The extremal fully loaded graphs with respect to Merrifield-Simmons index

Qigang Yu, Zhongxun Zhu*

Faculty of Mathematics and Statistics, South Central University for Nationalities,
Wuhan 430074, P.R. China

Abstract. The Merrifield-Simmons index, denoted by $i(G)$, of a graph G is defined as the total number of its independent sets of G. 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. Let $\mathscr{U}_n^1$ be the set of fully loaded unicyclic graphs. In this paper, we determine graphs with the largest, second-largest, and third-largest Merrifield-Simmons index in $\mathscr{U}_n^1$.
Keywords: Merrifield-Simmons index ; fully loaded unicyclic graph; independent set

AMS subject classification: 05C69, 05C05

1. Introduction

Graph theory has provided chemist with a variety of useful tools, such as topological indices. The *Merrifield-Simmons index* of a graph G is a prominent example of topological indices which is of interest in combinatorial chemistry. It is defined as the total number of independent vertex subsets, denoted by $i(G)$, of a graph G. Merrifield and Simmons showed the correlation between this index and boiling points. For detailed information on the chemical applications, we refer to [1, 2, 3] and the references therein.

Now there have been many papers studying the Merrifield-Simmons index. In [4], Prodinger and Tichy showed that the path P_n has the minimal Merrifield-Simmons index and the star S_n has the maximal Merrifield-Simmons index for all trees with n vertices. In [5, 6], The authors studied the Merrifield-Simmons indices of the unicyclic graphs. Li and Zhu [7] studied bounds for the Merrifield-Simmons index of unicyclic graphs with a given diameter. In [8, 9], Deng et al characterized the bicyclic graph with the maximal and smallest Merrifield-Simmons index. In [10], Li and

E-mail: zzxun73@mail.scuec.edu.cn (Z. Zhu)
* Corresponding author.

Zhu studied tricyclic graphs with maximal Merrifield-Simmons index. Gutman [11], Zhang and Tian [12] studied the Merrifield-Simmons indices of hexagonal chains and catacondensed systems, respectively.

In order to present our results, we introduce some notations and terminologies. For other undefined notation we refer to Bollobás [13]. All graphs considered here are both connected and simple. If $W \subset V(G)$, we denote by $G - W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E \subset E(G)$, we denote by $G - E$ the subgraph of G obtained by deleting the edges of E. If $W = \{v\}$ and $E = \{xy\}$, we write $G - v$ and $G - xy$ instead of $G - \{v\}$ and $G - \{xy\}$, respectively. We denote by $P_n, C_n, K_{1,n-1}$ the path, the cycle, the star on n vertices, respectively. Let $N(v) = \{u|uv \in E(G)\}$, $N[v] = N(v) \cup \{v\}$.

A fully loaded unicyclic graph [14] is a unicyclic graph with the property that there is no vertex with degree less than 3 in its unique cycle. Let $\mathscr{U}_n^1$ be the set of fully loaded unicyclic graphs, and $\mathscr{U}_n^1(l)$ be the subset of $\mathscr{U}_n^1$ in which every graph has a unique cycle of length l. Let the vertices of C_l be ordered successively as $u_1, u_2, \cdots, u_l$, $C_n^l(k_1, k_2, \cdots, k_l)$ be the graph obtained from C_l by attaching exactly k_i pendent edges to the vertex u_i for $i = 1, 2, \cdots, l$, where $k_i \geq 1$ and $\sum_{i=1}^{l} k_i = n - l$.

In this paper, we characterize graphs with the largest, second-largest, and third-largest Merrifield-Simmons index in $\mathscr{U}_n^1$.

We list some results that will be used in this paper.

