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Ordering Unicyclic Graphs with Respect to Hosoya Indices and Merrifield-Simmons Indices

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Abstract

Given a molecular graph G, the Hosoya index $z(G)$ and the Merrifield-Simmons index $\sigma(G)$ are defined as the total number of the independent edge-sets and the total number of the independent vertexsets of the graph G, respectively. Let $\mathscr{U}_{n,g}$ denote the set of unicyclic graphs with order n and girth $g \geq 3$. In this paper, we will give the first $\lfloor \frac{g}{2} \rfloor + 1$ Merrifield-Simmons indices and the last $\lfloor \frac{g}{2} \rfloor + 2$ Hosoya indices of all unicyclic graphs in the set $\mathscr{U}_{n,g}$ $(6 \leq g \leq n-8)$ and characterize corresponding extremal graphs. Moreover, for $g = n-2$, the first $\lfloor \frac{g}{2} \rfloor + 2$ Merrifield-Simmons indices and the last $\lfloor \frac{g}{2} \rfloor + 2$ Hosoya indices of unicyclic graphs in the set $\mathscr{U}_{n,g}$ are characterized.

1. Introduction

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The Hosoya index $z(G)$ and the Merrifield-Simmons index $\sigma(G)$ of a graph G are two prominent examples of topological indices which are of interest in combinatorial chemistry. They are defined as the number of matchings (independent edge subsets) and the number of independent vertex subsets of a graph, respectively.

The Hosoya index was introduced by Hosoya [13] in 1971, and it turned out to be applicable to several questions of molecular chemistry. For example, the connections with physico-chemical properties such as boiling point, entropy or heat of vaporization are well studied. Similar connections are known for the Merrifield-Simmons index, introduced by Merrifield and Simmons [22] in 1989. For detailed information on the chemical applications, we refer to [12, 14, 20, 21, 22, 26] and the references therein. Recently, many authors have investigated Hosoya indices and Merrifield-Simmons index (e.g., see [2]- [11], [15], [19], [23]-[28]).

In this paper, we will give the first $\lfloor \frac{g}{2} \rfloor + 1$ Merrifield-Simmons indices and the last $\lfloor \frac{g}{2} \rfloor + 2$ Hosoya indices of all unicyclic graphs in the set $\mathscr{U}_{n,g}$ $(6 \leq g \leq n-8)$ and characterize corresponding extremal graphs. Moreover, for $g = n-2$, the first $\lfloor \frac{g}{2} \rfloor + 2$ Merrifield-Simmons indices and the last $\lfloor \frac{g}{2} \rfloor + 2$ Hosoya indices of unicyclic graphs in the set $\mathscr{U}_{n,g}$ are characterized.

In order to discuss our results, we first introduced some terminologies and notations of graphs. For other undefined notations, the reader is referred to [1]. We only consider finite, undirected and simple graphs. For a vertex x of a graph G, we denote the neighborhood and the degree of x by $N_G(x)$ and $d_G(x)$, respectively. A *pendant vertex* is a vertex of degree 1. Denote $N_G[x] = N_G(x) \cup \{x\}$. Let C_q be a cycle of order q and P_s be a path of order s. The girth of a graph G is the length of a shortest cycle in G, with the girth of an acyclic graph being infinite. We will use $G - x$ or $G - xy$ to denote the graph that arises from G by deleting the vertex $x \in V(G)$ or the edge $xy \in E(G)$.

A unicyclic graph is a connected graph with n vertices and n edges. Let G be a unicyclic graph of order n and girth g. If $g = n$, then $G \cong C_n$, a cycle of order n; and if $g = n-1$, then $G \cong U_{n,n-1}$ (see Fig. 1). Therefore, we assume $3 \leq g \leq n-2$. Let $\mathscr{U}_{n,g} = \{U : U$ is a unicyclic graph of order n and girth g, $3 \leq g \leq n-2\}$.

2. Preliminaries

We first give some lemmas that will be used in the proof of our results.

Lemma 2.1 (see [12]). *Let $G = (V, E)$ be a graph.*
(i) If $uv \in E(G)$, then $\sigma(G) = \sigma(G - uv) - \sigma(G - (N_G[u] \cup N_G[v]))$

and $z(G) = z(G - uv) + z(G - \{u, v\})$;

(ii) If $v \in V(G)$, *then* $\sigma(G) = \sigma(G - v) + \sigma(G - N_G[v])$

and $z(G) = z(G - v) + \sum_{u \in N_G(v)} z(G - \{u, v\})$;

(iii) If $G_1, G_2, \ldots, G_\omega$ *are the components of a graph* G, *then* $\sigma(G) = \prod_{j=1}^{\omega} \sigma(G_j)$ *and* $z(G) = \prod_{j=1}^{\omega} z(G_j)$.

