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On the Calculation of the Path Numbers ^1Z, ^2Z and the Hosoya Z Index

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For acyclic molecules, Randić[4] introduced a family of topological indices, the path numbers ^mZ, m = 1, 2,..., which are deduced from the Hosoya matrix. The path-number concept was recently extended to molecules containing cycles. Relations between ^1Z, ^2Z and the Hosoya index Z were established.[6] In this work we point out several further relations for the path numbers, valid for both acyclic and cyclic systems. Using them, ^mZ can be calculated recursively, especially in the case m = 1 and m = 2. One of the conclusions of this study is that, from an algorithmic point of view, it is expedient to evaluate all the indices ^1Z, ^2Z,... simultaneously, and together with the Hosoya index Z.

INTRODUCTION

In a seminal paper[1] Randić created a new approach to topological indices by introducing the Wiener matrix $\boldsymbol{W} = \boldsymbol{W}(\mathrm{G}) = ||W_{ij}||$, the (i,j)-entry of which is the number of paths in G, containing the path P_{ij}. Here G is the molecular graph and P_{ij} denotes a path between the vertices i and j (for details see below). The Wiener-matrix-concept was eventually elaborated in due detail.[2,3]

Randić put forward[4] also the analogous Hosoya matrix $\boldsymbol{Z} = \boldsymbol{Z}(G) = ||Z_{ij}||$, the (i,j)-entry of which is the Hosoya index[5] of $G - P_{ij}$. Both $\boldsymbol{W}$ and $\boldsymbol{Z}$ are well-defined only in the case of acyclic systems, in which there is a unique path between each pair of vertices.

The m-th path number, $m = 1, 2,...$, is then defined as the sum of those entries of the Hosoya matrix which correspond to pairs of vertices at distance m.

In the case of molecular graphs containing cycles, the above definitions are not applicable. Recently, a modified approach to path numbers was proposed,[6,7] which in the case of acyclic molecular graphs reduces to Randić's, but which is straightforwardly usable also for cyclic systems. The m-th path number, pertaining to the molecular graph G, is now conceived as[6]

$$ {}^{m}Z = {}^{m}Z(G) = \sum_{{}^{m}P(G)} Z(G - {}^{m}P) \tag{1} $$

where ${}^{m}P$ is a path of length m and the summation goes over the set ${}^{m}P(G)$ of all such paths in graph G. It is assumed that the terminal vertices of ${}^{m}P$ are distinct, *i.e.*, that ${}^{m}P$ is not a closed path (*i.e.*, not a cycle). Further, $G - {}^{m}P$ is a subgraph of G, obtained by deleting from it all edges of the path ${}^{m}P$, but keeping all its vertices. Hence, G and $G - {}^{m}P$ have an equal number of vertices. (Recall that ${}^{m}P$ possesses $m + 1$ vertices – two of which are terminal – and m edges).

The main features of the topological indices ${}^{m}Z$, including their chemical applications were discussed elsewhere.[4,6,7] In this paper, we focus our attention on some mathematical properties of path numbers, especially those which may be useful for designing algorithms for their calculation.

Path numbers are intimately related to the Hosoya Z index[6] and various properties of the Hosoya index will be extensively used throughout this paper. Therefore, we will first briefly repeat a few basic facts from the theory of the Hosoya index.[5,8,9]

THE HOSOYA Z INDEX

We use the same notation as in our previous paper.[6] Thus, by $a(G,k)$ we denote the number of k-matchings of the molecular graph G. Then, Hosoya's[5] topological index Z and his Z-counting polynomial are defined as:

$$ Z = Z(G) = \sum_{k \geq 0} a(G, k) $$

and

$$Q(\mathrm{G}) = Q(\mathrm{G}; x) = \sum_{k \geq 0} a(\mathrm{G}, k)\, x^k .$$

Clearly, $Q(\mathrm{G}; 1) = Z(\mathrm{G})$.

Let $e = (u, v)$ be an edge of graph G, connecting vertices u and v. Let $\delta(u)$ be the degree (valency) of vertex u, namely the number of the first neighbours of u.

