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Original Scientific Paper

Hosoya Indices of Bicyclic Graphs

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Abstract. Given a molecular graph G, the Hosoya index $Z(G)$ of G is defined as the total number of the matchings of the graph. Let $\mathscr{B}_n$ denote the set of bicyclic graphs on n vertices. In this paper, the minimal, the second-, the third-, the fourth-, and the fifth-minimal Hosoya indices of bicyclic graphs in the set $\mathscr{B}_n$ are characterized.

Keywords: hosoya index, bicyclic graphs, pendent vertex

INTRODUCTION

Let G be a (molecular) graph on n vertices. Two edges of G are said to be independent if they are not adjacent in G. A k-matching of G is a set of k mutually independent edges. Denote by $Z(G,k)$ the number of k-matchings of G. For convenience, we regard the empty edge set as a matching. Then $Z(G,0)=1$ for any graph G. The Hosoya index of G, is defined as

$$Z(G)=\sum_{i=0}^{\frac{n}{2}} Z(G,k) .$$

Obviously, $Z(G)$ is equal to the total number of matchings of G.

The Hosoya index of a graph was introduced by Hosoya[7] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures .[9,14,15] Since then, many authors have investigated the Hosoya index .[3,9,11,17,19,20] An important direction is to determine the graphs with maximal or minimal Hosoya indices in a given class of graphs. Gutman[5] showed that linear hexagonal chain is the unique chain with minimal Hosoya index among all hexagonal chains. Zhang[18] showed that zig-zag hexagonal chain is the unique chain with maximal Hosoya indices among all hexagonal chains. Zhang and Tian[19] gave another proof of above mentioned results of Gutman and Zhang. Zhang and Tian[20] determined the graphs with minimal and second minimal Hosoya indices among catacondensed systems. As for n-vertex trees, it has been shown that the path has the maximal Hosoya index and the star has the minimal Hosoya index.[3] Recently, Hou[10] characterized the trees with a given size of matching and having minimal and second minimal Hosoya index, respectively. Yu and Tian[16] studied the graphs with given edge-independence number and cyclomatic number and having the minimal Merrifield-Simmons indices. Yu and Lv[17] characterized the trees with maximal Merrifield-Simmons indices and minimal Hosoya indices, respectively, among the trees with k pendent vertices. The present authors[11] determined the unicyclic graphs on n vertices having minimal, second-, third-, fourth-, fifth- and sixth-minimal Hosoya indices.

In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bondy and Murty.[1] We only consider finite, simple and undirected graphs. If $W \subseteq V(G)$, we denote by $G-W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E' \subseteq E(G)$, we denote by $G-E'$ the subgraph of G obtained by deleting the edges of E'. If $W=\{v\}$ and $E'=\{xy\}$, we write $G-v$ and $G-xy$ instead of $G-\{v\}$ and $G-\{xy\}$, respectively. For a vertex v of G, we denote $N(v)=\{u \mid uv \in E(G)\}$ and $N[v]=N(v)\cup\{v\}$. We denote by P_n, C_n and $K_{1,n-1}$ the path, cycle and the star on n vertices, respectively. If a path has endpoints u,*v, then we shall use $u \to^* v$ to denote this path.

A bicyclic graph is a connected graph with n vertices and $n+1$ edges. We shall by $\mathscr{B}_n$ denote the set of

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all bicyclic graphs on n vertices. Let G_1, G_2 be two connected graphs with $V(G_1) \cap V(G_2) = \{v\}$. Let $G = G_1 v G_2$ be a graph defined by $V(G) = V(G_1) \cup V(G_2)$ $V(G_1) \cap V(G_2) = \{v\}$ and $E(G) = E(G_1) \cup E(G_2)$. Two graphs are disjoint if they have no vertex in common.

We shall by $G^k_{n,a,b}$ denote the bicyclic graph constructed by attaching kleaves to the vertex v of $C_a v C_b$, and set $\mathscr{B}_{n,1} := \{B \in \mathscr{B}_n$: B is constructed by attaching k leaves to one vertex except v, say u, on $C_a v C_b$ }. For convenience, we let $G'^k_{n,a,b}$ be any one of the members in $\mathscr{B}_{n,1}$. Three internal disjoint paths P_x, P_y and P_c possessing common end vertices *u,v* form a bicyclic graph denoted by G″. We shall by $\tilde{G}^k_{n,x,y,c}$ denote the bicyclic graph constructed by attaching k leaves to the vertex v of G″, and set $\mathscr{B}_{n,2} := \{B' \in \mathscr{B}_n$: B′ G′ is constructed by attaching k leaves to one vertex except u and v, say w, of G″}. For convenience, let $G^k_{n,x,y,c}$ be any one of the members in $\mathscr{B}_{n,2}$. Graphs $G^k_{n,a,b}, G'^k_{n,a,b}, \tilde{G}^k_{n,x,y,c}$ and $G^k_{n,x,y,c}$ are depicted as in Figure 1. In this paper, we show that $\tilde{G}^{n-4}_{n,3,3,2}, G^{n-5}_{n,3,3}, \tilde{G}^{n-5}_{n,3,3,3}, G^{n-6}_{n,4,3}, G^{n-6}_{n,4,3,3}$ is the bicyclic graph with first-, second-, third-, fourth- and fifth-minimal Hosoya index in $\mathscr{B}_n$, respectively (see Figure 2).

