

# The extremal unicyclic graphs with perfect matching with respect to Hosoya index and Merrifield-Simmons index

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**Abstract.** The Hosoya index  $z(G)$  of  $G$  is defined as the total number of the matchings of  $G$  and the Merrifield-Simmons index  $i(G)$  of a graph  $G$  is defined as the total number of the independent sets of  $G$ . Although there are many known results on these two indices, there exists few on a given class of graphs with perfect matchings. In this paper, we first introduce two new strengthened transformations. Then we characterize the extremal unicyclic graphs with perfect matching which have minimal, second minimal Hosoya index, and maximal, second maximal Merrifield-Simmons index, respectively.

**Keywords:** perfect matching; Merrifield-Simmons index; Hosoya index

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## 1. Introduction

Let  $G = (V, E)$  be a simple connected graph. For a vertex  $v$  of  $G$ , denote the degree of  $v$  by  $d_G(v)$ . Two edges of  $G$  are said to be independent if they are not adjacent in  $G$ . A  $k$ -matching of  $G$  is a set of  $k$  mutually independent edges. Two vertices of  $G$  are said to be independent if they are not adjacent in  $G$ . An independent  $k$ -set is a set of  $k$  vertices, no two of which are adjacent.

In 1971 the Japanese chemist Haruo Hosoya introduced a molecular-graph based structure descriptor[5], which he named *topological index* and soon re-named into *Hosoya index*. The *Hosoya index*, denoted by  $z(G)$ , is defined to be the total number of matchings, namely,  $z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} z(G, k)$ , where  $z(G, k)$  is the number of  $k$ -matchings of  $G$ . Note that  $z(G, 0) = 1$  for any graph  $G$ . The *Merrifield-Simmons index* was introduced in 1982 in a paper of Prodinger and Tichy [6], although it is called Fibonacci number of a graph there. The *Merrifield-Simmons index*, denoted by  $i(G)$ , is defined to be the total number of independent sets of  $G$ , that is,  $i(G) = \sum_{k=0}^n i(G, k)$ , where  $i(G, k)$  is the number of  $k$ -independent sets of  $G$ . Note that  $i(G, 0) = 1$  for any graph  $G$ . *Hosoya index* was applied to correlations with boiling point, entropies, calculated bond orders, as well as for coding of chemical structures. Merrifield and Simmons developed a topological approach to structural chemistry. The cardinality of

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topological space in their theory turns out to be equal  $i(G)$  of respective molecular graph  $G$ .

Since then, many researchers have investigated these graphic invariants. An important direction is to determine the graphs with maximal or minimal indices in a given class of graphs. As for  $n$ -vertex trees, it has been shown that the path has the maximal Hosoya index and the star has the minimal Hosoya index [13]. Hou [23] characterized the trees with a given size of matching and having minimal and second minimal Hosoya index, respectively. In [2] Yu and Lv characterized the trees with  $k$  pendant vertices having minimal Hosoya index. In [8] Liu et al. studied trees with a prescribed diameter with respect to the Merrifield-Simmons indices and Hosoya indices. As for  $n$ -vertex unicyclic graphs, Deng and Chen [7] gave the sharp lower bound on the Hosoya index of unicyclic graphs. Ou [14] characterized extremal unicyclic molecular graphs with maximal Hosoya index. In [19], Li et al. characterized unicyclic graphs with minimal, second-minimal, third-minimal, fourth-minimal, fifth-minimal and sixth-minimal Hosoya index. In [20] Li and Zhu, studied the number of independent sets in unicyclic graphs with a given diameter. Wang and Hua [12] characterized the extremal (maximal and minimal) Merrifield-Simmons index of unicyclic graphs with a given girth, Xu and Xu [17] determined all the unicyclic graphs of order  $n$  and with given maximum degree maximizing the Hosoya index and minimizing the Merrifield-Simmons index. In particular, Yu and Tian [3] characterized the extremal graphs with minimal Hosoya indices and maximal Merrifield-Simmons indices, respectively, among all the connected graphs of order  $n$  and size  $n+t-1$  with  $0 \leq t \leq m-1$ , where  $m$  is the matching number. We refer readers to survey papers [1, 10, 11, 15, 16, 21, 18, 22] for further information.

