On the Relation between the Path Numbers ^1Z, ^2Z and the Hosoya Z Index

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The path numbers of the mth order, ^mZ, of a connected undirected graph are introduced and studied analitically. The definition of the ^1Z and ^2Z indices for acyclic graphs proposed earlier is generalized in order to cover cyclic graphs. The relationships between the path numbers ^1Z and ^2Z and the Hosoya Z index are discussed. It is shown that the path number ^1Z and the Hosoya Z index are closely related graph-theoretical invariants. The information contents of the ^1Z and ^2Z indices are only slightly overlapped, and hence the indices could be used as "independent" predictor variables in structure−property−activity studies.

1. INTRODUCTION

A fundamental concept of chemistry is molecular structure inasmuch as properties and behavior of molecules follow from their structures.[1−3] This statement has also been a subject of some criticisms.[4,5] If nonmetric properties of a molecule are considered, then the molecule can be represented by a (molecular) graph. In order to correlate property/activity of a molecule with its topology, first the graph is transformed into a more convenient mathematical representation (matrix, polynomial, etc.) and then by an algorithm the informational content of the graph is converted into a numerical characteristic. A scalar numerical descriptor uniquely determined by molecular graph is named topological (graph theoretical) index.[6]

Hosoya noticed the chemical significance of certain combinatorial properties of molecular graphs.[7] He investigated the selection of independent edges of a graph G and introduced the quantities $a(G,k)$ as the number of selections of k independent edges (k-matchings) in G. In order to avoid complicated manipulations with the set of $a(G,k)$'s Hosoya defined the Z-counting polynomial, $Q(G;x)$. The polynomial has a number of interesting properties and is still the subject of investigations.[6−12] Hosoya also proposed a graph invariant, the famous Z index. The Hosoya Z index, its modifications,[13−15] and its generalization[16] have found many applications particularly in quantitative structure−property relationship studies.[7,9,13−24]

In the past the selection of invariants of a graph matrix as molecular indices was limited to the adjacency matrix and the distance matrix.[25,26] The situation has been changing in the last few years, and quite a few novel matrices have been proposed.[27−31] Randić has recently put forward a novel matrix, the Hosoya $\mathbf{Z}$ matrix associated with connected acyclic molecular graphs (trees) as well as two molecular indices path numbers ^1Z and ^2Z, derived from it.[32] He also reported a few empirical regularities for the $\mathbf{Z}$ matrix entries in case of n-alkanes, and tested the new indices by examining the boiling points in octanes.

A great number of topological indices have been proposed so far.[33] Their efficiency as molecular descriptors and degree of their intercorrelation have been examined only for a small minority of them. To make an evaluation of the existing and the future indices easier, Randić put forth a set of desirable features of topological indices which will hopefully put some constraints on their unreasonable proliferation.[34] One out of 13 requirements that an index is not trivially related to or highly intercorrelated with other indices is particularly important. If an index does not fulfill this condition, then its infomational content is either entirely or in major part comprised of other indices.

In this article we will discuss relationship between the path numbers ^1Z, ^2Z and the Hosoya Z index.

2. DEFINITIONS OF Z, ^1Z, ^2Z, AND ^mZ INDICES AND CONSTRUCTION OF HOSOYA $\mathbf{Z}$ MATRIX

2.1. Z Index. The Hosoya Z index, $Z = Z(G)$, of an undirected graph G is derived by a combinatorial algorithm and is defined as

$$Z = \sum_{k=0}^{[N/2]} a(G,k) \tag{1}$$

where $a(G,k)$ is the number of k-matchings of G, N is the number of vertices of G, and the Gaussian brackets,[7,35] [ ], represent the integer part of $N/2$. For all graphs by definition $a(G,0) = 1$ and $a(G,1)$ is equal to the number of edges of G. The $a(G,k)$'s appear as coefficients in the Z-counting polynomial of G

$$Q(G;x) = \sum_{k=0}^{[N/2]} a(G,k)x^k \tag{2}$$

Clearly, the Z index can be obtained from the polynomial for $x = 1$

$$Z = Q(G;x=1) = Q(G;1) \tag{3}$$

2.2. Hosoya Z Matrix. The Hosoya $\mathbf{Z}$ matrix is defined only for tree graphs. The $\mathbf{Z}$ matrix entry z_{ij} corresponding to a pair of adjacent vertices (i,j) in a tree T is the Z index

