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On the Hosoya *Z* Index of General Graphs

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On the Hosoya *Z* Index of General Graphs[#]

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Abstract

Motivation. The *Z* index, proposed by Haruo Hosoya in 1971, has initially been applied only to simple graphs representing saturated hydrocarbons. Our aim in this report was to extend the *Z* index to general graphs that may be used to represent unsaturated systems and heterosystems and to investigate the behavior of the *Z* index in regard to their structural characteristics such as size, branching, cyclicity, multiple edges and loops.

Method. Chemical graph–theoretical concepts were used. The *Z* index was calculated by means of the *Z* counting polynomial and the matching polynomial. These polynomials were constructed using the appropriate recurrence relations. The structural behavior of the *Z* index was tested against the total walk count (*twc*) index.

Results. The *Z* index was obtained for a number of simple graphs and general graphs. It is shown that the *Z* index of these graphs follows their structural changes, that is, the *Z* index increases with the size, loops, multiple edges, cycles and is sensitive to branching. The *twc* index supports in most cases the structural behavior of the *Z* index. The relationship between the *Z* counting polynomial and the matching polynomial is discussed. The edge decomposition of the *Z* index is also commented.

Conclusions. The range of applicability of the Hosoya *Z* index is extended to general graphs. It is shown that this index accounts well for their structural characteristics.

Keywords. General graph; loop graph; loop multigraph; matching polynomial; multigraph; total walk count index; *Z* counting polynomial; Hosoya *Z* index.

1 INTRODUCTION

Haruo Hosoya introduced in 1971 a topological index that he called the *Z* index [1]. This topological index, also called the Hosoya *Z* index [2,3], has found an extensive use in quantitative structure–property relationships (QSPRs) and quantitative structure–activity relationships (QSARs) [2–5]. In some cases such as in simple linear regressions based on topological indices the *Z* index gives better QSPR and QSAR models than most indices [6]. It is also applicable to many different problems, not only in chemistry, but also in mathematics (*e.g.* combinatorial theory), chemoinformatics (*e.g.* coding and identification of molecules) and physics (*e.g.* dimer statistics) [7–10]. Originally the *Z* index was introduced for simple graphs representing saturated

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hydrocarbons. In the past there were some attempts to extend the *Z* index to edge–weighted graphs representing heterosystems [2,4,11,12]. Unfortunately, the systematic use of this index in the study of the structural characteristics of unsaturated systems and heterosystems has not yet been undertaken. In this paper we report on our work on the extension of the *Z* index to general graphs. The response of the Z index to various structural changes is tested against the total walk count (*twc*) [13].

Molecular graphs will be presented in the usual way [14] – atoms will be represented by vertices, bonds by edges. Saturated hydrocarbons will be represented by *simple* graphs [15] (also called *normal* graphs [16] or *schlicht* graphs [17]). These graphs do not contain multiple edges or loops. Two or more edges that join a pair of vertices in a graph are called multiple edges. A loop is an edge joining a vertex to itself [18]. Unsaturated hydrocarbons will be represented by graphs in which no loops are allowed but more than one edge can join two vertices. Such graphs are called *multigraphs* [18]. Saturated molecules containing heteroatoms are conventionally represented by *loopgraphs* [19], that is, graphs in which loops (representing heteroatoms [20]) are permitted but not multiple edges. Unsaturated heterosystems will be represented by *loopmultigraphs* [19] (also called *pseudographs* [18]). Multiple edges and loops are allowed in these graphs. A collective name for multigraphs, loopgraphs and loopmultigraphs is *general* graphs [21,22]. These graphs are of interest not only in chemistry but also in various fields of science and engineering, such as in the communication net theory [23].

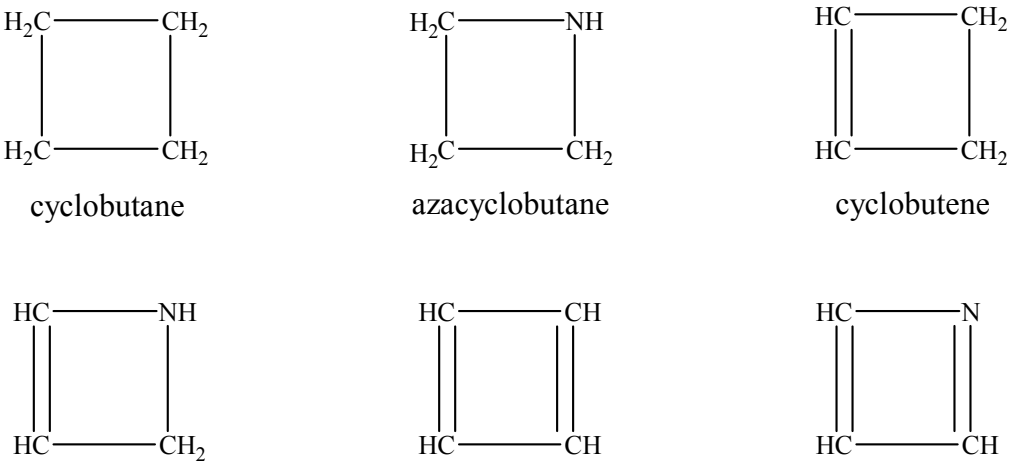


Figure 1. A set of monocyclic molecules.

As illustrative examples of the aforementioned classes of compounds, we give in Figure 1 a set of monocyclic molecules, starting with a saturated molecule (cyclobutane) and ending with an unsaturated heterosystem (azacyclobutadiene), and in Figure 2 the corresponding graphs: simple graph **1** for cyclobutane, loopgraph **2** for azacyclobutane, multigraphs **3** and **5** for cyclobutene and

cyclobutadiene respectively, and loopmultigraphs graphs **4** and **6** for azacyclobutene and azacyclobutadiene respectively.

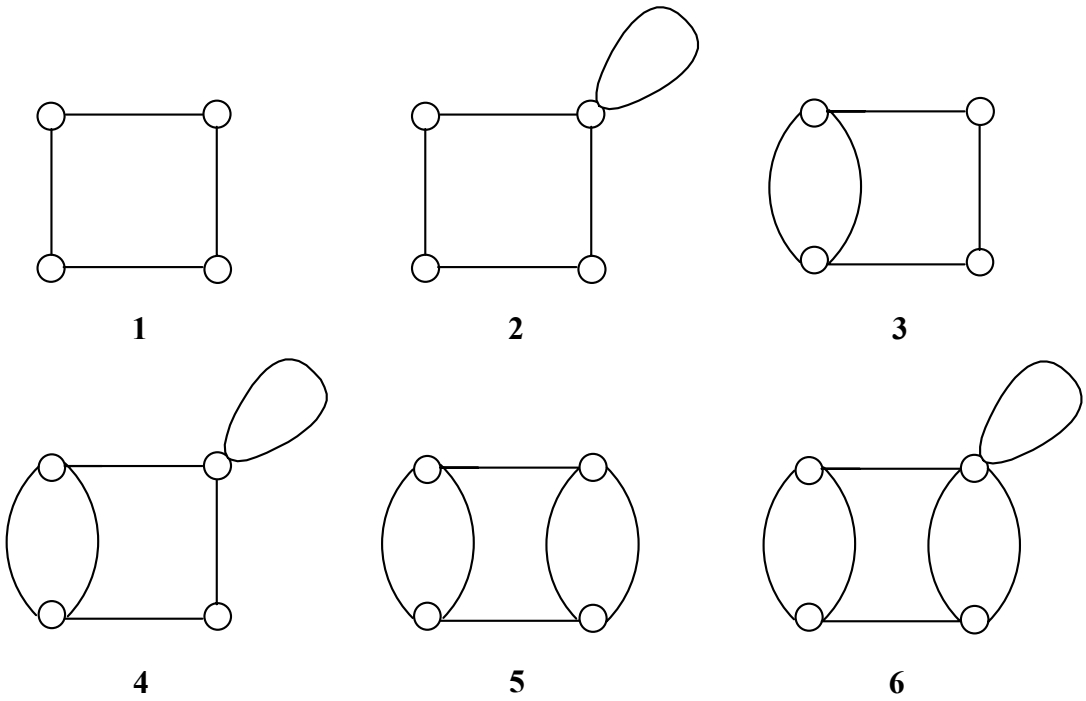


Figure 2. Molecular graphs corresponding to molecules of Figure 1.

