CROATICA CHEMICA ACTA
CCACAA **78** (2) 235–239 (2005)

ISSN-0011-1643
CCA-3003
Original Scientific Paper

Comparison of the Hosoya *Z*-Indices for Simple and General Graphs of the Same Size*

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RECEIVED JANUARY 11, 2005; REVISED MARCH 1, 2005; ACCEPTED MARCH 1, 2005

Keywords
general graphs
Hosoya *Z*-index
molecular graphs
simple graphs

In the extension of our previous work (Ref. 1), the average values of the *Z*-indices have been computed for the simple and general graphs of the same size. Three results have been obtained: (i) General graphs have always higher average values of the *Z*-indices than the corresponding simple graphs, (ii) Replacement of the non-cut-edge of the graph with a loop increases the value of the *Z*-index, and (iii) The value of the *Z*-index of a path with a loop attached to its second vertex is higher than or equal to the value of the *Z*-index of the cycle of the same size.

INTRODUCTION

We noticed in our previous report[1] that the loops and multiple edges contribute to the value of the Hosoya *Z*-index.[2] In that paper, the loops and multiple edges were added to simple graphs and they were thus transformed into general graphs. Simple (molecular) graphs are graphs without loops and multiple edges.[3] In general graphs, loops and multiple edges are allowed.[4] Note that a loop is an edge joining a vertex to itself and a multiple edge represents a connection between two vertices with more than one edge. All the graphs that we consider are connected.[5] It should also be noted that in the case of graphs with an even number of vertices, the last contribution to the *Z*-index equals the number of spanning trees.[6]

The above transformation from simple to general graphs resulted in an increase of the number of edges. This increase in the value of the *Z*-index was evidently the result of the size effect in terms of loops and multiple edges. In this note, we investigate the behavior of the *Z*-index when the size effect is avoided, that is, when simple graphs and general graphs of the same size are compared. Simple and general graphs of the same size have the same number of vertices and edges.

NOTATIONS[5,7]

Let G be any graph. We denote by V(G) the set of vertices of G and by E(G) the set of edges of G. Matching in G is any set of independent edges in G.

Let $v \in V$(G). Let G-v denote a subgraph of G obtained by deletion of a vertex v and all its adjacent edges. In addition, let $d_G(v)$ and $N_G(v)$ denote, respectively, the degree and the set of neighbors of vertex v in G.

Let $e \in E$(G). Let G-e denote a subgraph of G obtained by deletion of an edge e. Then the edge e is a cut-edge if G is connected and if G-e is not. Let CE(G) denote the set of cut-edges of G.

* Dedicated to Edward C. Kirby on the occasion of his 70th birthday.

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Let $e' \notin G$. Let $G+e'$ denote a graph obtained by adition of an edge e' to G and let P_n denote a path with n vertices and by C_n the cycle with n vertices. Let also $P_{n,k}$ denote a path with n vertices with a single loop attached to the k-th vertex of the path.

RESULTS AND DISCUSSION

The First Result

We first report a comparison of the Hosoya *Z*-indices for simple graphs and several classes of general graphs of the same size with 7 and 8 vertices and with the maximal vertex-degree 4. The considered classes of general graphs are: (i) general graphs with a single loop, (ii) general graphs with a single double edge, and (iii) general graphs with a single loop and a single double edge. Illustrative examples of these classes of general graphs and the corresponding simple graphs are given in Figure 1.

Table I gives the numbers of the considered graphs with 7 vertices and Table II the graphs with 8 vertices. These numbers have been obtained by the computer program given in the Appendix.

In the following two tables, we compare the values of average *Z*-indices for the graphs with the same number of vertices and edges. In Table III, we consider graphs with 7 vertices and in Table IV graphs with 8 vertices. Average values of the *Z*-indices have been also obtained by the computer program given in the Appendix.

From Tables III and IV, it is readily seen that the existence of loops and double bonds increases the value of the *Z*-index following the transformation from simple graphs into general graphs of the same size. Thus, the statement expressed in Ref. 1 has a much stronger significance.