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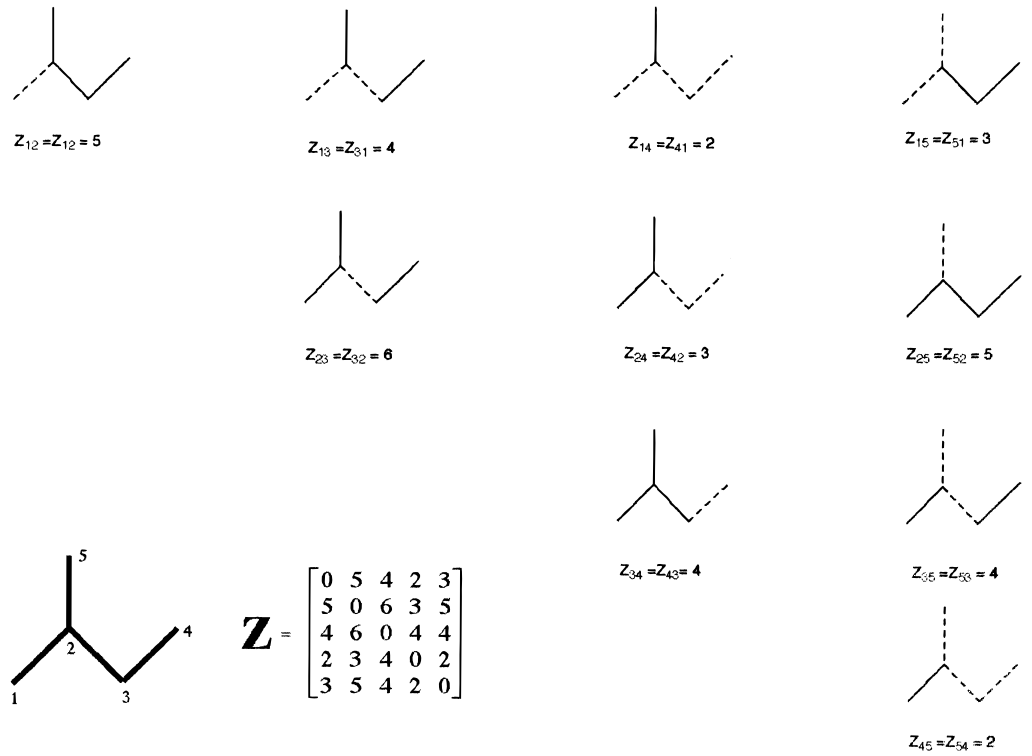

Figure 1. Calculation of the elements of the ***Z*** matrix of 2-methylbutane. The broken lines represent erased bonds.

of the graph T-e derived from T by erasing the edge e_{ij}. The constructional procedure for an entry corresponding to a pair of nonadjacent vertices (i,j) is similar. The path of length l, $^lp_{ij}$ connecting the vertices (i,j) is removed, and the Z index of the fragments is calculated. For tree graphs mapping f: $\upsilon \rightarrow \pi$, where υ is the set of pairs of vertices of T and π is the set of paths connecting them, is bijective, which means that every member of each set is uniquely paired with a member of the other. Therefore, the **Z** matrix of a labeled tree with N vertices is the square $N \times N$ symmetric matrix, $z_{ij} = z_{ji}$, with $z_{ii} = 0$ by definition. The process of finding the ***Z*** matrix is illustrated for 2-methylbutane in Figure 1.

2.3. Path Numbers ^1Z and ^2Z. Randić defined the path numbers ^1Z and ^2Z by means of the Hosoya ***Z*** matrix elements as

$$^1Z = \sum_{e_{ij}} {}^1z_{ij} \tag{4}$$

and

$$^2Z = \sum_{^2p_{ik}} {}^2z_{ik} \tag{5}$$

where the superscripts 1 and 2 associated with ***Z*** matrix elements denote that the distances between the vertices (i,j) and (i,k) are 1 and 2, respectively. The sum in eq 4 is over all edges in T, while the sum in eq 5 is over all paths of length two in T. These definitions unnecessarily restrict the domains of the indices to tree graphs. Hence, it is desirable to redefine ^1Z and ^2Z so as to extend their domains to other graphs of chemical interest.