Denote by $\mathrm{G} - e$ the subgraph obtained by deleting from G the edge e (but keeping its terminal vertices u and v). Denote by $\mathrm{G} - [e]$ the subgraph obtained by deleting from G the vertices u and v and, of course, the edge e as well as the edges incident to u and v. Hence, if G has N vertices, then $\mathrm{G} - e$ and $\mathrm{G} - [e]$ have N and N–2 vertices, respectively. If G has M edges, then $\mathrm{G} - e$ and $\mathrm{G} - [e]$ have $M - 1$ and $M - \delta(u) - \delta(v) + 1$ edges, respectively.

The following recursion relations are well known:[5]

If e is an arbitrary edge of graph G, then

$$Q(\mathrm{G}) = Q(\mathrm{G} - e) + x\, Q(\mathrm{G} - [e]). \tag{2}$$

If graph G is composed of two disconnected components G_1 and G_2, then

$$Q(\mathrm{G}) = Q(\mathrm{G}_1) \cdot Q(\mathrm{G}_2). \tag{3}$$

Relations (2) and (3), together with the initial conditions (4):

$$Q(\mathrm{G}; x) \equiv 1 \quad \text{if G has no edges} \tag{4}$$

enable the recursive calculation of the Z-counting polynomial of any graph.

We now define another, closely related, polynomial:

$$R(\mathrm{G}) = R(\mathrm{G}; x) = \sum_{k \geq 0} a(\mathrm{G}, k)\, x^{N-2k}$$

where N is the number of vertices of G. Recall that also $R(\mathrm{G}; 1) = Z(\mathrm{G})$. From Eqs. (2)–(4) it directly follows

$$R(\mathrm{G}) = R(\mathrm{G} - e) + R(\mathrm{G} - [e]) \tag{5}$$

$$R(\mathrm{G}) = R(\mathrm{G}_1) \cdot R(\mathrm{G}_2) \tag{6}$$

$$R(\mathrm{G}; x) = x^N \quad \text{if G has } N \text{ vertices, but no edges.} \tag{7}$$

The following analytical properties of the polynomials Q and R are known[10]

$$\frac{dQ(G;x)}{dx} = \sum_e Q(G-[e];x) \tag{8}$$

$$\frac{dR(G;x)}{dx} = \sum_v R(G-v;x). \tag{9}$$

The summation in (8) goes over all edges of G whereas the summation in (9) runs over all vertices.

By setting $x = 1$ in either Eqs. (2)–(4) or (5)–(7), we arrive at the (long known)[5] recurrence relations for the calculation of the Hosoya index:

$$Z(G) = Z(G-e) + Z(G-[e]) \tag{10}$$

$$Z(G) = Z(G1)\cdot Z(G2) \tag{11}$$

$$Z(G) = 1 \qquad \text{if G has no edges.} \tag{12}$$

An immediate consequence of relations (10)–(12) is the following:
If v is a vertex of graph G, incident to the edges $e_1, e_2, \ldots, e_{\delta(v)}$, then

$$Z(G) = Z(G-v) + \sum_{i=1}^{\delta(v)} Z(G-[e]). \tag{13}$$

An example of the application of Eqs. (10)–(12) is given in the last section.

A GENERAL RECURSION RELATION FOR ^mZ

In this section, we deduce a recursion relation for ^mZ that has a form analogous to Eq. (10).

Consider an edge $e = (u,v)$ of a graph G. Then, the set of paths of length m of graph G, ^{m}P (G), can be partitioned into four disjoint subsets:

^{m}P′(G) – consisting of paths that contain the edge e,

^{m}P″(G) – consisting of paths that touch the edge e, *i.e.*, contain a terminal vertex of the edge e (either vertex u or vertex v), but not the edge e itself,

^{m}P‴(G) – consisting of paths that contain the terminal vertices of the edge e (both vertex u and vertex v), but not the edge e itself, and

^{m}P⁗(G) – consisting of all other paths of length m of graph G; note that these paths do not contain any of the vertices u or v.