Let  $U$  be a unicyclic graph. The base of  $U$ , denoted by  $\widehat{U}$ , is the minimal unicyclic subgraph of  $U$ . Obviously,  $\widehat{U}$  is a cycle, and  $U$  can be obtained from  $\widehat{U}$  by planting trees to some vertices of  $\widehat{U}$ . Let  $\mathcal{U}(2m, m)$  be the set of all unicyclic graphs on  $2m(m \geq 2)$  vertices with perfect matchings. Although there are many known results on the Hosoya index and Merrifield-Simmons index, there exists few on a given class of graphs with perfect matchings. In this paper, we first introduce two new strengthened transformations. Then the extremal graphs in  $\mathcal{U}(2m, m)$  which have minimal, second minimal Hosoya index, and maximal, second maximal Merrifield-Simmons index, are characterized, respectively.

In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bollobás [4]. 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  $P_n, C_n$  and  $S_n$  the path, the cycle and the star on  $n$  vertices, respectively. Set  $N(v) = \{u | uv \in E(G)\}$ ,  $N[v] = N(v) \cup \{v\}$ .

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

Now we give some lemmas that will be used in the proof of our main results.

**Lemma 1.1** ([13]). Let  $G = (V, E)$  be a graph.

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

**Lemma 1.2** ([13]). 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  $G_1, G_2, \dots, G_t$  are the components of the graph  $G$ , then  $i(G) = \prod_{j=1}^t i(G_j)$ .

**Lemma 1.3** ([9]). 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)  $z(G_1^*) < z(G)$  or  $z(G_2^*) < z(G)$ ;
- (ii)  $i(G_1^*) > i(G)$  or  $i(G_2^*) > i(G)$ .

## 2. Main results

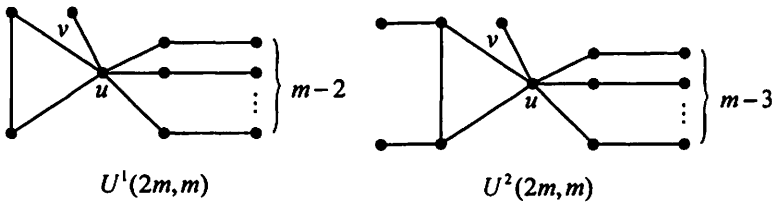


Figure 1: The graphs  $U^1(2m, m)$  and  $U^2(2m, m)$

**Lemma 2.1.** Let  $U^1(2m, m), U^2(2m, m)$  be graphs as shown in Figure 1.

- (i) For integer  $m \geq 2$ ,  $z(U^1(2m, m)) = (m + 4)2^{m-2}$  and  $i(U^1(2m, m)) = 2 \cdot 3^{m-1} + 2^{m-2}$ ;
- (ii) For integer  $m \geq 3$ ,  $z(U^2(2m, m)) = (5m + 13)2^{m-4}$  and  $i(U^2(2m, m)) = 16 \cdot 3^{m-3} + 2^{m-1}$ .

*Proof.* (i) By Lemma 1.1 and Lemma 1.2, we have

$$z(U^1(2m, m)) = z(U^1(2m, m) - u) + \sum_{x \in N(u)} z(U^1(2m, m) - u - x)$$

$$\begin{aligned}
&= z((m-1)P_2 \cup P_1) + z((m-1)P_2) + \\
&\quad 2z((m-2)P_2 \cup 2P_1) + (m-2)z((m-2)P_2 \cup 2P_1) \\
&= (m+4)2^{m-2}. \\
i(U^1(2m, m)) &= i(U^1(2m, m) - u) + i(U^1(2m, m) - N[u]) \\
&= i((m-1)P_2 \cup P_1) + i((m-2)P_1) = 2 \cdot 3^{m-1} + 2^{m-2}.
\end{aligned}$$

