



## The Largest $n - 1$ Hosoya Indices of Unicyclic Graphs

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**Abstract.** The Hosoya index  $Z(G)$  of a graph  $G$  is defined as the total number of edge independent sets of  $G$ . In this paper, we extend the research of [J. Ou, On extremal unicyclic molecular graphs with maximal Hosoya index, *Discrete Appl. Math.* 157 (2009) 391–397.] and [Y. Ye, X. Pan, H. Liu, Ordering unicyclic graphs with respect to Hosoya indices and Merrifield-Simmons indices, *MATCH Commun. Math. Comput. Chem.* 59 (2008) 191–202.] and order the largest  $n - 1$  unicyclic graphs with respect to the Hosoya index.

### 1. Introduction

In this paper, we follow the standard notation in graph theory in [1]. Let  $G = (V, E)$  be a simple connected graph of order  $n$ . Two distinct edges in a graph  $G$  are *independent* if they are not incident with a common vertex in  $G$ . A set of pairwise independent edges in  $G$  is called a *matching*. A  $k$ -matching of  $G$  is a set of  $k$  mutually independent edges.

In theoretical chemistry molecular structure descriptors are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds. The *Hosoya index*  $Z(G)$  of a graph  $G$  is defined as the total number of its matchings [8]. If  $m(G, k)$  denotes the number of its  $k$ -matchings, then

$$Z(G) = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G, k).$$

The Hosoya index has been studied intensively in the literature (see survey [19] and references [2, 6, 9, 13, 18, 21, 25]). It is shown in [7] that the linear hexagonal chain is the unique graph with minimal Hosoya index among all hexagonal chains, while in [23] and [24] the authors proved that zig-zag hexagonal chain is the unique chain with the maximal Hosoya index among all hexagonal chains. As for trees, it has been shown that the path has the maximal Hosoya index and the star has the minimal Hosoya index [5]. Recently, Hou [11] characterized the trees with a given size of matching having minimal and second minimal Hosoya index. Pan et al. in [15] characterized the trees with given diameter and having minimal Hosoya index. In [16] Ou used linear algebra theory on permanents to characterize the minimal and second

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minimal Hosoya index of unicyclic graphs with fixed girth. In [20] the authors considered the Hosoya and Merrifield-Simmons indices of unicyclic graphs with maximum degree  $\Delta$  and characterized the graphs with the maximal Hosoya index and the minimal Merrifield-Simmons index.

For  $v \in V(G)$ , we denote by  $G - v$  the graph obtained from  $G$  by deleting the vertex  $v$  together with their incident edges. For  $e \in E(G)$ , we denote by  $G - e$  the graph obtained from  $G$  by removing the edge  $e$ . Let  $\deg(v)$  denotes the vertex degree of  $v$ . We denote by  $P_n$ ,  $S_n$  and  $C_n$  the path, the star and the cycle on  $n$  vertices, respectively. By  $L_{n,k}$  we denote the graph obtained from  $C_k$  and  $P_{n-k+1}$  by identifying a vertex of  $C_k$  with one end vertex of  $P_{n-k+1}$ .

Let  $F_n$  denotes the  $n$ -th Fibonacci number. It is well-known that  $F_n$  satisfy the following recursive relations:

$$F_n = F_{n-1} + F_{n-2}, \quad F_1 = 1, F_0 = 0, n \geq 2 \quad (1)$$

$$F_n = F_k F_{n-k+1} + F_{k-1} F_{n-k}, \quad 1 \leq k \leq n \quad (2)$$

$$F_m F_{n+1} - F_n F_{m+1} = (-1)^n F_{m-n} \quad (3)$$

$$F_{-n} = (-1)^{n+1} F_n, \quad n \geq 0. \quad (4)$$

Let  $\mathcal{U}_{n,k}$  be the set of all unicyclic graphs of order  $n \geq 3$  with girth  $k \geq 3$ . It is easy to see that if  $k = n$  or  $n - 1$ , there is only one unicyclic graph. Therefore, we can assume that  $3 \leq k \leq n - 2$ . Deng et al. in [3] showed that the unique extremal unicyclic graph in  $\mathcal{U}_{n,k}$  with maximal Hosoya index is  $L_{n,k}$ . Ou in [17] proved the following:

**Theorem 1.1.** *Let  $G$  be a connected unicyclic graph of order  $n \geq 5$ . If  $G \not\cong C_n$ , then  $Z(G) \leq F_{n+1} + 2F_{n-3}$ , with the equality holding if and only if  $G \cong L_{n,4}$  or  $G \cong L_{n,n-2}$ .*

In [22], the authors presented the smallest  $\lfloor \frac{k}{2} \rfloor + 2$  Hosoya indices of unicyclic graphs with given girth  $k$ . A fully loaded unicyclic graph is a unicyclic graph with the property that there is no vertex with degree less than 3 in its unique cycle. Hua in [10] determined the extremal fully loaded unicyclic graphs with minimal, second-minimal and third-minimal Hosoya indices. Deng in [4] obtained the largest Hosoya index of  $(n, n + 1)$  graphs. Inspired by these results, in this paper we determine the first  $n - 1$  unicyclic graphs with the largest Hosoya index among all unicyclic graphs of order  $n$ .