Accordingly, ^mZ(G) can be written as:

$$^mZ(G) = \sum_{^mP'} Z(G - {}^mP') + \sum_{^mP''} Z(G - {}^mP'') + \sum_{^mP'''} Z(G - {}^mP''') + \sum_{^mP''''} Z(G - {}^mP''''). \quad (14)$$

Let us now apply the recursion relation (10) to the edge e of the subgraphs occurring in the four summations on the right-hand side of Eq. (14). This recursion cannot be applied to the first term, since $G - {}^mP'$ does not contain e. Thus, the first term is left unchanged. On the other hand, the subgraphs $G - {}^mP''$, $G - {}^mP'''$ and $G - {}^mP''''$ do contain the edge e, and by means of Eq. (10) the second, third and fourth summations on the right-hand side of Eq. (14) become

$$\sum_{^mP''} Z((G - {}^mP'') - e) + \sum_{^mP''} Z((G - {}^mP'') - [e]) + \sum_{^mP'''} Z((G - {}^mP''') - e) +$$

$$+ \sum_{^mP'''} Z((G - {}^mP''') - [e]) + \sum_{^mP''''} Z((G - {}^mP'''') - e) + \sum_{^mP''''} Z((G - {}^mP'''') - [e]). \quad (15)$$

By noticing that

$$(G - {}^mP'') - e = (G - e) - {}^mP''$$
$$(G - {}^mP''') - e = (G - e) - {}^mP'''$$
$$(G - {}^mP'''') - e = (G - e) - {}^mP''''$$

and

$$(G - {}^mP'''') - [e] = (G - [e]) - {}^mP''''$$

but that the analogous interchange cannot be done for $(G - {}^mP'') - [e]$ and $(G - {}^mP''') - [e]$, the expression (15) is rewritten as

$$\sum_{^mP''} Z((G - e) - {}^mP'') + \sum_{^mP'''} Z((G - e) - {}^mP''') + \sum_{^mP''''} Z((G - e) - {}^mP'''') +$$

$$+ \sum_{^mP''''} Z((G - [e]) - {}^mP'''') + \sum_{^mP'''} Z((G - {}^mP''') - [e]) + \sum_{^mP''} Z((G - {}^mP'') - [e]). \quad (16)$$

In view of the fact that $G - e$ does not contain ${}^mP'$, in the first three terms in (16) we recognise ${}^mZ(G - e)$. Similarly, as $G - [e]$ contains neither ${}^mP'$ nor ${}^mP''$ nor ${}^mP'''$, the fourth term in (16) is just ${}^mZ(G - [e])$. Hence, Eq. (14) results in

$$^mZ(G) = {}^mZ(G - e) + {}^mZ(G - [e]) +$$

$$+ \sum_{^mP'(G)} Z(G - {}^mP) + \sum_{^mP''(G)} Z((G - {}^mP) - [e]) + \sum_{^mP'''(G)} Z((G - {}^mP) - [e]) \quad (17)$$

which holds for all values of m, $m \geq 1$.

In the above recursion, the edges and vertices are subsequently deleted. If deletion ends in a graph G with no vertices, then ${}^mZ(G) = 1$, and if one formally deletes further, then ${}^mZ(G) = 0$. In order to apply the recursion relation (17), we have to find all the paths of G that either contain the edge e or touch it or contain both of its terminal vertices, but not the edge e itself. In the general case this turns out to be quite a tedious task. Nevertheless, as shown in the subsequent sections, if $m = 1$ or $m = 2$, the calculations required by Eq. (17) are still feasible.

CALCULATION OF ${}^mZ$ OF DISCONNECTED GRAPHS

First of all, note that the quantity ${}^mZ(G)$ is well defined irrespective of whether graph G is connected or disconnected. Although molecular graphs are (usually) connected, throughout the recursive evaluation of ${}^mZ$ we sooner-or-later encounter disconnected graphs. (For an example see the last section.)