Similarly, we can prove (ii). □

Let  $G$  be a connected graph with perfect matchings which, as shown in Figure 2, consists of a connected subgraph  $H$  and a tree  $T$  such that  $T$  is attached to a vertex  $r$  of  $H$ . The vertex  $r$  is called the root of the tree  $T$ , or the root-vertex of  $G$ . The distance between the root  $r$  and the vertex of  $T$  furthest from  $r$  is defined as the height of the tree  $T$ . Throughout the paper,  $|V(T)|$  is the number of vertices of an attached tree  $T$  not including the root  $r$  of  $T$ . If  $v$  is the vertex of  $T$  furthest from the root  $r$ , since  $G$  has perfect matchings, then  $v$  must be a pendant vertex and adjacent with a vertex  $u$  of degree 2.

**Transformation 1** First, take off the vertices  $u, v$  of  $G$  to obtain the graph  $G - u - v$ ; then attach a path of length 2, say  $ru'v'$ , to the root  $r$ . This procedure results in a graph  $G_1$  which still has perfect matchings and is displayed in Figure 2.

If  $|V(T - u - v)| > 2$ , we can repeat above transformation on  $G_1$ . And finally we get a graph  $G_0$  when  $|V(T)|$  is odd or a graph  $H_0$  when  $|V(T)|$  is even. Both  $G_0$  and  $H_0$  are shown in Figure 3.

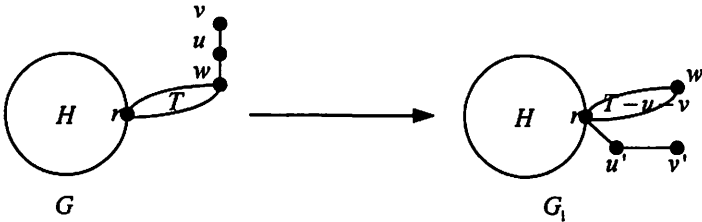


Figure 2: The graphs  $G$  and  $G_1$  in Transformation 1



Figure 3: The graphs  $G_0$  and  $H_0$

**Lemma 2.2.** Let  $G, G_0$  and  $H_0$  be graphs as shown in Figure 2 and Figure 3,

(i)  $z(G) \geq z(G_0)$ , the equality holds if and only if  $G \cong G_0$ ; or  $z(G) \geq z(H_0)$ , the equality holds if and only if  $G \cong H_0$ ;

(ii)  $i(G) \leq i(G_0)$  the equality holds if and only if  $G \cong G_0$ ; or  $i(G) \leq i(H_0)$ , the equality holds if and only if  $G \cong H_0$ .

*Proof.* The proof is by induction on  $|V(T) - \{r\}|$ . Let  $|V(T) - \{r\}| = k$ . For  $k = 1, 2$ , the results hold obviously since  $G \cong G_0$  when  $k = 1$  and  $G \cong H_0$  when  $k = 2$ . Now suppose further that the results hold for the positive integers smaller than  $k$ . We have to distinguish the following two cases.

**Case 1.**  $k$  is odd. By Lemma 1.1, we have

$$\begin{aligned} z(G) &= z(G - v) + z(G - u - v) \\ &= z(G - u - v - w) + 2z(G - u - v), \\ z(G_0) &= z(G_0 - v') + z(G_0 - u' - v') \\ &= z(G_0 - u' - v' - r) + 2z(G_0 - u' - v'). \end{aligned}$$

Obviously,  $G_0 - u' - v' - r = H - r \cup \frac{k-1}{2}P_2 \cup P_1$  is a proper spanning subgraph of  $G - u - v - w$ , then  $z(G - u - v - w) \geq z(G_0 - u' - v' - r)$ . Further by the induction hypothesis, we have  $z(G - u - v) \geq z(G_0 - u' - v')$ , then  $z(G) \geq z(G_0)$ .