At the end of this section, we list some known results which will be used in this paper.

Lemma 1.[3] Let G = (V, E) be a graph.

(i) If $uv \in E(G)$, then $Z(G) = Z(G - uv) + Z(G - \{u, v\})$;

(ii) If $v \in V(G)$, then $Z(G) = Z(G - v) + \sum_{u \in N(v)} Z(G - \{u, v\})$;

(iii) If $G_1, G_2, \ldots, G_t$ are the components of the graph G, then $Z(G) = \prod_{j=1}^{t} Z(G_j)$.

Lemma 2.[12] Let H, X, Y be three connected graphs disjoint in pair. Suppose that u, v are two vertices of H, v' is a vertex of X, u' is a vertex of Y. Let G be the graph obtained from H, X, Y by identifying v with v' and u with u', respectively. Let G_1^* be the graph obtained from H, X, Y by identifying vertices v, v', u' and G_2^* be the graph obtained from H, X, Y by identifying vertices u, v', u'; see Figure 3. Then

$$Z(G_1^*) < Z(G) \quad \text{or} \quad Z(G_2^*) < Z(G).$$

Lemma 3.[13] Let H be a connected graph and T_{l+1} be a tree with $l+1$ vertices such that $V(H) \cap V(T_{l+1}) = \{v\}$. Then $Z(HvT_{l+1}) \geq Z(HvK_{1,l})$.

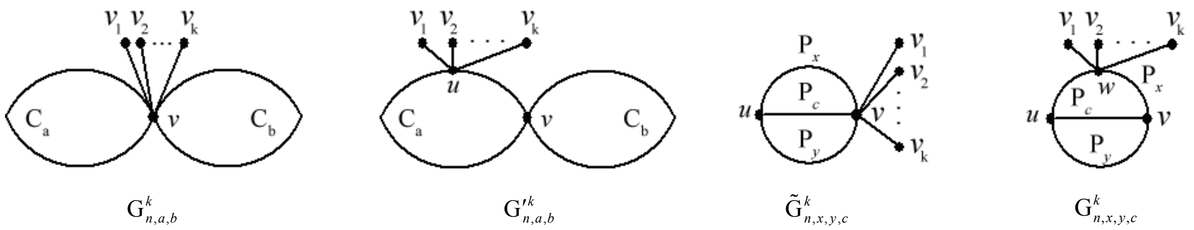

Figure 1. Graphs $G^k_{n,a,b}$, $G'^k_{n,a,b}$, $\tilde{G}^k_{n,x,y,c}$ and $G^k_{n,x,y,c}$.

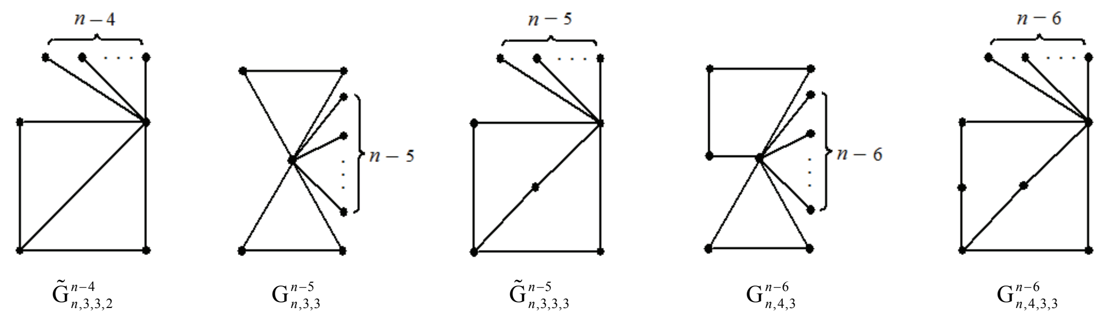

Figure 2. Graphs $\tilde{G}^{n-4}_{n,3,3,2}, G^{n-5}_{n,3,3}, \tilde{G}^{n-5}_{n,3,3,3}, G^{n-6}_{n,4,3}$ and $G^{n-6}_{n,4,3,3}$.

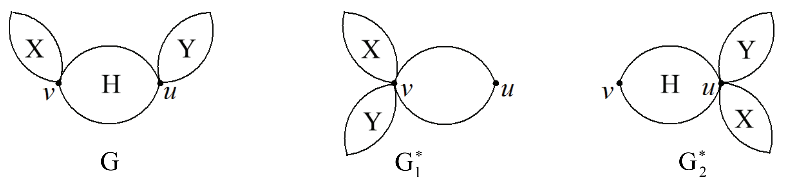

Figure 3. Graphs G, G_1^* and G_2^*.

LEMMAS AND MAIN RESULTS

According to the definitions of the Hosoya index, by Lemma 1, if v is a vertex of G and G contains at least one edge, then $Z(G) > Z(G-v)$. In particular, when v is a pendent vertex of G and u is the unique vertex adjacent to v, we have $Z(G) = Z(G-v) + Z(G-\{u,v\})$. So it is easy to see that $Z(P_0) = 1$, $Z(P_1) = 1$ and $Z(P_n) = Z(P_{n-1}) + Z(P_{n-2})$ for $n \geq 2$. Denote by F_n the n-th Fibonacci number. Recall that $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = 1$ and $F_1 = 1$. It is easy to get

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

Note that $F_{n+m} = F_n F_m + F_{n-1}F_{m-1}$. By Lemma 1, we obtain the following results.