The following result holds for all m, $m \geq 1$. Let G be composed of disconnected components G_1 and G_2. Then, parallel to Eq. (11) we have

$$ {}^mZ(G) = {}^mZ(G_1)\, Z(G_2) + {}^mZ(G_2)\, Z(G_1) \qquad (18) $$

which can be written also as

$$ \frac{{}^mZ(G)}{Z(G)} = \frac{{}^mZ(G_1)}{Z(G_1)} + \frac{{}^mZ(G_2)}{Z(G_2)} \, . $$

If G has several components, say G_1, G_2,......, G_p, then the above identity is immediately generalized as

$$ \frac{{}^mZ(G)}{Z(G)} = \frac{{}^mZ(G_1)}{Z(G_1)} + \frac{{}^mZ(G_2)}{Z(G_2)} + \ldots + \frac{{}^mZ(G_p)}{Z(G_p)} \, . \qquad (19) $$

In order to prove Eq. (18) observe that each path ${}^mP$ in graph G lies either fully in G_1 or fully in G_2. This implies that the set ${}^mP$ (G) is the union of the disjoint sets ${}^mP$ (G_1) and ${}^mP$ (G_2). Consequently, bearing in mind Eq. (1),

$$ {}^mZ(G) = \sum_{{}^mP(G_1)} Z(G_1 - {}^mP \cup G_2) + \sum_{{}^mP(G_2)} Z(G_1 \cup G_2 - {}^mP). $$

Using Eq. (11), we now obtain

$$^{m}Z(G) = Z(G_2) \sum_{^{m}P(G_1)} Z(G_1 - {}^{m}P) + Z(G_1) \sum_{^{m}P(G_2)} (G_2 - {}^{m}P)$$

from which formula (18) follows immediately.

Formulae (18) and (19) show that in order to calculate the m-th path number of a disconnected graph G, we must know the m-th path numbers of all components of G, as well as the Hosoya indices of all components of G.

CALCULATION OF ^1Z

The fundamental expression, connecting ^1Z with the Hosoya Z index is the previously reported:[6]

$$^{1}Z(G) = \sum_{e} Z(G - e). \tag{20}$$

As explained above, the polynomial $Q(G)$ can be calculated recursively. If this polynomial is known, then ^1Z is also known. Namely, the following identity is obeyed

$$^{1}Z(G) = M\, Q(G; 1) - Q'(G; 1) \tag{21}$$

where M is the number of edges of G. Another form of the same result is

$$\frac{^{1}Z(G)}{Z(G)} = M - \frac{d}{dx} \ln Q(G; x)\Big|_{x=1}.$$

The above formulae are obtained[6] by combining Eqs. (8), (10) and (20).

Let e be an edge of graph G and let $\delta(e)$ be the number of edges incident to e. Note that if $e = (u,v)$, then $\delta(e) = \delta(u) + \delta(v) - 2$.

For $x = 1$, Eq. (2) becomes

$$Q(G; 1) = Q(G - e; 1) + Q(G - [e]; 1)$$

whereas by differentiating Eq. (2) with respect to the variable x and then setting $x = 1$ we get

$$Q'(G; 1) = Q'(G - e; 1) + Q'(G - [e]; 1) + Q(G - [e]; 1).$$

When these relations are substituted back into (21), then by noting that the subgraphs $G - e$ and $G - [e]$ have $M - 1$ and $M - 1 - \delta(e)$ edges, respectively, we arrive at

$$^1Z(G) = [(M-1)\,Q(G-e;1) - Q'(G-e;1)] + Q(G-e;1) + $$
$$+ [(M-1-\delta(e))\,Q(G-[e];1) - Q'(G-[e];1)] +$$
$$+ [1+\delta(e)]\,Q(G-[e];1) - Q(G-[e];1)].$$

Because

$$(M-1)\,Q(G-e;1) - Q'(G-e;1) = {}^1Z(G-e)$$

and

$$(M-1-\delta(e))\,Q(G-[e];1) - Q'(G-[e];1) = {}^1Z(G-[e])$$

we finally obtain

$$^1Z(G) = {}^1Z(G-e) + {}^1Z(G-[e]) + Z(G-e) + \delta(e)\,Z(G-[e]) \qquad (22)$$

which enables a direct recursive calculation of ^1Z.