Lemma 1.1. *[11] Let $G = (V, E)$ be a graph.*

(i) *If $uv \in E(G)$, then $i(G) = i(G - uv) - i(G - \{N[u] \cup N[v]\})$;*
(ii) *If $v \in V(G)$, then $i(G) = i(G - v) + i(G - N[v])$;*
(iii) *If $G_1, G_2, \ldots, G_t$ are the components of the graph G, then $i(G) = \prod_{j=1}^{t} i(G_j)$.*

Lemma 1.2 ([15]). *Let H be a connected graph and T_l be a tree of order $l+1$ with $V(H) \cap T_l = \{v\}$. Then*

$$i(HvT_l) \leq i(HvK_{1,l}).$$

Lemma 1.3 ([16]). *Let H, X, Y be three connected graphs disjoint in pair. Suppose that u, v are two vertices of H, v' is a vertex of X, u' is a vertex of Y. Let G be the graph obtained from H, X, Y by identifying v with v' and u with u', respectively. Let G_1^* be the graph obtained from H, X, Y by identifying vertices v, v', u' and G_2^* be the graph obtained from H, X, Y by identifying vertices u, v', u'. Then*

$$i(G_1^*) > i(G) \qquad or \qquad i(G_2^*) > i(G).$$

Denote by F_n the nth Fibonacci number. Recall that $F_n = F_{n-1}+F_{n-2}$ with initial conditions $F_0 = 1$ and $F_1 = 1$. Then $i(P_n) = F_{n+1}$. For convenience, we let $F_n = 0$ for $n < 0$.

2. Graph in $\mathscr{U}_n^1$ with largest Merrifield-Simmons index

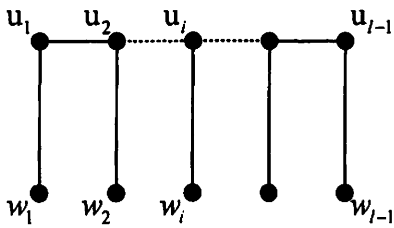

Figure 1: $B_{2(l-1)}^{l-1}$

Lemma 2.1. *Let $B_{2(l-1)}^{l-1}$ be graph in Figure 1, then* $i(C_n^l(1,\cdots,1,n-2l+1)) = 2^{n-2l+1}i(B_{2(l-1)}^{l-1}) + 4i(B_{2(l-3)}^{l-3})$.

Proof. In $C_n^l(1,\cdots,1,n-2l+1)$, let $\{v_1,\cdots,v_{n-2l+1}\}$ be the set of pendant vertices adjacent to u_l. By Lemma 1.1, we have

$$\begin{aligned}
& i(C_n^l(1,\cdots,1,n-2l+1) \\
= \;& i(C_n^l(1,\cdots,1,n-2l+1)-v_1)+i(C_n^l(1,\cdots,1,n-2l+1)-N[v_1]) \\
= \;& i(C_n^l(1,\cdots,1,n-2l+1)-v_1)+i((n-2l)P_1\cup B_{2(l-1)}^{l-1}) \\
= \;& \cdots \\
= \;& i(C_n^l(1,\cdots,1,n-2l+1)-v_1-\cdots-v_{n-2l+1})+ \\
& (2^{n-2l}+\cdots+2^0)i(B_{2(l-1)}^{l-1}) \\
= \;& i(C_n^l(1,\cdots,1,n-2l+1)-v_1-\cdots-v_{n-2l+1}-u_l)+ \\
& i(C_n^l(1,\cdots,1,n-2l+1)-v_1-\cdots-v_{n-2l+1}-N[u_l])+ \\
& (2^{n-2l}+\cdots+2^0)i(B_{2(l-1)}^{l-1}) \\
= \;& i(B_{2(l-1)}^{l-1})+i(2P_1\cup B_{2(l-3)}^{l-3})+(2^{n-2l}+\cdots+2^0)i(B_{2(l-1)}^{l-1}) \\
= \;& 2^{n-2l+1}i(B_{2(l-1)}^{l-1})+4i(B_{2(l-3)}^{l-3}).
\end{aligned}$$

□

Lemma 2.2. $i(C_n^l(1,\cdots,1,n-2l+1)) < i(C_n^{l-1}(1,\cdots,1,n-2l+3))$ *for* $l \geq 4$.