Lemma 4. Given positive integers *a, b, k* with *a, b* ≥ 3.

(i) $Z(G^k_{n,a,b}) = (k+1)F_{a-1}F_{b-1} + 2F_{a-2}F_{b-1} + 2F_{a-1}F_{b-2}$;

(ii) For graph $G'^k_{n,a,b}$, let $C_a = u \to^* v \to^* u = P_x \cup P_y$, then

$$Z(G'^k_{n,a,b}) = k(F_{x-1}F_{y-2}F_{b-1} + F_{x-2}F_{y-3}F_{b-1} + 2F_{x-2}F_{y-2}F_{b-2}) + F_{a-1}F_{b-1} + 2F_{a-2}F_{b-1} + 2F_{a-1}F_{b-2}.$$

Proof. (i) By Lemma 1,

$$\begin{aligned}
Z(G^k_{n,a,b}) &= Z(G^k_{n,a,b} - v_1) + \sum_{u\in N(v_1)} Z(G^k_{n,a,b} - \{u, v_1\}) \\
&= Z(G^{k-1}_{n-1,a,b}) + Z(P_{a-1} \cup P_{b-1} \cup \{v_2,\ldots,v_k\}) \\
&= Z(G^{k-1}_{n-1,a,b}) + F_{a-1}F_{b-1} \\
&= \cdots \\
&= Z(G^0_{n-k,a,b}) + kF_{a-1}F_{b-1} \\
&= Z(G^0_{n-k,a,b} - v) + \sum_{u\in N(v)} Z(G^0_{n-k,a,b} - \{u,v\}) + kF_{a-1}F_{b-1} \\
&= Z(P_{a-1} \cup P_{b-1}) + 2Z(P_{a-2} \cup P_{b-1}) + 2Z(P_{a-1} \cup P_{b-2}) + kF_{a-1}F_{b-1} \\
&= (k+1)F_{a-1}F_{b-1} + 2F_{a-2}F_{b-1} + 2F_{a-1}F_{b-2}
\end{aligned}$$

(ii) Let $Q = G'^k_{n,a,b} - \{u, v_1, \ldots, v_k\}$, $C_a = P_x \cup P_y$. By Lemma 1,

$$\begin{aligned}
Z(G'^k_{n,a,b}) &= Z(G'^k_{n,a,b} - v_1) + \sum_{u\in N(v_1)} Z(G'^k_{n,a,b} - \{u, v_1\}) \\
&= Z(G'^{k-1}_{n-1,a,b}) + Z(Q \cup \{v_2,\ldots,v_k\}) \\
&= Z(G'^{k-1}_{n-1,a,b}) + Z(Q) \\
&= \cdots \\
&= Z(G'^0_{n-k,a,b}) + kZ(Q) \\
&= Z(G'^0_{n-k,a,b} - v) + \sum_{u\in N(v)} Z(G'^0_{n-k,a,b} - \{v,u\}) + kZ(Q) \\
&= kZ(Q) + F_{a-1}F_{b-1} + 2F_{a-2}F_{b-1} + 2F_{a-1}F_{b-2}, \qquad (1)
\end{aligned}$$

where,

$$\begin{aligned}
Z(Q) &= Z(Q - v) + \sum_{v_j\in N(v)} Z(Q - \{v_j, v\}) \\
&= Z(P_{x-2} \cup P_{y-2} \cup P_{b-1}) + Z(P_{x-3} \cup P_{y-2} \cup P_{b-1}) \\
&\quad + Z(P_{x-2} \cup P_{y-3} \cup P_{b-1}) + 2Z(P_{x-2} \cup P_{y-2} \cup P_{b-2}) \\
&= F_{x-2}F_{y-2}F_{b-1} + F_{x-3}F_{y-2}F_{b-1} + F_{x-2}F_{y-3}F_{b-1} + 2F_{x-2}F_{y-2}F_{b-2} \\
&= F_{x-1}F_{y-2}F_{b-1} + F_{x-2}F_{y-3}F_{b-1} + 2F_{x-2}F_{y-2}F_{b-2}. \qquad (2)
\end{aligned}$$

Hence, by Eqs. (1) and (2) we have

$$Z(G'^k_{n,a,b}) = k(F_{x-1}F_{y-2}F_{b-1} + F_{x-2}F_{y-3}F_{b-1} + 2F_{x-2}F_{y-2}F_{b-2}) + F_{a-1}F_{b-1} + 2F_{a-2}F_{b-1} + 2F_{a-1}F_{b-2}.$$

This completes the proof.

Lemma 5. Given positive integers *x, c, y, k* with *x, c, y* ≥ 2.