Formula (22) could, of course, have been deduced also from Eq. (17). For this one has to notice that the subset $^1P'(G)$ has just a single element, for which $G - {}^1P \equiv G - e$. Further, the subset $^1P''(G)$ has $\delta(e)$ elements, each of which satisfying the condition $(G - {}^1P) - [e] \equiv G - [e]$.

Formula (22) should be compared with Eq. (10). In fact, comparison of (10) and (22) reveals that it is reasonable to evaluate the two indices Z and ^1Z simultaneously.

CALCULATION OF ^2Z

The fundamental expression, connecting ^2Z with the Hosoya index is:

$$^2Z(G) = \mu(G)\,Z(G) - \sum_v [\delta(v)-1]\,Z(G-v) \qquad (23)$$

where the auxiliary quantity $\mu(G)$ is defined as

$$\mu(G) = \sum_v \left[\binom{\delta(v)}{2} - \delta(v) + 1\right] = \frac{1}{2}\sum_v \delta(v)^2 + N - 3M$$

with summation going over all vertices of G.

In order to deduce Eq. (23), we have to observe that every path of length two embraces two edges. Consider a path ^2P consisting of the edges $e_1 = (u_1, v)$ and $e_2 = (u_2, v)$. Hence, $G - {}^2P \equiv G - e_1 - e_2$. From Eq. (10), it immediately follows:

$$Z(G) = Z(G - e_1) + Z(G - [e_1]) = Z(G - e_1 - e_2) + Z(G - e_1 - [e_2]) + Z(G - [e_1]).$$

Because, evidently, $G - e_1 - [e_2] \equiv G - [e_2]$, the above relation yields

$$Z(G - {}^2P) = Z(G) - Z(G - [e_1]) - Z(G - [e_2]). \tag{24}$$

Now, ${}^2Z(G)$ is obtained by summing the right-hand side of Eq. (24) over all paths of length two. Instead, we may sum over all vertices of G, taking into account that each vertex v is the non-terminal vertex of exactly $\binom{\delta(v)}{2}$ paths of length two. This results in

$${}^2Z(G) = \sum_v \binom{\delta(v)}{2} Z(G) - \sum_v [\delta(v) - 1] \sum_{i=1}^{\delta(v)} Z(G) - [e_i])$$

which, in view of Eq. (13), becomes

$${}^2Z(G) = \sum_v \binom{\delta(v)}{2} Z(G) - \sum_v [\delta(v) - 1]\,[Z(G) - Z(G - v)].$$

Now, Eq. (23) follows straightforwardly.

In the general case, the calculation of the right-hand side of Eq. (23) is not easy. The reason for this is, of course, the term $\delta(v) - 1$. If, however, G is a regular graph, *i.e.*, if all vertices of G have equal degrees (say, δ), then by bearing in mind the identity (9), Eq. (23) reduces to:

$${}^2Z(G) = \frac{(\delta - 1)(\delta - 2)N}{2} - (\delta - 1)\,R'(G; 1).$$

Hence, in this special case, it is possible to directly evaluate ${}^2Z(G)$ from the knowledge of the numbers $a(G, k)$, $k \geq 0$, or (what is the same) from the knowledge of the polynomials $Q(G; x)$ or $R(G; x)$.

Recall that the molecular graphs of fullerenes are regular of degree $\delta = 3$. Cycle C_N is also a regular graph, of degree $\delta = 2$.

AN ILLUSTRATION AND CONCLUDING REMARKS

In order to illustrate the applications of the present results, we consider the molecular graph of azulene (graph Az depicted in Figure 1). As preparation, we first calculate the Hosoya Z index and the path numbers of the path P_N, also depicted in Figure 1.