By Lemma 1.2, we have

$$\begin{aligned} i(G) &= i(G - v) + i(G - u - v) \\ &= i(G - u - v - w) + 2i(G - u - v) \\ i(G_0) &= i(G_0 - v') + i(G_0 - u' - v') \\ &= i(G_0 - u' - v' - r) + 2i(G_0 - u' - v') \end{aligned}$$

Note that  $G_0 - u' - v' - r = H - r \cup \frac{k-1}{2}P_2 \cup P_1$  is a proper spanning subgraph of  $G - u - v - w$ , then  $i(G - u - v - w) \leq i(G_0 - u' - v' - r)$ . Further by the induction hypothesis, we have  $i(G - u - v) \leq i(G_0 - u' - v')$ , then  $i(G) \leq i(G_0)$ .

Hence the results hold by induction in this case.

**Case 2.**  $k$  is even. The proof is similar to case 1.

This completes the proof.  $\square$

**Remark:** Let  $G, G_0$  be the graphs as shown in Figure 2 and 3, if  $H = K_1$ , by Lemma 2.2,  $G_0$  must be the extremal graph with minimal Hosoya index and maximal Merrifield-Simmons index among all trees with perfect matchings.

As shown in Figure 4, let  $G_2 \in \mathcal{U}(2m, m)$  be a unicyclic graph with  $|V(\widehat{G}_2)| \geq 4$ , it has only one root-vertex, say  $r$ , attached to only some paths of length 2, and the others root-vertices attached to only a pendant edge. Then at least one of adjacent vertex  $v$  of  $r$  on  $\widehat{G}$  has degree 2. Let  $G_3$  be the graph obtained from  $G_2$  by contracting the edge  $rv$ , and then attaching a pendant edge  $rv'$  to  $r$ .

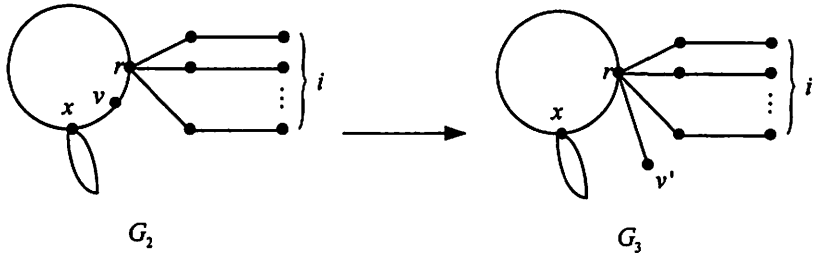


Figure 4: The graphs  $G_2$  and  $G_3$

**Lemma 2.3.** *Let  $G_2, G_3$  be graphs as shown in Figure 4. Then  $z(G_2) > z(G_3)$  and  $i(G_2) < i(G_3)$ .*

*Proof.* Let  $d_{G_2}(v) = \{r, x\}$ . By Lemma 1.1, we have

$$\begin{aligned}
 z(G_2) &= z(G_2 - rv) + z(G_2 - r - v) \\
 &= z(G_2 - rv - r) + \\
 &\quad \sum_{y \in N_{G_2 - rv}(r)} z(G_2 - rv - r - y) + z(G_2 - r - v) \\
 &= z(G_2 - rv - r - v) + z(G_2 - rv - r - v - x) + \\
 &\quad \sum_{y \in N_{G_2 - rv}(r)} z(G_2 - rv - r - y) + z(G_2 - r - v),
 \end{aligned}$$

$$\begin{aligned}
 z(G_3) &= z(G_3 - v') + z(G_3 - v' - r) \\
 &= z(G_3 - v' - r) + \sum_{y \in N_{G_3 - v'}(r) - x} z(G_3 - v' - r - y) + \\
 &\quad z(G_3 - v' - r - x) + z(G_3 - v' - r).
 \end{aligned}$$

Moreover, it is easy to see that we have

$$\begin{aligned}
 G_2 - r - v &= G_2 - rv - r - v \cong G_3 - v' - r, \\
 G_2 - rv - r - v - x &\cong G_3 - v' - r - x, \\
 N_{G_2 - rv}(r) &= N_{G_3 - v'}(r) - x, \\
 G_2 - rv - r - y &\supset G_3 - v' - r - y, y \in N_{G_3 - v'}(r) - x,
 \end{aligned}$$

then

$$\begin{aligned}
 z(G_2) - z(G_3) &= \sum_{y \in N_{G_2 - rv}(r)} z(G_2 - rv - r - y) - \\
 &\quad \sum_{y \in N_{G_3 - v'}(r) - x} z(G_3 - v' - r - y) > 0.
 \end{aligned}$$

Hence  $z(G_2) > z(G_3)$ .