(i) If $xcy \geq 18$, then

$$Z(\tilde{G}^k_{n,x,y,c}) = (k+1)[F_{x-1}F_{c-2}F_{y-2} + F_{x-2}F_{c-3}F_{y-2} + F_{x-2}F_{c-2}F_{y-3}] + 3F_{x-2}F_{y-2}F_{c-2} + 2F_{x-3}F_{y-2}F_{c-3} + 2F_{x-3}F_{y-3}F_{c-2} + 2F_{x-2}F_{y-3}F_{c-3};$$

(ii) If $cy \geq 6$ and in $G^k_{n,x,y,c}$ let $P_x = P_{x_1} w P_{x_2}$ (see Figure 1) then

$$\begin{aligned}
Z(G^k_{n,x,y,c}) &= kF_{x_1-1}(F_{x_2}F_{c-2}F_{y-2} + F_{x_2-2}F_{c-2}F_{y-3}) + \\
&\quad kF_{x_1-2}(F_{x_2-1}F_{c-3}F_{y-2} + F_{x_2-2}F_{c-4}F_{y-2} + \\
&\quad 2F_{x_2-2}F_{c-3}F_{y-3} + F_{x_2-1}F_{c-2}F_{y-3} + \\
&\quad F_{x_2-2}F_{c-2}F_{y-4}) + F_{x-1}F_{y-2}F_{c-2} + \\
&\quad F_{x-2}F_{y-2}F_{c-3} + F_{x-2}F_{y-3}F_{c-2} + \\
&\quad 3F_{x-2}F_{y-2}F_{c-2} + 2F_{x-3}F_{y-3}F_{c-2} + \\
&\quad 2F_{x-2}F_{y-3}F_{c-3}.
\end{aligned}$$

Proof. (i) Let $T = \tilde{G}^k_{n,x,y,c} - \{v, v_1, \ldots, v_k\}$. By Lemma 1,

$$\begin{aligned}
Z(\tilde{G}^k_{n,x,y,c}) &= Z(\tilde{G}^k_{n,x,y,c} - v_1) + \sum_{v\in N(v_1)} Z(\tilde{G}^k_{n,x,y,c} - \{v, v_1\}) \\
&= Z(\tilde{G}^{k-1}_{n-1,x,y,c}) + Z(T \cup \{v_2,\ldots,v_k\}) \\
&= Z(\tilde{G}^{k-1}_{n-1,x,y,c}) + Z(T) \\
&= \cdots
\end{aligned}$$

$$= Z(\tilde{G}^0_{n-k,x,y,c}) + kZ(T)$$
$$= Z(\tilde{G}^0_{n-k,x,y,c} - v) + \sum_{w_j \in N(v)} Z(\tilde{G}^0_{n-k,x,y,c} -$$
$$= \{w_j, v\}) + kZ(T)$$
$$= (k+1)Z(T) + \sum_{w_j \in N(v)} Z(\tilde{G}^0_{n-k,x,y,c} - \{w_j, v\}).$$

Furthermore, let $N(v) = \{w_1, w_2, w_3\}$ then

$$Z(T) = Z(T-u) + \sum_{w' \in N(u)} Z(Q - \{w', u\})$$
$$= Z(P_{x-2} \cup P_{y-2} \cup P_{c-2}) + Z(P_{x-3} \cup P_{y-2} \cup P_{c-2}) +$$
$$Z(P_{x-2} \cup P_{y-2} \cup P_{c-3}) + Z(P_{x-2} \cup P_{y-3} \cup P_{c-2})$$
$$= F_{x-2}F_{y-2}F_{c-2} + F_{x-3}F_{y-2}F_{c-2} + F_{x-2}F_{y-2}F_{c-3} +$$
$$F_{x-2}F_{y-3}F_{c-2}$$
$$= F_{x-1}F_{y-2}F_{c-2} + F_{x-2}F_{y-2}F_{c-3} + F_{x-2}F_{y-3}F_{c-2}.$$

On the other hand,

$$Z(\tilde{G}^0_{n-k,x,y,c} - \{v, w_1\}) = Z(\tilde{G}^0_{n-k,x,y,c} -$$
$$\{v, w_1\} - u) + \sum_{w' \in N(u)} Z(\tilde{G}^0_{n-k,a,b} - \{v, w_1\} - \{w', u\})$$
$$= F_{x-2}F_{y-2}F_{c-2} + F_{x-3}F_{y-2}F_{c-3} + F_{x-3}F_{y-3}F_{c-2},$$
$$Z(\tilde{G}^0_{n-k,x,y,c} - \{v, w_2\})$$
$$= F_{x-2}F_{y-2}F_{c-2} + F_{x-3}F_{y-2}F_{c-3} + F_{x-2}F_{y-3}F_{c-3},$$
$$Z(\tilde{G}^0_{n-k,x,y,c} - \{v, w_3\})$$
$$= F_{x-2}F_{y-2}F_{c-2} + F_{x-2}F_{y-3}F_{c-3} + F_{x-3}F_{y-3}F_{c-2}.$$

Hence, we have

$$Z(\tilde{G}^k_{n,x,y,c}) = (k+1)(F_{x-1}F_{y-2}F_{c-2} + F_{x-2}F_{y-2}F_{c-3} +$$
$$F_{x-2}F_{y-3}F_{c-2}) + F_{x-2}F_{y-2}F_{c-2} + F_{x-3}F_{y-2}F_{c-3} +$$
$$F_{x-3}F_{y-3}F_{c-2} + F_{x-2}F_{y-2}F_{c-2} + F_{x-3}F_{y-2}F_{c-3} +$$
$$F_{x-2}F_{y-3}F_{c-3} + F_{x-2}F_{y-2}F_{c-2} + F_{x-2}F_{y-3}F_{c-3} +$$
$$F_{x-3}F_{y-3}F_{c-2}$$
$$= (k+1)(F_{x-1}F_{c-2}F_{y-2} + F_{x-2}F_{c-3}F_{y-2} + F_{x-2}F_{c-2}F_{y-3}) +$$
$$3F_{x-2}F_{y-2}F_{c-2} + 2F_{x-3}F_{y-2}F_{c-3} +$$
$$2F_{x-3}F_{y-3}F_{c-2} + 2F_{x-2}F_{y-3}F_{c-3}.$$

Similarly, we can show that (ii) holds. This completes the proof of Lemma 5.

