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Some extremal unicyclic graphs with respect to Hosoya index and Merrifield-Simmons index*

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Abstract The Hosoya index of a graph is defined as the total number of the matchings, including the empty edge set, of the graph. The Merrifield-Simmons index of a graph is defined as the total number of the independent vertex sets, including the empty vertex set, of the graph. Let $\mathcal{U}(n,\Delta)$ be the set of connected unicyclic graphs of order n with maximum degree Δ. We consider the Hosoya indices and the Merrifield-Simmons indices of graphs from $\mathcal{U}(n,\Delta)$. In this paper, we characterize the graphs in $\mathcal{U}(n,\Delta)$ with the maximal Hosoya index and the minimal Merrifield-Simmons index, respectively, and determine the corresponding indices.

1 Introduction

The Hosoya index and the Merrifield-Simmons index of a graph G are two well-known topological indices in combinatorial chemistry. The former, denoted by $z(G)$, is defined as the total number of the matchings (independent edge subsets), including the empty edge set, of the graph, and the latter, denoted by $i(G)$, is defined as the total number of the independent vertex sets, including the empty vertex set, of the graph.

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The Hosoya index was introduced by Hosoya [1] in 1971. Since its first introduction the Hosoya index has received much attention (see [2, 3, 4, 5]). Moreover, it plays an important role in studying the relation between molecular structure and physical and chemical properties of certain hydrocarbon compounds. The Merrifield-Simmons index, introduced by Merrifield and Simmons [6] in 1989, is the other topological index whose mathematical properties can be found in some detail [7, 8, 9, 10]. In [6] it was shown that $i(G)$ is correlated with boiling points.

It is significant to determine the extremal (maximal or minimal) graphs with respect to these two indices. By now, many nice results can be found in [2, 3, 4, 5, 6, 7, 8, 9, 10, 11] concerning the extremal graphs with respect to these two indices. For examples, trees, unicyclic graphs, and so on, are of major interest. Especially, Wagner [3] characterizes the extremal trees with maximal Hosoya index and minimal Merrifield-Simmons index. Deng et al. [4] determine all the extremal unicyclic graphs with respect to these two indices. All graphs considered in this paper are finite and simple. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, we denote by $N_G(v)$ the neighbors of v in G, and $N_G[v] = \{v\} \bigcup N_G(v)$. $d_G(v) = |N_G(v)|$ is called the degree of v in G or written as $d(v)$ for short. For other undefined notations and terminology from graph theory, the readers are referred to [12].

Let $\mathcal{U}(n, \Delta)$ be the set of connected unicyclic graphs of order n with maximum degree Δ. In Section 2, we list some basic lemmas which will be used in the proofs. In Section 3, we characterize the graphs in $\mathcal{U}(n, \Delta)$ with the maximal Hosoya index and the minimal Merrifield-Simmons index, respectively, and determine their corresponding indices.

2 Some lemmas

We first list three lemmas, which can be found in [6, 8], as basic but necessary preliminaries.

Lemma 2.1. *Let G be a graph, and $v \in V(G)$, $uv \in E(G)$. Then we have*

(1) $z(G) = z(G - v) + \sum\limits_{w \in N_G(v)} z(G - \{w, v\})$, $z(G) = z(G - uv) + z(G - \{u, v\})$;

(2) $i(G) = i(G - v) + i(G - N_G[v])$.

Lemma 2.2. *If G_1, $G_2, \cdots$, G_t are the components of a graph G, we have*

(1) $i(G) = \prod\limits_{k=1}^{t} i(G_k)$;

(2) $z(G) = \prod\limits_{k=1}^{t} z(G_k)$.

Lemma 2.3. *Let F_n be the n_{th} Fibonacci number, that is, $F_0 = 0$, $F_1 = F_2 = 1$, and $F_n = F_{n-1} + F_{n-2}$ for $n \geq 3$. For a path P_n with n vertices (of length $n - 1$), we have $z(P_n) = F_{n+1}$ and $i(P_n) = F_{n+2}$.*

A tree is called a $d - pode$ (see [3]) if it contains only one vertex v of degree $d > 2$. v is called the *center*. Denote by $R(c_1, c_2, \cdots, c_d)$ the d-pode where $\sum\limits_{k=1}^{d} c_k = n - 1$, c_i is the length of the $i-$th "ray" going out from the center. That is to say, $R(c_1, c_2, \cdots, c_d) - v = \bigcup\limits_{k=1}^{d} P_{c_k}$. For convenience, if the number of c_k is l_k, we write it as $c_k^{l_k}$ in the following. For example, $R(2, 2, 3, 3, 5)$ will be written as $R(2^2, 3^2, 5^1)$ for short.

For some positive integers $k_1 \leq k_2 \leq \cdots \leq k_m$ we denote by $C_k(k_1^{l_1}, k_2^{l_2}, \cdots, k_m^{l_m})$ a graph obtained by attaching $l_1, l_2, \cdots, l_m$ paths of length $k_1, k_2, \cdots, k_m$, respectively, to one vertex of C_k. For convenience, we let $C_k = C_k(0^1)$ and $P_{k-1} = C_k((-1)^1)$. And let $C_k^{(l)}(k_1^{l_1}, k_2^{l_2}, \cdots, k_m^{l_m})$ be a graph obtained from identifying a vertex of C_k with a pendant vertex of P_l of the graph $R(k_1^{l_1}, k_2^{l_2}, \cdots, k_m^{l_m}, l^1)$ where $l \geq 1$ and the value of l is independent of those of $k_1, k_2, \cdots, k_m$. For examples, the graphs $C_5(2^2, 3^2, 4^1)$ and $C_5^{(2)}(2^1, 3^2, 4^1)$ are shown in Fig. 1.

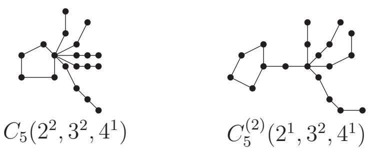

Fig. 1 The graphs $C_5(2^2, 3^2, 4^1)$ and $C_5^{(2)}(2^1, 3^2, 4^1)$

Lemma 2.4. *([3]) Let $G \neq K_1$ be a connected graph, $v \in V(G)$. $G(k, n-1-k)$ is the graph resulting from attaching at v two paths of length k and $n-1-k$, respectively. Let $n = 4m + j$ where $j \in \{1, 2, 3, 4\}$ and $m \geq 0$. Then*

$$z(G(1, n-2)) < z(G(3, n-4)) < \cdots < z(G(2m+2l-1, n-2m-2l)) <$$
$$z(G(2m, n-1-2m)) < \cdots < z(G(2, n-3)) < z(G(0, n-1)),$$

and

$$i(G(1, n-2)) > i(G(3, n-4)) > \cdots > i(G(2m+2l-1, n-2m-2l)) >$$
$$i(G(2m, n-1-2m)) > \cdots > i(G(2, n-3)) > i(G(0, n-1)).$$

Where $l = \lfloor \frac{i-1}{2} \rfloor$, and $G(0, n-1)$ can be also viewed as a graph obtained by attaching at $v \in V(G)$ a path of length $n-1$.

By repeating Lemma 2.4, the following remark is easily obtained.

Remark 2.1. *([3]) When a tree T of size t attached to a graph G is replaced by a path P_{t+1} as shown in Fig. 2, the Hosoya index increases, and the Merrifield-Simmons index decreases.*

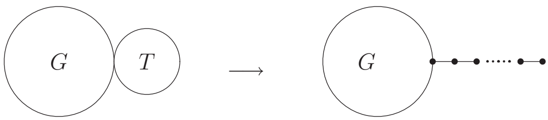

Fig. 2 The graphs in Remark 2.1

Lemma 2.5. *([2, 10]) Let $P = u_0u_1u_2 \cdots u_tu_{t+1}$ be a path or a cycle (if $u_0 = u_{t+1}$) in a graph G, where the degrees of $u_1, u_2, \cdots u_t$ in G are 2, $t \geq 1$. G_1 denotes the graph that results from identifying $u_r (0 \leq r \leq t)$ with the vertex v_k of a simple path $v_1v_2 \cdots v_k$, $G_2 = G_1 - u_ru_{r+1} + u_{r+1}v_1$ (see Fig. 3). Then we have $z(G_1) < z(G_2)$ and $i(G_1) > i(G_2)$.*

By the definition of the Fibonacci number, the following lemma can be obtained.

Lemma 2.6. *([4]) $F_n = F_kF_{n-k+1} + F_{k-1}F_{n-k}$ for $1 \leq k \leq n$.*

From Lemmas 2.1, 2.2, 2.3 and 2.6, the following two lemmas holds immediately.