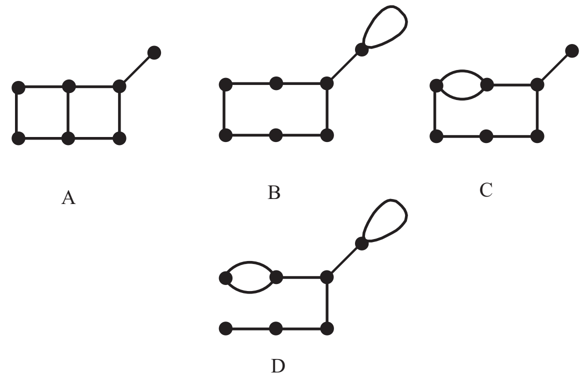

Figure 1. Examples of a simple graph (A) and of a general graph with a single loop (B), with a single double edge (C) and with a single loop and a single double edge (D) with 7 vertices and 8 edges and the maximal vertex-degree 4.

TABLE I. Numbers of graphs with 7 vertices, the maximal vertex-degree 4 and the prescribed number of edges

Number of edges	Number of simple graphs	Number of general graphs with a single loop	Number of general graphs with a single double edge	Number of general graphs with a single loop and a single double edge
6	9	0	0	0
7	29	52	28	0
8	56	151	109	135
9	79	242	214	455
10	79	261	263	719
11	59	183	209	643
12	31	87	101	324
13	9	24	28	78
14	2	2	3	6

TABLE II. Numbers of graphs with 8 vertices, the maximal vertex-degree 4 and the prescribed number of edges

Number of edges	Number of simple graphs	Number of general graphs with a single loop	Number of general graphs with a single double edge	Number of general graphs with a single loop and a single double edge
7	18	0	0	0
8	73	116	67	0
9	182	427	324	373
10	326	910	817	1580
11	430	1320	1344	3326
12	427	1332	1520	4267
13	298	943	1153	3466
14	134	420	542	1661
15	35	97	128	383
16	6	7	10	23

TABLE III. Average values of the Z-indices of graphs with 7 vertices, the maximal vertex-degree 4 and the prescribed number of edges

Number of edges	Average values of the Z-indices for simple graphs	Average values of the Z-indices for the general graphs with a single loop	Average values of the Z-indices for the general graphs with a single double edge	Average values of the Z-indices for the general graphs with a single loop and a single double edge
6	17.0000	not defined	not defined	not defined
7	22.6897	27.1346	22.7143	not defined
8	29.1786	35.6358	29.6697	36.2667
9	36.6962	45.4298	37.8131	46.5846
10	45.7215	56.8544	47.2471	58.7330
11	56.2881	70.3333	58.4737	72.8694
12	68.8710	85.9310	71.6436	89.3426
13	83.5556	103.7500	86.5714	108.2051
14	99.5000	124.0000	103.3333	129.0000

TABLE IV. Average values of the Z-indices of graphs with 8 vertices, the maximal vertex-degree 4 and the prescribed number of edges

Number of edges	Average values of the Z-indices for simple graphs	Average values of the Z-indices for the general graphs with a single loop	Average values of the Z-indices for the general graphs with a single double edge	Average values of the Z-indices for the general graphs with a single loop and a single double edge
7	26.2222	not defined	not defined	not defined
8	35.1233	41.9138	35.4328	not defined
9	45.3022	55.2998	46.1728	56.3941
10	57.2607	70.7681	58.9070	72.6165
11	71.7093	88.9818	74.0573	91.8545
12	89.0211	110.7793	92.2296	114.6703
13	109.5503	136.5143	113.8725	141.8009
14	134.0000	166.7119	139.1771	173.5707
15	162.4000	201.7423	168.2344	209.7311
16	195.8333	241.7143	199.8000	249.3043

The Second Result

In this section, we prove that the value of the Z-index of a path with a single loop is higher or equal to the value of the Z-index of a cycle of the same size.