Lemma 6. $Z(G^k_{n,a,b}) < Z(G'^k_{n,a,b})$.

Proof. Note that $a = x + y - 2$, by Lemma 4,

$$Z(G'^k_{n,a,b}) - Z(G^k_{n,a,b}) = k(F_{x-1}F_{y-2}F_{b-1} + F_{x-2}F_{y-3}F_{b-1} +$$
$$2F_{x-2}F_{y-2}F_{b-2}) - F_{a-1}F_{b-1}) = k(F_{x-1}F_{y-2}F_{b-1} +$$
$$F_{x-2}F_{y-3}F_{b-1} + 2F_{x-2}F_{y-2}F_{b-2}) - F_{x+y-3}F_{b-1})$$
$$= 2kF_{x-2}F_{y-2}F_{b-2}.$$

Note that $x \geq 2$, $y \geq 2$, $b \geq 3$ therefore $2kF_{x-2}F_{y-2}F_{b-2} > 0$, i.e., $Z(G^k_{n,a,b}) < Z(G'^k_{n,a,b})$.

Lemma 7. For positive integers *x, y, c* with $x \geq 3$, $cy \geq 6$, we have $Z(G^k_{n,x,y,c}) > Z(\tilde{G}^k_{n,x,y,c})$.

Proof. Note that $x = x_1 + x_2 - 1$, then by Lemma 5,

$$Z(G^k_{n,x,y,c}) - Z(\tilde{G}^k_{n,x,y,c}) =$$
$$k\,[F_{x_1-1}(F_{x_2-1}F_{c-2}F_{y-2} + F_{x_2-2}F_{c-2}F_{y-2} + F_{x_2-2}F_{c-2}F_{y-3}) +$$
$$F_{x_1-2}(F_{x_2-1}F_{c-3}F_{y-2} + F_{x_2-2}F_{c-4}F_{y-2} + 2F_{x_2-2}F_{c-3}F_{y-3} +$$
$$F_{x_2-1}F_{c-2}F_{y-3} + F_{x_2-2}F_{c-2}F_{y-4})] - k(F_{x-2}F_{c-2}F_{y-2} +$$
$$F_{x-3}F_{c-2}F_{y-2} + F_{x-2}F_{c-3}F_{y-2} + F_{x-2}F_{c-2}F_{y-3})$$
$$= k\,[F_{x_1-3}F_{x_2-2}(F_{c-2}F_{y-3} + F_{c-4}F_{y-4}) +$$
$$F_{x_1-2}F_{x_2-2}F_{c-4}F_{y-2} + F_{x_1-4}F_{x_2-2}F_{c-3}F_{y-3} +$$
$$F_{x_1-2}F_{x_2-2}F_{c-4}F_{y-4} + F_{x_1-2}F_{x_2-2}F_{c-3}F_{y-2} +$$
$$F_{x_1-2}F_{x_2-2}F_{c-2}F_{y-3}] \geq kF_{x_1-2}F_{x_2-2}(F_{c-3}F_{y-2} + F_{c-2}F_{y-3}) > 0$$

for $x_1, x_2 \geq 2$ and $cy \geq 6$. Hence, we have $Z(G^k_{n,x,y,c}) > Z(\tilde{G}^k_{n,x,y,c})$. This completes the proof.

Lemma 8. $G \in \mathscr{B}_n$,

(i) if G contains exactly two cycles, say C_a and C_b, then

$$Z(G) \geq (k+1)F_{a-1}F_{b-1} + 2F_{a-2}F_{b-1} + 2F_{a-1}F_{b-2},$$

the equality holds if and only if $G \cong G^k_{n,a,b}$.

(ii) if G contains exactly three cycles C_{k_1}, C_{k_2} and C_{k_3} with $C_{k_1} = P_x \cup P_c$, $C_{k_2} = P_x \cup P_y$, $C_{k_3} = P_c \cup P_y$, then

$$Z(G) \geq (k+1)(F_{x-1}F_{c-2}F_{y-2} + F_{x-2}F_{c-3}F_{y-2} +$$
$$F_{x-2}F_{c-2}F_{y-3}) + 3F_{x-2}F_{y-2}F_{c-2} +$$
$$2F_{x-3}F_{y-2}F_{c-3} + 2F_{x-3}F_{y-3}F_{c-2} + 2F_{x-2}F_{y-3}F_{c-3},$$

the equality holds if and only if $G \cong \tilde{G}^k_{n,x,y,c}$.