From Lemma 2.1, if v is a vertex of G, then $\sigma(G) > \sigma(G - v)$. Moreover, if G is a graph with at least one edge incident with v, then $z(G) > z(G - v)$.

Lemma 2.2 (see [18]). *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 let* G_2^* *be the graph obtained from* H, X, Y *by identifying vertices* u, v', u' *(see Fig. 1). Then*

(i) $\sigma(G_1^*) > \sigma(G)$ *or* $\sigma(G_2^*) > \sigma(G)$;

(ii) $z(G_1^*) < z(G)$ *or* $z(G_2^*) < z(G)$.

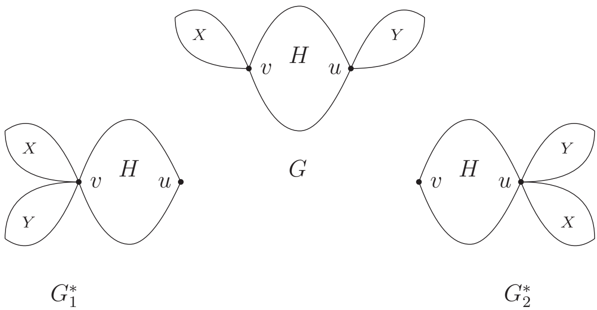

Fig. 1

Corollary 2.3. *Let* G *be a graph and* $v, u \in V(G)$. *Suppose that* $G_{s,t}$ *be a graph obtained from* G *by attaching* s, t *pendant vertices to* v, u, *respectively. Then*

$\sigma(G_{s+i,t-i}) > \sigma(G_{s,t})$ *for* $1 \le i \le t$ *or* $\sigma(G_{s-i,t+i}) > \sigma(G_{s,t})$ *for* $1 \le i \le s$ *and* $z(G_{s+i,t-i}) < \sigma(G_{s,t})$ *for* $1 \le i \le t$; *or* $z(G_{s-i,t+i}) < \sigma(G_{s,t})$ *for* $1 \le i \le s$.

Let $H_1,\ H_2$ be two connected graphs with $V(H_1) \cap V(H_2) = \{v\}$. Let $G = H_1 v H_2$ be a graph defined by $V(G) = V(H_1) \cup V(H_2)$ and $E(G) = E(H_1) \cup E(H_2)$.

Lemma 2.4 (see [19]). *Let H be a connected graph and T_l be a tree of order l with $V(H) \cap V(T_l) = \{v\}$. Then*

$$\sigma(HvT_l) \leq \sigma(HvK_{1,l-1}) \quad \textit{and} \quad z(HvT_l) \geq z(HvK_{1,l-1})$$

and equality holds if and only if $HvT_l \cong HvK_{1,l-1}$, where v is identified with the center of the star $K_{1,l-1}$ in $HvK_{1,l-1}$.

3. Main Results

In this section, we will give the first $\lfloor \frac{g}{2} \rfloor + 1$ Merrifield-Simmons indices and the last $\lfloor \frac{g}{2} \rfloor + 2$ Hosoya indices of unicyclic graphs in the set $\mathscr{U}_{n,g}$ $(3 \leq g \leq n-2)$.

In order to formulate our results, we need to define some unicyclic graphs (see Fig. 1) as follows.

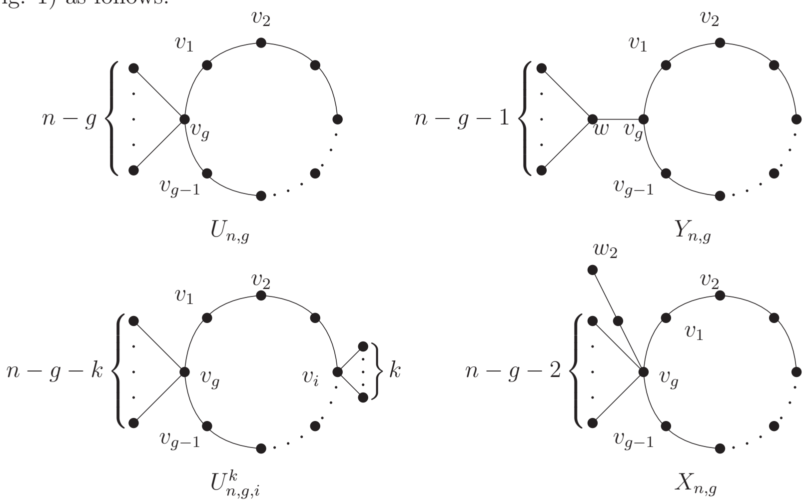

Fig. 1

Let $U_{n,g}(p_1, p_2, \ldots, p_{g-1}, p_g)$ be a unicyclic graph of order n created from a cycle $C_g = v_1 v_2 \cdots v_g v_1$ by attaching p_i pendant vertices to v_i, $1 \leq i \leq g$, respectively, where $n = g + \sum_{i=1}^{g} p_i$, $p_i \geq 0$, $i = 1, \ldots, g$.