Note that $Z(P_1)=1$, $Z(P_2)=2$ and that $Z(P_{n+2}) = Z(P_{n+1})+Z(P_n)$. Solving the recurrent relation, we obtain:

Proposition 1. –

$$Z(P_n) = \frac{5+3\sqrt{5}}{5(1+\sqrt{5})}\left(\frac{1+\sqrt{5}}{2}\right)^n + \frac{-1+\sqrt{5}}{2\sqrt{5}}\left(\frac{1-\sqrt{5}}{2}\right)^n$$

Substituting $p_i = Z(P_i)$ and $p_0 = 1$, and noting that $p_{i+2} = p_{i+1} + p_i$ for each $i \geq 2$, we prove the following theorem.

Theorem 2. – $Z(C_n) < Z(P_{n,k})$ for each $n \geq 3$, $k \leq n$ and $k \neq 2$, $n - 1$. For $k = 2$, $n - 1$, we have $Z(C_n) = Z(P_{n,k})$.

Proof. Note that $P_{n,k} \cong P_{n,n+1-k}$. Hence, $Z(P_{n,k}) = Z(P_{n,n+1-k})$. Therefore, we may assume that $k \leq n/2$. Distinguish three cases:

CASE 1: $n = 1$

$Z(P_{n,1}) = 2p_{n-1} + p_{n-2} \geq p_{n-1} + 2p_{n-2} = Z(C_n)$.

CASE 2: $n = 2$

$Z(P_{n,2}) = 3p_{n-2} + p_{n-3} = 2p_{n-2} + (p_{n-2} + p_{n-3}) = 2p_{n-2} + p_{n-1} = Z(C_n)$.

CASE 3: $n \geq 3$

$Z(P_{n,k}) = 2p_{k-1}p_{n-k} + p_{k-1}p_{n-k-1} + p_{k-2}p_{n-k} = 2p_{k-1}(p_{n-k-1}+p_{n-k-2}) + p_{k-1}p_{n-k-1} + p_{k-2}(p_{n-k-1}+p_{n-k-2}) = p_{k-1}p_{n-k-1} + p_{k-2}p_{n-k-1} + p_{k-2}p_{n-k-2} + 2p_{k-1}p_{n-k-2} + 2p_{k-1}p_{n-k-1} = p_{k-1}p_{n-k-1} + p_{k-2}p_{n-k-1} + p_{k-2}p_{n-k-2} + 2p_{k-1}p_{n-k-2} + 2p_{k-1}(p_{n-k-2} + p_{n-k-3}) = p_{k-1}p_{n-k-1} + p_{k-2}p_{n-k-1} + p_{k-2}p_{n-k-2} + 3p_{k-1}p_{n-k-2} + 2p_{k-1}p_{n-k-3} + p_{k-1}p_{n-k-2} = p_{k-1}p_{n-k-1} + p_{k-2}p_{n-k-1} + p_{k-2}p_{n-k-2} + 3p_{k-1}p_{n-k-2} + 2p_{k-1}p_{n-k-3} + (p_{k-2}+p_{k-3})p_{n-k-2} = (p_{k-1}p_{n-k-1} + p_{k-2}p_{n-k-1} + p_{k-1}p_{n-k-2}) + 2(p_{k-1}p_{n-k-2} + p_{k-1}p_{n-k-3} + p_{k-2}p_{n-2-k}) + p_{k-3}p_{n-k-2} = p_{n-1} + 2p_{n-2} + p_{k-3}p_{n-k-2} = Z(C_n) + p_{k-3}p_{n-k-2} > Z(C_n)$

This proves the theorem. ■

The Third Result

In this section, we prove that replacing the non-cut-edge of a graph with a loop increases the value of the *Z*-index.

We start our proof with an auxiliary lemma:

Lemma 3. – Let G be a graph and let $v \in V(G)$ such that $d_G(v) \geq 1$. Then, $Z(G) > Z(G-v)$

Proof. Denote by u an arbitrary neighboring vertex of v. Note that each matching of G–v is matching in G, but each matching in G that contains edge uv is not matching in G–v (it is not even a subgraph of G–v). ■

Theorem 4. – Let G be a connected graph and let $uv \in E(G) \setminus CE(G)$. Then, $Z(G - uv + vv) > Z(G)$.