Proof. (i) By Lemma 4 (i), we have

$$Z(G^k_{n,a,b}) = (k+1)F_{a-1}F_{b-1} + 2F_{a-2}F_{b-1} + 2F_{a-1}F_{b-2}.$$

Assume that G contains two edge-disjoint cycles, say C_a and C_b. Then assume C_a connects C_b by a path P_{c+2} for $c \geq -1$. It is easy to see, when $c = -1$, then C_a and C_b have exactly one vertex in common; when $c = 0$, then C_a connects C_b by an edge with one end vertex on C_a and the other one on C_b. The subgraph $C_a \cup P_{c+2} \cup C_b$ of G is as follows.

Let $C_a = u_1^1u_2^1 \ldots u_a^1u_1^1, C_b = u_1^2u_2^2 \ldots u_b^2u_1^2$ and $P_{c+2} = u_a^1u_1^3u_2^3 \ldots u_c^3u_b^2$. Set $V^*(G) := \{u_i^1 : d(u_i^1) \geq 3,$ $1 \leq i \leq a-1\} \cup \{u_i^3 : d(u_i^3) \geq 3, 1 \leq i \leq c\} \cup \{u_i^2 : d(u_i^2) \geq$ $3, 1 \leq i \leq b-1\} \cup \{u_a^1 : d(u_a^1) \geq 4\} \cup \{u_b^2 : d(u_b^2) \geq 4\}$

Assume $|V^*(G)| = k$ and hence relabel the vertices in $V^*(G)$ as $v_1', v_2', \ldots, v_k'$.

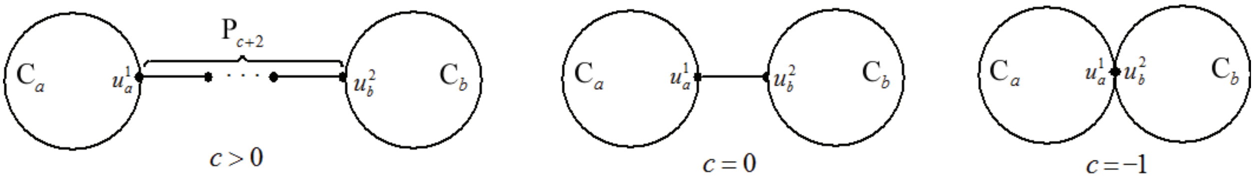

Figure 4. Graphs $\tilde{G}^{n-4}_{n,3,3,2}$, $G^{n-5}_{n,3,3}$, $\tilde{G}^{n-5}_{n,3,3,3}$, $G^{n-6}_{n,4,3}$ and $G'^{n-6}_{n,4,3,3}$.

Set $v_i' \in V^*(G)$ and let T_i be a subtree of $G - E(C_a \cup P_{c+2} \cup C_b)$ which contains v_i' and $|V(T_i)| = p_i + 1$. Denote

$$H = C_a \cup P_{c+2} \cup C_b \cup \left(\bigcup_{1\le j\le k, j\ne i} T_j \right).$$

Then $G = Hv_i'T_i$. By Lemma 3, we have $Z(Hv_i'T_i) \ge Z(Hv_i'K_{1,p_i})$. Thus repeated using Lemma 3,

$$Z(G) \ge Z(B_n(p_1, p_2, \ldots, p_k)),$$

where $B_n(p_1, p_2, \ldots, p_k)$ is a bicyclic graph with n vertices created from $C_a u_a^1 P_{c+2} u_b^2 C_b$ (see Figure 4) by attaching p_i pendent vertices to $v_i \in V^*(G), 1 \le i \le k$, respectively. Denote

$$X = K_{1,p_i},\ Y = K_{1,p_j},\ \text{and}\ H' = G - E(K_{1,p_i}) - E(K_{1,p_j}).$$

Then $B_n(p_1, p_2, \ldots, p_k) = X \cup Y \cup H'$. By Lemma 3, we have either

$$Z(G) \ge Z(B_n(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_k)) > Z(B_n(p_1, \ldots, p_i + p_j, \ldots, 0, \ldots, p_k)),$$

or

$$Z(G) \ge Z(B_n(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_k)) > Z(B_n(p_1, \ldots, 0, \ldots, p_i + p_j, \ldots, p_k)).$$

Repeated using above step, we obtain either

$$Z(G) \ge Z(B_n(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_k)) > \cdots > Z(G^k_{n,a,b}),$$

or

$$Z(G) \ge Z(B_n(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_k)) > \cdots > Z(G'^k_{n,a,b}).$$

By Lemma 6, we obtain that if bicyclic graph G has two edge-disjoint cycles, then

$$Z(G) \ge Z(G^k_{n,a,b}).$$

Therefore, if $G \in \mathscr{B}_n$ contains exactly two cycles, then

$$Z(G) \ge (k+1)F_{a-1}F_{b-1} + 2F_{a-2}F_{b-1} + 2F_{a-1}F_{b-2},$$

the equality holds if and only if $G \cong G^k_{n,a,b}$.

(ii) By Lemma 4 (ii), we have

$$Z(\tilde{G}^k_{n,x,y,c}) = (k+1)(F_{x-1}F_{c-2}F_{y-2} + F_{x-2}F_{c-3}F_{y-2} + F_{x-2}F_{c-2}F_{y-3}) + 3F_{x-2}F_{y-2}F_{c-2} + 2F_{x-3}F_{y-2}F_{c-3} + 2F_{x-3}F_{y-3}F_{c-2} + 2F_{x-2}F_{y-3}F_{c-3}.$$

The three cycles are formed by three paths, say P_x, P_y and P_c, from u_a^1 to u_b^1 being internal disjoint; see Figure 5.