2 THE *Z* INDEX FOR SIMPLE GRAPHS

One way to calculate the *Z* index for simple graphs is by means of the *Z* counting polynomial. The *Z* counting polynomial, $Q(G; x)$, of a simple connected graph *G* is defined [1] as:

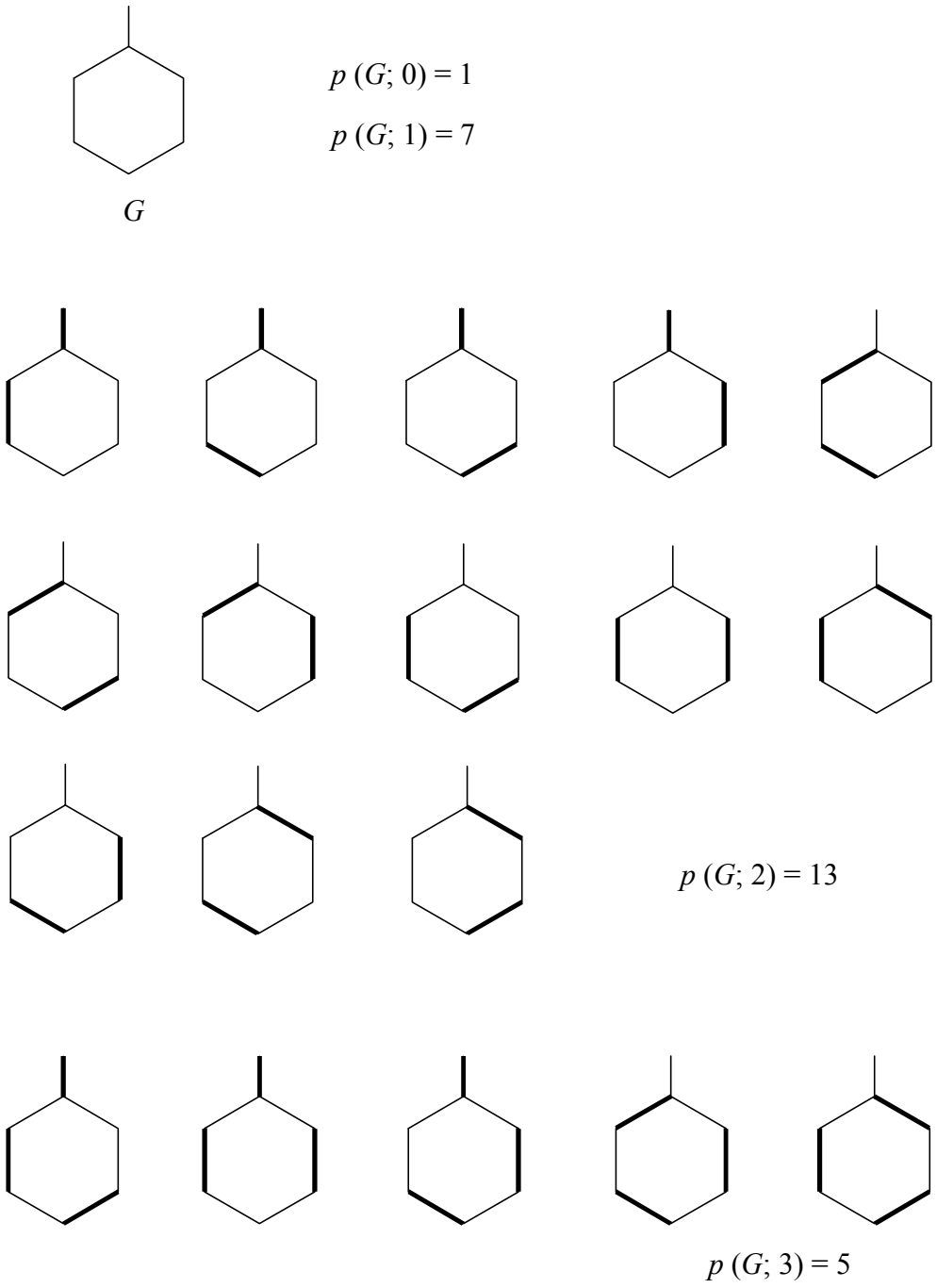
$$Q(G;x) = \sum_{k=0}^{[V/2]} p(G;k)x^k \tag{1}$$

where the coefficient $p(G; k)$ is the number of independent sets of *k* edges of *G*. A set *S* of *k* edges is independent (*k*–matching) if no two edges of the set *S* are adjacent in *G*. The Gaussian brackets [ ] above the summation in Eq. (1) denote the integer part of *V*/2, where *V* is the number of vertices in *G*. The empty set and all singleton sets are independent, hence $p(G; 0)=1$ and $p(G; 1)$ equals the number of edges in *G*. The *Z* index of *G*, $Z = Z(G)$, is defined by the expression:

$$Z = \sum_{k=0}^{[V/2]} p(G;k) \tag{2}$$

Obviously, the *Z* index is equal to the value of the *Z* counting polynomial for $x = 1$:

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



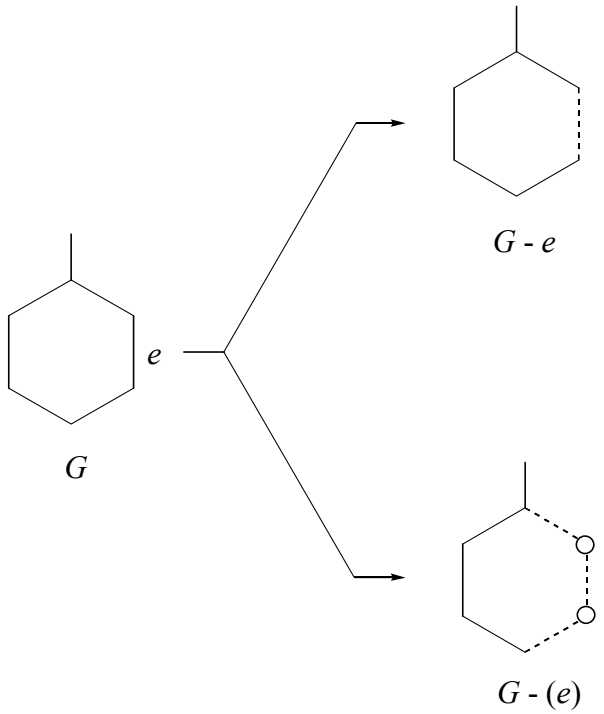
$$Q(G; x) = 1 + 7x + 13x^2 + 5x^3$$

$$Z(G) = 26$$

Figure 3. The graphical construction of the *Z* counting polynomial for a simple graph representing methylcyclohexane.