This paper is organized as follows. In Section 2, we give basic results concerning Hosoya index and some useful lemmas. In Section 3, we characterize unicyclic graphs in  $\mathcal{U}_{n,k}$  with the second maximal Hosoya index. Finally in Section 4, we order the largest  $n - 1$  unicyclic  $n$ -vertex graphs with respect to the Hosoya index.

## 2. Preliminary Results

We list some basic results from [5] concerning Hosoya index of a graph  $G$ :

(i) Let  $e = uv$  be an edge of a graph  $G$ . Then

$$Z(G) = Z(G - e) + Z(G - \{u, v\}). \quad (5)$$

(ii) Let  $v$  be a vertex of a graph  $G$ . Then

$$Z(G) = Z(G - v) + \sum_{u \sim v} Z(G - \{u, v\}), \quad (6)$$

where the summation extends over all vertices adjacent to  $v$ .

In particular, if  $v$  is a pendant vertex of  $G$  and  $u$  is the only vertex adjacent to  $v$ , we have  $Z(G) = Z(G - v) + Z(G - u - v)$ .

(iii) If  $G_1, G_2, \dots, G_k$  are connected components of  $G$ , then  $Z(G) = \prod_{i=1}^k Z(G_i)$ .

(iv) For paths, stars and cycles, we have

$$Z(P_0) = 0, Z(P_1) = 1, \quad Z(P_n) = F_{n+1}, \quad n \geq 2.$$

$$Z(S_n) = n; \quad Z(C_n) = F_{n-1} + F_{n+1}.$$

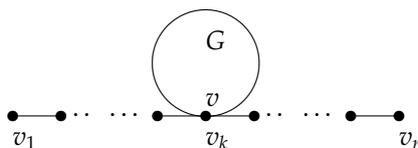
**Lemma 2.1.** [12] Let  $T_n$  be a tree of order  $n$ . Then  $Z(S_n) \leq Z(T_n) \leq Z(P_n)$ , with the left equality holding if and only if  $T_n \cong S_n$  and the right equality holding if and only if  $T_n \cong P_n$ .

**Lemma 2.2.** [3] Let  $U_{n,k} \in \mathcal{U}_{n,k}$  be a unicyclic graph with girth  $k \geq 3$ . Then  $Z(U_{n,k}) \leq Z(L_{n,k}) = F_{n+1} + F_{k-1}F_{n-k+1}$ , with the equality holding if and only if  $U_{n,k} \cong L_{n,k}$ .

**Lemma 2.3.** [18] Let  $G$  be a connected graph and  $v \in V(G)$ . Suppose  $P(n, k, G, v)$  denotes the graph obtained from  $G$  by identifying  $v$  with the vertex  $v_k$  of a simple path  $v_1v_2 \dots v_n$  (see Fig. 1). Let  $n = 4m + i$  ( $i \in \{0, 1, 2, 3\}, m \geq 0$ ). Then

$$\begin{aligned} Z(P(n, 2, G, v)) &< Z(P(n, 4, G, v)) < \dots < Z(P(n, 2m, G, v)) < \\ &< Z(P(n, 2m - 1 + 2l, G, v)) < \dots < Z(P(n, 3, G, v)) < Z(P(n, 1, G, v)), \end{aligned}$$

where  $l = \lfloor \frac{i}{2} \rfloor$ .



**Figure 1.** The graph  $P(n, k, G, v)$ .

Similarly, one can verify that for  $n = 4m + i$  ( $i \in \{0, 1, 2, 3\}$ ) and  $l = \lfloor \frac{i}{2} \rfloor$ , the following chain of inequalities holds

$$F_0F_n < F_2F_{n-2} < F_4F_{n-4} < \dots < F_{2m}F_{2m+i} < F_{2m-1+2l}F_{2m+i+1-2l} < \dots < F_3F_{n-3} < F_1F_{n-1}. \tag{7}$$

By repeated use of Lemma 2.3, the extremal unicyclic graph with the maximal Hosoya index has only paths attached to some vertices of a cycle.

**Lemma 2.4.** [3] Let  $P = uu_1u_2 \dots u_tv$  be a path in  $G$  and  $G \neq P$ , the degrees of  $u_1, u_2, \dots, u_t$  in  $G$  are 2. Let  $G_1$  denotes the graph that results from identifying  $u$  with the vertex  $v_k$  of a simple path  $v_1v_2 \dots v_k$  and identifying  $v$  with the vertex  $v_{k+1}$  of a simple path  $v_{k+1}v_{k+2} \dots v_n$ ,  $1 < k < n - 1$ ;  $G_2$  is obtained from  $G_1$  by deleting  $v_{k-1}v_k$  and adding  $v_1v_n$ ;  $G_3$  is obtained from  $G_1$  by deleting  $v_{k+1}v_{k+2}$  and adding  $v_1v_n$ . Then  $Z(G_1) < Z(G_2)$  or  $Z(G_1) < Z(G_3)$ .

Note that the previous lemma holds also for  $t = 0$  (if the vertices  $u_1, u_2, \dots, u_t$  do not exist).

### 3. The Second Maximal Hosoya Index of Unicyclic Graphs

In order to get the main result, we firstly determine unicyclic graphs with the second maximal Hosoya index in  $\mathcal{U}_{n,k}$ .

**Lemma 3.1.** Let  $U_{n,k} \in \mathcal{U}_{n,k}$  be a unicyclic graph with the second maximal Hosoya index and girth  $k$  ( $3 \leq k \leq n - 2$ ). Then  $U_{n,k}$  must be of the form  $H_i$  ( $i = 1, 2, 3$ ) (see Fig. 2), where  $s + t + k = n$ .