Proof. By Lemma 1.1, we have

$$\begin{aligned} i(B_{2(l-1)}^{l-1}) &= i(B_{2(l-1)}^{l-1} - w_1) + i(B_{2(l-1)}^{l-1} - N[w_1]) \\ &= i(B_{2(l-1)}^{l-1} - w_1 - u_1) + i(B_{2(l-1)}^{l-1} - w_1 - N[u_1]) + i(B_{2(l-2)}^{l-2}) \\ &= 2i(B_{2(l-3)}^{l-3}) + 2i(B_{2(l-2)}^{l-2}) \end{aligned}$$

By Lemma 2.1, we have $i(C_n^{l-1}(1,\cdots,1,n-2l+3) = 2^{n-2l+3}i(B_{2(l-2)}^{l-2}) + 4i(B_{2(l-4)}^{l-4})$.

$$\begin{aligned} & i(C_n^{l-1}(1,\cdots,1,n-2l+3) - i(C_n^l(1,\cdots,1,n-2l+1)) \\ = \; & 2^{n-2l+3}i(B_{2(l-2)}^{l-2}) + 4i(B_{2(l-4)}^{l-4}) - [2^{n-2l+1}i(B_{2(l-1)}^{l-1}) + 4i(B_{2(l-3)}^{l-3})] \\ = \; & 2^{n-2l+1}[4i(B_{2(l-2)}^{l-2}) - i(B_{2(l-1)}^{l-1})] + 4[i(B_{2(l-4)}^{l-4}) - i(B_{2(l-3)}^{l-3})] \\ = \; & 2^{n-2l+1}[4i(B_{2(l-2)}^{l-2}) - (2i(B_{2(l-3)}^{l-3}) + 2i(B_{2(l-2)}^{l-2}))] + \\ & 4[i(B_{2(l-4)}^{l-4}) - i(B_{2(l-3)}^{l-3})] \\ = \; & 2^{n-2l+1}[2i(B_{2(l-2)}^{l-2}) - 2i(B_{2(l-3)}^{l-3})] + 4[i(B_{2(l-4)}^{l-4}) - i(B_{2(l-3)}^{l-3})] \\ = \; & 2^{n-2l+1}[i(B_{2(l-2)}^{l-2}) + (2i(B_{2(l-3)}^{l-3}) + 2i(B_{2(l-4)}^{l-4})) - 2i(B_{2(l-3)}^{l-3})] \\ & +4[i(B_{2(l-4)}^{l-4}) - i(B_{2(l-3)}^{l-3})] \\ > \; & 2^{n-2l+1}i(B_{2(l-2)}^{l-2}) + 4[i(B_{2(l-4)}^{l-4}) - i(B_{2(l-3)}^{l-3})] \\ \geq \; & 2i(B_{2(l-2)}^{l-2}) + 4[i(B_{2(l-4)}^{l-4}) - i(B_{2(l-3)}^{l-3})] \\ = \; & 2[2i(B_{2(l-4)}^{l-4}) + 2i(B_{2(l-3)}^{l-3})] + 4[i(B_{2(l-4)}^{l-4}) - i(B_{2(l-3)}^{l-3})] \\ = \; & 8i(B_{2(l-4)}^{l-4}) > 0 \end{aligned}$$

Hence $i(C_n^l(1,\cdots,1,n-2l+1)) < i(C_n^{l-1}(1,\cdots,1,n-2l+3))$ for $l \geq 4$. □

By direct calculation, we have $i(C_n^3(1,1,n-5)) = 2^{n-2}+4$.

Corollary 2.3. $i(C_n^l(1,\cdots,1,n-2l+1)) < i(C_n^3(1,1,n-5)) = 2^{n-2}+4$ *for* $l \geq 4$.

Lemma 2.4. *For any graph* $G \in \mathscr{U}_n^1(l)$, *we have* $i(G) \leq i(C_n^l(1,\cdots,1,n-2l+1))$. *The equality holds if and only if* $G \cong C_n^l(1,\cdots,1,n-2l+1)$.

Proof. For any graph $G \in \mathscr{U}_n^1(l)$, by Lemma 1.2 repeatedly, we have $i(G) \le i(C_n^l(k_1, \cdots, k_l))$, where $k_i + 1$ be order of the tree attaching at $u_i, i = 1, \cdots, l$.