Denote $U_{n,g} = U_{n,g}(\underbrace{0, \ldots, 0}_{g-1}, n-g)$ and $U^k_{n,g,i} = U_{n,g}(\underbrace{0, \ldots, 0}_{i-1}, k, 0, \ldots, 0, n-g-k)$ for $1 \leq k \leq n-g-k$ (see Fig. 1). Then $U^k_{n,g,i} \cong U^k_{n,g,g-i}$ and $U^k_{n,g,i} \cong U^{n-g-k}_{n,g,i}$.

Let $X_{n,g}$ (see Fig. 1) be a graph obtained from $U_{n-1,g}$ by attaching a pendant vertex to one pendant vertex of $U_{n-1,g}$.

Let $Y_{n,g}$ (see Fig. 1) be a graph obtained from $U_{g+1,g}$ by attaching $n-g-1$ pendant vertices to one pendant vertex of $U_{g+1,g}$.

Denote $\mathscr{U}^k_{n,g} = \{U^k_{n,g,i} \ : \ 1 \le i \le g-1\}$.

Let F_n be the nth Fibonacci number, i.e., $F_0 = F_1 = 1$, $F_n = F_{n-1} + F_{n-2}$, $n \ge 2$. Note that $\sigma(P_n) = F_{n+1}$, $z(P_n) = F_n$. By Lemma 2.1, we have the following results.

Lemma 3.1. *Let $U^k_{n,g,i}$, $X_{n,g}$, $Y_{n,g}$ be the graphs shown in Figure 1, where $1 \le i \le g-1$. Denote $U^0_{n,g,0} = U_{n,g}$ and $F_{-1} = 0$. Then*

(i) $\sigma(U^k_{n,g,i}) = (2^{n-g-k} + 2^k)F_g - F_{g-1} + (2^{n-g} - 2^{n-g-k} - 2^k + 1)F_iF_{g-i}$ and $z(U^k_{n,g,i}) = 2F_g + (n-g-1)F_{g-1} + k(n-g-k)F_{i-1}F_{g-i-1}$ for $k, i \ge 0$;

(ii) $\sigma(X_{n,g}) = 3 \cdot 2^{n-g-2}F_g + 2F_{g-2}$ and $z(X_{n,g}) = 4F_g + (2n-2g-5)F_{g-1}$;

(iii) $\sigma(Y_{n,g}) = F_g + 2^{n-g-1}(F_g + F_{g-2})$ and $z(Y_{n,g}) = 2F_g + (n-g-1)(F_g + F_{g-2})$.

By Lemma 3.1, we have the following results.

Lemma 3.2. *Let $U^k_{n,g,i}$, $X_{n,g}$, $Y_{n,g}$ be the graphs shown in Figure 1. Then*

(i) $\sigma(U^k_{n,g,i}) > \sigma(U^{k+1}_{n,g,i})$ and $z(U^k_{n,g,i}) < z(U^{k+1}_{n,g,i})$ for $k < \frac{n-g-1}{2}$;

(ii) $\sigma(U^1_{n,g,3}) > \sigma(U^2_{n,g,2})$ and $z(U^1_{n,g,3}) < z(U^2_{n,g,2})$ for $6 \le g \le n-5$ or $g = n-4 \ge 7$;

(iii) $\sigma(U^2_{n,g,2}) > \sigma(U^1_{n,g,1})$ and $z(U^2_{n,g,2}) > z(U^1_{n,g,1})$ for $6 = g \le n-8$ or $7 \le g \le n-7$;

(iv) $\sigma(U^1_{n,g,1}) > \sigma(X_{n,g})$ and $z(U^1_{n,g,1}) < z(X_{n,g})$;

(v) $\sigma(X_{n,g}) \ge \sigma(Y_{n,g})$ and $z(X_{n,g}) \le z(Y_{n,g})$.

Proof. Note that $F_g = F_iF_{g-i} + F_{i-1}F_{g-i-1}$.