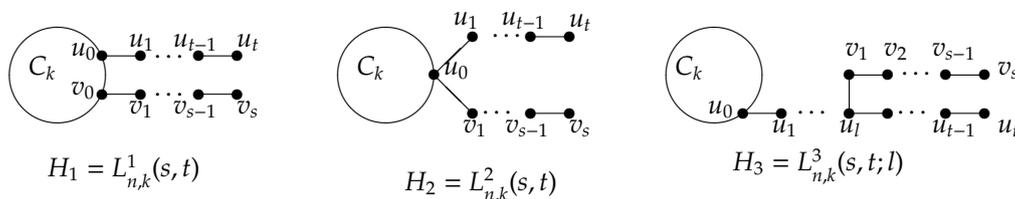
*Proof.* Let  $C_k$  be the unique cycle of  $U_{n,k}$ .

If there are at least three vertices on  $C_k$  of degree greater than 2, then by Lemma 2.3 and Lemma 2.4, there exists a graph  $G_1$  of the form  $H_1$  such that  $Z(U_{n,k}) < Z(G_1) < Z(L_{n,k})$ , which contradicts to the fact that  $U_{n,k}$  has the second maximal Hosoya index. Hence, there are at most two vertices in  $C_k$  of degree at least 3 and let  $u$  be a vertex of  $C_k$  of degree greater than 2.

If  $deg(u) \geq 5$ , by Lemma 2.3 and Lemma 2.4, there exists a graph  $G_2$  of the form  $H_2$  such that  $Z(U_{n,k}) < Z(G_2) < Z(L_{n,k})$ , which contradicts to the fact that  $U_{n,k}$  has the second maximal Hosoya index. Hence,  $3 \leq deg(u) \leq 4$ . Let  $v$  be a vertex of degree greater than 2, different from  $u$ . We consider the following two subcases.

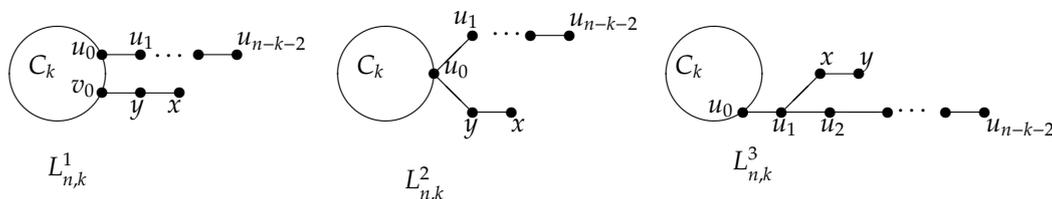
Assume first that  $v \in V(C_k)$ . Similarly as above, we have  $3 \leq deg(v) \leq 4$ . If at least one of the vertices  $u$  and  $v$  has degree 4, then by Lemma 2.3, there exists a graph  $G_3$  of the form  $H_1$  such that  $Z(U_{n,k}) < Z(G_3) < Z(L_{n,k})$ , which is a contradiction. Therefore,  $deg(u) = deg(v) = 3$  and all other vertices of  $U_{n,k}$  have degree 1 or 2.

Let now  $v \notin V(C_k)$ . If there are other vertices different from  $v$  and not in  $C_k$  with degree greater than 2, then by Lemma 2.4, we can get a graph  $G_4$  of the form  $H_3$  such that  $Z(U_{n,k}) < Z(G_4) < Z(L_{n,k})$ , which is impossible. Hence, we can assume that  $u$  and  $v$  are the only vertices of degree greater than 2 in  $U_{n,k}$ . Similarly as above, we can conclude that  $deg(u) = deg(v) = 3$ .  $\square$



**Figure 2.** Three classes of unicyclic graphs.

Let  $\mathcal{L}_{n,k}^i$  be the set of all unicyclic graphs of the form like  $H_i$  ( $i = 1, 2, 3$ ) (as shown in Fig. 3), respectively.



**Figure 3.** The extremal unicyclic graphs.

**Lemma 3.2.** Let  $n \geq 10$ .

- (i) If  $k > 3$ ,  $L_{n,k}^i$  ( $i = 1, 2, 3$ ) (see Fig. 3) is the unique graph with the maximal Hosoya index in  $\mathcal{L}_{n,k}^i$  ( $i = 1, 2, 3$ ), respectively. In  $L_{n,k}^1$ , the vertices  $u_0$  and  $v_0$  are adjacent;
- (ii) If  $k = 3$ ,  $L_{n,3}^3(2, n-5; 3)$  and  $L_{n,3}^3$  (see Fig. 3) are the graphs with the maximal Hosoya index in  $\mathcal{L}_{n,3}^3$ ;  $L_{n,3}^i$  ( $i = 1, 2$ ) (see Fig. 3) is the unique graph with the maximal Hosoya index in  $\mathcal{L}_{n,3}^i$  ( $i = 1, 2$ ), respectively. In  $L_{n,3}^1$ , the vertices  $u_0$  and  $v_0$  are adjacent.

*Proof.* We distinguish the following three cases.