If $k_1 = 1$, $i(C_n^l(k_1, \cdots, k_l)) = i(C_n^l(1, k_2, k_3, \cdots, k_l))$;

If $k_1 \ge 2$, then $k_2 \ge 2$, let $H = C_{n-k_1-k_2-2}^l(1, 1, k_3 \cdots, k_l)$, $X = K_{1,k_1-1}$, $Y = K_{1,k_2-1}$, by Lemma 1.3, we have

$$i(C_n^l(k_1, \cdots, k_l)) < i(C_n^l(1, k_1 + k_2 - 1, k_3, \cdots, k_l)).$$

Using this procedure repeatedly, we have $i(G) \le i(C_n^l(1, \cdots, 1, n - 2l + 1))$. □

By Corollary 2.3 and Lemma 2.4, we have the following theorem.

Theorem 2.5. *For any graph $G \in \mathscr{U}_n^1$, we have $i(G) \le 2^{n-2} + 4$, the equality holds if and only if $G \cong C_n^3(1, 1, n - 5)$.*

3. Graphs in $\mathscr{U}_n^1$ with second- and third-largest Merrifield-Simmons index

Let $C_3 = u_1u_2u_3$ be the unique triangle of $C_n^3(k_1, k_2, k_3)$, without loss of generality, let $k_1 \le k_2 \le k_3$, and $N(u_1) = \{u_2, u_3, v_1, \cdots, v_{k_1}\}$, $N(u_2) = \{u_1, u_3, w_1, \cdots, w_{k_2}\}$, $N(u_3) = \{u_1, u_2, z_1, \cdots, z_{k_3}\}$.

Lemma 3.1. *Let $n \ge 8$ and $G \in \mathscr{U}_n^1(3) - C_n^3(1, 1, n - 5)$, then $i(G) \le 14 \cdot 2^{n-6} + 8$. The equality holds if and only if $G \cong C_n^3(1, 2, n - 6)$.*

Proof. By direct calculation, we have $i(C_n^3(1, 2, n - 6)) = 14 \cdot 2^{n-6} + 8$.

Case 1 If $G \cong C_n^3(k_1, k_2, k_3)$.

Since $G \ncong C_n^3(1, 1, n - 5)$, then $(k_1, k_2, k_3) \ne (1, 1, n - 5)$.

Subcase 1.1 If $k_1 = 1$, then $k_3 \ge k_2 \ge 2$. If $k_2 = 2$, we have $i(C_n^3(1, k_2, k_3)) = i(C_n^3(1, 2, n - 6))$; if $k_2 \ge 3$, let $H = C_n^3(1, k_2, k_3) - \{w_3, \cdots, w_{k_2}, z_3, \cdots, z_{k_3}\}$, $X = K_{1,k_2-2}$ and $Y = K_{1,k_3-2}$, by Lemma 1.3, we have $i(C_n^3(1, k_2, k_3)) < i(C_n^3(1, 2, k_2 + k_3 - 2)) = i(C_n^3(1, 2, n - 6))$.

Subcase 1.2 If $k_1 \ge 2$, then $k_3 \ge k_2 \ge 2$. Let $H = C_n^3(k_1, k_2, k_3) - \{v_2, \cdots, v_{k_1}, w_2, \cdots, w_{k_2}\}$, $X = K_{1,k_1-1}$ and $Y = K_{1,k_2-1}$, by Lemma 1.3, we have $i(C_n^3(k_1, k_2, k_3)) < i(C_n^3(1, k_1 + k_2 - 1, k_3))$. According to subcase 1.1, we have $i(C_n^3(1, k_1 + k_2 - 1, k_3)) < i(C_n^3(1, 2, n - 6))$. Hence $i(C_n^3(k_1, k_2, k_3)) < i(C_n^3(1, 2, n - 6))$.

Case 2 If $G \ncong C_n^3(k_1, k_2, k_3)$.

Subcase 2.1 $C_n^3(1,1,n-5)$ can't be obtained from G only by Lemma 1.2.

Repeatedly using Lemma 1.2 on G, we finally obtain the graph $C_n^3(k_1,k_2,k_3)$ $((k_1,k_2,k_3) \neq (1,1,n-5))$ and $i(G) < i(C_n^3(k_1,k_2,k_3))$, by case 1, we have $i(G) < i(C_n^3(1,2,n-6))$.