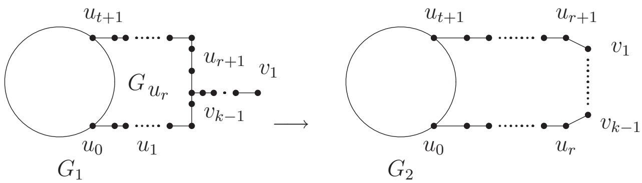

Fig. 3 The graphs in Lemma 2.5

Lemma 2.7. $z(R(2^{\Delta-2},l,m)) = 2^{\Delta-2}F_{l+m+2} + (\Delta-2)2^{\Delta-3}F_{l+1}F_{m+1}$

$i(R(2^{\Delta-2},l,m)) = 3^{\Delta-2}F_{l+2}F_{m+2} + 2^{\Delta-2}F_{l+1}F_{m+1}.$

Lemma 2.8. $z(C_k(k_1^{l_1},k_2^{l_2},\cdots,k_m^{l_m})) = (F_{k+1}+F_{k-1}+\sum_{j=1}^{m}\frac{l_jF_kF_{k_j}}{F_{k_j+1}})\prod_{j=1}^{m}F_{k_j+1}^{l_j},$

$i(C_k(k_1^{l_1},k_2^{l_2},\cdots,k_m^{l_m})) = F_{k+1}\prod_{j=1}^{m}F_{k_j+2}^{l_j} + F_{k-1}\prod_{j=1}^{m}F_{k_j+1}^{l_j}.$

Lemma 2.9. *For two positive integers k and m, we have*

$$F_kF_m - F_{k-1}F_{m+1} = \begin{cases} (-1)^{k-1}F_{m-k+1} & if \quad k \le m; \\ (-1)^{m-1}F_{k-m-1} & if \quad k > m. \end{cases}$$

Proof. We only prove the case when $k \le m$, and the proof for the case when $k > m$ is similar and is therefore omitted.

$$\begin{aligned} & F_kF_m - F_{k-1}F_{m+1} \\ = \; & (F_{k-1}+F_{k-2})F_m - F_{k-1}(F_m + F_{m-1}) \\ = \; & (-1)^1(F_{k-1}F_{m-1} - F_{k-2}F_m) \\ = \; & (-1)^1[(F_{k-2}+F_{k-3})F_{m-1} - F_{k-2}(F_{m-1}+F_{m-2})] \\ = \; & (-1)^2[F_{k-2}F_{m-2} - F_{k-3}F_{m-1}] \\ = \; & \cdots\cdots \\ = \; & (-1)^{k-2}[F_2F_{m-(k-2)} - F_1F_{m-(k-3)}] \\ = \; & (-1)^{k-1}F_{m-k+1}. \end{aligned}$$

Thus the proof is completed. □

3 Main results

Now we start to consider the maximal Hosoya index and minimal Merrifield-Simmons index of graphs in $\mathcal{U}(n,\Delta)$. If $\Delta = 2$, only one graph, the cycle C_n, belongs to $\mathcal{U}(n,\Delta)$. When $\Delta = n-1$, the set $\mathcal{U}(n,\Delta)$ consists of a single graph $C_3(1^{n-3})$, which is a graph obtained from the star S_n by adding an edge. So, in the following, we always assume that $2 < \Delta < n-1$.

In order to continue our study, we first choose two subsets of $\mathcal{U}(n,\Delta)$. Denote by $\mathcal{U}_1(n,\Delta)$ the set of all graphs $C_k^{(l)}(k_1^{l_1}, k_2^{l_2})$ where $1 \le k_2 \le 2$ when $k_1 = 1$, $k_2 \ge 2$ when $k_1 = 2$, and $l_2 = 1$ when $k_2 > 2$. And we denote by $\mathcal{U}_2(n,\Delta)$ the set of all graphs $C_k(k_1^{l_1}, k_2^{l_2})$ where $1 \le k_2 \le 2$ when $k_1 = 1$, $k_2 \ge 2$ when $k_1 = 2$, and $l_2 = 1$ when $k_2 > 2$.

Lemma 3.1. *Suppose that G^* from $\mathcal{U}(n,\Delta)$ has maximal Hosoya index or minimal Merrifield-Simmons index. Then, either $G^* \in \mathcal{U}_1(n,\Delta)$ or $G^* \in \mathcal{U}_2(n,\Delta)$.*

Proof. Suppose that the unique cycle in G^* is C_0.

If all vertices of maximum degree Δ are not on the cycle C_0, Let T_1 be a subtree such that $V(T_1) \setminus V(C_0)$ contains a vertex of degree Δ. By Remark 2.1, if we replace all subtrees attached at C_0 by paths of the same order, the Hosoya index will increase. Therefore, after removing the paths attached at C_0 but not in T_1 and enlarging the length of C_0 while the obtained graph is still in $\mathcal{U}(n,\Delta)$, in view of Remark 2.1 and Lemma 2.5, the Hosoya index will increase again. By Lemma 2.4, all paths attached at the vertex of degree Δ in T_1 must be of the lengths 1 or 2 except a unique possible path of length $k > 2$. So G^* belongs to $\mathcal{U}_1(n,\Delta)$. Note that if all the vertices of degree Δ have $\Delta - 1$ neighbors of degree 1, then it is the case when $k_1 = k_2 = 1$.

If there exists a vertex of degree Δ which is on the cycle C_0, by a similar argument, we have $G^* \in \mathcal{U}_2(n,\Delta)$. The proof for the Merrifield-Simmons index is completely analogous and is omitted. This completes the proof. $\square$

Lemma 3.2. *If $\Delta \ge \frac{n-1}{2}$, and $G_1 \in \mathcal{U}_1(n,\Delta)$, then there exists a graph $G_2 \in \mathcal{U}_2(n,\Delta)$ such that $z(G_2) > z(G_1)$ and $i(G_1) > i(G_2)$.*

Proof. Suppose that $G_1 = C_k^{(l)}(k_1^{l_1}, k_2^{l_2})$. First we claim that $k_1 = 1$ in G_1. Otherwise, by Lemma 2.4, the graph $R(k_1^{l_1}, k_2^{l_2}, l)$ in G_1 must be $R(2^{\Delta-1}, l)$, we find that the order of G_1 is $2(\Delta-1)+1+l+k-1 > 2\Delta-1+1+2 = 2\Delta+2 > 2\Delta+1 \geq n$ $(l \geq 1, k \geq 3)$, a contradiction.

Consider a graph $G_2 = C_{k+l+1}(1^{l_1-1}, 2^{l_2})$ from $\mathcal{U}_2(n, \Delta)$ as shown in Fig. 4. By applying (1) of Lemma 2.1 to the edges v_0v_1 and v_1v_2 of G_1 and G_2, respectively, we have

$$z(G_1) = z(G_1 - v_0v_1) + z(P_{k-2})z(R(1^{l_1}, 2^{l_2}, l-1))$$

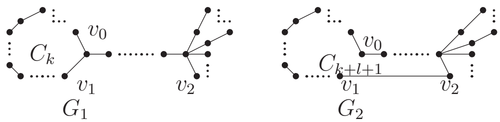

Fig. 4 The graphs G_1 and G_2 for $\Delta \geq \frac{n-1}{2}$

and

$$\begin{aligned} z(G_2) &= z(G_2 - v_1v_2) + z(G_2 - \{v_1, v_2\}) \\ &= z(G_2 - v_1v_2) + z(P_{k-2})z(R(1^{l_1-1}, 2^{l_2}, l)) + z(P_{k-3})z(R(1^{l_1-1}, 2^{l_2}, l-1)). \end{aligned}$$

Note that $G_1 - v_0v_1 \cong G_2 - v_1v_2$, and by Lemma 2.4, $z(R(1^{l_1-1}, 2^{l_2}, l)) > z(R(1^{l_1}, 2^{l_2}, l-1))$, so we have $z(G_2) > z(G_1)$.

By Lemmas 2.1 and 2.8, we get

$$\begin{aligned} i(G_1) &= 2^{l_1}3^{l_2}i(C_k((l-1)^1)) + 2^{l_2}i(C_k((l-2)^1)) \\ &= 2^{l_1}3^{l_2}(F_{k+l+1} - F_{k-2}F_l) + 2^{l_2}(F_{k+l} - F_{k-2}F_{l-1}) \end{aligned}$$

and

$$i(G_2) = 2^{l_1-1}3^{l_2}F_{k+l+2} + 2^{l_2}F_{k+l}.$$

When $l = 1$ or 2, a simple calculation shows the validity of the formula of $i(G_1)$. So, by Lemma 2.6, we have

$$\begin{aligned} i(G_1) - i(G_2) &= 2^{l_1-1}3^{l_2}(2F_{k+l+1} - 2F_{k-2}F_l - F_{k+l+2}) + 2^{l_2}(F_{k+l} - F_{k-2}F_{l-1} - F_{k+l}) \\ &= 2^{l_1-1}3^{l_2}(F_{k+l-1} - 2F_{k-2}F_l) - 2^{l_2}F_{k-2}F_{l-1} \\ &= 2^{l_1-1}3^{l_2}(F_{k-1}F_{l+1} - F_{k-2}F_l) - 2^{l_2}F_{k-2}F_{l-1} \\ &= 2^{l_1-1}3^{l_2}(F_{k-1}F_l + F_{k-1}F_{l-1} - F_{k-2}F_l) - 2^{l_2}F_{k-2}F_{l-1} \end{aligned}$$

$$= 2^{l_1-1}3^{l_2}(F_{k-1}F_l - F_{k-2}F_l) + 2^{l_1-1}3^{l_2}F_{k-1}F_{l-1} - 2^{l_2}F_{k-2}F_{l-1} > 0.$$

If $k_1 = k_2 = 1$, it implies that $l_2 = 0$. Obviously, $z(G_2) > z(G_1)$ and $i(G_1) > i(G_2)$.

