of the edge e_i be v_{2i-1} and v_{2i}, $i = 1, 2, ..., k$. Then the vertices contained in M are v_1, v_2, ..., v_{2k}. Consequently, the vertices not contained in M are v_{2k+1}, ..., v_n.

In ref 16 a weight

$$\prod_{j=2k+1}^{n} \deg(v_j) \tag{14}$$

is associated to the k matching M and $m_T(k)$ is the sum of such weights of all k matchings of T.

AN ALTERNATIVE INTERPRETATION OF THE IMMANANT FORMULA

Bearing in mind eq 2, expression 14 is transformed as follows:

$$\prod_{j=2k+1}^{n} \deg(v_j) = \prod_{j=1}^{n} \deg(v_j) \prod_{i=1}^{2k} \frac{1}{\deg(v_i)} = S(T) \prod_{i=1}^{2k} \frac{1}{\deg(v_i)}$$

We further see that

$$(-1)^k \prod_{i=1}^{2k} \frac{1}{\deg(v_i)} = (-1)^k \prod_{i=1}^{k} \frac{1}{\deg(v_{2i-1})\deg(v_{2i})} = \prod_{i=1}^{k}\left[-\frac{1}{\deg(v_{2i-1})\deg(v_{2i})}\right]$$

may be understood (in the sense of eq 9) as the weight of the matching M of the weighted graph T_w in which the weight of the edge e_i is chosen to be $-1/[\deg(v_{2i-1})\deg(v_{2i})]$. In other words, if an edge e_j connects the vertices v_r and v_s, then its weight in T_w is

$$w_j = -\frac{1}{\deg(v_r)\deg(v_s)} \tag{15}$$

If eq 15 applies to all edges of the molecular graph T_w then

$$m_T(k) = (-1)^k\, S(T)\, m(T_w,k) \tag{16}$$

and formula 12 may be rewritten as

$$W(T) = \frac{S(T)}{4} \sum_{k\geq 0} (-1)^k\, \chi_3(k)\, m(T_w,k) + \binom{n}{2} \tag{17}$$

Needless to say that $m(T_w,k)$ in the expressions 16 and 17 satisfies the conditions (10) and (11).

CONNECTIONS

Combining (17) with (13) we arrive at

$$W(T) = \frac{S(T)}{4} \sum_{k\geq 0}\left[\frac{1}{2}(n-2k-1)(n-2k-2) - k\right] m(T_w,k) + \binom{n}{2} \quad (18)$$

or, in expanded form

$$W(T) = \frac{S(T)}{8}[(n^2 - 3n + 2) + (n^2 - 7n + 10)\, m(T_w,1) + (n^2 - 11n + 26)\, m(T_w,2) + (n^2 - 15n + 50)\, m(T_w,3) + \ldots] + \binom{n}{2}$$

Hexanes form the first larger family of alkane isomers. Thus for trees of interest in chemical graph theory, $n \geq 6$ and usually[27] $n \approx 10$. Bearing this in mind we readily conclude that the multiplier

$$[{}^1/_2(n-2k-1)(n-2k-2) - k]$$

occurring in eq 18, attains its maximum value at $k = 0$ and its next largest value at $k = 1$. (Recall that $0 \leq k \leq n/2$.) It is therefore worth noting that the contribution to the Wiener number, associated with $k = 0$ in eq 18 is a simple function of Narumi's index, namely

$$\frac{n^2 - 3n + 2}{8} S(T)$$

The respective contribution coming from $k = 1$ reads

$$-\frac{n^2 - 7n + 10}{8} S(T) \sum_{(i,j)} \frac{1}{\deg(v_i)\, \deg(v_j)} \quad (19)$$

where we have taken into account (11) and (15). There is a striking similarity between the sum occurring in expression 19 and the right-hand side of formula 3 for Randić's connectivity index.

By taking into account formulas 4 and 8, identity 18 is transformed into

$$W(T) = \frac{(n-1)(n-2)}{8} S(T)\, Z(T_w) - \frac{n-2}{2} S(T)\, Z_1(T_w) + \frac{1}{2} S(T)\, Z_2(T_w) + \binom{n}{2} \quad (20)$$

which is a mathematically exact result, provided the edges of the molecular graph T are weighted according to eq 15.

Hence we reached a somewhat surprising conclusion:

In the case of acyclic molecules the Wiener number (which is a distance-based structure descriptor) can be expressed in terms of four other topological indices: the Narumi index (which is a vertex-degree-based structure descriptor), the Hosoya index, and its two closely related derivatives (which are based on counting sets of independent edges).

For such an algebraic connection a certain price is to be paid: instead of the simple molecular graph, one has to consider its appropriately weighted variant, with edge weights chosen according to eq 15. In spite of this, the present analysis indicates that the algebraic (and therefore also conceptual) connections between various currently used topological indices may be much deeper than hitherto anticipated. If these connections are not straightforward and if they involve more than two indices (as is the case with formula 20), then they hardly could be comprehended without employing a pertinent mathematical apparatus. In particular, eq 20 was deduced within the framework of the recently developed immanant-based approach to the Wiener number.[14]

The obvious question at this point is how the present results can be extended to cycle-containing molecular graphs. This task seems to be far from easy because at the present moment the entire immanant approach is limited to trees. Nevertheless, it is reasonable to expect that in the future algebraic connections between various topological indices (e.g., W, S, χ, and Z) will be established also if the molecular graph is not a tree.

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