As an example of the construction of the *Z* counting polynomial we give in Figure 3 the "pedestrian" (graphical) construction of the *Z* counting polynomial for a simple graph representing methylcyclohexane. The graphical construction of the *Z* counting polynomial is of a conceptual

value, but computationally is impractical for larger graphs.



$$Q(G; x) = Q(G - e; x) + xQ(G -(e); x)$$

$$\begin{array}{rl} & Q\,(G - e; x) = 1 + 6x + 9x^2 + 2x^3 \\ + & xQ\,(G - (e); x) = \quad x + 4x^2 + 3x^3 \\ \hline & Q\,(G; x) = 1 + 7x + 13x^2 + 5x^3 \end{array}$$

Figure 4. The construction of the *Z* counting polynomial for the graph *G* of Figure 3 using the recurrence relation (4).

A much easier and faster way to compute $Q(G; x)$ is by the recurrence relation [1]:

$$Q(G;x) = Q(G-e;x) + xQ(G-(e);x) \tag{4}$$

where *G*–*e* and *G*–(*e*) denote spanning subgraphs of *G* obtained by erasing an edge *e*, and the edge *e* and all edges adjacent to *e* respectively. Since *G* is connected, its spanning graph *G*–*e* is connected if and only if *G* contains at least one cycle and the edge *e* is one of the edges making up the cycle(s). The spanning subgraph *G*–(*e*) is always disconnected. The *Z* counting polynomial of a disconnected graph *D* with components D_i (i=1, . . . , n), that is:

$$D = \bigcup_{i=1}^{n} D_i \tag{5}$$

is defined by the expression:

$$Q(D;x) = \prod_{i=1}^{n} Q(D_i;x) \tag{6}$$

and consequently the *Z* index for the graph *D* is given by:

$$Z(D) = \prod_{i=1}^{n} Z(D_i) \tag{7}$$

The idea behind the recurrence relation, Eq. (4), is to reduce *G* to smaller fragments for which the *Z* counting polynomials can easily be computed. In Figure 4, we give the construction of the *Z* counting polynomial for the graph of Figure 3 using Eq. (4).

3 THE RELATIONSHIP BETWEEN THE MATCHING POLYNOMIAL AND THE *Z* COUNTING POLYNOMIAL FOR SIMPLE GRAPHS

When Hosoya introduced the *Z* counting polynomial in 1971, the matching [24] (acyclic [25,26], reference [27]) polynomial was unknown in chemistry. The matching polynomial became an object of research interest of mathematical chemists after the topological resonance energy (TRE) had been introduced in 1975–1977 by the Zagreb Group [25,26] and by Aihara [27]. This polynomial is a key concept in the TRE theory of aromaticity [25–28].

The matching polynomial, $\alpha(G; x)$, of a simple connected graph *G* is given by [24]:

$$\alpha(G;x) = \sum_{k=0}^{[V/2]} (-1)^k \, p(G;k) x^{V-2k} \tag{8}$$

The expression for the matching polynomial of a disconnected graph is analogous to the one given for the *Z* counting polynomial, Eq. (6). It should be noted that for an acyclic structure, represented by a tree *T*, $\alpha(T; x)$ is equal to its characteristic polynomial $P(T; x)$.

If one compares Eq. (1) with Eq. (8), one sees a great similarity between these two equations. The relationship between the matching polynomial and the *Z* counting polynomial is [29]:

$$\alpha(G;x) = x^V Q(G; x = -x^{-2}) \tag{9}$$

or

$$Q(G;x) = (i\sqrt{x})^V \, \alpha(G; x = i/\sqrt{x}) \tag{10}$$

where $i = \sqrt{-1}$.

Thus, for example, the matching polynomial of the cyclobutane graph **1** of Figure 2:

$$\alpha(\mathbf{1};x) = x^4 - 4x^2 + 2 \tag{11}$$

converts immediately *via* Eq. (9) into the *Z* counting polynomial of **1**:

$$Q(\mathbf{1};x) = 1 + 4x + 2x^2 \tag{12}$$

Because of the relationship (9), the *Z* index can also be obtained from the matching polynomial by means of the following expression [29]:

$$Z(G) = (-i)^V \alpha(G; x = i) \tag{13}$$

This expression eliminated the use of the *Z* counting polynomial for calculating the *Z* index. Hereafter we will use the matching polynomial for calculating the *Z* index. There are also available computer programs for getting matching polynomials of simple graphs and fullerenes [*e.g.*, 30,31], but not for general graphs.

4 THE *Z* INDEX FOR GENERAL GRAPHS

We constructed the matching polynomial of a general connected graph using the following recurrence formula [14,25,26]:

$$\alpha(G;x) = \alpha(G - e;x) - \alpha(G - [e];x) \tag{14}$$

where *G*–*e* denotes a subgraph of *G* obtained by removing an edge *e* from *G* and *G*–[*e*] is a subgraph obtained by removal of the edge *e* and incident vertices from *G*. Therefore, Eq. (14) differs from Eq. (4).

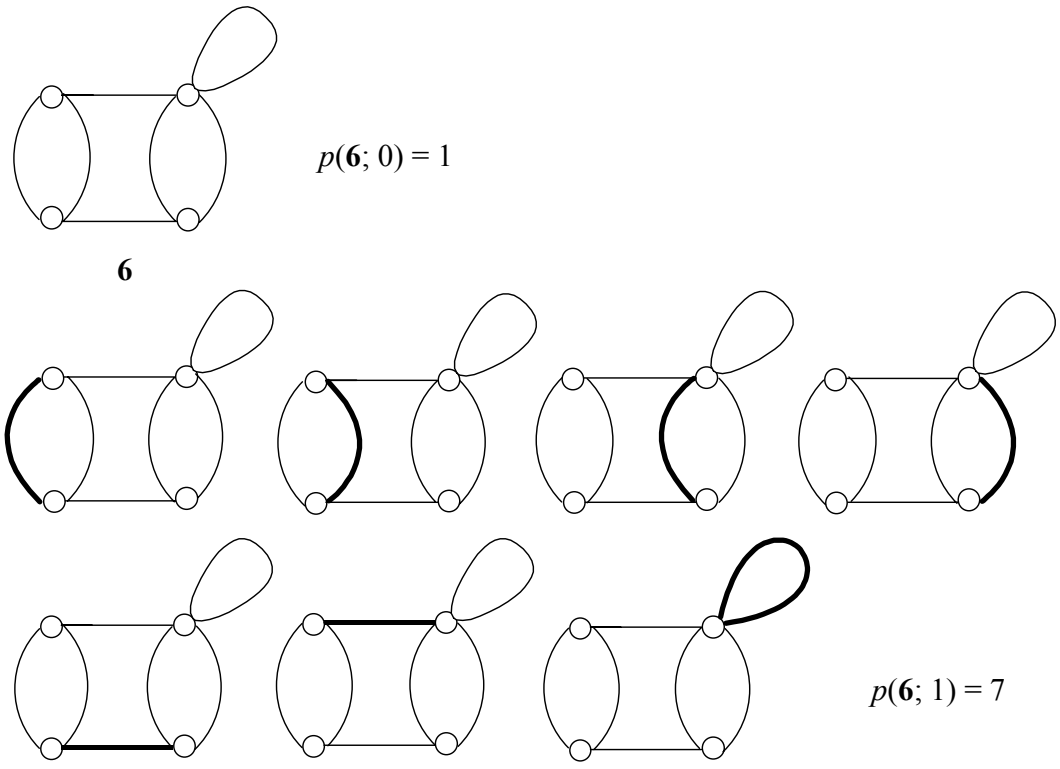
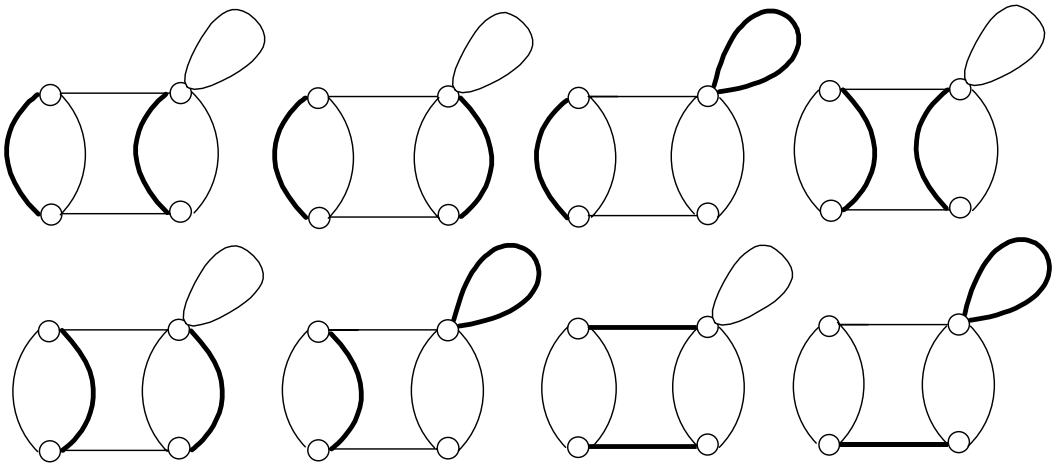