This completes the proof. $\square$

Lemma 3.3. *If $\Delta < \frac{n-1}{2}$, and $G_1 \in \mathcal{U}_1(n,\Delta)$, then there exists a graph $G_2 \in \mathcal{U}_2(n,\Delta)$ such that $i(G_1) > i(G_2)$.*

Proof. Suppose that $G_1 = C_k^{(l)}(k_1^{l_1}, k_2^{l_2})$. If $k_1 = 1$ and $k_2 = 2$, or $k_1 = k_2 = 1$, with a similar method as in Lemma 3.2, our result follows.

Suppose that $k_1 = 2$. Then the graph G_1 is isomorphic to $C_k^{(l)}(2^{\Delta-2}, m^1)$ where $m \geq 2$. We choose a graph $G_2 = C_{k+l+m}(2^{\Delta-2})$ from $\mathcal{U}_2(n,\Delta)$ as shown in Fig. 5.

By Lemmas 2.1 and 2.8, we have

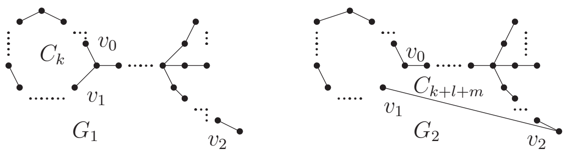

Fig. 5 The graphs G_1 and G_2 for $\Delta < \frac{n-1}{2}$

$$i(G_1) = 3^{\Delta-2}F_{m+2}i(C_k((l-1)^1) + 2^{\Delta-2}F_{m+1}i(C_k((l-2)^1))$$
$$= 3^{\Delta-2}F_{m+2}(F_{k+l+1} - F_{k-2}F_l) + 2^{\Delta-2}F_{m+1}(F_{k+l} - F_{k-2}F_{l-1})$$

and

$$i(G_2) = 3^{\Delta-2}F_{k+l+m+1} + 2^{\Delta-2}F_{k+l+m-1}.$$

Note that the formula of $i(G_1)$ holds if $l = 1$ or $l = 2$. So we have

$$i(G_1) - i(G_2) = 3^{\Delta-2}[F_{m+2}(F_{k+l+1} - F_{k-2}F_l) - F_{k+l+m+1}]$$
$$+ 2^{\Delta-2}[F_{m+1}(F_{k+l} - F_{k-2}F_{l-1}) - F_{k+l+m-1}]$$

Set $A_1 = F_{m+2}(F_{k+l+1} - F_{k-2}F_l) - F_{k+l+m+1}$ and $A_2 = F_{m+1}(F_{k+l} - F_{k-2}F_{l-1}) - F_{k+l+m-1}$. Then, by Lemma 2.6, we have

$$A_1 = F_{m+2}F_{k+l+1} - F_{m+2}F_{k-2}F_l - (F_{k+l+1}F_{m+1} + F_{k+l}F_m)$$
$$= F_mF_{k+l+1} - F_{m+2}F_{k-2}F_l - F_{k+l}F_m$$
$$= F_mF_{k+l-1} - F_{m+2}F_{k-2}F_l$$

$$
\begin{aligned}
&= F_m(F_{k-1}F_{l+1} + F_{k-2}F_l) - (F_{m+1} + F_m)F_{k-2}F_l \\
&= F_mF_{k-1}F_{l+1} - F_{m+1}F_{k-2}F_l \\
&= F_m(F_{k-2} + F_{k-3})F_l + F_mF_{k-1}F_{l-1} - F_mF_{k-2}F_l - F_{m-1}F_{k-2}F_l \\
&= F_mF_{k-3}F_l + F_mF_{k-1}F_{l-1} - F_{m-1}F_{k-2}F_l \\
&= \tfrac{1}{2}(F_m2F_{k-3}F_l - F_{m-1}F_{k-2}F_l + F_mF_{k-1}2F_{l-1} - F_{m-1}F_{k-2}F_l) > 0
\end{aligned}
$$

and

$$
\begin{aligned}
A_2 &= F_{m+1}F_{k+l} - F_{m+1}F_{k-2}F_{l-1} - (F_{m+1}F_{k+l-1} + F_mF_{k+l-2}) \\
&= F_{m+1}F_{k+l-2} - F_{m+1}F_{k-2}F_{l-1} - F_mF_{k+l-2} \\
&= F_{m-1}F_{k+l-2} - F_{m+1}F_{k-2}F_{l-1} \\
&= F_{m-1}(F_{k-1}F_l + F_{k-2}F_{l-1}) - (F_m + F_{m-1})F_{k-2}F_{l-1} \\
&= F_{m-1}F_{k-1}F_l - F_mF_{k-2}F_{l-1}.
\end{aligned}
$$

Note that $A_1 > 0$, thus, by Lemma 2.6, we get

$$
\begin{aligned}
i(G_1) - i(G_2) &= 3^{\Delta-2}A_1 + 2^{\Delta-2}A_2 \\
&> 2^{\Delta-2}(A_1 + A_2) \\
&= 2^{\Delta-2}(F_mF_{k-1}F_{l+1} - F_{m+1}F_{k-2}F_l + F_{m-1}F_{k-1}F_l - F_mF_{k-2}F_{l-1}) \\
&= 2^{\Delta-2}(F_{k-1}F_{m+l} - F_{k-2}F_{m+l}) > 0.
\end{aligned}
$$

Therefore $i(G_1) > i(G_2)$ as desired. By now we complete the proof. $\square$

Lemma 3.4. *Suppose that $4 \le \Delta < \frac{n-1}{2}$. Let G be the graph from $\mathcal{U}(n,\Delta)$ with maximal Hosoya index. Then $G \in \mathcal{U}_2(n,\Delta)$, or*

(1) $G \in \{C^{(1)}_{n-2\Delta+1}(2^{\Delta-1})\} \bigcup \mathcal{U}_2(n,\Delta)$ *if* $n = 2\Delta+2$ *or* $n > 2\Delta+3$ *and* $\Delta > 4$*;*

(2) $G \in \{C^{(1)}_4(2^{\Delta-2}, (n-2\Delta-1)^1), C^{(1)}_{n-2\Delta+1}(2^{\Delta-1})\}$ *if* $n = 2\Delta+3$*, or* $\Delta = 4$.

Proof. From Lemma 3.1, $G \in \mathcal{U}_1(n,\Delta)$ or $G \in \mathcal{U}_2(n,\Delta)$. If the latter holds, we are done. If $G \cong C^{(l)}_k(k_1^{l_1}, k_2^{l_2}) \in \mathcal{U}_1(n,\Delta)$, we claim that $k_1 = 2$. Otherwise, suppose that $k_1 = 1$. With a similar argument that as used in the proof of Lemma 3.2, we can find a graph G_2 from $\mathcal{U}_2(n,\Delta)$ such that $z(G_2) > z(G)$, a contradiction to the choice of G.