(i) By Lemma 3.1, we have

$$\begin{aligned}
\sigma(U^k_{n,g,i}) - \sigma(U^{k+1}_{n,g,i}) &= (2^{n-g-k-1} - 2^k)(F_g - F_iF_{g-i}) \\
&= (2^{n-g-k-1} - 2^k)F_{i-1}F_{g-i-1} > 0; \\
z(U^k_{n,g,i}) - z(U^{k+1}_{n,g,i}) &= k(n-g-k)F_{i-1}F_{g-i-1} - (k+1)(n-g-k-1)F_{i-1}F_{g-i-1} \\
&= [k(n-g-k) - (k+1)(n-g-k-1)]F_{i-1}F_{g-i-1} \\
&= -(n-g-2k-1)F_{i-1}F_{g-i-1} < 0.
\end{aligned}$$

(ii) By Lemma 3.1, we have

$$\begin{aligned} \sigma(U^1_{n,g,3}) - \sigma(U^2_{n,g,2}) &= 2^{n-g-1}(F_g + 3F_{g-3}) + F_{g-2} + 2F_{g-4} \\ &\quad -2^{n-g-2}(F_g + 6F_{g-2}) - F_{g-1} - 2F_{g-3} \\ &= 2^{n-g-2}(2F_{g-5} - F_{g-6}) - F_{g-6} - 4F_{g-5} \\ &> 0 \qquad \text{for } 6 \le g \le n-5 \text{ or } g = n-4 \ge 7; \\ z(U^1_{n,g,3}) - z(U^2_{n,g,2}) &= -2[(n-g-3)F_{g-5} - F_{g-6}] < 0. \end{aligned}$$

(iii) By Lemma 3.1, we have

$$\begin{aligned} \sigma(U^2_{n,g,2}) - \sigma(U^1_{n,g,1}) &= 2^{n-g-2}(F_g + 6F_{g-2}) + F_{g-1} + 2F_{g-3} - 2^{n-g-1}F_{g+1} - 2F_{g-2} \\ &= 2^{n-g-2}F_{g-6} + 2F_{g-3} - F_{g-4} > 0; \\ z(U^2_{n,g,2}) - z(U^1_{n,g,1}) &= 2(n-g-2)F_{g-3}F_1 - (n-g-1)F_{g-2}F_0 \\ &= (n-g-5)F_{g-5} - 2F_{g-6} \\ &> 0 \qquad \text{for } 6 = g \le n-8 \text{ or } 7 \le g \le n-7. \end{aligned}$$

(iv) By Lemma 3.1, we have

$$\begin{aligned} \sigma(U^1_{n,g,1}) - \sigma(X_{n,g}) &= 2^{n-g-1}F_{g+1} + 2F_{g-2} - 3 \cdot 2^{n-g-2}F_g - 2F_{g-2} \\ &= 2^{n-g-2}F_{g-3} > 0; \\ z(U^1_{n,g,1}) - z(X_{n,g}) &= 2F_g + (n-g-1)F_{g-1} + (n-g-1)F_{g-2} \\ &\quad -4F_g - (2n-2g-5)F_{g-1} \\ &= -2F_g - (n-g-4)F_{g-1} + (n-g-1)F_{g-2} \\ &= -2F_g - 5F_{g-1} - (n-g-1)F_{g-3} < 0. \end{aligned}$$

(v) By Lemma 3.1, we have

$$\begin{aligned} \sigma(X_{n,g}) - \sigma(Y_{n,g}) &= 3 \cdot 2^{n-g-2}F_g + 2F_{g-2} - (2^{n-g-1}+1)F_g - 2^{n-g-1}F_{g-2} \\ &= 2^{n-g-2}F_{g-3} + 2F_{g-2} - F_g \\ &= (2^{n-g-2} - 1)F_{g-3} \ge 0; \\ z(X_{n,g}) - z(Y_{n,g}) &= -(n-g-3)F_g + (2n-2g-5)F_{g-1} - (n-g-1)F_{g-2} \\ &= (n-g-2)F_{g-1} - 2(n-g-2)F_{g-2} \\ &= -(n-g-2)F_{g-4} \le 0. \end{aligned}$$

■

Lemma 3.3 (see [16, 17]). *Let $n = 4s + r$, where n, s and r are integers with $0 \leq r \leq 3$.*

(i) For $r \in \{0, 1\}$, we have

$$\begin{aligned} F_0F_n &> F_2F_{n-2} > F_4F_{n-4} > \cdots > F_{2s}F_{2s+r} > F_{2s-1}F_{2s+r+1} \\ &> F_{2s-3}F_{2s+r+3} > \cdots > F_3F_{n-3} > F_1F_{n-1}; \end{aligned}$$

(ii) For $r \in \{2, 3\}$, we have

$$\begin{aligned} F_0F_n &> F_2F_{n-2} > F_4F_{n-4} > \cdots > F_{2s}F_{2s+r} > F_{2s+1}F_{2s+r-1} \\ &> F_{2s-1}F_{2s+r+1} > \cdots > F_3F_{n-3} > F_1F_{n-1}. \end{aligned}$$