Figure 5. The construction of the matching polynomial for the graph **6** of Figure 2 using the graphical approach.

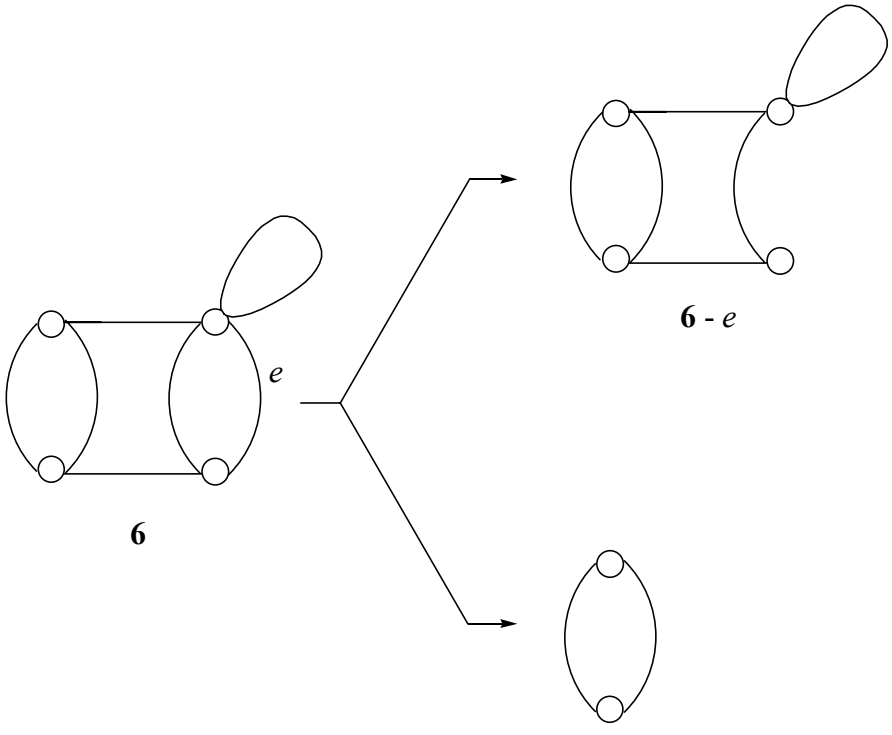


$p(\mathbf{6}; 2) = 8$

$\alpha(\mathbf{6}; x) = x^4 - 7x^2 + 8$

$Z(\mathbf{6}) = 16$

Figure 5. (Continued).



$$\alpha(\mathbf{6} - e; x) = x^4 - 6x^2 + 6$$
$$+ \quad -\alpha(\mathbf{6} - [e]; x) = \quad - x^2 + 2$$
$$\alpha(\mathbf{6}; x) = x^4 - 7x^2 + 8$$
$$Z(\mathbf{6}) = 16$$

Figure 6. The construction of the matching polynomial for the graph **6** of Figure 2 using the recurrence relation (14).

After we obtain the matching polynomial of the general graph *G*, the *Z* index is simply equal to the sum of absolute values of the matching polynomial coefficients:

$$Z(G) = \sum_{k=0}^{[V/2]} \left| (-1)^k \, p(G;k) \right| = \sum_{k=0}^{[V/2]} p(G;k) \tag{15}$$

In Figure 5 we present the construction of the matching polynomial for the graph **6** of Figure 2, using graphical approach and in Figure 6 by applying the recurrence relation (14).

5 THE EDGE CONTRIBUTIONS TO THE *Z* INDEX

The *Z* index at first sight appears as a topological index that cannot be decomposed into the edge contributions. However, the decomposition of the *Z* index of a simple connected acyclic graph (tree) into edge contributions has been done by means of superimposing all the diagrams representing independent sets of edges of the tree [32].

The decomposition of *Z* index into edge contributions is possible not only for trees but for all kinds of connected and disconnected graphs. The correctness of this claim is easy to see bearing in mind that for a general graph *G* holds the identity [33]:

$$\sum_{e} p_e(G;k) = k \, p(G;k) \tag{16}$$

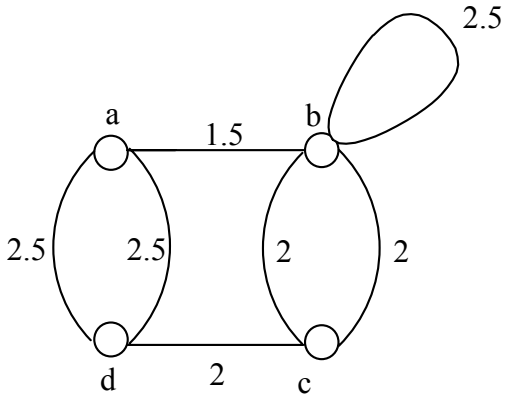
where $p_e(G; k)$ represents the number of independent sets of *k* edges of *G* that contain the edge *e*. The summation goes over all edges of *G*. Dividing Eq. (16) by *k* and then summing over *k* one immediately obtains the sought after analytical expression for the decomposition of *Z* index into edge contributions:

$$\sum_{e} \sum_{k=1}^{[V/2]} \frac{p_e(G;k)}{k} = \sum_{k=1}^{[V/2]} p(G;k) = Z(G) - 1 \tag{17}$$

The quantities $p_e(G; k)$ associated with a given edge *e* can be found just from the spanning subgraph *G*–(*e*). To wit, the relationship between *Z*(*G*–(*e*)) and quantities $p_e(G; k)$ is given by the expression:

$$Z(G - (e)) = \sum_{k=1}^{[V/2]} p_e(G;k) \tag{18}$$

If one assigns the quantities $\sum_k (p_e(G;k)/k)$ to the corresponding edges in *G* then one creates the edge–weighted graph *G*. An example of such weighting of a graph is given on the loopmultigraph **6**, shown bellow:



6 HOW THE STRUCTURE OF (MOLECULAR) MULTIGRAPHS, LOOPGRAPHS AND LOOPMULTIGRAPHS AFFECTS THE VALUE OF THE *Z* INDEX

In this section we discuss how the structural characteristics of (molecular) multigraphs, loopgraphs and loopmultigraphs, such as size (in terms of the number of vertices and edges), branching, cyclicity, multiple edges and loops, influence the value of *Z* index. It is clear that the *Z* index increases with the size in terms of either the number of multiple edges and loops or the number of vertices (the increase in the number of vertices reflects in the increase in the number of edges in connected graphs of any kind) because already the value of $p(G; 1)$ increases with these numbers. This is also seen when graphs in Figure 2 are compared. In Table 1 we give the expressions for the matching polynomial and the corresponding values of the *Z* index for a set of graphs shown in Figure 2.