Suppose that $k_1 = 2$. Then, G is isomorphic to $C^{(l)}_k(2^{\Delta-2}, m^1)$ where $m \ge 2$. For convenience, we denote G by G_1. Next we claim that $l = 1$. Suppose to the contrary that $l \ge 2$. We choose a graph $G_2 = C_{k+l+m}(2^{\Delta-2})$ from $\mathcal{U}_2(n,\Delta)$ as shown in Fig. 4. By applying Lemma 2.1 to G_1 and G_2 (in a same way as in the proof of Lemma 3.2, denote by G_0 the isomorphic couple $G_1 - v_0v_1$ and $G_2 - v_1v_2$), from Lemmas 2.6 and 2.7, we have

$$\begin{aligned} z(G_1) &= z(G_0) + z(P_{k-2})z(R(2^{\Delta-2}, l-1, m)) \\ &= z(G_0) + 2^{\Delta-2}F_{k-1}F_{l+m+1} + (\Delta-2)2^{\Delta-3}F_lF_{m+1}F_{k-1} \end{aligned}$$

and

$$\begin{aligned} z(G_2) &= z(G_0) + z(R(2^{\Delta-2}, k+l-2, m-1) \\ &= z(G_0) + 2^{\Delta-2}F_{k+l+m-1} + (\Delta-2)2^{\Delta-3}F_{k+l-1}F_m. \end{aligned}$$

So, by Lemma 2.6, we have

$$\begin{aligned} z(G_2) - z(G_1) &= 2^{\Delta-2}(F_{k+l+m-1} - F_{k-1}F_{l+m+1}) + (\Delta-2)2^{\Delta-3}(F_{k+l-1}F_m - F_lF_{m+1}F_{k-1}) \\ &= 2^{\Delta-2}(F_{k-1}F_{l+m+1} + F_{k-2}F_{l+m} - F_{k-1}F_{l+m+1}) \\ &\quad + (\Delta-2)2^{\Delta-3}(F_{k+l-1}F_m - F_lF_{m+1}F_{k-1}) \\ &= 2^{\Delta-2}F_{k-2}F_{l+m} + (\Delta-2)2^{\Delta-3}(F_{k+l-1}F_m - F_lF_{m+1}F_{k-1}) \end{aligned}$$

Set $A = F_{k+l-1}F_m - F_lF_{m+1}F_{k-1}$. Then, from Lemma 2.6, we have

$$\begin{aligned} A &= (F_kF_l + F_{k-1}F_{l-1})F_m - F_{k-1}F_l(F_m + F_{m-1}) \\ &= F_kF_lF_m - F_{k-1}F_mF_{l-2} - F_{k-1}F_lF_{m-1} \\ &= (F_{k-1} + F_{k-2})F_lF_m - F_{k-1}F_mF_{l-2} - F_{k-1}F_lF_{m-1} \\ &= F_{k-1}(F_{l-1} + F_{l-2})(F_{m-1} + F_{m-2}) + F_{k-2}F_lF_m - F_{k-1}F_{l-2}(F_{m-1} + F_{m-2}) \\ &\quad - F_{k-1}(F_{l-1} + F_{l-2})F_{m-1} \\ &= F_{k-1}F_{l-1}F_{m-2} + F_{k-2}F_lF_m - F_{k-1}F_{l-2}F_{m-1} \\ &= \tfrac{1}{2}(F_{k-1}F_{l-1}2F_{m-2} + 2F_{k-2}F_lF_m - 2F_{k-1}F_{l-2}F_{m-1}) \\ &> \tfrac{1}{2}(F_{k-1}F_{l-1}F_{m-1} - F_{k-1}F_{l-2}F_{m-1} + F_{k-1}F_lF_m - F_{k-1}F_{l-2}F_{m-1}) > 0. \end{aligned}$$

So $z(G_2) - z(G_1) > 0$. A contradiction to the maximality of $z(G_1)$. Therefore $G \cong C_k^{(1)}(2^{\Delta-2}, m^1)$.

Set $B = z(G_2) - z(G_1)$. From the above computation and by Lemma 2.9, we have

$$\begin{aligned} B &= z(C_{k+1+m}(2^{\Delta-2})) - z(C_k^{(1)}(2^{\Delta-2}, m^1)) \\ &= 2^{\Delta-2}F_{k-2}F_{m+1} + (\Delta-2)2^{\Delta-3}(F_kF_m - F_{m+1}F_{k-1}) \\ &= \begin{cases} 2^{\Delta-2}F_{k-2}F_{m+1} + (-1)^{k-1}(\Delta-2)2^{\Delta-3}F_{m-k+1} & if \quad k \le m; \\ 2^{\Delta-2}F_{k-2}F_{m+1} + (-1)^{m-1}(\Delta-2)2^{\Delta-3}F_{k-m-1} & if \quad k > m. \end{cases} \end{aligned}$$

It is easy to see that $B > 0$ if $k \le m$ and k is odd, or $m < k$ and m is odd, or $k = 3$, or $k = m+1$. By the choice of G, we only consider the cases where $4 \le k \le m$ and k is even, or $k \ge m+2$ and m is even. By Lemmas 2.1, 2.3 and 2.6, we have

$$\begin{aligned}
z(C_k^{(1)}(2^{\Delta-2}, m^1)) &= z(C_k)z(R(2^{\Delta-2}, m^1) + z(P_{k-1})2^{\Delta-2}F_{m+1} \\
&= (F_{k+1}+F_{k-1})[2^{\Delta-2}(F_{m+1}+F_m)+(\Delta-2)2^{\Delta-3}F_{m+1}]+2^{\Delta-2}F_kF_{m+1} \\
&= 2^{\Delta-2}[(F_{k+1}+F_k+F_{k-1})F_{m+1}+(F_{k+1}+F_{k-1})F_m] \\
&\quad + (\Delta-2)2^{\Delta-3}F_{m+1}(F_{k+1}+F_{k-1}) \\
&= 2^{\Delta-2}[2F_{k+1}F_{m+1}+2F_kF_m+(F_{k+1}+F_{k-1}-2F_k)F_m] \\
&\quad + (\Delta-2)2^{\Delta-3}F_{m+1}(F_{k+1}+F_{k-1}) \\
&= 2^{\Delta-2}[2F_{k+m+1}+F_{k-3}F_m]+(\Delta-2)2^{\Delta-3}F_{m+1}(F_{k+1}+F_{k-1}) \\
&= 2^{\Delta-1}F_{k+m+1}+2^{\Delta-3}[2F_{k-3}F_m+(\Delta-2)F_{m+1}(F_{k+1}+F_{k-1})].
\end{aligned}$$

When $m \ge 4$ and $k \ge m+2$, we have

$$\begin{aligned}
&z(C_{k+m-2}^{(1)}(2^{\Delta-2}, 2^1)) - z(C_k^{(1)}(2^{\Delta-2}, m^1)) \\
&= 2^{\Delta-1}F_{k+m+1}+2^{\Delta-3}[2F_{k+m-5}F_2+(\Delta-2)F_3(F_{k+m-1}+F_{k+m-3})] \\
&\quad - 2^{\Delta-1}F_{k+m+1}+2^{\Delta-3}[2F_{k-3}F_m+(\Delta-2)F_{m+1}(F_{k+1}+F_{k-1})] \\
&= 2^{\Delta-3}[2(F_{k+m-5}-F_{k-3}F_m)+(\Delta-2)(2F_{k+m-1}+2F_{k+m-3}-F_{m+1}F_{k+1}-F_{m+1}F_{k-1})]
\end{aligned}$$

Set $B_1 = F_{k+m-5} - F_{k-3}F_m$ and $B_2 = 2F_{k+m-1} + 2F_{k+m-3} - F_{m+1}F_{k+1} - F_{m+1}F_{k-1}$. Then, by Lemma 2.6, we have

$$\begin{aligned}
B_1 &= F_{k-3}F_{m-1}+F_{k-4}F_{m-2}-F_{k-3}F_m \\
&= F_{k-4}F_{m-2}-F_{k-3}F_{m-2} = -F_{k-5}F_{m-2}, \\
B_2 &= 2(F_{k+1}F_{m-1}+F_kF_{m-2})-F_{m+1}F_{k+1}+2(F_{k-1}F_{m-1}+F_{k-2}F_{m-2})-F_{m+1}F_{k-1} \\
&= F_{k+1}(2F_{m-1}-F_{m+1})+F_{k-1}(2F_{m-1}-F_{m+1})+2F_{m-2}(F_k+F_{k-2}) \\
&= -(F_{k+1}+F_{k-1})F_{m-2}+2F_{m-2}(F_k+F_{k-2}) \\
&= (2F_k-F_{k+1}+2F_{k-2}-F_{k-1})F_{m-2} \\
&= (F_{k-2}+F_{k-4})F_{m-2}.
\end{aligned}$$

So, for $m \ge 4$ and $k \ge m+2$, it follows that

$$\begin{aligned}
z(C_{k+m-2}^{(1)}(2^{\Delta-2}, 2^1)) - z(C_k^{(1)}(2^{\Delta-2}, m^1)) &= 2^{\Delta-3}(2B_1+B_2) \\
&= 2^{\Delta-3}(F_{k-2}+F_{k-4}-2F_{k-5})F_{m-2} > 0 \ (*).
\end{aligned}$$