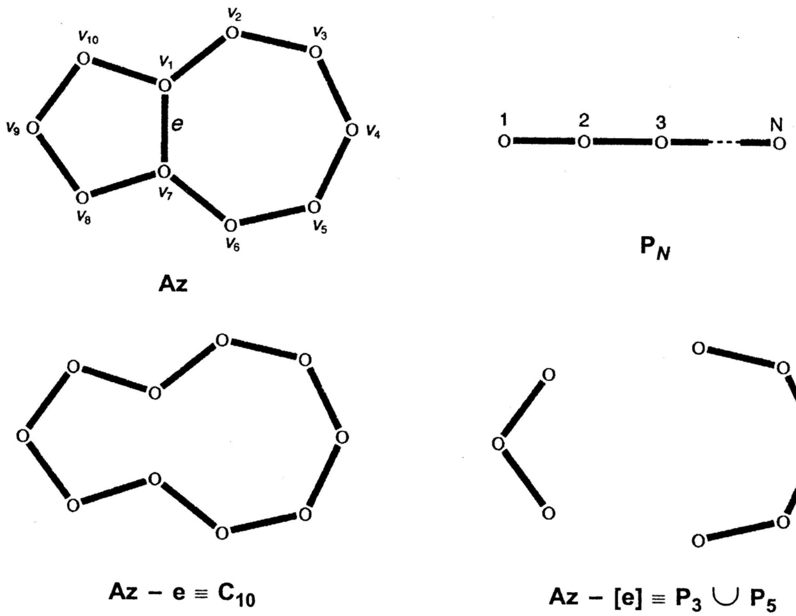

Figure 1. The molecular graph of azulene (Az) and some auxiliary graphs needed for the calculation of its Hosoya index and path numbers.

From Eqs. (10) and (11) one directly obtains

$$Z(\mathrm{P}_N) = Z(\mathrm{P}_{N-1}) + Z(\mathrm{P}_{N-2})$$

which, together with the initial conditions $Z(\mathrm{P}_1) = 1$ and $Z(\mathrm{P}_2) = 2$ leads to the conclusion[5] that the Z index of the N-vertex path graph is just the N-th Fibonacci number, F_N. Recall that $F_3 = 2 + 1 = 3$, $F_4 = 3 + 2 = 5$, $F_5 = 5 + 3 = 8$, *etc.* The first few values of $Z(\mathrm{P}_N)$ are reproduced in Table I. From Eq. (20) it now follows

$$^1Z(\mathrm{P}_N) = \sum_{k=1}^{N-1} F_k \, F_{N-k} \ . \tag{25}$$

Bearing in mind the identity

$$F_N = F_k \, F_{N-k} + F_{k-1} \, F_{N-k-1}$$

formula (25) is transformed into

TABLE I

The Hosoya index and the first five path numbers of the graphs P_N , $1 \leq N \leq 12$; $Z(P_N)$ is the N-th Fibonacci number; observe that the value 566 for $^1Z(P_{10})$ is obtained by summing $Z(P_{10}) = 89$, $^1Z(P_9) = 310$ and $^1Z(P_8) = 167$

N	$Z(P_N)$	$^1Z(P_N)$	$^2Z(P_N)$	$^3Z(P_N)$	$^4Z(P_N)$	$^5Z(P_N)$
1	1	0	0	0	0	0
2	2	1	0	0	0	0
3	3	4	1	0	0	0
4	5	10	4	1	0	0
5	8	22	10	4	1	0
6	13	45	22	10	4	1
7	21	88	45	22	10	4
8	34	167	88	45	22	10
9	55	310	167	88	45	22
10	89	566	310	167	88	45
11	144	1020	566	310	167	88
12	233	1819	1020	566	310	167

$$^1Z(P_N) = (N-1)\,Z(P_N) - 2Z(P_{N-2}) - {}^1Z(P_{N-2})$$

from which the ^1Z-values of P_N are calculated recursively; the initial conditions are $^1Z(P_1) = 0$ and $^1Z(P_2) = 1$. The respective results up to $N = 12$ are presented in Table I.

The higher path numbers of P_N are deduced from the relations[6]

$$^1Z(P_N) = {}^2Z(P_{N+1}) = {}^3Z(P_{N+2}) = \ \dots = {}^mZ(P_{N+m-1})$$

and $^mZ(P_N) = 0$ whenever $N \leq m$. Since the values of $^1Z(P_N)$ have previously been established, no extra calculation is required at all; see Table I for illustration.