Table 1. Matching polynomials and values of *Z* index and total walk count (*twc*) index for six graphs of Figure 2.

Molecular graph	Matching polynomial	Z	twc
1	$x^4 - 4x^2 + 2$	7	120
2	$x^4 - 5x^2 + 4$	10	350
3	$x^4 - 5x^2 + 3$	9	282
4	$x^4 - 6x^2 + 6$	13	552
5	$x^4 - 6x^2 + 5$	12	480
6	$x^4 - 7x^2 + 8$	16	992

Multiple edges and loops individually increase the value of the *Z* index (compare graphs **1**, **3** and **5**, and graphs **1** and **2**). Multiple edges affect less the *Z* index than loops (compare graphs **2** and **3**, and **4** and **5**). When both the multiple edge(s) and loop(s) are simultaneously present in the graph, their joint influence is greater on the *Z* index than their individual influences. The *Z* index orders graphs of Figure 2 in the following way: its value increases on going from the simple graph **1**, to the multigraph **3**, to the loopgraph **2**, to the graph **5** with two multiple edges, to the graph **4** with one multiple edge and one loop, and finally to the loopmultigraph **6** with two multiple edges and one loop. In order to check this observation, we computed the total walk count (*twc*) index for the graphs **1**–**6** taking into account all walks with length of 4 using our computer program [22]. A walk

in a (general) graph is any sequence of consecutive edges (and loops). The *twc* index produced the same order: **1** < **3** < **2** < **5** < **4** <**6**. We used the *twc* index as a standard because it has been found that *twc* is a suitable quantity to order molecules according to the structural characteristics of their graphs [34,35].

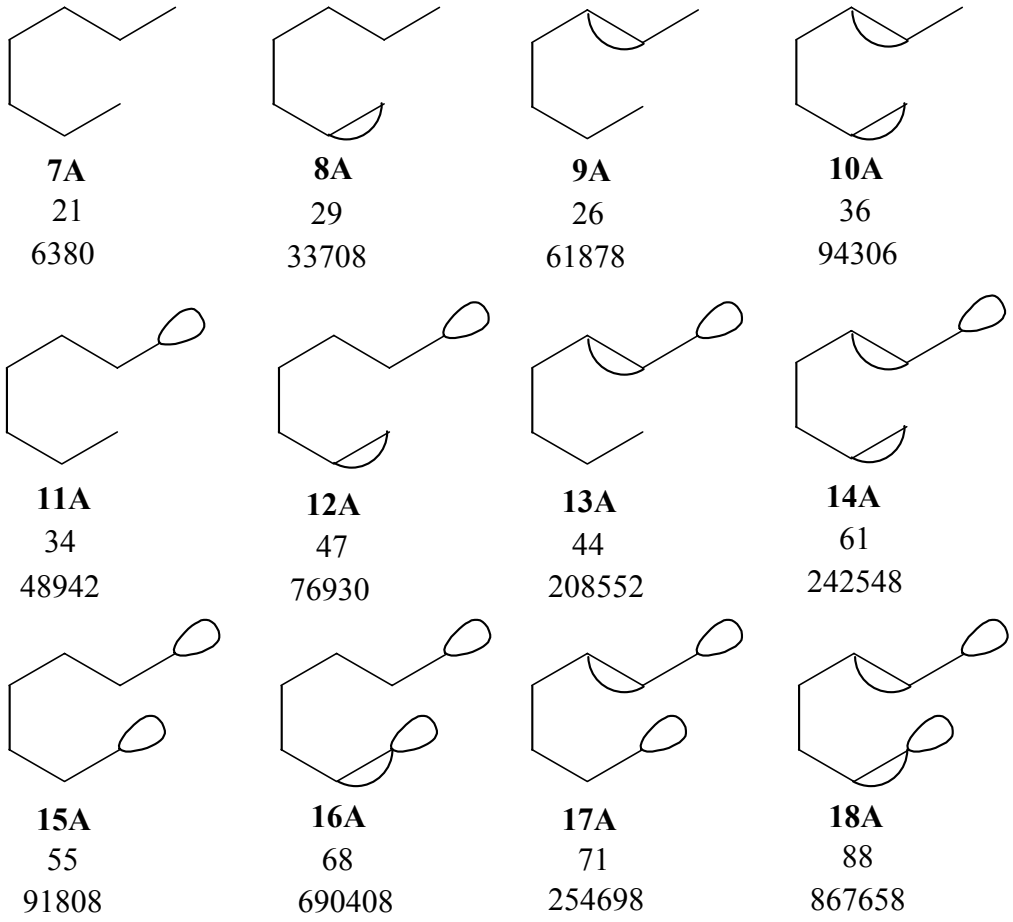


Figure 7. A set of unbranched simple graphs, multigraphs, loopgraphs, and loopmultigraphs. Below each graph the values of *Z* index and *twc* index (computed for walks up to the length of 10) are given.

We investigated in more detail the influence of branching on the *Z* index using the set of acyclic unbranched and branched multigraphs, loopgraphs and loopmultigraphs with seven vertices, starting with the parent simple graphs. In Figure 7 we give unbranched graphs and in Figure 8 their branched isomers. From these figures we see that the *Z* index indeed increases with the increase in the size in terms of the number of edges and loops. We also noted as before that loops always bring a greater increase in the value of *Z* index than multiple edges. Regarding branching, Hosoya stated that the *Z* index of the acyclic unbranched simple graphs is the *largest* among the isomeric graphs. We observed that this statement holds for simple graphs and loopgraphs, but *not* for all multigraphs and loopmultigraphs; compare, for example, the values of the *Z* index for **9A** and **9B**, **10A** and **10B**, **13A** and **13B**, **14A** and **14B**, **17A** and **17B**, and **18A** and **18B**. In Figures 9 and 10 we give graphical enumeration of the *Z* indices for multigraphs **9A** and **9B**.