Subcase 2.2 $C_n^3(1,1,n-5)$ can be obtained from G only by Lemma 1.2, repeatedly.

Since $G \not\cong C_n^3(1,1,n-5)$, then G must have the form as indicated in Figure 2, where $T_i, i = 1,2,3$ all are trees, denote G by $G(T_1,T_2,T_3)$. Let $|V(T_i)| = t_i+1, t_i \in [0,n-7] (i = 1,2,3)$. Replace T_i by K_{1,t_i} for $i = 1,2,3$, by Lemma 1.2, we have $i(G(T_1,T_2,T_3)) \leq i(G(K_{1,t_1},K_{1,t_2},K_{1,t_3}))$.

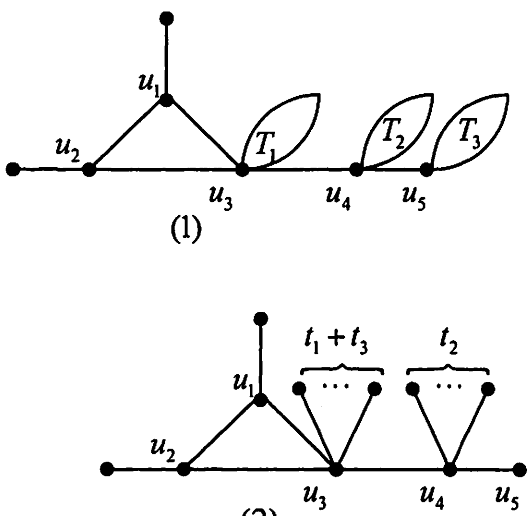

Figure 2: (1) $G(T_1,T_2,T_3)$ and (2) $\tilde{G}$

If $t_3 \geq 1$, let $H = K_{1,t_2+2}, X = C_{n-t_2-t_3-2}(1,1,t_1), Y = K_{1,t_3}$, then $G(K_{1,t_1},K_{1,t_2},K_{1,t_3}) \cong Xu_3Hu_5Y$, by Lemma 1.3, we have

$$i(G(K_{1,t_1},K_{1,t_2},K_{1,t_3})) < i(\tilde{G}),$$

where $\tilde{G}$ show in Figure 2;

If $t_3 = 0$, $G(K_{1,t_1},K_{1,t_2},K_{1,t_3}) \cong \tilde{G}$, hence $i(G(K_{1,t_1},K_{1,t_2},K_{1,t_3})) = i(\tilde{G})$.

By Lemma 1.1, it is easy to obtain that

$$i(\tilde{G}) = 8 \cdot 2^{n-6} + 2^{n-4-t_2} + 2^{t_2+3},$$

where $t_2 \in [0, n-7]$. Hence

$$f(t_2) = i(\tilde{G}) - i(C_n^3(1,2,n-6)) = 2^{n-4-t_2} + 2^{t_2+3} - 6 \cdot 2^{n-6} - 8.$$

But

$$\frac{df(t_2)}{dt_2} = (2^{t_2+3} - 2^{n-4-t_2}) \ln 2,$$

then $\frac{df(t_2)}{dt_2} > 0$ if $t_2 > \lceil \frac{n-7}{2} \rceil$; $\frac{df(t_2)}{dt_2} < 0$ if $t_2 < \lceil \frac{n-7}{2} \rceil$. Hence $f(t_2) \leq \max\{f(0), f(n-7)\}$. Since $f(0) = f(n-7) = -2^{n-5}$, so $i(\tilde{G}) < i(C_n^3(1,2,n-6))$.