**Case 1.** For graphs in  $\mathcal{L}_{n,k}^1$ .

By formula (5), we have

$$\begin{aligned} Z(L_{n,k}^1(s, t)) &= Z(L_{n,k}^1(s, t) - v_0v_1) + Z(L_{n,k}^1(s, t) - v_0 - v_1) \\ &= Z(P_s)Z(L_{n-s,k}) + Z(P_{s-1})Z(T_{n-s-1}) \\ &\leq Z(P_s)Z(L_{n-s,k}) + Z(P_{s-1})Z(P_{n-s-1}), \end{aligned}$$

where  $T_{n-s-1}$  is a tree of order  $n - s - 1$ . The equality holds if and only if  $T_{n-s-1} \cong P_{n-s-1}$  and consequently  $u_0$  and  $v_0$  must be adjacent in  $L_{n,k}^1(s, t)$  (see Fig. 5). In the following, we assume  $u_0$  and  $v_0$  are adjacent in  $L_{n,k}^1(s, t)$ .

$$\begin{aligned} Z(L_{n,k}^1(s, t)) &= Z(P_s)Z(L_{n-s,k}) + Z(P_{s-1})Z(P_{n-s-1}) \\ &= F_{s+1}(F_{n-s+1} + F_{k-1}F_{n-s-k+1}) + F_s F_{n-s} \\ &= F_{s+1}F_{n-s+1} + F_s F_{n-s} + F_{k-1} \cdot F_{s+1}F_{n-s-k+1} \\ &= F_{n+1} + F_{k-1} \cdot F_{s+1}F_{n-s-k+1}. \end{aligned}$$

If  $s$  is odd,  $Z(L_{n,k}^1(s, t))$  is strictly increasing with respect to  $s$ . If  $s$  is even,  $Z(L_{n,k}^1(s, t))$  is strictly decreasing with respect to  $s$ . Therefore, it follows that

$$\begin{aligned} Z(L_{n,k}^1(2, n - k - 2)) &> Z(L_{n,k}^1(4, n - k - 4)) > \dots > Z(L_{n,k}^1(2m, 2m + i)) > \\ &> Z(L_{n,k}^1(2m - 1 + 2l, 2m + i + 1 - 2l)) > \dots > Z(L_{n,k}^1(3, n - k - 3)) > Z(L_{n,k}^1(1, n - k - 1)), \end{aligned}$$

where  $n - k = 4m + i$ ,  $i \in \{0, 1, 2, 3\}$  and  $l = \lfloor \frac{i}{2} \rfloor$ . Finally, we get that  $L_{n,k}^1$  is the only graph with the maximal Hosoya index in  $\mathcal{L}_{n,k}^1$ .

**Case 2.** For graphs in  $\mathcal{L}_{n,k}^2$ .

We can easily get the result from Lemma 2.3. It follows that  $L_{n,k}^2$  is the only graph with the maximal Hosoya index in  $\mathcal{L}_{n,k}^2$ .

**Case 3.** For graphs in  $\mathcal{L}_{n,k}^3$ .

In order to prove the  $L_{n,k}^3$  is the only graph with the maximal Hosoya index in  $\mathcal{L}_{n,k}^3$ , it suffices to verify that  $Z(L_{n,k}^3(s, t; l)) \leq Z(L_{n,k}^3)$ . For  $s \geq 1$ , by Lemma 2.3, there is an integer  $l_0$  such that  $Z(L_{n,k}^3(2, n - k - 2; l_0)) \geq Z(L_{n,k}^3(s, t; l))$ . For convenience, we denote  $G = L_{n,k}^3(2, n - k - 2; l_0)$ .

By formula (6), we have

$$\begin{aligned} Z(G) &= Z(G - v_2) + Z(G - v_2 - v_1) \\ &= Z(G - v_2 - v_1) + Z(G - v_2 - v_1 - u_{l_0}) + Z(G - v_2 - v_1) \\ &= 2Z(L_{n-2,k}) + Z(P_{l_0-1})Z(L_{n-l_0-2,k}). \end{aligned}$$

$$\begin{aligned} Z(L_{n,k}^3) &= Z(L_{n,k}^3 - y) + Z(L_{n,k}^3 - x - y) \\ &= Z(L_{n,k}^3 - x - y) + Z(L_{n,k}^3 - x - y - u_1) + Z(L_{n,k}^3 - x - y) \\ &= 2Z(L_{n-2,k}) + Z(C_k)Z(P_{n-k-3}). \end{aligned}$$

Therefore, it follows that

$$\begin{aligned} Z(L_{n,k}^3) - Z(G) &= Z(C_k)Z(P_{n-k-3}) - Z(P_{l_0-1})Z(L_{n-l_0-2,k}) \\ &= Z(C_k)Z(P_{n-k-3}) - Z(P_{l_0-1})[Z(C_k)Z(P_{n-k-l_0-2}) + Z(P_{k-1})Z(P_{n-k-l_0-3})] \\ &= Z(C_k)F_{n-k-2} - F_{l_0}[Z(C_k)F_{n-k-l_0-1} + F_k F_{n-k-l_0-2}] \\ &= Z(C_k)[F_{n-k-2} - F_{l_0}F_{n-k-l_0-1}] - F_{l_0}F_k F_{n-k-l_0-2} \\ &= Z(C_k)F_{l_0-1}F_{n-k-l_0-2} - F_{l_0}F_k F_{n-k-l_0-2} \\ &= [F_{k+1}F_{l_0-1} + F_{k-1}F_{l_0-1} - F_{l_0}F_k]F_{n-k-l_0-2} \\ &= [2F_{k-1}F_{l_0-1} - F_k F_{l_0-2}]F_{n-k-l_0-2} \\ &\geq [2F_{k-1}F_{l_0-1} - F_k F_{l_0-1}]F_{n-k-l_0-2} \\ &= [F_{k-1}F_{l_0-1} - F_{k-2}F_{l_0-1}]F_{n-k-l_0-2} \\ &= F_{k-3}F_{l_0-1}F_{n-k-l_0-2} \geq 0. \end{aligned}$$

As above, it is easy to find that the equality holds if and only if  $s = 2$  and  $l_0 = n - k - 2$ , or  $k = 3, s = 2$  and  $l_0 = 3$ .