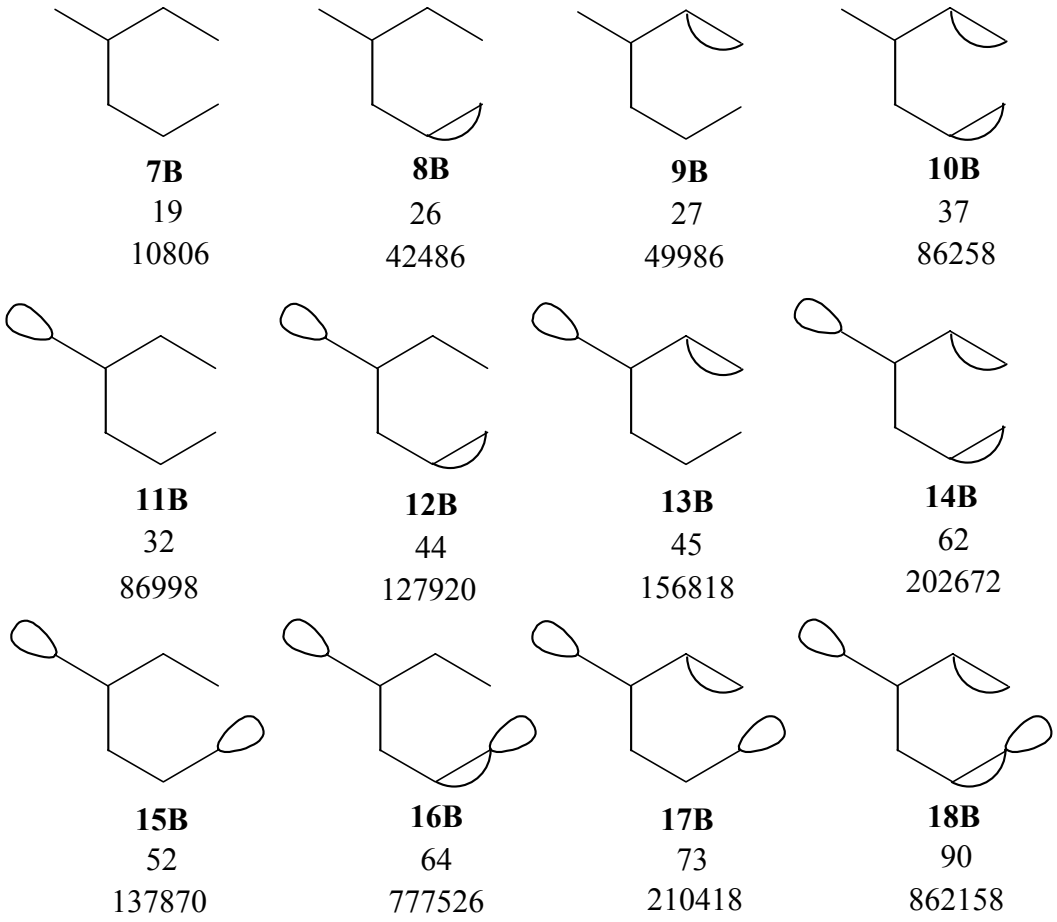
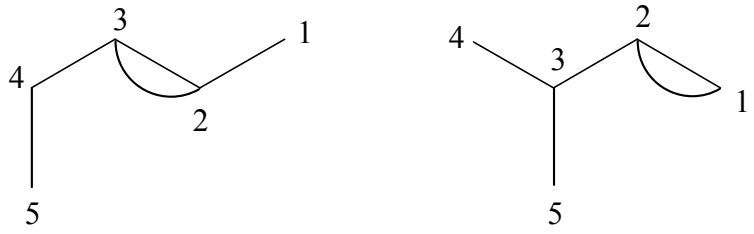


Figure 8. A set of branched simple graphs, multigraphs, loopgraphs and loopmultigraphs related to graphs of Figure 7. Below each graph the values of *Z* index and *twc* index (computed for walks up to the length of 10) are given.

The difference in the value of *Z* index for **9A** and **9B** is caused by different values of the $p(G; 3)$, while values of $p(G; 0)$, $p(G; 1)$ and $p(G; 2)$ are identical. Therefore, the values of *Z* index for pairs of smaller unbranched and branched multigraphs obtained from **9A** and **9B**, such as pair **19A** and **19B**, given below, are expected to be identical.



19A **19B**

10 10

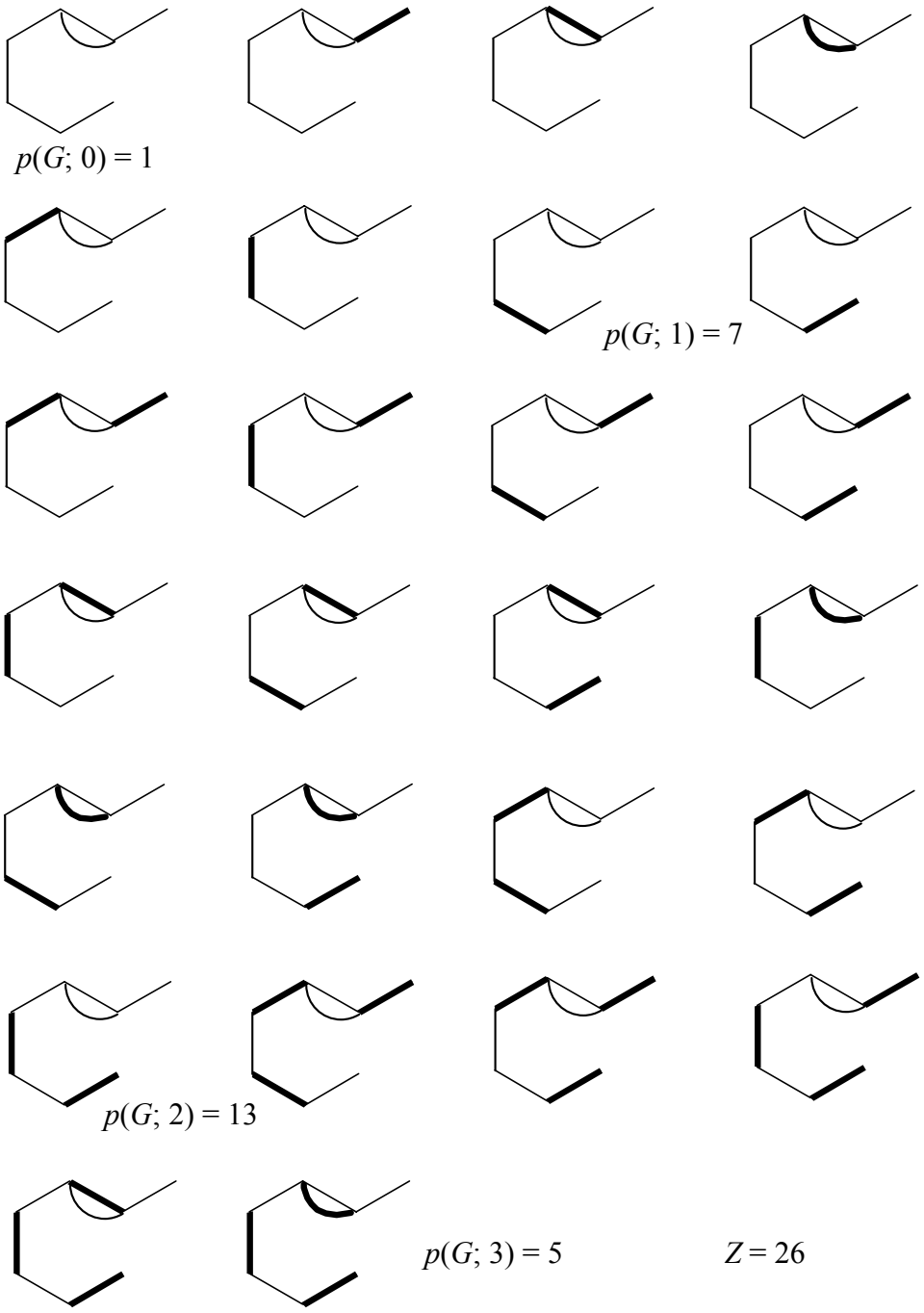


Figure 9. Computing the *Z* index for **9A** using graphical approach.

Apparently, in the case of multigraphs and loopmultigraphs the values of the *Z* index depend strongly on the mutual position of multiple edges and loops. In some positions multiple edges and loops offer greater combinatorial possibilities to unbranched multigraphs and loopmultigraphs and in some other positions to branched multigraphs and loopmultigraphs.