By Lemmas 3.1 and 3.3, we have

Lemma 3.4. *Let $g = 4t + r$, where t and r are integers with $t \geq 1$ and $0 \leq r \leq 3$.*
(i) For $r \in \{0, 1\}$, we have

$$\begin{aligned} \sigma(U^k_{n,g,2}) &> \sigma(U^k_{n,g,4}) > \cdots > \sigma(U^k_{n,g,2t}) > \sigma(U^k_{n,g,2t-1}) \\ &> \sigma(U^k_{n,g,2t-3}) > \cdots > \sigma(U^k_{n,g,1}) \\ \text{and} \quad z(U^k_{n,g,2}) &< z(U^k_{n,g,4}) < \cdots < z(U^k_{n,g,2t}) < z(U^k_{n,g,2t-1}) \\ &< z(U^k_{n,g,2t-3}) < \cdots < z(U^k_{n,g,1}). \end{aligned}$$

(ii) For $r \in \{2, 3\}$, we have

$$\begin{aligned} \sigma(U^k_{n,g,2}) &> \sigma(U^k_{n,g,4}) > \cdots > \sigma(U^k_{n,g,2t}) > \sigma(U^k_{n,g,2t+1}) \\ &> \sigma(U^k_{n,g,2t-1}) > \cdots > \sigma(U^k_{n,g,1}) \\ \text{and} \quad z(U^k_{n,g,2}) &< z(U^k_{n,g,4}) < \cdots < z(U^k_{n,g,2t}) < z(U^k_{n,g,2t+1}) \\ &< z(U^k_{n,g,2t-1}) < \cdots < z(U^k_{n,g,1}). \end{aligned}$$

By Lemmas 3.2 and 3.4, we have the following:

Corollary 3.5. *The unicyclic graphs with the first $\lfloor \frac{g}{2} \rfloor + 2$ Merrifield-Simmons indices or the last $\lfloor \frac{g}{2} \rfloor + 2$ Hosoya indices in the set $\mathscr{U}_{n,g}$, $g = n - 2 = 4t + r$, $t \geq 1$, $0 \leq r \leq 3$ are as follows:*

$$\begin{aligned} &U_{n,g}, U^1_{n,g,2}, U^1_{n,g,4}, \ldots, U^1_{n,g,2t}, U^1_{n,g,2t-1}, U^1_{n,g,2t-3}, \ldots, U^1_{n,g,1}, X_{n,g}, \ \text{when } r \in \{0, 1\}; \\ &U_{n,g}, U^1_{n,g,2}, U^1_{n,g,4}, \ldots, U^1_{n,g,2t}, U^1_{n,g,2t+1}, U^1_{n,g,2t-1}, \ldots, U^1_{n,g,1}, X_{n,g}, \ \text{when } r \in \{2, 3\}. \end{aligned}$$

Note that $\mathscr{U}_{n,n-2}$ contains no other unicyclic graphs than the above listed.

Lemma 3.6. *Let $G \in \mathscr{U}_{n,g} \setminus (\mathscr{U}^1_{n,g} \cup \{U^2_{n,g,2}, U_{n,g}\})$ with $6 = g \le n-8$ or $7 \le g \le n-7$. Then*

$$\sigma(G) < \sigma(U^2_{n,g,2}) \quad \textit{and} \quad z(G) > z(U^2_{n,g,2}).$$

Proof. Let $C_g = v_1 v_2 \cdots v_g v_1$ be a cycle of length g of G. Let $V^*(G) = \{v_i : d(v_i) \ge 3, 1 \le i \le g\}$. Since $n > g$, we have $V^*(G) \ne \emptyset$. Without loss of generality, we assume that $v_g \in V^*(G)$. We consider two cases.

Case 1. $|V^*(G)| \ge 2$.

In this case, let $v_i \in V^*(G)$ and let T_i be a subtree of $G - E(C_g)$ which containing v_i and $|V(T_i)| = p_i + 1$. Let $t = |\{p_i \ : \ p_i > 0\}|$. Then $t \ge 2$.

We first show there is a unicyclic graph $G^1 = U_{n,g}(p_1, \ldots, p_g)$ such that $\sigma(G) \le \sigma(G^1)$ (or $z(G) \ge z(G^1)$, resp.) and equality holds if and only if $G \cong G^1$. Denote $H = C_g \cup \left(\bigcup\limits_{1 \le k \le g, k \ne i} T_{p_k} \right)$. Then $G = H v_i T_i$. By Lemma 2.4, we have $\sigma(HvT_i) \le \sigma(HvK_{1,p_i-1})$ (or $z(HvT_i) \ge z(HvK_{1,p_i-1})$, resp.). Thus $\sigma(G) \le \sigma(U_{n,g}(p_1, \ldots, p_g))$ (or $z(G) \ge z(U_{n,g}(p_1, \ldots, p_g))$, resp.). Denote $G^1 = U_{n,g}(p_1, \ldots, p_g)$.