Hence, the results hold. □

Theorem 3.2. *Let $n \geq 8$, $C_n^3(1,2,n-6)$ has the second-largest Merrifield-Simmons index among all graphs in $\mathscr{U}_n^1$.*

Proof. For any graph $G \in \mathscr{U}_n^1 - C_n^3(1,1,n-5)$, let C_l be its unique cycle. If $l \geq 4$, by Lemma 2.4, we have $i(G) \leq i(C_n^l(1,\cdots,1,n-2l+1))$. Furthermore, by Lemma 2.2, we have $i(C_n^l(1,\cdots,1,n-2l+1)) \leq i(C_n^4(1,1,1,n-7)) = 11 \cdot 2^{n-6} + 12 < 14 \cdot 2^{n-6} + 8 = i(C_n^3(1,2,n-6))$. If $l = 3$, by Lemma 3.1, we have $i(G) \leq i(C_n^3(1,2,n-6))$. Hence, we obtain the desirable result. □

Now we consider the third largest upper bound of fully loaded graphs with respect to the Merrifield-Simmons index in $\mathscr{U}_n^1$. Let $\check{G}$ be graph as shown in Figure 3.

Lemma 3.3. *Let $n \geq 8$ and $G \in \mathscr{U}_n^1(3) - C_n^3(1,1,n-5) - C_n^3(1,2,n-6)$, then $i(G) \leq 13 \cdot 2^{n-6} + 16$. The equality holds if and only if $G \cong C_n^3(1,3,n-7)$.*

Proof. By Lemma 1.1, it is easy to obtain that $i(C_n^3(1,3,n-7)) = 13 \cdot 2^{n-6} + 16, i(\check{G}) = 13 \cdot 2^{n-6} + 6$.

Case 1. $G \cong C_n^3(k_1,k_2,k_3)$.

Since $G \not\cong C_n^3(1,1,n-5), C_n^3(1,2,n-6)$, then $(k_1,k_2,k_3) \neq (1,1,n-5),(1,2,n-6)$.

subcase 1.1. $k_1 = 1$, then $k_2 \geq 3$.

If $k_2 = 3$, then $i(G) = i(C_n^3(1,3,n-7))$;

If $k_2 \geq 4$, let $H = C_{10}^3(1,3,3), X = K_{1,k_2-3}, Y = K_{1,k_3-3}$, then $G = Xu_2Hu_3Y$, by Lemma 1.3, we have $i(G) < i(C_n^3(1,3,n-7))$.

subcase 1.2. $k_1 = 2$, then $k_2 \geq 2$.

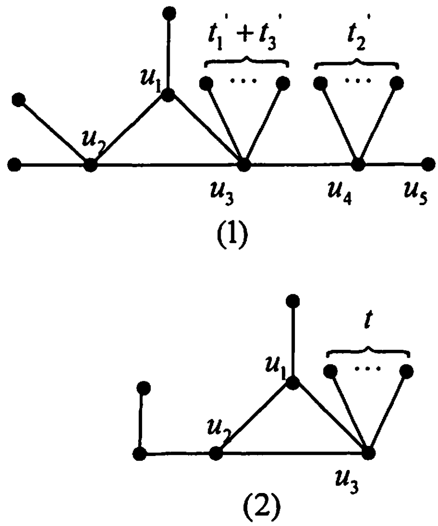

Figure 3: (1) $\hat{G}$ and (2) $\check{G}$

If $k_2 = 2$, then $G = C_n^3(2,2,n-7)$, let $H = C_{n-2}^3(1,1,n-7), X = K_{1,1}, Y = K_{1,1}$, then $G = Xu_1Hu_2Y$, by Lemma 1.3, we have $i(G) < i(C_n^3(1,3,n-7))$.

If $k_2 \geq 3$, then $k_3 \geq 3$, let $H = C_{n-k_2}^3(1,1,n-k_2-5), X = K_{1,1}, Y = K_{1,k_2-1}$, then $G = Xu_1Hu_2Y$, by Lemma 1.3, we have $i(G) < i(C_n^3(1,k_2,n-k_2-5))$. By subcase 1.1, we obtain $i(G) < i(C_n^3(1,3,n-7))$.

Similarly, we can prove the case when $k_1 \geq 3$.