2.4. Path Number ^mZ. We will generally define the path number of the mth order, $^mZ = {}^mZ(G)$, of a connected undirected graph G with N vertices as

$$^mZ = \sum_{^mp_{ij}} Z(G - {}^mp_{ij}) \quad 1 \le m \le N-1 \tag{6}$$

where $Z(G - {}^mp_{ij})$ is the Z index of the graph $G - {}^mp_{ij}$ derived from G by erasing a path of length m connecting the pair of vertices (i,j). The sum in eq 6 is over all paths of length m in G.

Clearly, if G is a tree and m is equal to 1 or 2, then eq 6 reduces to eqs 4 and 5, respectively. Equation 6 enables the creation of a novel basis of structurally ralated molecular indices which may offer a simpler interpretation of the regression equations, in comparison with a basis of ad hoc descriptors,[36] in structure−property−activity studies.

3. RELATIONSHIP BETWEEN ^1Z, ^2Z AND Z INDICES

We have tested the path numbers ^1Z and ^2Z on the set of all nonanes C_9H_{20} as well as on the series of cycloalkanes and alkylbenzenes, by examining their boiling points.[37] The close resemblance in quality between the regressions with the ^1Z index as predictor variable and regressions based on the Z index suggests that the indices encode the very similar information on molecular topology. The plot of the ^1Z index versus the Hosoya Z index for nonanes is illustrated in Figure 2 and shows strong linear intercorrelation. The high value of the correlation coefficient ($r^2 = 0.999$) hints that a formal relationship might exist between the two indices. We will show that there is indeed a close connection between the path number ^1Z and the Hosoya Z index.

3.1. Relationship between ^1Z and Z. Equation 6 for m equal to 1 gives the general definition of the path number ^1Z

$$^1Z = \sum_{e_{ij}} Z(G - e_{ij}) \tag{7}$$

Let G be a connected undirected graph with N vertices and

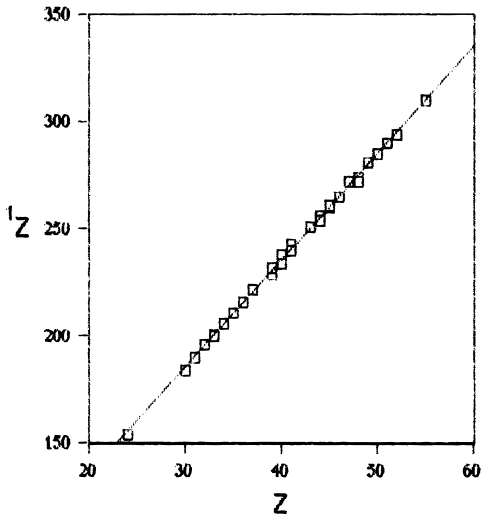

Figure 2. Plot of ^1Z *vs* Z for nonanes. The regression equation and the statistical parameters are $^1Z = 4.974(\pm 0.032)Z + 36.531$ (± 1.311); $n = 35$; $r^2 = 0.999$; $s = 1.299$; $F^{1,33} = 24699$.

R rings. The basic recursion relation for the Hosoya Z index of G is

$$Z(G) = Z(G - e_{ij}) + Z(G - e_{ij} - A_{e_{ij}}) \tag{8}$$

where $A_{e_{ij}}$ is the set of edges incident to the edge e_{ij}. The first term in eq 8 is the number of independent sets of G that do not contain edge e_{ij}. The number of the remaining independent sets of G can be expressed as

$$Z(G - e_{ij} - A_{e_{ij}}) = \sum_{k=1}^{[N/2]} a_{e_{ij}}(G,k) \tag{9}$$

where $a_{e_{ij}}(G,k)$ is the number of independent sets of edges of cardinality k (the number of elements in a set is called its cardinality) that contain edge e_{ij}. Combining eqs 7−9 with the identity[12]