Proof. Denote $N_G(v) = \{u, u_2, u_3 \ldots, u_{d_G(v)}\}$. We need to prove that $Z(G - uv + vv) - Z(G) > 0$. We have:

$$Z(G-uv+vv)-Z(G)=\begin{bmatrix} 2\cdot Z\big((G-uv+vv)-v\big)+ \\ \sum_{i=2}^{d_G(v)} Z\big((G-uv+vv)-u_i-v\big)\end{bmatrix}-\begin{bmatrix} Z(G-v)+Z(G-u-v)+ \\ \sum_{i=2}^{d_G(v)} Z(G-u_i-v)\end{bmatrix}. \qquad (1)$$

Note that $(G - uv + vv) - u_i - v = G - u_i - v$ for each $i = 2, \ldots d_G(v)$ and that $(G - uv + vv) - v = G - v$. Hence, the relation (1) reduces to

$Z(G - uv + vv) - Z(G) = Z((G - uv + vv) - v) - Z(G - u - v) = Z(G - v) - Z(G - u - v) >$ {from the previous Lemma} > 0.

This proves the theorem.■

CONCLUDING REMARKS

We found again that general graphs, that is, graphs with loops and multiple edges have a higher value of the *Z*-index. This indicates that the statement expressed in Ref. 1 has a much stronger significance and is not just a consequence of the increase in the number of edges. As the first result, we demonstrated this on the families of connected graphs with 7 and 8 vertices and with the maximal vertex-degree 4, and with the prescribed number of edges. As the second result, we proved that the value of *Z*-index of a path with a single loop is higher or equal to the value of *Z*-index of the cycle with the same number of vertices and, as the third result, we proved that replacing the non-cut-edge of graph with a loop increases the value of *Z*-index. We have also shown that this equality holds only if the loop is attached to the second vertex (counting from any end-vertex of the path).

Acknowledgement. – We thank the Ministry of Science, Education and Sports of Croatia for support.

APPENDIX

Description of the Computer Program

The number of vertices n is the input data while the output data are:

(i) The average value of the *Z*-index of the simple connected graph with n vertices with the maximal degree at most 4, and with the prescribed number of edges

$$\left(=\frac{NumMatchesSimpleGraphs}{NumSimpleGraphs}\right).$$

(ii) The average value of *Z*-index of the connected graph with n vertices and with the maximal vertex-degree at most 4, and with a single loop and without double edges, and with the prescribed number of edges

$$\left(=\frac{NumMatchesLoopGraphs}{NumLoopGraphs}\right).$$

(iii) The average value of the *Z*-index of the connected graph with n vertices and with the maximal vertex-degree at most 4, with a single double edge and without loops, and with the prescribed number of edges

$$\left(=\frac{NumMatchesDBGraphs}{NumDBGraphs}\right).$$

(iv) The average value of the *Z*-index of the connected graph with n vertices and with the maximal vertex--degree at most 4, with a single double edge and a single loop, and with the prescribed number of edges

$$\left(=\frac{NumMatchesLoopDBGraphs}{NumLoopDBGraphs}\right).$$

For each matrix $\boldsymbol{M}$, the *Z*-index of the graph that corresponds to matrix $\boldsymbol{M}$ is denoted by $ZM(\boldsymbol{M})$

At the start of the program, we set the values of *NumMatchesSimpleGraphs*, *NumSimpleGraphs*, *NumMatchesLoopGraphs*, *NumLoopGraphs*, *NumMatchesDBGGraphs*, *NumDBGGraphs*, *NumMatchesLoopDBGGraphs* and *NumLoopDBGGraphs* to zero. These eight values are calculated in three iterations. The first iteration is concerned with graphs whose simple underlying graph has the maximal vertex-degree $MaxDeg = 2$, the second iteration is concerned with graphs whose simple underlying graph has the maximal vertex-degree, $MaxDeg = 3$ and the third iteration is concerned with graphs whose simple underlying graph has the maximal vertex-degree $MaxDeg = 4$.