Case 2. $G \not\cong C_n^3(k_1,k_2,k_3)$.

subcase 2.1. Neither $C_n^3(1,1,n-5)$ nor $C_n^3(1,2,n-6)$ can be obtained from G only by Lemma 1.2. Repeatedly using Lemma 1.2 on G, we finally obtain the graph $C_n^3(k_1,k_2,k_3), (k_1,k_2,k_3) \neq (1,1,n-5), (1,2,n-6)$, and $i(G) < i(C_n^3(k_1,k_2,k_3))$, by case 1, we have $i(G) < i(C_n^3(1,3,n-7))$.

subcase 2.2. $C_n^3(1,1,n-5)$ can be obtained from G only by using Lemma 1.2, repeatedly.

As the proof of subcase 2.2 of Lemma 3.1, we have $i(G) < i(\tilde{G})$.

$$g(t_2) = i(\tilde{G}) - i(C_n^3(1,3,n-7)) = 2^{n-4-t_2} + 2^{t_2+3} - 5 \cdot 2^{n-6} - 16.$$

But

$$\frac{dg(t_2)}{dt_2} = (2^{t_2+3} - 2^{n-4-t_2}) \ln 2,$$

if $t_2 > \lceil\frac{n-7}{2}\rceil$, $\frac{dg(t_2)}{dt_2} > 0$; if $t_2 < \lceil\frac{n-7}{2}\rceil$, $\frac{dg(t_2)}{dt_2} < 0$. Hence $g(t_2) \leq \max\{g(0), g(n-7)\} < 0$. Since $g(0) = g(n-7) = -8 - 2^{n-6} < 0$, then $i(\tilde{G}) < i(C_n^3(1,3,n-7))$, hence $i(G) < i(C_n^3(1,3,n-7))$.

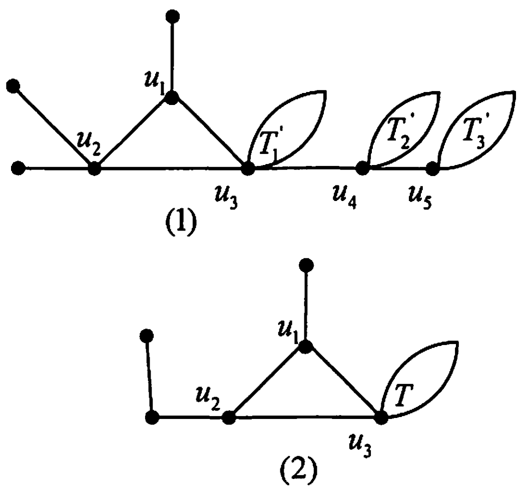

Figure 4: (1) $\hat{G}(T_1', T_2', T_3')$ and (2) $\check{G}(T)$

subcase 2.3. $C_n^3(1,2,n-6)$ can be obtained from G only by using Lemma 1.2, repeatedly.

Then $G \cong \hat{G}(T_1', T_2', T_3')$, or $G \cong \check{G}(T)$, as shown in Figure 4, where $T_i'(i = 1,2,3)$ and T all are trees. Let $|V(T_i')| = t_i' + 1, |V(T)| = t + 1$, then $t_i' \in [0, n-8](i = 1,2,3), t \in [1, n-6]$.

(1) $G \cong \check{G}(T)$.

By Lemma 1.2, we have $i(\check{G}(T)) \leq i(\check{G}) < i(C_n^3(1,3,n-7))$.

(2) $G \cong \hat{G}(T_1', T_2', T_3')$.

If $n = 8$, then $G \cong \hat{G} \cong \check{G}$, then next we only consider $n \geq 9$.

By Lemma 1.2, we have $i(G) \leq i(G(K_{1,t_1'}, K_{1,t_2'}, K_{1,t_3'}))$.