Since $G \notin \mathscr{U}^1_{n,g} \cup \{U_{n,g}\}$, we have $t \ge 2$ and $p_i \ge 2$ for at least two i. If $t = 2$, then, by Corollary 2.3, there is a unicyclic graph $G^2 \in \mathscr{U}^2_{n,g}$ such that $\sigma(G^1) \le \sigma(G^2)$ (or $z(G^1) \ge z(G^2)$, resp.) and equality holds if and only if $G^1 \cong G^2$. Note that $G \ncong U^2_{n,g,2}$, and hence, by Lemma 3.4, $\sigma(G) \le \sigma(G^1) \le \sigma(G^2) < \sigma(U^2_{n,g,2})$ (or $z(G) \ge z(G^1) \ge z(G^2) > z(U^2_{n,g,2})$, resp.). If $t \ge 3$, let $p_k, p_l, p_m \ne 0$, $1 \le k < l < m \le d-1$. By Corollary 2.3, we have either

$$\sigma(U_{n,g}(p_1, \ldots, p_k, \ldots, p_l, \ldots, p_{d-1})) < \sigma(U_{n,g}(p_1, \ldots, p_k + p_l, \ldots, 0, \ldots, p_{d-1}))$$

(or $z(U_{n,g}(p_1, \ldots, p_k, \ldots, p_l, \ldots, p_{d-1})) > z(U_{n,g}(p_1, \ldots, p_k + p_l, \ldots, 0, \ldots, p_{d-1}))$, resp.) or $\sigma(U_{n,g}(p_1, \ldots, p_k, \ldots, p_l, \ldots, p_{d-1})) < \sigma(U_{n,g}(p_1, \ldots, 0, \ldots, p_k + p_l, \ldots, p_{d-1}))$ (or $z(U_{n,g}(p_1, \ldots, p_k, \ldots, p_l, \ldots, p_{d-1})) > z(U_{n,g}(p_1, \ldots, 0, \ldots, p_k + p_l, \ldots, p_{d-1}))$, resp.).

Repeated the above step, we obtain a sequence unicyclic graphs

$$G^2, G^3, \ldots, G^{t-1} \in \mathscr{U}^2_{n,g}$$

such that $\sigma(G^1) < \sigma(G^2) < \cdots < \sigma(G^{t-1})$ (or $z(G^1) > z(G^2) > \cdots > z(G^{t-1})$, resp.). Hence by Lemma 3.4, we have $\sigma(G) \le \sigma(G^1) < \cdots < \sigma(G^{t-1}) < \sigma(U^2_{n,g,2})$ (or $z(G) \ge z(G^1) > \cdots > z(G^{t-1}) > z(U^2_{n,g,2})$, resp.).

Case 2. $|V^*(G)| = 1$.

In this case, we let $v_i \in V^*(G)$ and $N(v_i) \setminus \{v_{i-1}, v_{i+1}\} = \{x_1, \ldots, x_s\}$ with $d(x_j) \geq 2,\ 1 \leq j \leq r$, and $d(x_{r+1}) = \cdots = d(x_s) = 1$. Then $r \geq 1$ as $T \ncong U_{n,g}$. Let $T_i(x_j)$ be subtrees of $G - v_i$ which contain x_j, and $|V(T_i(x_j))| = s_j + 1,\ 1 \leq j \leq r$.

Let G' be a unicyclic graph created from $U_{g+s,g}$ by attaching s_j pendant vertices to x_j, $1 \leq j \leq r$, respectively. Then, by Lemma 2.4, we have $\sigma(G) \leq \sigma(G')$ (or $z(G) \geq z(G')$, resp.).

Denote G^* be a graph obtained from G' by deleting s_1 pendant vertices to x_1 and s_2 pendant vertices to x_2 if $r \geq 2$ or $G^* = U_{g+1,g}$ for $r = 1$, then $G' = G^*_{s_1,s_2}$ or $G' = G^*_{s_1,s-1}$. Thus, by Corollary 2.3, we have $\sigma(G') \leq \sigma(X_{n,g})$ (or $z(G') \geq z(X_{n,g})$, resp.) or $\sigma(G') \leq \sigma(Y_{n,g})$ (or $z(G') \geq z(Y_{n,g})$, resp.). Thus, by Lemmas 3.2 and 3.4, we have $\sigma(G) \leq \sigma(G') \leq \sigma(X_{n,g}) < \sigma(U^2_{n,g,2})$ (or $z(G) \geq z(G') \geq z(X_{n,g}) > z(U^2_{n,g,2})$, resp.) or $\sigma(G) \leq \sigma(G') \leq \sigma(Y_{n,g}) < \sigma(U^2_{n,g,2})$ (or $z(G) \geq z(G') \geq z(Y_{n,g}) > z(U^2_{n,g,2})$, resp.).