We further need the Z and ^mZ indices of the cycle C_N. These are easily obtained[6] from the data collected in Table 1:

$$Z(C_N) = Z(P_N) + Z(P_{N-2})$$
$$^mZ(C_N) = (N - m + 1)\,Z(P_N - m + 1); \quad m = 1, 2, \dots$$

In particular, $Z(C_{10}) = 89 + 34 = 123$, $^1Z(C_{10}) = 10 \cdot 89 = 890$, $^2Z(C_{10}) = 9 \cdot 55 = 495$, $^3Z(C_{10}) = 8 \cdot 34 = 272$, *etc.*

Consider now the azulene graph Az, Figure 1. Let e be the edge connecting its vertices v_1 and v_7. Then, $Az - e \equiv C_{10}$ and $Az - [e\,] \equiv P_3 \cup P_5$, see Figure 1.

From Eqs. (10) and (11):

$$Z(\mathrm{Az}) = Z(\mathrm{C}_{10}) + Z(\mathrm{P}_3) \cdot Z(\mathrm{P}_5) = 123 + 3 \cdot 8$$

resulting in

$$Z(\mathrm{Az}) = 147.$$

From Eqs. (22) and (18):

$$\begin{aligned} {}^1Z(\mathrm{Az}) &= {}^1Z(\mathrm{C}_{10}) + {}^1Z(\mathrm{P}_3 \cup \mathrm{P}_5) + Z(\mathrm{C}_{10}) + 4 \cdot Z(\mathrm{P}_3 \cup \mathrm{P}_5) = \\ &= {}^1Z(\mathrm{C}_{10}) + {}^1Z(\mathrm{P}_3)\, Z(\mathrm{P}_5) + {}^1Z(\mathrm{P}_5)\, Z(\mathrm{P}_3) + Z(\mathrm{C}_{10}) + 4 \cdot Z(\mathrm{P}_3)\, Z(\mathrm{P}_5) = \\ &= 890 + 4 \cdot 8 + 22 \cdot 3 + 123 + 4 \cdot 3 \cdot 8 \end{aligned}$$

which gives

$${}^1Z(\mathrm{Az}) = 1207.$$

In order to calculate ${}^2Z(\mathrm{Az})$ *via* Eq. (17), $m = 2$, we have to find the subsets ${}^2\mathrm{P}'(\mathrm{Az})$ and ${}^2\mathrm{P}''(\mathrm{Az})$. For the choice $e = (v_1, v_7)$ we have:

$$\begin{aligned} {}^2\mathrm{P}'(\mathrm{Az}) &= \{\pi_1, \pi_2, \pi_3, \pi_4\} \\ {}^2\mathrm{P}''(\mathrm{Az}) &= \{\pi_5, \pi_6, \pi_7, \pi_8\} \end{aligned}$$

where

$$\begin{array}{llll} \pi_1 = (v_1, v_7, v_6) & \pi_2 = (v_1, v_7, v_8) & \pi_3 = (v_2, v_1, v_7) & \pi_4 = (v_7, v_1, v_{10}) \\ \pi_5 = (v_1, v_2, v_3) & \pi_6 = (v_1, v_{10}, v_9) & \pi_7 = (v_7, v_6, v_5) & \pi_8 = (v_7, v_8, v_9)\,. \end{array}$$

Further, for $i = 1, 2, 3, 4$,

$$\mathrm{Az} - \pi_i = \mathrm{P}_{10} \qquad Z(\mathrm{Az} - \pi_i) = 89$$

for $i = 5, 7$

$$\mathrm{Az} - \pi_i - [e] = \mathrm{P}_1 \cup \mathrm{P}_3 \cup \mathrm{P}_4 \qquad Z(\mathrm{Az} - \pi_i - [e]) = 1 \cdot 3 \cdot 5 = 15$$

whereas for $i = 6, 8$

$$\mathrm{Az} - \pi_i - [e] = \mathrm{P}_1 \cup \mathrm{P}_2 \cup \mathrm{P}_5 \qquad Z(\mathrm{Az} - \pi_i - [e]) = 1 \cdot 2 \cdot 8 = 16.$$