When $k \ge 4$ and $m \ge k$, we have

$$z(C_4^{(1)}(2^{\Delta-2}, (m+k-4)^1)) - z(C_k^{(1)}(2^{\Delta-2}, m^1))$$

$$= 2^{\Delta-1}F_{k+m+1} + 2^{\Delta-3}[2F_1F_{k+m-4} + (\Delta-2)(F_5+F_3)F_{k+m-3}]$$
$$- 2^{\Delta-1}F_{k+m+1} + 2^{\Delta-3}[2F_{k-3}F_m + (\Delta-2)F_{m+1}(F_{k+1}+F_{k-1})]$$
$$= 2^{\Delta-3}[2(F_{k+m-4} - F_{k-3}F_m) + (\Delta-2)(7F_{k+m-3} - F_{m+1}F_{k+1} - F_{m+1}F_{k-1})]$$
$$= 2^{\Delta-3}2(F_{k-3}F_m + F_{k-4}F_{m-1} - F_{k-3}F_m)$$
$$+ 2^{\Delta-3}(\Delta-2)[7(F_{m-3}F_{k-1} + F_{m-2}F_k) - F_{m+1}F_{k+1} - F_{m+1}F_{k-1}]$$
$$= 2^{\Delta-3}2F_{k-4}F_{m-1} + 2^{\Delta-3}(\Delta-2)[(7F_{m-3} - F_{m+1})F_{k-1} + 7F_{m-2}F_k - F_{m+1}F_{k+1}]$$
$$= 2^{\Delta-2}F_{k-4}F_{m-1}$$
$$+ 2^{\Delta-3}(\Delta-2)[(7F_{m-3} - F_4F_{m-2} - F_3F_{m-3})F_{k-1} + 7F_{m-2}F_k - F_{m+1}F_k - F_{m+1}F_{k-1}]$$
$$= 2^{\Delta-2}F_{k-4}F_{m-1}$$
$$+ 2^{\Delta-3}(\Delta-2)[(5F_{m-3} - 3F_{m-2} - F_{m+1})F_{k-1} + (7F_{m-2} - F_3F_{m-1} - F_2F_{m-2})F_k]$$
$$= 2^{\Delta-2}F_{k-4}F_{m-1} + 2^{\Delta-3}(\Delta-2)[(2F_{m-3} - 3F_{m-4} - F_{m+1})F_{k-1} + (6F_{m-2} - 2F_{m-1})F_k]$$
$$= 2^{\Delta-2}F_{k-4}F_{m-1}$$
$$+ 2^{\Delta-3}(\Delta-2)[(2F_{m-3} - 3F_{m-4} - F_{m+1})F_{k-1} + (2F_{m-2} + 2F_{m-4})(F_{k-1} + F_{k-2})]$$
$$= 2^{\Delta-2}F_{k-4}F_{m-1}$$
$$+2^{\Delta-3}(\Delta-2)[(2F_{m-3} - 3F_{m-4} + 2F_{m-2} + 2F_{m-4} - F_{m+1})F_{k-1} + (2F_{m-2} + 2F_{m-4})F_{k-2}]$$
$$= 2^{\Delta-2}F_{k-4}F_{m-1} + 2^{\Delta-3}(\Delta-2)[-(F_{m-2} + F_{m-4})F_{k-1} + (F_{m-2} + F_{m-4})2F_{k-2}]$$
$$= 2^{\Delta-2}F_{k-4}F_{m-1} + 2^{\Delta-3}(\Delta-2)(F_{m-2} + F_{m-4})(2F_{k-2} - F_{k-1}) > 0 \quad (**).$$

By the inequalities (*) and (**), we find that $z(C_k^{(1)}(2^{\Delta-2}, m^1))$ reaches its maximal value at $m = 2$ or $k = 4$. Here $k \geq m+2$ and m is even, or $4 \leq k \leq m$ and k is even.

Note that $k + m = n - 2\Delta + 3$. So the couple $C_{k+m-2}^{(1)}(2^{\Delta-2}, 2^1)$ and $C_4^{(1)}(2^{\Delta-2}, (m+k-4)^1)$ are just $C_{n-2\Delta+1}^{(1)}(2^{\Delta-1})$ and $C_4^{(1)}(2^{\Delta-2}, (n-2\Delta-1)^1)$, respectively. Finally, we will show that $z(C_{n-2\Delta+1}^{(1)}(2^{\Delta-1})) \geq z(C_4^{(1)}(2^{\Delta-2}, (n-2\Delta-1)^1))$ with the equality holding if and only if $n = 2\Delta+3$ or $\Delta = 4$. In fact, we have, for $n \geq 2\Delta+3$,

$$z(C_{n-2\Delta+1}^{(1)}(2^{\Delta-1})) - z(C_4^{(1)}(2^{\Delta-2}, (n-2\Delta-1)^1))$$
$$= 2^{\Delta-3}[2(F_{n-2\Delta-2} - F_{n-2\Delta-1}) + (\Delta-2)(2F_{n-2\Delta+2} + 2F_{n-2\Delta} - 7F_{n-2\Delta})]$$
$$= 2^{\Delta-3}[-2F_{n-2\Delta-3} + (\Delta-2)(2F_{n-2\Delta+2} - 5F_{n-2\Delta})]$$
$$= 2^{\Delta-3}[-2F_{n-2\Delta-3} + (\Delta-2)(2F_{n-2\Delta+1} - 3F_{n-2\Delta})]$$
$$= 2^{\Delta-3}[-2F_{n-2\Delta-3} + (\Delta-2)F_{n-2\Delta-3}]$$
$$= 2^{\Delta-3}(\Delta-4)F_{n-2\Delta-3} \geq 0,$$

and for $n = 2\Delta + 2$,

$$z(C^{(1)}_{n-2\Delta+1}(2^{\Delta-1})) - z(C^{(1)}_4(2^{\Delta-2}, (n-2\Delta-1)^1)) = 2^{\Delta-3}[-2F_1 + (\Delta-2)(2F_4 + 2F_2 - 7F_2)]$$
$$= 2^{\Delta-3}(\Delta - 4) \geq 0.$$

The proof is completed. $\square$

Next we will prove the following four theorems, in which the graphs from $\mathcal{U}(n, \Delta)$ are characterized with maximal Hosoya index and minimal Merrifield-Simmons index.

Theorem 3.1. *If $\Delta \geq \frac{n+1}{2} > 3$, the graph from $\mathcal{U}(n, \Delta)$ with maximal Hosoya index and minimal Merrifield-Simmons index is $C_3(2^{n-1-\Delta}, 1^{2\Delta-1-n})$. And $z(C_3(2^{n-1-\Delta}, 1^{2\Delta-1-n}))$ $= (3\Delta - n + 1)2^{n-1-\Delta}$, $i(C_3(2^{n-1-\Delta}, 1^{2\Delta-1-n})) = 2^{n-1-\Delta} + 3^{n-\Delta}2^{2\Delta-1-n}$.*

Proof. Suppose that a graph G from $\mathcal{U}(n, \Delta)$ has the maximal Hosoya index or the minimal Merrifield-Simmons index. By Lemmas 3.1 and 3.2, , we have $G \in \mathcal{U}_2(n, \Delta)$.

Thanks to Lemma 2.4, we find that G is $C_{n-\Delta+2}(1^{\Delta-2})$ or of the form $C_k(k_1^{l_1}, k_2^{l_2})$ where $k_1 = 1$, $k_2 = 2$. First we prove that G is not $C_{n-\Delta+2}(1^{\Delta-2})$ by comparing the two indices of $C_{n-\Delta+2}(1^{\Delta-2})$ and $C_{n-\Delta+1}(1^{\Delta-3}, 2^1)$. By Lemma 2.8, we have

$$z(C_{n-\Delta+2}(1^{\Delta-2})) = (\Delta - 1)F_{n-\Delta+2} + 2F_{n-\Delta+1},$$
$$z(C_{n-\Delta+1}(1^{\Delta-3}, 2^1)) = (2\Delta - 3)F_{n-\Delta+1} + 4F_{n-\Delta},$$

and

$$i(C_{n-\Delta+2}(1^{\Delta-2})) = 2^{\Delta-2}F_{n-\Delta+3} + F_{n-\Delta+1},$$
$$i(C_{n-\Delta+1}(1^{\Delta-3}, 2^1)) = 3 \cdot 2^{\Delta-3}F_{n-\Delta+2} + 2F_{n-\Delta}.$$

So we get

$$z(C_{n-\Delta+1}(1^{\Delta-3}, 2^1)) - z(C_{n-\Delta+2}(1^{\Delta-2}))$$
$$= (2\Delta - 3)F_{n-\Delta+1} - (\Delta - 1)F_{n-\Delta+2} + 2(2F_{n-\Delta} - F_{n-\Delta+1})$$
$$= (\Delta - 1)(2F_{n-\Delta+1} - F_{n-\Delta+2}) - F_{n-\Delta+1} + 2F_{n-\Delta-2}$$
$$= (\Delta - 1)F_{n-\Delta-1} - F_{n-\Delta+1} + 2F_{n-\Delta-2}$$
$$= (\Delta - 3)F_{n-\Delta-1} + 2F_{n-\Delta} - F_{n-\Delta+1} > 0,$$

and

$$i(C_{n-\Delta+2}(1^{\Delta-2})) - i(C_{n-\Delta+1}(1^{\Delta-3}, 2^1))$$
$$= 2^{\Delta-3}(2F_{n-\Delta+3} - 3F_{n-\Delta+2}) + F_{n-\Delta+1} - 2F_{n-\Delta}$$

$= 2^{\Delta-3}(2F_{n-\Delta+1} - F_{n-\Delta+2}) - F_{n-\Delta-2}$
$= 2^{\Delta-3}F_{n-\Delta-1} - F_{n-\Delta-2} > 0.$

So we claim that G is of the form $C_k(k_1^{l_1}, k_2^{l_2})$ where $k_1 = 1$ and $k_2 = 2$. Secondly, we claim that

$$z(C_{n-\Delta+1-l}(1^{\Delta-3-l}, 2^{l+1})) > z(C_{n-\Delta+2-l}(1^{\Delta-2-l}, 2^l))$$

and

$$i(C_{n-\Delta+1-l}(1^{\Delta-3-l}, 2^{l+1})) < i(C_{n-\Delta+2-l}(1^{\Delta-2-l}, 2^l))$$

that is to say, after decreasing the length of C_k in $C_k(1^{l_1}, 2^{l_2})$ by 1 and increasing the number of attached P_3's in $C_k(1^{l_1}, 2^{l_2})$ by 1, the Hosoya index increases and the Merrifield–Simmons index decreases.