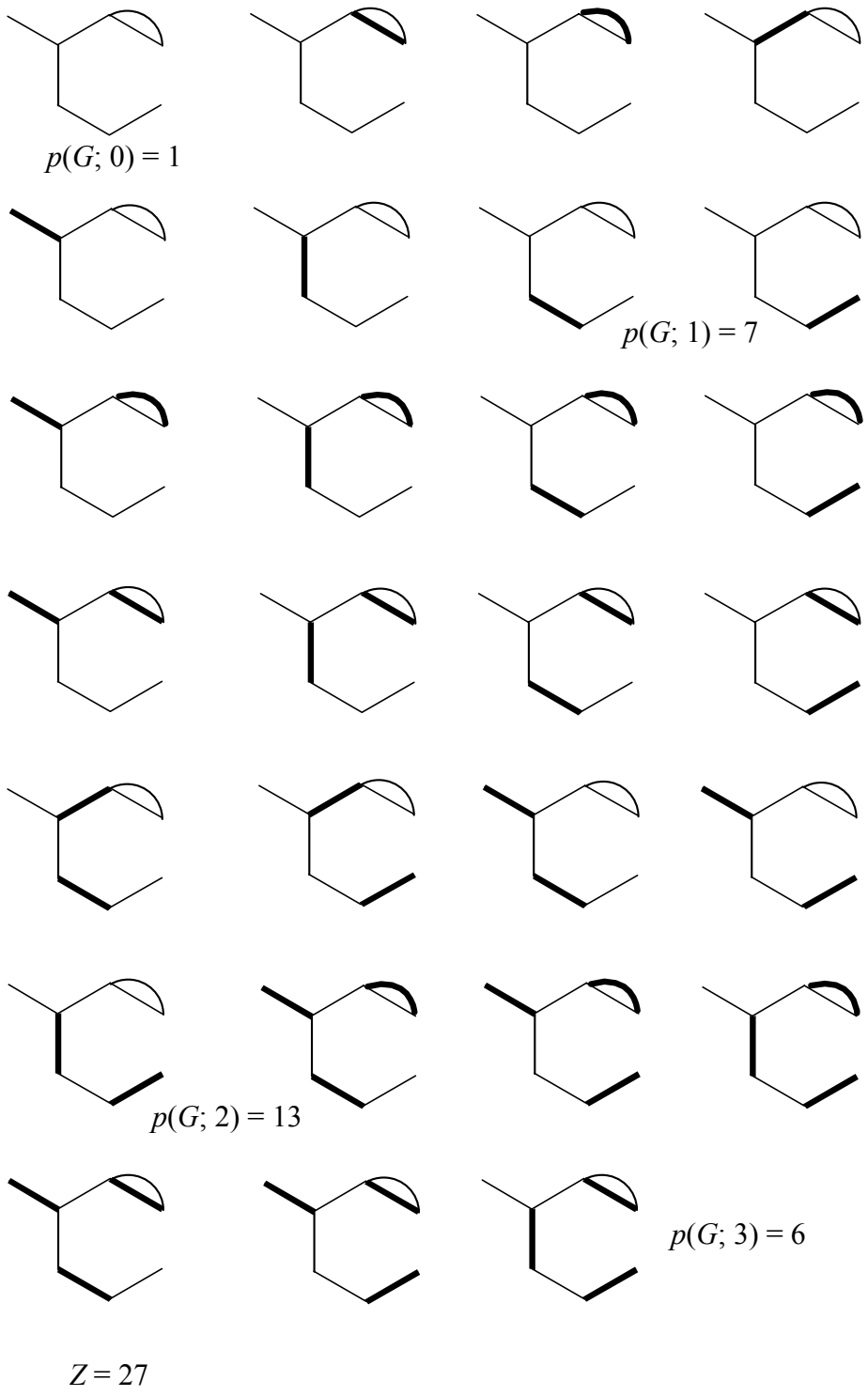


Figure 10. Computing the *Z* index for **9B** using graphical approach.

The *twc* index supports only in part the response of the *Z* index to branching. In the case of simple graphs *twc* is always greater for the branched isomer [35]. The same appears to be true for loopgraphs, but not for all multigraphs and loopmultigraphs. In some cases branched multigraphs and loopmultigraphs have smaller values of *twc* than unbrached counterparts (compare **9A** and **9B**, **10A** and **10B**, **13A** and **13B**, **14A** and **14B**, **17A** and **17B**, **18A** and **18B**).

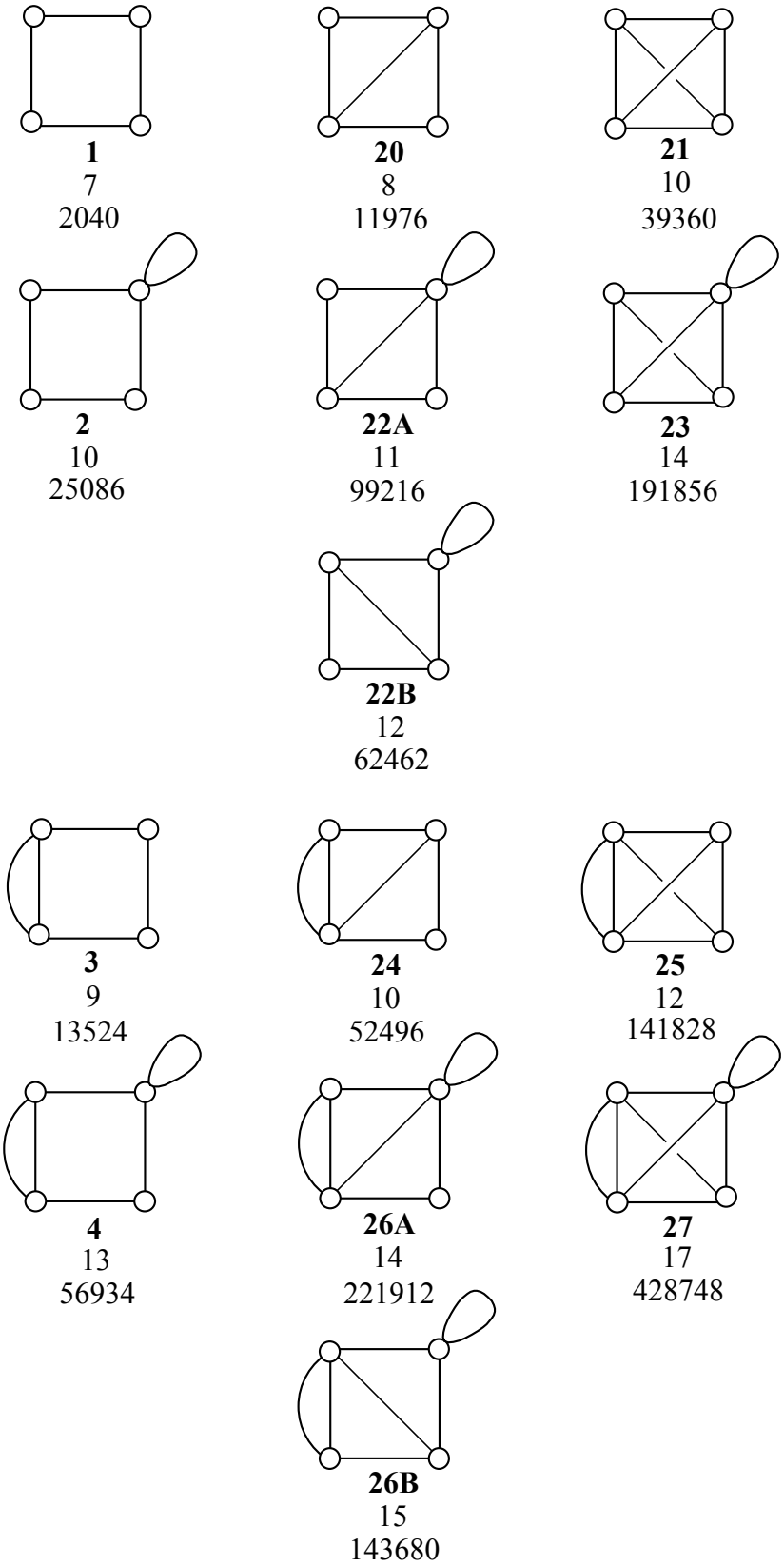


Figure 11. A set of cyclic graphs with four vertices and the values of their *Z* indices and tw*c* indices (computed for walks with up to length of 8).