For  $k = 3$ , we have

$$Z(L_{n,3}^3) = 2Z(L_{n-2,3}) + 4F_{n-5};$$

$$Z(L_{n,3}^3(2, n - 5; 3)) = 2Z(L_{n-2,3}) + 2Z(L_{n-5,3}).$$

It is easy to verify that

$$\begin{aligned} Z(L_{n,3}^3) - Z(L_{n,3}^3(2, n - 5; 3)) &= 4F_{n-5} - 2Z(L_{n-5,3}) \\ &= 4F_{n-5} - 2F_{n-4} - 2F_{n-7} \\ &= 0. \end{aligned}$$

This completes the proof.  $\square$

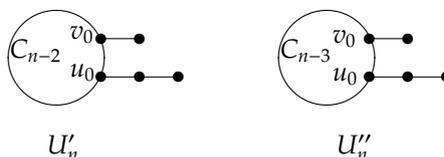


Figure 4. Extremal graphs for  $k = n - 2$  and  $k = n - 3$ .

**Lemma 3.3.** Let  $U_{n,k} \in \mathcal{U}_{n,k} \setminus \{L_{n,k}\}$  be a unicyclic graph with girth  $k$  ( $3 \leq k \leq n - 2$ ) and  $n \geq 10$ .

- (i) If  $k = n - 2$ , then  $Z(U_{n,k}) \leq Z(U'_n) = F_{n+1} + F_{n-3}$ , with equality if and only if  $U_{n,k} \cong U'_n$ .
- (ii) If  $k = n - 3$ , then  $Z(U_{n,k}) \leq Z(U''_n) = F_{n+1} + 2F_{n-4}$ , with equality if and only if  $U_{n,k} \cong U''_n$ .
- (iii) If  $3 \leq k \leq \frac{n-1}{2}$  and  $k \neq \frac{n-2}{2}$ , then  $Z(U_{n,k}) \leq F_{n+1} + 2F_{k-1}F_{n-k-1}$  for  $k$  odd, with equality if and only if  $U_{n,k} \cong L_{n,k}^1$ ;  $Z(U_{n,k}) \leq 2F_{n-1} + F_{k-1}F_{n-k+1} + F_{k+1}F_{n-k-2}$  for  $k$  even, with equality if and only if  $U_{n,k} \cong L_{n,k}^3$ .
- (iv) If  $k = \frac{n-2}{2}$ , then  $Z(U_{n,k}) \leq F_{n+1} + 2F_{k-1}F_{n-k-1}$ , with equality if and only if  $U_{n,k} \cong L_{n,k}^1$  or  $U_{n,k} \cong L_{n,k}^3$ .
- (v) If  $\frac{n-1}{2} < k \leq n - 4$ , then  $Z(U_{n,k}) \leq F_{n+1} + 2F_{k-1}F_{n-k-1}$  for  $k$  and  $n$  having the same parity, with equality if and only if  $U_{n,k} \cong L_{n,k}^1$ ; otherwise,  $Z(U_{n,k}) \leq 2F_{n-1} + F_{k-1}F_{n-k+1} + F_{k+1}F_{n-k-2}$ , with equality if and only if  $U_{n,k} \cong L_{n,k}^3$ .

The graphs  $U'_n, U''_n, L_{n,k}^1, L_{n,k}^3$  are shown in Fig. 3 and Fig. 4.

*Proof.* For  $k = n - 2$ , from Lemma 3.2 the unique extremal graph is  $U'_n \cong L_{n,n-2}^1(1, 1)$ . For  $k = n - 3$ , from Lemma 3.2 and direct verification we have that the unique extremal graph is  $U''_n \cong Z(L_{n,n-3}^1)$ . For  $k = 3$ , we can easily verify that  $Z(L_{n,3}^1) > Z(L_{n,3}^2)$ , and  $Z(L_{n,3}^1) > Z(L_{n,3}^3(2, n - 5; 3))$ .

For  $3 < k \leq n - 4$ , by Lemma 3.2, it suffices to compare the values  $Z(L_{n,k}^1)$ ,  $Z(L_{n,k}^2)$  and  $Z(L_{n,k}^3)$ .