By Lemma 1.2,

$$\begin{aligned} i(G_2) &= i(G_2 - v) + i(G_2 - N[v]) \\ i(G_3) &= i(G_3 - v') + i(G_3 - N[v']) \\ &= i(G_3 - v' - xr) - i(G_3 - v' - N[x] \cup N[r]) + i(G_3 - N[v'] - x) \\ &\quad + i(G_3 - N[v'] - N[x]), \end{aligned}$$

and

$$\begin{aligned} G_2 - v &\cong G_3 - v' - xr, \\ G_2 - N[v] &\cong G_3 - N[v'] - x, \\ G_3 - N[v'] - N[x] &\supset G_3 - v' - N[x] \cup N[r], \end{aligned}$$

hence

$$i(G_3) - i(G_2) = i(G_3 - N[v'] - N[x]) - i(G_3 - v' - N[x] \cup N[r]) > 0.$$

Hence  $i(G_2) < i(G_3)$ . □

**Lemma 2.4.** *For any graph  $G \in \mathcal{U}(2m, m)$  with  $|V(\widehat{G})| \geq 4$ , there exists a graph  $U_0 \in \mathcal{U}(2m, m)$  which satisfies  $z(G) \geq z(U_0)$  and  $i(G) \leq i(U_0)$ , where  $U_0$  is a graph with some root-vertex attached to a pendant edge and all paths of length 2, and the others roots of  $U_0$  attached to only one pendant edge. The equality holds if and only if  $G \cong U_0$ .*

*Proof.* For any graph  $G \in \mathcal{U}(2m, m)$ , it can be obtained from  $\widehat{G}$  by planting trees to some vertices of  $\widehat{G}$ . Repeatedly by Transformation 1,  $G$  can be transformed into a graph  $G_a$  at each root-vertex of  $G$  attached to a pendant edge and all paths of length 2, or only paths of length 2. Moving all the paths of length 2 to some root-vertex, say  $r$ , then the others root-vertices of  $G$  has at most a pendant edge, denote the resulted graph by  $G_b$ . Obviously,  $G_b \in \mathcal{U}(2m, m)$ , by Lemma 1.3,  $z(G) \geq z(G_a) \geq z(G_b)$  and  $i(G) \leq i(G_a) \leq i(G_b)$ , the equality holds if and only if  $G \cong G_a \cong G_b$ .

If there is a pendant edge at  $r$  in  $G_b$ ,  $G_b$  is desirable. Otherwise, by Lemma 2.3,  $G_3$  is desirable. □

Let  $U_0$  be the graph described in Lemma 2.4, we distinguish the following two cases:

(i)  $\widehat{U}_0 \cong C_3$ . Then  $U_0$  must be one of two graphs  $U^1(2m, m)$  and  $U^2(2m, m)$ .

(ii)  $\widehat{U}_0 \not\cong C_3$ . Then we have  $|V(\widehat{U}_0)| \geq 4$ . Assume that  $u$  is the vertex adjacent to the root  $r$  on  $\widehat{U}_0$  clockwise. If  $u$  is not a root-vertex, then  $u$  is a vertex of degree 2, and so is its other adjacent vertex, say  $v_0$ , on  $\widehat{U}_0$ , and the edge  $uv_0$  belongs to perfect matchings of  $U_0$ .