By Lemma 2.8, we have

$z(C_{n-\Delta+2-l}(1^{\Delta-2-l}, 2^l)) = 2^{l-1}[(2\Delta - 2 - l)F_{n-\Delta+2-l} + 4F_{n-\Delta+1-l}],$
$z(C_{n-\Delta+1-l}(1^{\Delta-3-l}, 2^{l+1})) = 2^l[(2\Delta - 3 - l)F_{n-\Delta+1-l} + 4F_{n-\Delta-l}],$

and

$i(C_{n-\Delta+2-l}(1^{\Delta-2-l}, 2^l)) = 3^l 2^{\Delta-2-l}F_{n-\Delta+3-l} + 2^l F_{n-\Delta+1-l},$
$i(C_{n-\Delta+1-l}(1^{\Delta-3-l}, 2^{l+1})) = 3^{l+1}2^{\Delta-3-l}F_{n-\Delta+2-l} + 2^{l+1}F_{n-\Delta-l}.$

So we get

$z(C_{n-\Delta+1-l}(1^{\Delta-3-l}, 2^{l+1})) - z(C_{n-\Delta+2-l}(1^{\Delta-2-l}, 2^l))$
$= 2^{l-1}[(4\Delta - 6 - 2l)F_{n-\Delta+1-l} + 8F_{n-\Delta-l} - (2\Delta - 2 - l)F_{n-\Delta+2-l} - 4F_{n-\Delta+1-l}]$
$= 2^{l-1}[(4\Delta - 10 - 2l)F_{n-\Delta+1-l} + 8F_{n-\Delta-l} - (2\Delta - 2 - l)F_{n-\Delta+2-l}]$
$= 2^{l-1}[(4\Delta - 18 - 2l)F_{n-\Delta+1-l} + 8F_{n-\Delta-l+2} - (2\Delta - 2 - l)F_{n-\Delta+2-l}]$
$= 2^{l-1}[(2\Delta - 9 - l)2F_{n-\Delta+1-l} - (2\Delta - 10 - l)F_{n-\Delta+2-l}] > 0,$

and

$i(C_{n-\Delta+2-l}(1^{\Delta-2-l}, 2^l)) - i(C_{n-\Delta+1-l}(1^{\Delta-3-l}, 2^{l+1}))$
$= 3^l 2^{\Delta-3-l}[2F_{n-\Delta+3-l} - 3F_{n-\Delta+2-l}] + 2^l[F_{n-\Delta+1-l} - 2F_{n-\Delta-l}]$
$= 3^l 2^{\Delta-3-l}F_{n-\Delta-1-l} - 2^l F_{n-\Delta-l-2} > 0.$

Therefore, for $\Delta \geq \frac{n+1}{2} > 3$, G is $C_3(2^{n-1-\Delta}, 1^{2\Delta-1-n})$. By Lemma 2.8, with a simple calculation, we have

$$z(C_3(2^{n-1-\Delta}, 1^{2\Delta-1-n})) = (3\Delta - n + 1)2^{n-1-\Delta}$$

and

$$i(C_3(2^{n-1-\Delta}, 1^{2\Delta-1-n})) = 2^{n-1-\Delta} + 3^{n-\Delta}2^{2\Delta-1-n}$$

ending the proof. □

Theorem 3.2. *If* $3 < \Delta < \frac{n+1}{2}$*, the graph from* $\mathcal{U}(n,\Delta)$ *with minimal Merrifield-Simmons index is* $C_3(2^{\Delta-3},(n-2\Delta+3)^1)$*. And* $i(C_3(2^{\Delta-3},(n-2\Delta+3)^1)) = 3^{\Delta-2}F_{n-2\Delta+5} + 2^{\Delta-3}F_{n-2\Delta+4}$.

Proof. Suppose that a graph G from $\mathcal{U}(n,\Delta)$ has the minimal Merrifield-Simmons index. By Lemmas 3.1, 3.2 and 3.3, we have $G \in \mathcal{U}_2(n,\Delta)$.

Combining the arguments in the proof of Theorem 3.1, we find that if $3 < \Delta < \frac{n+1}{2}$, G is of the form $C_k(2^{l_1}, k_2^{l_2})$ where $k_2 \geq 2$. In the next step, we will show that, in $G \cong C_k(2^{l_1}, k_2^{l_2})$, $2 \leq k_2 < n-2\Delta+3$ is impossible when $3 < \Delta < \frac{n+1}{2}$.

For $n-2\Delta+3 > l \geq 3$, by Lemmas 2.6 and 2.8, we have

$i(C_{n-2\Delta+6-l}(2^{\Delta-3}, l^1)) = 3^{\Delta-3}F_{n-2\Delta+7-l}F_{l+2} + 2^{\Delta-3}F_{n-2\Delta+5-l}F_{l+1}$,

$i(C_{n-2\Delta+4}(2^{\Delta-2})) = 3^{\Delta-2}F_{n-2\Delta+5} + 2^{\Delta-2}F_{n-2\Delta+3}$.

So for $n-2\Delta+3 > l \geq 3$, we have

$$\begin{aligned}
&i(C_{n-2\Delta+6-l}(2^{\Delta-3}, l^1)) - i(C_{n-2\Delta+4}(2^{\Delta-2}))\\
&= 3^{\Delta-3}(F_{n-2\Delta+7-l}F_{l+2} - 3F_{n-2\Delta+5}) + 2^{\Delta-3}(F_{n-2\Delta+5-l}F_{l+1} - 2F_{n-2\Delta+3})\\
&= 3^{\Delta-3}[F_{n-2\Delta+7-l}F_{l+2} - 3(F_{l+2}F_{n-2\Delta+4-l} + F_{l+1}F_{n-2\Delta+3-l})]\\
&\quad + 2^{\Delta-3}[F_{n-2\Delta+5-l}F_{l+1} - 2(F_{l+1}F_{n-2\Delta+3-l} + F_lF_{n-2\Delta+2-l})]\\
&= 3^{\Delta-3}[2F_{n-2\Delta+3-l}F_{l+2} - 3F_{l+1}F_{n-2\Delta+3-l}] + 2^{\Delta-3}(F_{l+1} - 2F_l)F_{n-2\Delta+2-l}\\
&= 3^{\Delta-3}(2F_l - F_{l+1})F_{n-2\Delta+3-l} - 2^{\Delta-3}(2F_l - F_{l+1})F_{n-2\Delta+2-l} > 0.
\end{aligned}$$

Thus, for $n-2\Delta+3 > l \geq 3$, we have $i(C_{n-2\Delta+4}(2^{\Delta-2})) < i(C_{n-2\Delta+6-l}(2^{\Delta-3}, l^1))$. Finally, we look for the form of G by comparing the Hosoya indices of $C_{n-2\Delta+4}(2^{\Delta-2})$ and $C_3(2^{\Delta-3},(n-2\Delta+3)^1)$. Similarly, we have

$$\begin{aligned}
i(C_3(2^{\Delta-3},(n-2\Delta+3)^1)) &= 3^{\Delta-3}F_4F_{n-2\Delta+5} + 2^{\Delta-3}F_2F_{n-2\Delta+4}\\
&= 3^{\Delta-2}F_{n-2\Delta+5} + 2^{\Delta-3}F_{n-2\Delta+4}.
\end{aligned}$$

Obviously, we get

$$i(C_{n-2\Delta+4}(2^{\Delta-2})) - i(C_3(2^{\Delta-3},(n-2\Delta+3)^1)) = 2^{\Delta-3}(2F_{n-2\Delta+3} - F_{n-2\Delta+4}) > 0.$$

Therefore, if $3 < \Delta < \frac{n+1}{2}$, G is $C_3(2^{\Delta-3}, (n-2\Delta+3)^1)$, and $i(C_3(2^{\Delta-3}, (n-2\Delta+3)^1)) = 3^{\Delta-2}F_{n-2\Delta+5} + 2^{\Delta-3}F_{n-2\Delta+4}$, which finishes the proof. $\square$