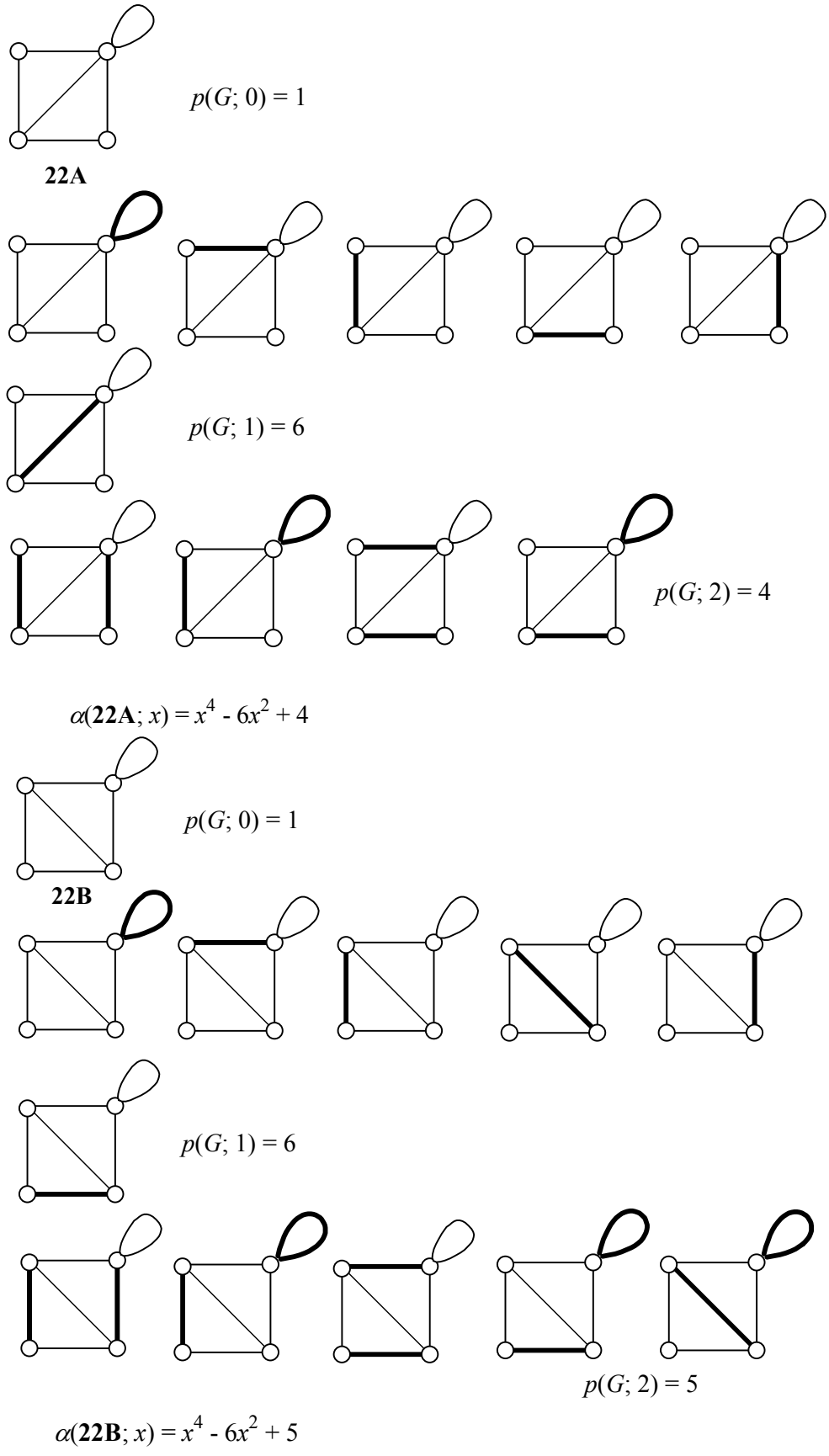


Figure 12. Construction of the matching polynomial for **22A** and **22B**.

In these examples the *twc* index opposes the *Z* index. Loops increase the value of the *twc* index (and the *Z* index) much more than multiple edges (compare, for example, **7B** and **8B** and **7B** and **11B**). Especially explosive increase in the values of the *twc* index occurs when the loop and multiple edges are adjacent (compare **16A** and **17A**, and **16B** and **17B**). This is not observed in the case of the *Z* index, graphs with the adjacent loop and multiple edges possess smaller values of the *Z* index than graphs with the non–adjacent loop and multiple edges.

Cyclicity is a structural characteristic that cannot be isolated from other structural characteristics. The change in the number of cycles usually results in the size change. We selected a set of cyclic simple graphs, multigraphs, loopgraphs and loopmultigraphs with four vertices. They are presented in Figure 11 together with their *Z* indices and *twc* indices values, whilst their matching polynomails are given in Table 2. Note that matching polynomials for the graphs **1**, **2**, **3**, and **4** are already given in Table 1.

Table 2. Matching polynomials for the graphs of Figure 11.

Graph	Matching polynomial
20	$x^4 - 5x^2 + 2$
21	$x^4 - 6x^2 + 3$
22A	$x^4 - 6x^2 + 4$
22B	$x^4 - 6x^2 + 5$
23	$x^4 - 7x^2 + 6$
24	$x^4 - 6x^2 + 3$
25	$x^4 - 7x^2 + 4$
26A	$x^4 - 7x^2 + 6$
26B	$x^4 - 7x^2 + 7$
27	$x^4 - 8x^2 + 8$

The value of the *Z* index increases with the increase in the number of cycles. The same is true for the *twc* index. It can again be seen that a loop increases more the values of the *Z* and *twc* indices than a multiple edge. The *Z* index and *twc* disagree in the cases such as **22A** and **22B**, and **26A** and **26B**, where the loop is placed either on the vertex adjacent to three or two vertices. Apparently the combinatorial possibilities for the *Z* index are greater when the vertex carrying the loop has only two adjacent vertices (see Figure 12), whilst the reverse is true for *twc*.

7 CONCLUSIONS

The Hosoya *Z* index was generated for selected sets of acyclic and cyclic simple graphs, multigraphs, loopgraphs, and loopmultigraphs. The influence of structural characteristics, such as the size, branching, cyclicity, of studied graphs on the *Z* index was analyzed. In most cases the results for simple graphs parallel the results obtained for the multigraphs, loopgraphs and loopmultigraphs. However, it has been found for some multigraphs and loopmultigraphs that the branched structure has a greater value of the *Z* index than the unbranched isomer, thus, *opposing* the observation for the simple graphs where the branched structure has always smaller value of the *Z*

index than the unbranched isomer. In most cases the *twc* index supports results obtained by the *Z* index, that is, the values of the indices increase with the size in terms of multiple edges and loops, they are sensitive to branching, but *twc* is not always in agreement with the *Z* index, and loops cause a considerable increase in their values. It also appears that the position of the loop is important for both *Z* index and *twc*.

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