By formula (6), we have

$$\begin{aligned} Z(L_{n,k}^1) &= 2Z(L_{n-2,k}) + Z(P_{n-3}), \\ Z(L_{n,k}^2) &= 2Z(L_{n-2,k}) + Z(P_{k-1})Z(P_{n-k-2}), \\ Z(L_{n,k}^3) &= 2Z(L_{n-2,k}) + Z(C_k)Z(P_{n-k-3}). \end{aligned}$$

It is not difficult to verify that  $Z(L_{n,k}^1) - Z(L_{n,k}^2) = F_{n-2} - F_k F_{n-k-1} > F_{n-2} - F_3 F_{n-4} = F_{n-5} > 0$  for  $n > 5$ .

$$\begin{aligned} Z(L_{n,k}^1) - Z(L_{n,k}^3) &= Z(P_{n-3}) - Z(C_k)Z(P_{n-k-3}) \\ &= F_{n-2} - (F_{k+1} + F_{k-1})F_{n-k-2} \\ &= F_k F_{n-k-1} + F_{k-1} F_{n-k-2} - F_{k+1} F_{n-k-2} - F_{k-1} F_{n-k-2} \\ &= F_k F_{n-k-1} - F_{k+1} F_{n-k-2} \\ &= (-1)^{k+1} F_{n-2k-2} \quad \text{by formula (3).} \end{aligned}$$

If  $3 < k \leq \frac{n-1}{2}$  and  $k \neq \frac{n-2}{2}$ , then  $n \geq 2k + 1$ . For  $n > 2k - 2$  it follows that  $F_{n-2k-2} > 0$ , and for  $n = 2k + 1$  it follows that  $F_{-1} = 1 > 0$ . Therefore, in both cases if  $k$  is odd, then  $Z(L_{n,k}^1) - Z(L_{n,k}^3) > 0$ ; if  $k$  is even, then  $Z(L_{n,k}^1) - Z(L_{n,k}^3) < 0$ .

If  $k = \frac{n-2}{2}$ , then  $F_{n-2k-2} = F_0 = 0$  and  $Z(L_{n,k}^1) = Z(L_{n,k}^3)$ .

If  $\frac{n-1}{2} < k \leq n - 4$ , then we have

$$(-1)^{k+1} F_{n-2k-2} = (-1)^{k+1} (-1)^{2k+3-n} F_{2k+2-n} = (-1)^{n+k} F_{2k+2-n}.$$

So, if  $k$  and  $n$  have the same parity, then  $Z(L_{n,k}^1) - Z(L_{n,k}^3) > 0$ ; otherwise,  $Z(L_{n,k}^1) - Z(L_{n,k}^3) < 0$ .

This completes the proof.  $\square$

#### 4. Ordering of Unicyclic Graphs with Respect to Hosoya Index

In this section, we extend the result in [17] and order the first  $n - 1$  unicyclic graphs with respect to the Hosoya index for  $n \geq 11$ . For  $5 \leq n \leq 10$ , using exhaustive computer search among all unicyclic graphs (with the help of Nauty [14]), we have the following:

If  $n = 5$ , then  $Z(C_5) = 11 > Z(L_{5,4}) = Z(L_{5,3}) = 10 > Z(U'_5) = 9$ .

If  $n = 6$ , then  $Z(C_6) = 18 > Z(L_{6,4}) = 17 > Z(L_{6,5}) = Z(L_{6,3}) = 16 > Z(U''_6) = Z(U'_6) = 15$ .

If  $n = 7$ , then  $Z(C_7) = 29 > Z(L_{7,4}) = Z(L_{7,5}) = 27 > Z(L_{7,3}) = Z(L_{7,6}) = 26 > Z(L_{7,3}^1) = Z(U''_7) = 25$ .

If  $n = 8$ , then  $Z(C_8) = 47 > Z(L_{8,4}) = Z(L_{8,6}) = 44 > Z(L_{8,5}) = 43 > Z(L_{8,3}) = Z(L_{8,7}) = Z(L_{8,4}^1) = 42$ .

If  $n = 9$ , then  $Z(C_9) = 76 > Z(L_{9,4}) = Z(L_{9,7}) = 71 > Z(L_{9,6}) = Z(L_{9,5}) = 70 > Z(L_{9,8}) = Z(L_{9,3}) = Z(L_{9,4}^3) = 68$ .

If  $n = 10$ , then  $Z(C_{10}) = 123 > Z(L_{10,4}) = Z(L_{10,8}) = 115 > Z(L_{10,6}) = 114 > Z(L_{10,7}) = Z(L_{10,5}) = 113 > Z(L_{10,9}) = Z(L_{10,3}) = 110 > Z(L_{10,4}^3) = Z(L_{10,4}^1) = Z(L_{10,6}^1) = 109$ .

All other unicyclic graphs have strictly smaller Hosoya index.

**Theorem 4.1.** For  $n \geq 11$ , the first  $n - 1$  largest Hosoya indices of unicyclic graphs are:  $Z(C_n) > Z(L_{n,4}) > Z(L_{n,6}) > \dots > Z(L_{n,2m}) > Z(L_{n,2m+1+2l}) > \dots > Z(L_{n,5}) > Z(L_{n,3}) > Z(L_{n,4}^3)$ , where  $n = 4m + i$ ,  $i \in \{0, 1, 2, 3\}$ ,  $l = \lfloor \frac{i}{2} \rfloor$ , and  $Z(L_{n,k}) = Z(L_{n,n-k+2})$ .