**Transformation 2** Assume that  $|V(\widehat{U}_0)| \geq 4$ . Let  $u$  be not a root-vertex which is adjacent to the root  $r$  on  $\widehat{U}_0$  clockwise, and its other adjacent

vertex on  $\widehat{U}_0$  be  $v_0$ . Contract  $uv_0$  into a single vertex  $u(v_0)$  and add a pendant edge  $u(v_0)v$ , denote the resulted graph by  $U_1$ . If  $|V(\widehat{U}_1)| \geq 4$ , we continue to carry out the following transformation on  $U_1$ : first, take off the vertex  $v$  from  $U_1$  to obtain the graph  $U_1 - v$ ; then contract the edge  $ru(v_0)$ , and attach a path of length 2, say  $ru'v'$ , to the root  $r$ . The resulted graph is denoted by  $U_2$ . This procedure is shown in Figure 5.

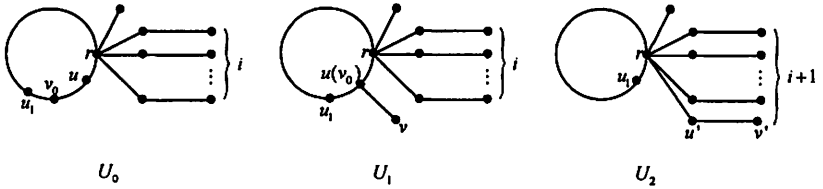


Figure 5: The graphs  $U_0, U_1$  and  $U_2$

**Lemma 2.5.** Let  $U_0, U_1$  and  $U_2$  be graphs as shown in Figure 5,

- (i)  $z(U_0) > z(U_1)$  and  $z(U_1) > z(U_2)$ ;
- (ii)  $i(U_0) < i(U_1)$  and  $i(U_1) < i(U_2)$ .

*Proof.* (i) By Lemma 1.1, we have

$$\begin{aligned} z(U_0) &= z(U_0 - ur) + z(U_0 - u - r) \\ z(U_1) &= z(U_1 - u(v_0)r) + z(U_1 - u(v_0) - r) \end{aligned}$$

Moreover, it is easy to see that we have

$$\begin{aligned} U_0 - ur &\cong U_1 - u(v_0)r, \\ U_0 - u - r &\supset U_1 - u(v_0) - r, \end{aligned}$$

Hence  $z(U_0) > z(U_1)$ .

Similarly,

$$\begin{aligned} z(U_1) &= z(U_1 - u(v_0)) + z(U_1 - u(v_0) - v) + z(U_1 - u(v_0) - r) + \\ &\quad z(U_1 - u(v_0) - u_1) \\ &= z(U_1 - u(v_0)) + z(U_1 - u(v_0) - v) + z(U_1 - u(v_0) - r) + \\ &\quad z((U_1 - u(v_0) - u_1 - v) \cup P_1) \\ &= z(U_1 - u(v_0)) + z(U_1 - u(v_0) - v) + z(U_1 - u(v_0) - r) + \\ &\quad z(U_1 - u(v_0) - u_1 - v), \end{aligned}$$

$$\begin{aligned} z(U_2) &= z(U_2 - u_1r) + z(U_2 - u_1 - r) \\ &= z(U_2 - u_1r - v') + z(U_2 - u_1r - v' - u') + z(U_2 - u_1 - r) \\ &= z(U_2 - u_1r - v' - u') + z(U_2 - u_1r - v' - u' - r) + \\ &\quad z(U_2 - u_1r - v' - u') + z(U_2 - u_1 - r), \end{aligned}$$



and

$$\begin{aligned} U_1 - u(v_0) &\cong U_2 - u_1r - v' - u' \cup P_1, \\ U_1 - u(v_0) - r &\cong U_2 - u_1r - v' - u' - r \cup P_1, \\ U_1 - u(v_0) - v &\cong U_2 - u_1r - v' - u', \end{aligned}$$