If $t_3' \geq 1$, let $H = K_{1,t_2'+2}, X = C^3_{n-t_2'-t_3'-2}(1,2,t_1'), Y = K_{1,t_3'}$, then $G(K_{1,t_1'}, K_{1,t_2'}, K_{1,t_3'}) \cong X u_3 H u_5 Y$, by Lemma 1.3, we have

$$i(G(K_{1,t_1'}, K_{1,t_2'}, K_{1,t_3'})) < i(\hat{G});$$

If $t_3 = 0$, $G(K_{1,t_1'}, K_{1,t_2'}, K_{1,t_3'}) \cong \hat{G}$, hence $i(G(K_{1,t_1'}, K_{1,t_2'}, K_{1,t_3'})) = i(\hat{G})$

By direct calculation, we have

$$i(\hat{G}) = 14 \cdot 2^{n-7} + 14 \cdot 2^{n-8-t_2'} + 2^{t_2'+4}.$$

Hence

$$h(t_2) = i(\tilde{G}) - i(C_n^3(1,3,n-7)) = 14 \cdot 2^{n-8-t_2'} + 2^{t_2'+4} - 6 \cdot 2^{n-6} - 16.$$

But

$$\frac{dh(t_2')}{dt_2'} = (2^{t_2'+4} - 14 \cdot 2^{n-8-t_2}) \ln 2,$$

if $t_2' > \lceil \frac{n-12+\frac{\ln 14}{\ln 2}}{2} \rceil$, $\frac{dh(t_2')}{dt_2'} > 0$; if $t_2' < \lceil \frac{n-12+\frac{\ln 14}{\ln 2}}{2} \rceil$, $\frac{dh(t_2')}{dt_2'} < 0$. Hence $h(t_2) \leq \max\{h(0), h(n-8)\}$. Since $h(0) = -5 \cdot 2^{n-7} < 0, h(n-8) = -2 - 2^{n-5} < 0$, then $i(\tilde{G}) < i(C_n^3(1,3,n-7))$. Hence $i(G) \leq i(C_n^3(1,3,n-7))$.

We thus complete the proof here. □

Theorem 3.4. *Among all graphs in $\mathscr{U}_n^1 - C_n^3(1,1,n-5) - C_n^3(1,2,n-6)$, we have $i(G) \leq 13 \cdot 2^{n-6} + 16$, the equality holds if and only if $G \cong C_n^3(1,3,n-7)$. That is, $C_n^3(1,3,n-7)$ has the third-largest Merrifield-Simmons index in $\mathscr{U}_n^1$.*

Proof. For any graph $G \in \mathscr{U}_n^1 - C_n^3(1,1,n-5) - C_n^3(1,2,n-6)$, let C_l be its unique cycle. If $l \geq 4$, by Lemma 2.4, we have $i(G) \leq i(C_n^l(1,\cdots,1,n-2l+1))$. Furthermore, by Lemma 2.2, we have $i(C_n^l(1,\cdots,1,n-2l+1)) \leq i(C_n^4(1,1,1,1,n-7)) = 11 \cdot 2^{n-6} + 12 < 13 \cdot 2^{n-6} + 16$. If $l = 3$, by Lemma 2.7, $i(G) \leq 13 \cdot 2^{n-6} + 16$. Hence, we obtain the desirable result. □

References

[1] R.E. Merrifield, H.E. Simmons, Topological Methods in Chemistry (Wiley, New York, 1989).

[2] I. Gutman, O.E. Polansky, Mathmatical Concepts in Organic Chemistry, Springer, Berlin, 1986.

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

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

[5] A.S. Pedersen, P.D. Vestergaard, The number of independent sets in unicyclic graphs, Discrete Appl. Math. 152 (2005) 246-256.

[6] 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.

[7] S. Li, Z. Zhu, The number of independent sets in unicyclic graphs with a given diameter, Discrete Appl. Math. 157 (2009) 1387-1395.

[8] H. Deng, S. Chen, J. Zhang, The Merrifield-Simmons index in $(n, n+1)-$graphs, J. Math. Chem. 43 (1) (2008) 75-91.

[9] H. Deng, The smallest Merrifield-Simmons index of $(n, n+1)-$graphs, Mathematical and Computer Modelling 49 (2009) 320-326.

[10] S. Li, X. Li, Z. Zhu, Tricyclic graphs with maximum Merrifield-Simmons index, Discrete Appl. Math., 158 (2010) 204-212.

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

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

[13] B. Bollobás, Modern Graph Theory (Springer-Verlag, 1998).

[14] H. Hua, Minimizing a class of unicyclic graphs by means of Hosoya index, Mathematical and Computer Modelling 48 (2008) 940-948.

[15] 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.

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