$$\sum_{e_{ij}} a_{e_{ij}}(G,k) = ka(G,k) \tag{10}$$

the relationship between the path number ^1Z and the Hosoya Z index follows immediately

$$^1Z = (N + R - 1)Z - \sum_{k=1}^{[N/2]} ka(G,k) \tag{11}$$

what can be rewritten also as

$$^1Z = \sum_{k=0}^{[N/2]} (N + R - 1 - k)a(G,k) \tag{12}$$

Since the second term in eq 11 is just the derivative of $Q(G;x)$ for $x = 1$, $Q'(G;1)$, the path number ^1Z can be also expressed by means of the Z-counting polynomial and its first derivative as

$$^1Z = (N + R - 1)Q(G;1) - Q'(G;1) \tag{13}$$

For computing the value of the ^1Z index of an arbitrary connected undirected graph, it is necessary and sufficient to have knowledge of the number of vertices and the number of rings as well as the number of k-matchings. The first two demands are trivial, but the third, if we think about general explicit analytical expressions for computing the number of k-matchings, is not. It is possible to find out formulas for $a(G,k)$'s but only for some special classes of compounds (graphs).

3.1.1. Trees. We have derived formulas for computing the first few a(G,k)'s for tree graphs. Before we state them it is worth noting that in the case of trees, $a(G,k)$ is equal to (plus or minus) the $(2k)$th coefficient of the characteristic polynomial of G.[38] Results similar to ours were previously communicated for these coefficients[39,40] especialy for $k = 2$.[41,42] From eq 10 one derives the explicit expression for $a(T,2)$

$$a(T,2) = {}^1/_2 \sum_{e_{ij}}^{N-1} a_{e_{ij}}(T,2) = {}^1/_2 \sum_{e_{ij}}^{N-1} [(a(T,1) - (v_i + v_j - 1)]$$

$$= {}^1/_2[N(N-1) - \sum_i v_i^2] \tag{14}$$

where v_i and v_j are valences of the vertices i and j connected by the edge e_{ij}, and N is the number of vertices in T. The expression for $a(T,3)$ is derived as follows:

$$a(T,3) = {}^1/_3 \sum_{e_{ij}}^{N-1} a_{e_{ij}}(T,3) = {}^1/_3 \sum_{e_{ij}}^{N-1} [a(T,2) - \sum_{e_{ij}}^{e_{ij}+v_{e_{ij}}} a_{e_{ij}}(T,2) +$$

$$(v_i + 1)(v_j + 1)] = {}^1/_3[(N-1)(a(T,2) + N + 1) +$$

$$\sum_i v_i^3 - (N+2)\sum_i v_i^2 + 3\sum_{e_{ij}} v_i v_j] \tag{15}$$

where $^v e_{ij}$ represents valency of the edge e_{ij} (the number of edges incident to e_{ij}). The formula for $a(T,4)$ is derived in a similar way as the expression for a(T,3)

$$a(T,4) = {}^1/_4[(N-1)(a(T,2) + a(T,3) + 2N + 3) -$$

$$\sum_i V_i^4 + (N+3)\sum_i v_i^3 - (a(T,2) + 3N + 7)\sum_i v_i^2 +$$

$$(3N+13)\sum_{e_{ij}} v_i v_j - 4\sum_{^2p_{kl}} v_k v_l - 4\sum_{e_{ij}} v_i v_j (v_i + v_j)] \tag{16}$$

where v_i is the valency of vertex i, and $^2p_{kl}$ denotes the path of length two with terminal vertices k and l.

A special case of tree graphs is the path graph (tree with minimum number of terminals), P_N. The number of k-matchings of P_N is given by[22,26]

$$a(P_N,k) = \binom{N-k}{k} \quad 0 \le k \le [N/2] \tag{17}$$

and the formula for computing the $^1Z(P_N)$ is

$$^1Z(P_N) = \sum_{k=0}^{[N/2]} (N - 1 - \mathrm{k})\binom{N-k}{k} \tag{18}$$

Combining eq 13 modified for P_N ($G = P_N$, $R = 0$) with

$$Q(P_N;x) = Q(P_{N-1};x) + xQ(P_{N-2};x) \tag{19}$$

one deduces a noteworthy recursion relation

$$^1\mathrm{Z}(P_N) = {}^1Z(P_{N-1}) + {}^1Z(P_{N-2}) + Z(P_N) \tag{20}$$

3.1.2. Cycles. The ^1Z index of a cycle (regular graph of degree 2) with N vertices, C_N can be computed using the relation