Let  $W = U_1 - u(v_0) - u_1 - v$ . Obviously,  $U_2 - u_1 - r \cong (W - r) \cup P_2$ . By Lemma 1.1,

$$z(W) = z(W - r) + \sum_{y \in N_W(r)} z(W - r - y)$$

Let  $rx$  be the pendant edge in  $U_1$ , then  $z(W - r - x) = z(W - r)$ , so

$$\begin{aligned} z(U_1) - z(U_2) &= z(U_1 - u(v_0) - u_1 - v) - z(U_2 - u_1 - r) \\ &= z(W) - 2z(W - r) \\ &= \sum_{y \in N_W(r)} z(W - r - y) - z(W - r) \\ &= \sum_{y \in N_W(r) - x} z(W - r - y) + z(W - r - x) - z(W - r) \\ &= \sum_{y \in N_W(r) - x} z(W - r - y) > 0. \end{aligned}$$

Hence  $z(U_1) > z(U_2)$ .

(ii) By Lemma 1.2, we have

$$\begin{aligned} i(U_0) &= i(U_0 - ur) - i(U_0 - N[u] \cup N[r]), \\ i(U_1) &= i(U_1 - u(v_0)r) - i(U_1 - N[u(v_0)] \cup N[r]) \end{aligned}$$

Moreover, it is easy to see that we have

$$\begin{aligned} U_0 - ur &\cong U_1 - u(v_0)r, \\ U_0 - N[u] \cup N[r] - u_1 &= U_1 - N[u(v_0)] \cup N[r]. \end{aligned}$$

Then

$$i(U_0 - N[u] \cup N[r]) > i(U_1 - N[u(v_0)] \cup N[r]).$$

Hence

$$i(U_1) - i(U_0) = i(U_0 - N[u] \cup N[r]) - i(U_1 - N[u(v_0)] \cup N[r]) > 0,$$

that is,  $i(U_0) < i(U_1)$ .

Furthermore,

$$\begin{aligned} i(U_1) &= i(U_1 - u(v_0)) + i(U_1 - N[u(v_0)]), \\ i(U_2) &= i(U_2 - u') + i(U_2 - N[u']) \\ &= i(U_2 - u' - u_1r) - i(U_2 - u' - N[u_1] \cup N[r]) + \\ &\quad i(U_2 - N[u'] - u_1) + i(U_2 - N[u'] - N[u_1]), \end{aligned}$$

and

$$\begin{aligned}U_1 - u(v_0) &\cong U_2 - u' - u_1r, \\U_1 - N[u(v_0)] &\cong U_2 - N[u'] - u_1, \\U_2 - N[u'] - N[u_1] &\supset U_2 - u' - N[u_1] \cup N[r],\end{aligned}$$

then

$$i(U_2) - i(U_1) = i(U_2 - N[u'] - N[u_1]) - i(U_2 - u' - N[u_1] \cup N[r]) > 0$$

Hence  $i(U_2) > i(U_1)$ . □

In order to obtain the minimal Hosoya index and maximal Merrifield-Simmons index in  $\mathcal{U}(n, m)$ , by *Translation 1* and Lemma 2.2, 2.3, we only want to consider the graph  $U_0$  described in Lemma 2.4. Furthermore, by *Translation 2* and Lemma 2.5, we only want to discuss the graph  $U_0$  in  $\mathcal{U}(n, m)$  with base  $C_3$ , then  $U_0 \cong U^1(2m, m)$  or  $U_0 \cong U^2(2m, m)$ . By Lemma 2.1, we obtain our main results:

**Theorem 2.6.** *Let  $G \in \mathcal{U}(2m, m)(m \geq 2)$ ,  $z(G) \geq (m + 4)2^{m-2}$  and  $i(G) \leq 2 \cdot 3^{m-1} + 2^{m-2}$ . The equality holds if and only if  $G \cong U^1(2m, m)$ .*

**Theorem 2.7.** *Let  $G \in \mathcal{U}(2m, m) \setminus U^1(2m, m)(m \geq 3)$ , then  $z(G) \geq (5m + 13)2^{m-4}$  and  $i(G) \leq 16 \cdot 3^{m-3} + 2^{m-1}$ . The equality holds if and only if  $G \cong U^2(2m, m)$ .*

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