Therefore the proof of the lemma is complete. ■

From Lemmas 3.2 and 3.4, we have

Theorem 3.7. *The unicyclic graphs with the first* $\lfloor \frac{g}{2} \rfloor + 1$ *Merrifield-Simmons indices or the last* $\lfloor \frac{g}{2} \rfloor + 1$ *Hosoya indices in the set* $\mathscr{U}_{n,g}$ *for* $g = 3$ *are* $U_{n,g},\ U^1_{n,g,1}$*; and for* $g \in \{4, 5\}$ *are* $U_{n,g},\ U^1_{n,g,2},\ U^1_{n,g,1}$.

By Lemmas 3.2, 3.4 and 3.6, we have the following results.

Theorem 3.8. *For* $6 = g \leq n - 8$ *or* $7 \leq g \leq n - 7$ *with* $g = 4t + r,\ t \geq 1,\ 0 \leq r \leq 3$.

(i) The unicyclic graphs with first $\lfloor \frac{g}{2} \rfloor + 1$ *Merrifield-Simmons indices in the set* $\mathscr{U}_{n,g}$ *are follows:*

$U_{n,g}, U^1_{n,g,2}, U^1_{n,g,4}, \ldots, U^1_{n,g,2t}, U^1_{n,g,2t-1}, U^1_{n,g,2t-3}, \ldots, U^1_{n,g,3}, U^2_{n,g,2},$ *when* $r \in \{0, 1\}$*;*
$U_{n,g}, U^1_{n,g,2}, U^1_{n,g,4}, \ldots, U^1_{n,g,2t}, U^1_{n,g,2t+1}, U^1_{n,g,2t-1}, \ldots, U^1_{n,g,3}, U^2_{n,g,2},$ *when* $r \in \{2, 3\}$.

(ii) The unicyclic graphs with the last $\lfloor \frac{g}{2} \rfloor + 2$ *Hosoya indices in the set* $\mathscr{U}_{n,g}$ *are follows:*

$U_{n,g}, U^1_{n,g,2}, \ldots, U^1_{n,g,2t}, U^1_{n,g,2t-1}, U^1_{n,g,2t-3}, \ldots, U^1_{n,g,3}, U^1_{n,g,1}, U^2_{n,g,2},$ *when* $r \in \{0, 1\}$*;*
$U_{n,g}, U^1_{n,g,2}, \ldots, U^1_{n,g,2t}, U^1_{n,g,2t+1}, U^1_{n,g,2t-1}, \ldots, U^1_{n,g,3}, U^1_{n,g,1}, U^2_{n,g,2},$ *when* $r \in \{2, 3\}$.

Remark. In [23], Ou determined the unicycle graphs with the minimum Hosoya index and the second-minimum Hosoya index in the set $\mathscr{U}_{n,g}$.

4. Notes

By Theorems 3.7 and 3.8, we have that the graph with k-minimum Hosoya index is also almost the graph with k-maximum Merrifield-Simmons index in the set $\mathscr{U}_{n,g}$ for $g = n-2$, or $6 = g \le n-8$, or $7 \le g \le n-7$, where $k \le \lfloor \frac{g}{2} \rfloor$. But in the other cases, we illustrate two examples to show that the graph with larger Merrifield-Simmons index is the graph with smaller Hosoya index.

Example 4.1. $\sigma(U^1_{10,6,2}) = 192 > \sigma(U^2_{10,6,2}) = 186$ and $z(U^1_{10,6,2}) = 59 < z(U^2_{10,6,2}) = 61$.

Example 4.2. $\sigma(U^1_{10,6,3}) = 185 < \sigma(U^1_{10,6,2}) = 192$ and $z(U^1_{10,6,3}) = 62 > z(U^1_{10,6,2}) = 59$.

However, from Theorem 3.8, we known that $z(U^1_{n,g,1}) < z(U^2_{n,g,2})$ and $\sigma(U^1_{n,g,1}) < \sigma(U^2_{n,g,2})$ for $6 = g \le n-8$, or $7 \le g \le n-7$.

Also, the unicycle graphs in the set $\mathscr{U}_{n,g}$ for $g \in \{n-3, n-4, n-5, n-6\}$ may be ordered according to Merrifield-Simmons indices or Hosoya indices by detailed calculations.

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References

[1] J.A. Bondy and U.S.R. Murty, *Graph Theory with Applications*, MacMillan, New York, 1976.