Bearing the above in mind we obtain

$$\sum_{^2\mathrm{P}'(\mathrm{Az})} Z(\mathrm{Az} - {}^2\mathrm{P}) + \sum_{^2\mathrm{P}''(\mathrm{Az})} Z((\mathrm{Az} - {}^2\mathrm{P}) - [e]) =$$

$$= [89 + 89 + 89 + 89] + [15 + 16 + 15 + 16] = 418.$$

Since, in addition, ${}^2\mathrm{Z}(\mathrm{Az} - e) = {}^2\mathrm{Z}(\mathrm{C}_{10}) = 495$ and ${}^2\mathrm{Z}(\mathrm{Az} - [e]) = {}^2\mathrm{Z}(\mathrm{P}_3 \cup \mathrm{P}_5)$ $= {}^2\mathrm{Z}(\mathrm{P}_3)\, Z(\mathrm{P}_5) + {}^2\mathrm{Z}(\mathrm{P}_5)\, Z(\mathrm{P}_3) = 1 \cdot 8 + 10 \cdot 3 = 38$, formula (17) yields ${}^2\mathrm{Z}(\mathrm{Az})$ $= 495 + 38 + 418$, *i.e.*,

$${}^2\mathrm{Z}(\mathrm{Az}) = 951.$$

By comparing the families of formulae (10), (17), (22); (11), (18) as well as (20), (23) we see that with increasing the value of m, the calculation of ${}^mZ$ becomes more and more tedious. On the other hand, these formulae, as well as the above example, suggest a general strategy for such calculations: it is expedient to evaluate all the indices ${}^1Z$, ${}^2Z$, ... simultaneously, and together with the Hosoya index Z.

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REFERENCES

1. M. Randić, *Chem. Phys. Lett.* **211** (1993) 478–483.
2. M. Randić, X. Guo, T. Oxley, and H. Krishnapriyan, *J. Chem. Inf. Comput. Sci.* **33** (1993) 709–716.
3. M. Randić, X. Guo, T. Oxley, H. Krishnapriyan, and L. Naylor, *J. Chem. Inf. Comput. Sci.* **34** (1994) 361–367.
4. M. Randić, *Croat. Chem. Acta* **67** (1994) 415–429.
5. H. Hosoya, *Bull. Chem. Soc. Jpn.* **44** (1971) 2332–2339.
6. D. Plavšić, M. Šoškić, I. Landeka, I. Gutman, and A. Graovac, *J. Chem. Inf. Comput. Sci.* **36** (1996) 1118–1122.
7. D. Plavšić, M. Šoškić, Z. Đaković, I. Gutman, and A. Graovac, *J. Chem. Inf. Comput. Sci.* **37** (1997) 529–534.
8. H. Hosoya, in: N. Trinajstić (Ed.), *Mathematics and Computational Concepts in Chemistry*, Horwood, Chichester, 1986, pp. 110–123.
9. I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, 1986.
10. I. Gutman, *Commun. Math. Chem. (MATCH)* **28** (1992) 139–150.

SAŽETAK

Računanje staznih brojeva ^{1}Z, ^{2}Z i Hosoyina Z indeksa

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Za acikličke molekule Randić[4] je uveo niz novih topologijskih indeksa, stazne brojeve ^{m}Z, $m = 1, 2, \ldots$, koji se izvode iz Hosoyine matrice. Koncept staznog broja nedavno je proširen na molekule koje sadrže prstenove. Nađene su relacije koje povezuju ^{1}Z, ^{2}Z s Hosoyinim indeksom Z.[6] U ovom radu ukazujemo na još neke relacije staznih brojeva, koje vrijede za acikličke i cikličke sustave, i omogućuju rekurzivno računanje indeksa ^{m}Z, posebice za $m = 1$ i $m = 2$. S algoritamskog stajališta korisno je izračunati sve indekse ^{1}Z, ^{2}Z, ... istovremeno i zajedno s Hosoyinim indeksom Z.