Theorem 3.3. *Suppose that $3 < \Delta < \frac{n+1}{2}$. Let $G \in \mathcal{U}(n, \Delta)$ be a graph with the maximal Hosoya index. Then*

(1) G is $C_{n-2\Delta+4}(2^{\Delta-2})$ if $3 < \Delta < 6$, or $\frac{n-2}{2} \leq \Delta < \frac{n+1}{2}$,, or $\Delta = \frac{n-4}{2} < 10$, or $\frac{n-4}{2} > \Delta \in \{6, 7\}$, or $\frac{n-5}{2} > \Delta = 8$;

(2) G is $C_{n-2\Delta+4}(2^{\Delta-2})$ or $C^{(1)}_{n-2\Delta+1}(2^{\Delta-1})$ if $\Delta = 6 = \frac{n-3}{2}$, or $\Delta = 8 = \frac{n-5}{2}$, or $\Delta = 10 = \frac{n-4}{2}$;

(3) G is $C^{(1)}_{n-2\Delta+1}(2^{\Delta-1})$ if $\Delta = \frac{n-3}{2} > 6$, or $\Delta = \frac{n-4}{2} > 10$, or $8 < \Delta < \frac{n-4}{2}$.

And $z(C_{n-2\Delta+4}(2^{\Delta-2})) = 2^{\Delta-3}(\Delta F_{n-2\Delta+4} + 4F_{n-2\Delta+3})$, $z(C^{(1)}_{n-2\Delta+1}(2^{\Delta-1})) = 2^{\Delta-1} F_{n-2\Delta+4} + 2^{\Delta-2}F_{n-2\Delta-2} + 2^{\Delta-2}(\Delta-2)(F_{n-2\Delta+2} + F_{n-2\Delta})$.

Proof. Note that if $\frac{n-1}{2} \leq \Delta < \frac{n+1}{2}$, the graph G must be in $\mathcal{U}_2(n, \Delta)$ from the application of Lemma 3.2. By Lemma 3.4, for $3 < \Delta < \frac{n-1}{2}$, we find that G is either in $\mathcal{U}_2(n, \Delta)$, or $C^{(1)}_{n-2\Delta+1}(2^{\Delta-1})$ or $C^{(1)}_4(2^{\Delta-2}, (n-2\Delta-1)^1)$.

First we will show that if G is in $\mathcal{U}_2(n, \Delta)$, then G must be $C_{n-2\Delta+4}(2^{\Delta-2})$. Considering the arguments in the proof of Theorem 3.1, we find that G is of the form $C_k(2^{l_1}, k_2^{l_2})$ where $k_2 \geq 2$ if $G \in \mathcal{U}_2(n, \Delta)$. Next we will show that, in $C_k(2^{l_1}, k_2^{l_2})$, $k_2 > 2$ is impossible when $3 < \Delta < \frac{n-1}{2}$. For $l \geq 3$, by Lemmas 2.6 and 2.8, we have

$$\begin{aligned} z(C_{n-2\Delta+6-l}(2^{\Delta-3}, l^1)) &= (F_{n-2\Delta+7-l}+F_{n-2\Delta+5-l})2^{\Delta-3}F_{l+1}+(\Delta-3)2^{\Delta-4}F_{l+1}F_{n-2\Delta+6-l} \\ &\quad + 2^{\Delta-3}F_lF_{n-2\Delta+6-l} \\ &= 2^{\Delta-3}(F_{n-2\Delta+7}+F_{l+1}F_{n-2\Delta+5-l})+(\Delta-3)2^{\Delta-4}F_{l+1}F_{n-2\Delta+6-l}, \end{aligned}$$

$$z(C_{n-2\Delta+4}(2^{\Delta-2})) = (F_{n-2\Delta+5} + F_{n-2\Delta+3})2^{\Delta-2} + (\Delta-2)2^{\Delta-3}F_{n-2\Delta+4}.$$

So we obtain

$$\begin{aligned} & z(C_{n-2\Delta+4}(2^{\Delta-2})) - z(C_{n-2\Delta+6-l}(2^{\Delta-3}, l^1)) \\ &= 2^{\Delta-3}(2F_{n-2\Delta+5} + 2F_{n-2\Delta+3} - F_{n-2\Delta+7} - F_{l+1}F_{n-2\Delta+5-l}) + 2^{\Delta-3}F_{n-2\Delta+4} \\ &\quad + (\Delta-3)2^{\Delta-4}(2F_{n-2\Delta+4} - F_{l+1}F_{n-2\Delta+6-l}) \\ &= 2^{\Delta-3}(2F_{n-2\Delta+3} - F_{n-2\Delta+4} - F_{l+1}F_{n-2\Delta+5-l}) + 2^{\Delta-3}F_{n-2\Delta+4} \end{aligned}$$

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

Set $D_1 = 2F_{n-2\Delta+3} - F_{l+1}F_{n-2\Delta+5-l}$ and $D_2 = 2F_{n-2\Delta+4} - F_{l+1}F_{n-2\Delta+6-l}$. Note that $n-2\Delta+6-l \geq 3$ in $C_{n-2\Delta+6-l}(2^{\Delta-3}, l^1)$, that is to say, $l \leq n-2\Delta+3$. If $l = n-2\Delta+3$, then $D_1 = 2F_{n-2\Delta+3} - F_{n-2\Delta+4}F_2 = F_{n-2\Delta+1} > 0$, and $D_2 = 0$, so

$$z(C_{n-2\Delta+4}(2^{\Delta-2})) - z(C_{n-2\Delta+6-l}(2^{\Delta-3}, l^1)) = 2^{\Delta-3}D_1 + (\Delta - 3)2^{\Delta-4}D_2 > 0.$$

If $l \leq n - 2\Delta + 2$, by Lemma 2.6, we have

$$\begin{aligned} D_1 &= 2F_{n-2\Delta+3} - (F_{n-2\Delta+5} - F_lF_{n-2\Delta+4-l}) \\ &= F_lF_{n-2\Delta+4-l} - F_{n-2\Delta+2} \\ &= F_lF_{n-2\Delta+4-l} - (F_lF_{n-2\Delta+3-l} + F_{l-1}F_{n-2\Delta+2-l}) \\ &= F_lF_{n-2\Delta+2-l} - F_{l-1}F_{n-2\Delta+2-l} \geq 0, \end{aligned}$$

$$\begin{aligned} D_2 &= 2F_{l+1}F_{n-2\Delta+4-l} + 2F_lF_{n-2\Delta+3-l} - F_{l+1}F_{n-2\Delta+6-l} \\ &= 2F_lF_{n-2\Delta+3-l} - F_{l+1}F_{n-2\Delta+3-l} > 0. \end{aligned}$$

Then we also have

$$z(C_{n-2\Delta+4}(2^{\Delta-2})) - z(C_{n-2\Delta+6-l}(2^{\Delta-3}, l^1)) = 2^{\Delta-3}D_1 + (\Delta - 3)2^{\Delta-4}D_2 > 0.$$

Therefore G must be $C_{n-2\Delta+4}(2^{\Delta-2})$ if it is in $\mathcal{U}_2(n, \Delta)$, and $z(C_{n-2\Delta+4}(2^{\Delta-2})) = 2^{\Delta-3}(\Delta F_{n-2\Delta+4} + 4F_{n-2\Delta+3})$. Thus we have $G \cong C_{n-2\Delta+4}(2^{\Delta-2})$ if $\frac{n-1}{2} \leq \Delta < \frac{n+1}{2}$. By Lemma 3.4, we find that G must be $C_4^{(1)}(2^{\Delta-2}, (n - 2\Delta - 1)^1)$ or $C_{n-2\Delta+1}^{(1)}(2^{\Delta-1})$ if it does not belong to $\mathcal{U}_2(n, \Delta)$. From the proof of Lemma 3.4, we have $z(C_{n-2\Delta+1}^{(1)}(2^{\Delta-1})) = 2^{\Delta-1}F_{n-2\Delta+4} + 2^{\Delta-3}[2F_{n-2\Delta-2} + 2(\Delta - 2)(F_{n-2\Delta+2} + F_{n-2\Delta})]$. Now we start to determine the graph from $\mathcal{U}(n, \Delta)$ with maximal Hosoya index for $3 < \Delta < \frac{n-1}{2}$. First set $E = z(C_{n-2\Delta+4}(2^{\Delta-2})) - z(C_{n-2\Delta+1}^{(1)}(2^{\Delta-1}))$. Then we have

$$\begin{aligned} E &= 2^{\Delta-1}F_{n-2\Delta+3} + \Delta 2^{\Delta-3}F_{n-2\Delta+4} - 2^{\Delta-1}F_{n-2\Delta+4} \\ &\quad - 2^{\Delta-3}[2F_{n-2\Delta-2} + 2(\Delta - 2)(F_{n-2\Delta+2} + F_{n-2\Delta})] \\ &= -2^{\Delta-1}F_{n-2\Delta+2} + 2^{\Delta-3}[\Delta F_{n-2\Delta+4} - 2F_{n-2\Delta-2} - 2(\Delta - 2)(F_{n-2\Delta+2} + F_{n-2\Delta})] \\ &= -2^{\Delta-1}F_{n-2\Delta+2} + 2^{\Delta-3}(\Delta F_{n-2\Delta+1} - 2\Delta F_{n-2\Delta} + 4F_{n-2\Delta+2} + 2F_{n-2\Delta} + 2F_{n-2\Delta-1}) \\ &= 2^{\Delta-3}(\Delta F_{n-2\Delta+1} - 2\Delta F_{n-2\Delta} + 4F_{n-2\Delta+2} + 2F_{n-2\Delta+1} - 4F_{n-2\Delta+2}) \\ &= 2^{\Delta-3}(2F_{n-2\Delta+1} - \Delta F_{n-2\Delta-2}). \end{aligned}$$