[2] O. Chan, I. Gutman, T.K. Lam and R. Merris, Algebraic connections between topological indices, *J. Chem. Inform. Comput. Sci.*, 38(1998) 62-65.

[3] S.J. Cyvin and I. Gutman, Hosoya index of fused molecules, *MATCH Commun. Math. Comput. Chem.*, 23(1988) 89-94.

[4] S.J. Cyvin, I. Gutman and N. Kolakovic, Hosoya index of some polymers, *MATCH Commun. Math. Comput. Chem.*, 24(1989) 105-117.

[5] I. Gutman, Independent vertex sets in some compound graphs, *Publ. Inst. Math. (Beograd)*, 52(1992) 5-9.

[6] I. Gutman, Fragmentation formulas for the number of Kekulé structures, Hosoya and Merrifield-Simmons indices and related graph invariants, *Coll. Sci. Pap. Fac. Sci. Kragujevac*, 11(1990) 11-18.

[7] I. Gutman, Topological properties of benzenoid systems. Merrifield-Simmons indices and independence polynomials of unbranched catafusenes, *Rev. Roum. Chim.*, 36(1991) 379-388.

[8] I. Gutman, Independent vertex sets in some compound graphs, *Publ. Inst. Math. (Beograd)*, 52(1992) 5-9.

[9] I. Gutman, H. Hosoya, G. Uraković and L. Ristić, Two variants of the topological index and the relations between them, *Bull. Chem. Soc. Jpn*, 65(1992) 14-18.

[10] I. Gutman, N. Kolaković, Hosoya index of the second kind of molecules containing a polyacene fragment, *Bull. Acad. Serbe Sci. Arts (Cl. Math. Natur.)*, 102(1990) 39-46.

[11] I. Gutman, Extremal hexagonal chains, *J. Math. Chem.*, 12(1993) 197-210.

[12] I. Gutman and O.E. Polansky, *Mathematical Concepts in Organic Chemistry,*Springer, Berlin, 1986.

[13] 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.

[14] X. Li, Z.M. Li and L.S. Wang, The inverse problems for some topological indices in combinatorial chemistry, *J. Comput. Biol.*, 10(2003) 47-55.

[15] X. Li, H. Zhao and I. Gutman, On the Merrifield-Simmons index of trees, *MATCH Commun. Math. Comput. Chem.*, 54(2005) 389-402.

[16] X. Li and H.X. Zhao, On the Fibonacci numbers of trees, *Fibonacci Quarterly*, 44(2006) 32-38.

[17] S. B. Lin and C. Lin, Trees and forests with large and small independent indices, *Chinese J. Math.*, 23(3)(1995) 199-210.

[18] H.-Q. Liu and M. Lu, A unified approach to extremal cacti for different indices, *MATCH Commun. Math. Comput. Chem.*, 58(2007) 193-204.

[19] H.-Q. Liu, X. Yan and Z. Yan, On the Merrifield-Simmons indices and Hosoya indices of trees with a prescribed diameter, *MATCH Commun. Math. Comput. Chem.*, 57(2007) 371-384.

[20] R.E. Merrifield and H.E. Simmons, Enumeration of structure-sensitive graphical subsets: Theory, *Proc. Natl. Acad. Sci. USA*, 78(1981) 692-695.

[21] R.E. Merrifield and H.E. Simmons, Enumeration of structure-sensitive graphical subsets: Calculations, *Proc. Natl. Acad. Sci. USA*, 78(1981) 1329-1332.

[22] R.E. Merrifield and H.E. Simmons, *Topological Methods in Chemistry,* Wiley, New York, 1989.

[23] J. Ou, On extremal unicyclic molecular graphs with prescribed girth and minimal Hosoya index, *J. Math. Chem.*, DOI: 10.1007/s10910-006-9112-y.

[24] X.-F. Pan, J.-M. Xu, C. Yang and M.-J. Zhou, Some graphs with minimum Hosoya index and maximum Merrifield-Simmons index, *MATCH Commun. Math. Comput. Chem.*, 57(2007) 235-242.

[25] H. Prodinger, R. F. Tichy, Fibonacci numbers of graphs, Fibonacci Quart, 20(1982) 16-21.

[26] L. Türker, Contemplation on the Hosoya indices, *J. Mol. Struct.(Theochem)*, 623(2003) 75-77.

[27] A.-M. Yu and F. Tian, A kind of graphs with minimal Hosoya indices and maximal Merrifield-Simmons indices, *MATCH Commun. Math. Comput. Chem.*, 55(2006) 103-118.

[28] L.-Z. Zhang and F. Tian, Extremal catacondensed benzenoids, *J. Math. Chem.*, 34(2003) 111-122.