Let $P_x = u_a^1 u_2^1 \ldots u_b^1, P_y = u_a^1 u_2^2 \ldots u_b^1$ and $P_c = u_a^1 u_2^3 u_3^3 \ldots u_b^1$. Set $V^*(G) := \{u : d(u) \ge 3$ and $u \in V(P_x \cup P_y \cup P_c) \setminus \{u_a^1, u_b^1\}\} \cup \{u_a^1 : d(u_a^1) \ge 4\} \cup \{u_b^1 : d(u_b^1) \ge 4\}$. Assume $|V^*(G)| = k$ and hence relabel the vertices in $V^*(G)$ as $v_1', v_2', \ldots, v_k'$.

Set $v_i' \in V^*(G)$ and let T_i be a subtree of $G - E(P_x \cup P_y \cup P_c)$ which contains v_i' and $|V(T_i)| = p_i + 1$. Denote

$$H = P_x \cup P_y \cup P_c \cup \left(\bigcup_{1\le j\le k, j\ne i} T_j \right).$$

Then $G = Hv_i'T_i$. By Lemma 3, we have $Z(Hv_i'T_i) \ge Z(Hv_i'K_{1,p_i})$. Thus repeated using Lemma 3,

$$Z(G) \ge Z(B_n'(p_1, p_2, \ldots, p_k)),$$

where $B_n'(p_1, p_2, \ldots, p_k)$ is a bicyclic graph with n vertices created from G' (see Figure 5) by attaching p_i pendent vertices to $v_i \in V^*(G), 1 \le i \le k$, respectively. Denote

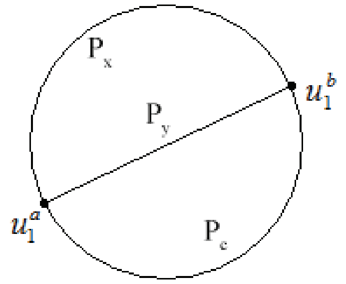

Figure 5. Graph G' formed by three internal disjoint paths P_x, P_y, P_c.

$$X = K_{1,p_i},\ Y = K_{1,p_j}, \text{ and}$$
$$H' = G - E(K_{1,p_i}) - E(K_{1,p_j}).$$

Then $B'_n(p_1, p_2, \ldots, p_k)) = X \cup Y \cup H'$. By Lemma 3, we have either

$$Z(G) \geq Z(B'_n(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_k)) > Z(B'_n(p_1, \ldots, p_i + p_j, \ldots, 0, \ldots, p_k)),$$

or

$$Z(G) \geq Z(B'_n(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_k)) > Z(B'_n(p_1, \ldots, 0, \ldots, p_i + p_j, \ldots, p_k)).$$

Repeated using above step, we obtain either

$$Z(G) \geq Z(B'_n(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_k)) > \cdots > Z(\tilde{G}^k_{n,x,y,c}),$$

or

$$Z(G) \geq Z(B'_n(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_k)) > \cdots > Z(G^k_{n,x,y,c}).$$

By Lemma 8, we obtain that if bicyclic graph G has exactly three cycles, then

$$Z(G) \geq (k+1)(F_{x-1}F_{c-2}F_{y-2} + F_{x-2}F_{c-3}F_{y-2} + F_{x-2}F_{c-2}F_{y-3}) + 3F_{x-2}F_{y-2}F_{c-2} + 2F_{x-3}F_{y-2}F_{c-3} + 2F_{x-3}F_{y-3}F_{c-2} + 2F_{x-2}F_{y-3}F_{c-3},$$

the equality holds if and only if $G \cong \tilde{G}^k_{n,x,y,c}$. This completes the proof.

Lemma 9. $Z(G^{k+1}_{n,a-1,b}) < Z(G^k_{n,a,b})$ for $a \geq 4,\ b \geq 3$.

Proof. By Lemma 5,

$$Z(G^{k+1}_{n,a-1,b}) - Z(G^k_{n,a,b}) = (k+2)F_{a-2}F_{b-1} + 2F_{a-3}F_{b-1} + 2F_{a-2}F_{b-2} - [(k+1)F_{a-1}F_{b-1} + 2F_{a-2}F_{b-1} + 2F_{a-1}F_{b-2}] = F_{b-1}[k(F_{a-2} - F_{a-1}) + (F_{a-3} - F_{a-2})] + 2F_{b-2}(F_{a-2} - F_{a-1}).$$

Note that $a \geq 4,\ b \geq 3$, therefore

$$F_{b-1}[k(F_{a-2} - F_{a-1}) + (F_{a-3} - F_{a-2})] + 2F_{b-2}(F_{a-2} - F_{a-1}) < 0,$$

and so $Z(G^{k+1}_{n,a-1,b}) < Z(G^k_{n,a,b})$ for $a \geq 4,\ b \geq 3$.

Let $\mathscr{B}_n = \mathscr{B}_n^2 \cup \mathscr{B}_n^3$, where $\mathscr{B}_n^2$ is the set of bicyclic graph with n vertices having exactly two cycles and $\mathscr{B}_n^3$ is the set of bicyclic graph with n vertices possessing exactly three cycles.