*Proof.* Let  $\mathcal{U}_n$  be the set of all connected unicyclic graphs on  $n$  vertices. Since  $\mathcal{U}_n$  is the union of all  $\mathcal{U}_{n,k}$ , where  $k = 3, 4, \dots, n$ , we need to order the extremal graphs  $L_{n,k}^1$ ,  $L_{n,k}^3$  and  $L_{n,k}$ ,  $k = 3, 4, \dots, n$  based on the Hosoya index. It follows that for  $n \geq 11$ , the second to the  $(n - 2)$ -th largest Hosoya indices are exactly graphs  $L_{n,k}$ ,  $k = 3, 4, \dots, n - 1$ , while the  $(n - 1)$ -th largest Hosoya index is achieved uniquely by the unicyclic graph  $L_{n,4}^3$ .

**Claim 1.**  $Z(L_{n,4}^1) > Z(L_{n,6}^1) > \dots > Z(L_{n,2m}^1) > Z(L_{n,2m-1+2l}^1) > \dots > Z(L_{n,5}^1) > Z(L_{n,3}^1)$ , where  $n = 4m + i$ ,  $i \in \{0, 1, 2, 3\}$ , and  $l = \lfloor \frac{i}{2} \rfloor$ .

First note that  $Z(L_{n,k}^1) = Z(L_{n,n-k}^1)$ , so we can assume  $k \leq \frac{n}{2}$ . From the proof of Lemma 3.3 and Lemma 2.2, we have

$$\begin{aligned} Z(L_{n,k}^1) - Z(L_{n,k-1}^1) &= 2 \cdot (Z(L_{n-2,k}) - Z(L_{n-2,k-1})) \\ &= 2 \cdot (F_{k-1} F_{n-k-1} - F_{k-2} F_{n-k}) \\ &= 2(-1)^k \cdot F_{n-2k+1} \quad \text{by formula (3).} \end{aligned}$$

Hence, if  $k$  is even,  $Z(L_{n,k}^1) - Z(L_{n,k-1}^1) > 0$ ; if  $k$  is odd,  $Z(L_{n,k}^1) - Z(L_{n,k-1}^1) < 0$ .

$$\begin{aligned} Z(L_{n,k}^1) - Z(L_{n,k-2}^1) &= Z(L_{n,k}^1) - Z(L_{n,k-1}^1) + Z(L_{n,k-1}^1) - Z(L_{n,k-2}^1) \\ &= 2(-1)^k \cdot (F_{n-2k+1} - F_{n-2k+3}). \end{aligned}$$

Hence, if  $k$  is even,  $Z(L_{n,k}^1) - Z(L_{n,k-2}^1) < 0$ ; if  $k$  is odd,  $Z(L_{n,k}^1) - Z(L_{n,k-2}^1) > 0$ .

**Claim 2.**  $Z(L_{n,4}) > Z(L_{n,6}) > \dots > Z(L_{n,2m}) > Z(L_{n,2m+1+2l}) > \dots > Z(L_{n,5}) > Z(L_{n,3})$ , where  $n = 4m + i$ ,  $i \in \{0, 1, 2, 3\}$ , and  $l = \lfloor \frac{i}{2} \rfloor$ .

For the extremal graphs  $L_{n,k}$ , we have  $Z(L_{n,k}) = Z(L_{n,n-k+2})$  and

$$\begin{aligned} Z(L_{n,k}) - Z(L_{n,k-1}) &= F_{k-1}F_{n-k+1} - F_{k-2}F_{n-k+2} \\ &= (-1)^k \cdot F_{n-2k+3}. \end{aligned}$$

Using the formula (7), we complete the result.

**Claim 3.**  $Z(L_{n,k}^3) \leq Z(L_{n,4}^3)$  for  $3 \leq k \leq n - 4$ , with equality if and only if  $k = 4$ .

Note that  $Z(L_{n,k}^3) = 2F_{n-1} + F_{k-1}F_{n-k+1} + F_{k+1}F_{n-k-2}$  and  $Z(L_{n,4}^3) = 2F_{n-1} + F_3F_{n-3} + F_5F_{n-6}$ . From formula (7), we have

$$F_3F_{n-3} > F_{k-1}F_{n-(k-1)} \quad \text{for } 3 \leq k \leq n - 4, \quad k \neq 4,$$

and

$$F_5F_{n-5} > F_{k+1}F_{n-(k+1)} \quad \text{for } 3 \leq k \leq n - 4, \quad k \neq 4, n - 5.$$

For the special case  $k = n - 5$ , we have  $Z(L_{n,n-5}^3) = 2F_{n-1} + F_{n-6}F_6 + F_{n-4}F_3$  and obviously  $Z(L_{n,4}^3) - Z(L_{n,n-5}^3) = F_3F_{n-5} - F_4F_{n-6} = 2F_{n-5} - 3F_{n-6} = F_{n-9} > 0$ . Therefore, it follows that  $Z(L_{n,k}^3) < Z(L_{n,4}^3)$ , for  $3 \leq k \leq n - 4$  and  $k \neq 4$ .