At start, we consider the set $\boldsymbol{M}_1$ of matrices $\boldsymbol{A} = [a_{ij}]$ of type $n \times n$ such that $a_{1i} = a_{i1} = 1$, for each $i = 2, \ldots, MaxDeg + 1$ and such that $\sum_{i=1}^{n} a_{ij} \leq MaxDeg$ for each $j =$

$1,\ldots,n$ and $\sum_{i=1}^{n} a_{ji} \le MaxDeg$ for each i, $j = 1,\ldots,n$. Note that in set $\boldsymbol{M}_1$ there are duplicates, *i.e.*, there are matrices that correspond to isomorphic graphs. By eliminating these duplicates, we reach the set $\boldsymbol{M}_2$. Since we are only interested in the connected graphs that represent molecules, in the next step we eliminate all matrices that correspond to disconnected graphs. In such a way, we get the set of matrices $\boldsymbol{M}_3$. Now, for each matrix $\boldsymbol{M}$ in $\boldsymbol{M}_3$ we perform the following calculations:

1) Find *Aut* ($\boldsymbol{M}$) the set of all automorphisms of a graph that correspond to matrix $\boldsymbol{M}$.

2) Increase *NumSimpleGraphs* by 1 and *NumMatchesSimpleGraphs* by *ZM* ($\boldsymbol{M}$).

3) Let L_1 ($\boldsymbol{M}$) be the set of all graphs obtained by adding one loop to a single vertex in such a way that the maximal vertex-degree of the corresponding graph does not exceed 4. Using *Aut* ($\boldsymbol{M}$), we eliminate all duplicates from L_1 ($\boldsymbol{M}$). In this way, we obtain L_2 ($\boldsymbol{M}$). For each matrix $\boldsymbol{M'} \in L_2$ ($\boldsymbol{M}$), *NumLoopGraphs* increases by 1 and *NumMatchesLoopGraphs* by *ZM* ($\boldsymbol{M'}$).

4) Let D_1 ($\boldsymbol{M}$) be the set of all graphs obtained by replacing one edge by a double bond in such a way that the maximal vertex-degree in the corresponding graph does not exceed 4. Using *Aut* ($\boldsymbol{M}$), we eliminate all duplicates from D_1 ($\boldsymbol{M}$). In this way, we obtain D_2 ($\boldsymbol{M}$). For each matrix $\boldsymbol{M'} \in D_2$ ($\boldsymbol{M}$), *NumDBGGraphs* increases by 1 and *NumMatchesDBGGraphs* by *ZM* ($\boldsymbol{M'}$).

5) Let LD_1 ($\boldsymbol{M}$) be the set of all graphs obtained by replacing one edge by a double edge and adding a single loop in such a way that the maximal vertex-degree in the corresponding graph does not exceed 4. Using *Aut* ($\boldsymbol{M}$), we eliminate all duplicates from LD_1 ($\boldsymbol{M}$). In this way, we obtain LD_2 ($\boldsymbol{M}$). For each matrix $\boldsymbol{M'} \in LD_2$ ($\boldsymbol{M}$), *NumLoopDBGGraphs* increases by 1 and *NumMatchesLoopDBGGraphs* by *ZM* ($\boldsymbol{M'}$).

Finally, at the end of the program, the values

$$\left(= \frac{NumMatchesSimpleGraphs}{NumSimpleGraphs} \right),$$

$$\left(= \frac{NumMatchesLoopGraphs}{NumLoopGraphs} \right),$$

$$\left(= \frac{NumMatchesDBGraphs}{NumDBGraphs} \right), \text{ and}$$

$$\left(= \frac{NumMatchesLoopDBGraphs}{NumLoopDBGraphs} \right) \text{ are outputted.}$$

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SAŽETAK

Usporedba Hosoyina *Z*-indeksa za jednostavne i opće grafove iste veličine

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Ovaj se članak nadovezuje na članak (vidi referenciju 1) u kojem su prosječne vrijednosti *Z*-indeksa bile izračunane za jednostavne i opće grafove različite veličine. U ovom su članku prosječne vrijednosti *Z*-indeksa izračunane za jednostavne i opće grafove iste veličine. Tri su rezultata dobivena: (i) opći grafovi imaju veće vrijednosti *Z*-indeksa od odgovarajućih jednostavnih grafova, (ii) zamjena brida s petljom povećava vrijednost *Z*-indeksa i (iii) vrijednost *Z*-indeksa staze s petljom na drugom čvoru veća je ili jednaka vrijednosti *Z*-indeksa ciklusa iste veličine.