Corollary 10. Let $G \in \mathscr{B}_n^2$, then $Z(G) \geq Z(G^{n-5}_{n,3,3})$, the equality holds if and only if $G \cong G^{n-5}_{n,3,3}$.

Lemma 11. For positive integers k, x, y, c, if $x \geq 4,\ y, c \geq 2,\ yc \geq 6$, then $Z(\tilde{G}^{k+1}_{n,x-1,y,c}) < Z(\tilde{G}^k_{n,x,y,c})$.

Proof. By Lemma 5,

$$Z(\tilde{G}^{k+1}_{n,x-1,y,c}) - Z(\tilde{G}^k_{n,x,y,c}) = -k(F_{x-3}F_{c-2}F_{y-2} + F_{x-4}F_{c-3}F_{y-2} + F_{x-4}F_{c-2}F_{y-3}) - 2F_{x-4}F_{c-2}F_{y-2} - F_{x-5}F_{c-3}F_{y-2} - 2F_{x-4}F_{c-3}F_{y-3} + [F_{x-2}F_{c-2}F_{y-2} + F_{x-3}F_{c-3}F_{y-2} + (F_{x-5} + F_{x-4})F_{c-3}F_{y-2} + (F_{x-5} + F_{x-4})F_{c-2}F_{y-3}] = -k(F_{x-3}F_{c-2}F_{y-2} + F_{x-4}F_{c-3}F_{y-2} + F_{x-4}F_{c-2}F_{y-3}) - 2F_{x-4}F_{c-2}F_{y-2} - F_{x-5}F_{c-3}F_{y-2} - 2F_{x-4}F_{c-3}F_{y-3}.$$

Note that $x \geq 4,\ y, c \geq 2$ and $yc \geq 6$; we have

$$-k(F_{x-3}F_{c-2}F_{y-2} + F_{x-4}F_{c-3}F_{y-2} + F_{x-4}F_{c-2}F_{y-3}) - 2F_{x-4}F_{c-2}F_{y-2} - F_{x-5}F_{c-3}F_{y-2} - 2F_{x-4}F_{c-3}F_{y-3} < 0.$$

This completes the proof of Lemma 11.

Corollary 12. Let $G \in \mathscr{B}_n^3$ then $Z(G) \geq Z(\tilde{G}^{n-4}_{n,3,3,2})$, the equality holds if and only if $G \cong \tilde{G}^{n-4}_{n,3,3,2}$.

Lemma 13. $Z(\tilde{G}^{n-4}_{n,3,3,2}) < Z(G^{n-5}_{n,3,3})$ for $n > 4$.

Proof. By Lemma 4, we have

$$Z(\tilde{G}^{n-4}_{n,3,3,2}) = 3n - 4, Z(G^{n-5}_{n,3,3}) = 4n - 8.$$

Therefore, $Z(\tilde{G}^{n-4}_{n,3,3,2}) < Z(G^{n-5}_{n,3,3})$.

Note that, by Lemma 5, we have:

$$Z(\tilde{G}^{n-5}_{n,3,3,3}) = 4n - 7,\ Z(G^{n-6}_{n,4,3}) = 6n - 16,\ Z(\tilde{G}^{n-6}_{n,4,3,3}) = 7n - 21.$$

Furthermore, by Lemmas 9, 11 and Corollary 12, we immediately get our main results:

Theorem 14. Let $G \in \mathscr{B}_n$.

(i) $Z(G) \geq 3n - 4$, the equality holds if and only if $G \cong \tilde{G}^{n-4}_{n,3,3,2}$ for $n > 4$.

(ii) if G is not isomorphic to any member in $\{\tilde{G}^{n-6}_{n,4,3,3}, G^{n-6}_{n,4,3}, \tilde{G}^{n-5}_{n,3,3,3}, G^{n-5}_{n,3,3}, \tilde{G}^{n-4}_{n,3,3,2}\}$, then

$$Z(G) > Z(\tilde{G}^{n-6}_{n,4,3,3}) > Z(G^{n-6}_{n,4,3}) > Z(\tilde{G}^{n-5}_{n,3,3,3}) > Z(G^{n-5}_{n,3,3}) > Z(\tilde{G}^{n-4}_{n,3,3,2})$$

for $n \geq 6$.

CONCLUSION

Among $\mathscr{B}_n$, we determine that $\tilde{G}^{n-4}_{n,3,3,2}$, $G^{n-5}_{n,3,3}$, $\tilde{G}^{n-5}_{n,3,3,3}$, $G^{n-6}_{n,4,3}$, $\tilde{G}^{n-6}_{n,4,3,3}$, respectively, is the bicyclic graph with minimal, the second-, the third-, the fourth-, and the fifth-minimal Hosoya indices.

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SAŽETAK

Hosoyini indeksi bicikličkih grafova

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Hosoyin indeks, *Z*(G), definiran je kao ukupan broj sparivanja u molekulskom grafu G. Neka $\mathscr{B}_n$ označava skup bicikličkih grafova s *n* čvorova. U radu su određeni biciklički grafovi iz skupa $\mathscr{B}_n$ s prvim, drugim, trećim, četvrtim i petim najmanjim Hosoyinim indeksom.