**Claim 4.** The cycle  $C_n$  has the largest Hosoya index among unicyclic graphs [17]. By using the above three claims, in order to prove that the extremal graphs  $L_{n,k}$  ( $k = 3, 4, \dots, n - 1$ ) are the next  $n - 3$  unicyclic graphs with the largest Hosoya index, we need to compare the following Hosoya indices

$$\begin{aligned} Z(L_{n,k}) = Z(L_{n,n-k+2}) &= F_{n+1} + F_{k-1}F_{n-k+1}, \\ Z(L_{n,4}^1) = Z(L_{n,n-4}^1) &= F_{n+1} + 4F_{n-5}, \\ Z(L_{n,4}^3) &= 2F_{n-1} + 2F_{n-3} + 5F_{n-6}, \\ Z(U'_n) &= F_{n+1} + F_{n-3}, \\ Z(U''_n) &= F_{n+1} + 2F_{n-4}. \end{aligned}$$

It is easy to verify that  $Z(L_{n,4}^1) > Z(U''_n) > Z(U'_n)$  and  $Z(L_{n,4}^3) > Z(L_{n,4}^1)$ . Therefore, we need to estimate the difference

$$\Delta = Z(L_{n,k}) - Z(L_{n,4}^3) = F_{n+1} + F_{k-1}F_{n-k+1} - (2F_{n-1} + 2F_{n-3} + 5F_{n-6}).$$

Note that for  $k \geq 3$ ,  $F_{k-1}F_{n-(k-1)} \geq F_2F_{n-2} = F_{n-2}$ . Hence,

$$\begin{aligned} \Delta &\geq F_{n+1} + F_{n-2} - 2F_{n-1} - 2F_{n-3} - 5F_{n-6} \\ &= 2F_{n-2} - 2F_{n-3} - 5F_{n-6} \\ &= 2F_{n-5} - 3F_{n-6} \\ &= 2F_{n-7} - F_{n-6} \\ &= F_{n-9} > 0. \end{aligned}$$

This completes the proof.  $\square$

## References

- [1] J. A. Bondy, U. S. R. Murty, *Graph Theory with Applications*, Macmillan Press, New York, 1976.
- [2] O. Chan, I. Gutman, T.K. Lam, R. Merris, Algebraic connections between topological indices, *J. Chem. Inform. Comput. Sci.* 38 (1998) 62–65.
- [3] H. Deng, S. Chen, The extremal unicyclic graphs with respect to Hosoya index and Merrifield-Simmons index, *MATCH Commun. Math. Comput. Chem.* 59 (2008) 171–190.
- [4] H. Deng, The largest Hosoya index of  $(n, n + 1)$ -graphs, *Comp. Math. Appl.* 56 (2008) 2499–2506.
- [5] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.
- [6] I. Gutman, On the Hosoya index of very large molecules, *MATCH Commun. Math. Comput. Chem.* 23 (1988) 95–103.
- [7] I. Gutman, Extremal hexagonal chains, *J. Math. Chem.* 12 (1993) 197–210.
- [8] H. Hosoya, Topological index: a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.* 44 (1971) 2332–2339.
- [9] H. Hua, Hosoya index of unicyclic graphs with prescribed pendent vertices, *J. Math. Chem.* 43 (2008) 831–844.
- [10] H. Hua, Minimizing a class of unicyclic graphs by means of Hosoya index, *Math. Comput. Model.* 48 (2008) 940–948.
- [11] Y. Hou, On acyclic systems with minimal Hosoya index, *Discrete Appl. Math.* 119 (2002) 251–257.
- [12] X. Li, J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* 54 (2005) 195–208.
- [13] S. Li, Z. Zhu, The number of independent sets in unicyclic graphs with a given diameter, *Discrete Appl. Math.* 157 (2009) 1387–1395.
- [14] B. McKay, *Nauty*, <http://cs.anu.edu.au/~bdm/nauty/>.
- [15] X. Pan, J. Xu, C. Yang, M. Zhou, Some graphs with minimum Hosoya index and maximum Merrifield-Simmons index, *MATCH Commun. Math. Comput. Chem.* 57 (2007) 235–242.
- [16] J. Ou, On extremal unicyclic molecular graphs with prescribed girth and minimal Hosoya index, *J. Math. Chem.* 42 (2007) 423–432.
- [17] J. Ou, On extremal unicyclic molecular graphs with maximal Hosoya index, *Discrete Appl. Math.* 157 (2009) 391–397.
- [18] S. Wagner, Extremal trees with respect to Hosoya index and Merrifield-Simmons index, *MATCH Commun. Math. Comput. Chem.* 57 (2007) 221–233.
- [19] S. Wagner, I. Gutman, Maxima and minima of the Hosoya index and the Merrifield-Simmons index: A survey of results and techniques, *Acta Appl. Math.* 112 (2010) 323–346.
- [20] K. Xu, B. Xu, Some extremal unicyclic graphs with respect to Hosoya index and Merrifield-Simmons index, *MATCH Commun. Math. Comput. Chem.* 62 (2009) 629–648.
- [21] K. Xu, On the Hosoya index and the Merrifield-Simmons index of graphs with a given clique number, *Appl. Math. Lett.* 23 (2010) 395–398.
- [22] Y. Ye, X. Pan, H. Liu, Ordering unicyclic graphs with respect to Hosoya indices and Merrifield-Simmons indices, *MATCH Commun. Math. Comput. Chem.* 59 (2008) 191–202.
- [23] L. Zhang, The proof of Gutman's conjectures concerning extremal hexagonal chains, *J. Sys. Math. Sci.* 18 (1998) 460–465.
- [24] L. Zhang, F. Tian, Extremal hexagonal chains concerning largest eigenvalue, *Sci. China Ser. A* 44 (2001) 1089–1097.
- [25] L. Zhang, F. Tian, Extremal catacondensed benzenoids, *J. Math. Chem.* 34 (2003) 111–122.