$$^1Z(C_N) = NZ(P_N) \tag{21}$$

Since $Z(P_N)$ is equal to the Nth Fibonacci number, F_N, and this holds for all N (the initial conditions for the Fibonacci recursion, $F_N = F_{N-1} + F_{N-2}$, are $F_0 = F_1 = 1$) the expression for $Z(P_N)$ is given by the Binét formula.[7,22] The explicit formula for $^1Z(C_N)$ is

$$^1Z(C_N) = N\{((1 + \sqrt{5})/2)^{N+1} - ((1 - \sqrt{5})/2)^{N+1}\}/\sqrt{5} \tag{22}$$

3.2. Relationship between ^2Z and Z. The general definition of the path number ^2Z is

$$^2Z = \sum_{^2p_{ik}} Z(G - {}^2p_{ik}) \tag{23}$$

Suppose that G is a connected undirected graph with N vertices and R rings. Using the recursion relation, eq 8, one can write

$$\begin{aligned} Z(G - {}^2p_{\mathrm{ik}}) &= Z(G - e_{ij}) - Z(G - e_{jk} - A_{e_{jk}}) \\ &= Z(G - e_{ij}) + Z(G - e_{jk}) - Z(G) \end{aligned} \tag{24}$$

where $^2p_{ik}$ is the path of length two of G, connecting the vertices i and k and passing through the vertex j. The cardinality the of the set $A_{e_{\mathrm{jk}}}$ is the valency of the edge e_{jk}. Combining eq 23 and eq 24 with the expression for the number of paths, ^2p, of length two in G

$$^2p = {}^1/_2\sum_{i=1}^{N} v_i^2 - (N + R - 1) = {}^1/_2 \sum_{e_{ij}=1}^{N+R-1} v_{e_{ij}} \tag{25}$$

one obtains the relationship between ^2Z and the Hosoya Z index

$$\begin{aligned} {}^2\mathrm{Z} &= \sum_{e_{\mathrm{ij}}} v_{e_{ij}} Z(\mathrm{G} - \mathrm{e_{ij}}) - {}^2pZ(G) \\ &= \sum_{e_{ij}} v_{\mathrm{e_{ij}}}(Z(G - e_{ij}) - {}^1/_2 Z(G)) \end{aligned} \tag{26}$$

3.2.1. Paths. If G is a path graph, P_N, then the path number ^mZ, for $m \geq 2$ can be calculated using the following relation

$$^mZ(P_N) = {}^{m-1}Z(P_{N-1}) = \ldots = {}^1Z(P_{N-m+1}); \quad 2 \leq m \leq N - 1 \tag{27}$$

In particular, the explicit analytical expression for ^2Z can be derived from eq 18 by the replacement of all N by $N - 1$.

3.2.2. Cycles. The path number ^2Z of a cycle C_N can be calculated using the relation

$$^2Z(C_N) = NZ(P_{N-1}) \tag{28}$$

or explicitly

$$^2Z(C_N) = N\{((1 + \sqrt{5})/2)^N - ((1 - \sqrt{5})/2)^{\mathrm{N}}\}/\sqrt{5} \tag{29}$$

The ^2Z index is only slightly intercorrelated with the path number ^1Z. The respective correlation coefficients are 0.498 and 0.228 for octanes and nonanes, respectively. It also poorly correlates with boiling points of the investigated compounds. Nevertheless,the ^2Z index embodies a certain piece of structural information that in combination with ^1Z or/and other indices significantly improve regression. For example, in case of nonanes the two parameter linear regression equation with predictor variables ^1Z and ^2Z ($r = 0.910$; $s = 2.703$) fits much better boiling points in comparison with the regression equation based on a single predictor variable ^1Z ($r = 0.830$; $s = 3.490$). Hence, the path number ^2Z can be considered as an important additional descriptor in a multiple regression.

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