Let $M = 2F_{n-2\Delta+1} - \Delta F_{n-2\Delta-2}$. From Lemma 3.4, it is obvious that G is $C_{n-2\Delta+4}(2^{\Delta-2})$

if $M > 0$, G is $C^{(1)}_{n-2\Delta+1}(2^{\Delta-1})$ if $M < 0$, and G is $C_{n-2\Delta+4}(2^{\Delta-2})$ or $C^{(1)}_{n-2\Delta+1}(2^{\Delta-1})$ if $M = 0$. We only need to consider the value of M. If $3 < \Delta < 6$, it follows that $M > 0$. Also we easily obtain that $M > 0$ when $n = 2\Delta + 2$, i.e. $\Delta = \frac{n-2}{2}$. So in the following we always assume that $6 \leq \Delta < \frac{\Delta-2}{2}$. We distinguish the following three cases.

Case 1. $n = 2\Delta + 3$.

In this case, we have $\Delta = \frac{n-3}{2}$. So $M = 2F_4 - \Delta F_1 = 6 - \Delta$. Obviously, $M < 0$ if $\Delta > 6$ and $M = 0$ if $\Delta = 6$.

Case 2. $n = 2\Delta + 4$.

In this case, we have $\Delta = \frac{n-4}{2}$. So $M = 2F_5 - \Delta F_2 = 10 - \Delta$. Obviously, $M > 0$ if $6 \leq \Delta < 10$ and $M = 0$ if $\Delta = 10$ and $M < 0$ if $\Delta > 10$.

Case 3. $n > 2\Delta + 4$.

In this case, we have $\Delta < \frac{n-4}{2}$. So, by Lemma 2.6, we obtain

$$\begin{aligned} M &= 2(F_{n-2\Delta-2}F_4 + F_{n-2\Delta-3}F_3) - \Delta F_{n-2\Delta-2} \\ &= (6 - \Delta)F_{n-2\Delta-2} + 4F_{n-2\Delta-3}. \end{aligned}$$

Then it is easy to see that $M > 0$ if $6 \leq \Delta \leq 7$. And obviously, $M > 0$ if $\Delta = 8$ and $n > 2\Delta + 5$; $M = 0$ if $\Delta = 8$ and $n = 2\Delta + 5$. If $\Delta \geq 9$, we have

$$M \leq 4F_{n-2\Delta-3} + (6 - 9)F_{n-2\Delta-2} < 0.$$

Combining all the above cases, our results follow. □

Theorem 3.4. *If $\Delta = 3$, the graphs from $\mathcal{U}(n, \Delta)$ with maximal Hosoya index is $C_4((n-4)^1)$ or $C_{n-2}(2^1)$, $z(C_4((n-4)^1)) = z(C_{n-2}(2^1)) = F_{n+1} + 2F_{n-3}$; the graph from $\mathcal{U}(n, \Delta)$ with minimal Merrifield-Simmons index is $C_3((n-3)^1)$, $i(C_3((n-3)^1)) = F_{n+1} + F_{n-1}$.*

Proof. By Lemma 3.1 and Remark 2.1, we find that the graph from $\mathcal{U}(n, 3)$ with maximal Hosoya index and minimal Merrifield-Simmons index is of the form $C_k((n-k)^1)$ where $3 \leq k \leq n-1$.

From Lemmas 2.6 and 2.8, we have

$$\begin{aligned} z(C_k((n-k)^1)) &= F_{n-k+1}(F_{k-1} + F_{k+1}) + F_k F_{n-k} \\ &= F_{n-k+1}F_{k-1} + (F_{n-k+1}F_{k+1} + F_{n-k}F_k) \\ &= F_{k-1}F_{n-(k-1)} + F_{n+1}, \end{aligned}$$

and

$$\begin{aligned} i(C_k((n-k)^1)) &= F_{k+1}F_{n-k+2} + F_{k-1}F_{n-k+1} \\ &= F_{k+1}F_{n-k+2} + F_kF_{n-k+1} - F_kF_{n-k+1} + F_{k-1}F_{n-k+1} \\ &= F_{n+2} - F_{k-2}F_{n+1-k}. \end{aligned}$$

Then, obviously, $z(C_k((n-k)^1)) = z(C_{n-k+2}((k-2)^1))$ for $3 \le k \le n-1$, and $i(C_k((n-k)^1)) = i(C_{n-k+3}((k-3)^1))$ for $4 \le k \le n-1$.

For $3 < k < n-1$, in view of Lemma 2.6, we have

$$\begin{aligned} F_3F_{n-3} - F_kF_{n-k} &= F_3(F_{k-2}F_{n-k} + F_{k-3}F_{n-k-1}) - F_kF_{n-k} \\ &= F_{n-k}(F_3F_{k-2} - F_k) + F_{k-3}F_{n-k-1}F_3 \\ &= -F_{n-k}F_{k-3} + 2F_{k-3}F_{n-k-1} \\ &= F_{k-3}(2F_{n-k-1} - F_{n-k}) > 0, \end{aligned}$$

and

$$\begin{aligned} F_1F_n - F_kF_{n+1-k} &= F_kF_{n+1-k} + F_{k-1}F_{n-k} - F_kF_{n+1-k} \\ &= F_{k-1}F_{n-k} > 0. \end{aligned}$$

So we have $F_kF_{n-k} < F_3F_{n-3}$ and $F_kF_{n+1-k} < F_1F_n$ for $3 < k < n-1$. Then it is easy to see that $F_{k-1}F_{n-(k-1)} < F_3F_{n-3}$ and $F_{k-2}F_{n+1-k} < F_1F_n$ for $4 < k < n-1$. That is to say, the maximal values of $F_{k-1}F_{n-(k-1)}$ and $F_{k-2}F_{n+1-k}$ are attained at $k = 4$ or $n-2$, and $k = 3$, respectively. Therefore, the graph from $\mathcal{U}(n,\Delta)$ with maximal Hosoya index is $C_4((n-4)^1)$ or $C_{n-2}(2^1)$, and the graph from $\mathcal{U}(n,\Delta)$ with minimal Merrifield-Simmons index is $C_3((n-3)^1)$. By Lemma 2.8, we have $z(C_4((n-4)^1)) = z(C_{n-2}(2^1)) = F_{n+1} + 2F_{n-3}$ and $i(C_3((n-3)^1)) = F_{n+1} + F_{n-1}$. This completes the proof. $\square$

Now all the extremal graphs from $\mathcal{U}(n,\Delta)$ maximizing the Hosoya index or minimizing the Merrifield-Simmons index are completely characterized. Finally, we would like to end this paper with the following remark which presents an interesting property of the graph from $\mathcal{U}(n,\Delta)$ with maximal Hosoya index and minimal Merrifield-Simmons index.

Remark 3.1. *In [3], the author showed that, among all trees of order n and with maximum degree Δ, the tree with with maximal Hosoya index and minimal Merrifield-Simmons index is $R(2^{n-1-\Delta}, 1^{2\Delta-n+1})$ if $\Delta \ge \frac{n-1}{2}$ or $R(2^{\Delta-1}, (n-2\Delta+1)^1)$ if $\Delta \le \frac{n-1}{2}$. Note that, when*

$\Delta \geq \frac{n+1}{2}$, the graph from $\mathcal{U}(n,\Delta)$ with maximal Hosoya index and minimal Merrifield-Simmons index is a graph obtained from $R(2^{n-1-\Delta}, 1^{2\Delta-n+1})$ by adding an edge at two pendant vertices of two "rays" of length 1. But for $3 \leq \Delta < \frac{n+1}{2}$ the graphs from $\mathcal{U}(n,\Delta)$ with maximal Hosoya index and minimal Merrifield-Simmons index are not always unique.

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