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

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Abstract

The Hosoya index and the Merrifield-Simmons index of a graph are defined as the total numbers of its matchings and its independent sets, respectively. In this paper, we characterize the unicyclic graphs with extremal Hosoya indices and Merrifield-Simmons indices, respectively.

1 Introduction

The Hosoya index or Z-index $Z(G)$ and the Merrifield-Simmons index or σ-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 total number of matchings (independent edge subsets) and the total number of independent vertex subsets of a graph, respectively. The Z-index was introduced by Hosoya [1,2] in 1971, and it turned out to be applicable to several questions of molecular chemistry. For example, the connections with physic-chemical properties such as boiling point, entropy or heat of vaporization are well studied.

Similar connections are known for the σ-index, introduced by Merrifield and Simmons [3] in 1989. For detailed information on the chemical applications, we refer to [3,4,5].

Several papers deal with the characterization of the extremal graphs with respect to these two indices in several given graph classes, usually, trees, unicyclic graphs, bicyclic graphs and certain structures involving pentagonal and hexagonal cycles are of major interest [6-26]. It turns out that typically the graphs of smallest Hosoya index coincide with those of largest Merrifield-Simmons index and vice versa. In view of the similar definitions, this might not be too surprising; however, the correlations between these two indices are not fully understood yet.

In this paper, we first deal with the characterization of the extremal unicyclic graphs of girth $r \geq 3$ with the largest Hosoya index and the smallest Merrifield-Simmons index in unicyclic graphs, then we characterize the unicyclic graphs with the largest and the second largest Merrifield-Simmons index and the smallest and the second smallest Hosoya index. These turn out again that the unicyclic graphs of largest (smallest) Hosoya index coincide with those of smallest (largest) Merrifield-Simmons index.

Let $G = (V, E)$ be a simple connected graph with the vertex set V and the edge set E. For any $v \in V$, $N_G(v)$ denotes the neighbors of v, and $d_G(v) = |N(v)|$ is the degree of v, $N_G[v] = \{v\} \cup \{u|uv \in E(G)\}$. A leaf is a vertex of degree one.

If $E' \subseteq E(G)$ and $W \subseteq V(G)$, then $G - E'$ and $G - W$ denote the subgraphs of G obtained by deleting the edges of E' and the vertices of W, respectively. If a graph G has components $G_1, G_2, \cdots, G_t$, then G is denoted by $\bigcup_{i=1}^{t} G_i$. We denote P_n the path on n vertices, C_n the cycle on n vertices, and S_n the star consisting of one center vertex adjacent to $n-1$ leaves.

The following basic results will be used and can be found in the references cited.

(i) If v is a vertex of G, then

$$Z(G) = Z(G - \{v\}) + \sum_{x \in N_G(v)} Z(G - \{v, x\})$$

$$i(G) = i(G - \{x\}) + i(G - N_G[x])$$

(ii) If uv is an edge of G, then

$$Z(G) = Z(G - uv) + Z(G - \{u, v\})$$

$$i(G) = i(G - uv) + i(G - \{N_G[u] \cup N_G[v]\})$$

(iii) If G is a graph with components G_1, G_2, $\cdots$, G_k, then

$$Z(G) = \prod_{i=1}^{k} Z(G_i) \text{ and } i(G) = \prod_{i=1}^{k} i(G_i)$$

(v) $Z(C_n) = f(n-1) + f(n+1)$; $Z(P_0) = 0$, $Z(P_1) = 1$ and $Z(P_n) = f(n+1)$ for $n \geq 2$.

$i(P_n) = f(n+2)$ for any $n \in \mathbb{N}$; $i(C_n) = f(n-1) + f(n+1)$ for any $n \geq 3$

where f(0)=0, $f(1) = 1$ and $f(n) = f(n-1) + f(n-2)$ for $n \geq 2$ denotes the sequence of Fibonacci numbers.

Lemma 1.1. $f(n) = f(k)f(n-k+1) + f(k-1)f(n-k)$ for $1 \leq k \leq n$.
Proof. We prove this result by induction on k.
$f(1)f(n) + f(0)f(n-1) = f(n)$.

Suppose that $f(k-1)f(n-k+2)+f(k-2)f(n-k+1)=f(n)$. Then

$$\begin{aligned} & f(k)f(n-k+1)+f(k-1)f(n-k) \\ = \; & f(k-1)f(n-k+1)+f(k-1)f(n-k)+f(k-2)f(n-k+1) \\ = \; & f(k-1)f(n-k+2)+f(k-2)f(n-k+1) \\ = \; & f(n). \end{aligned}$$

2 Transformations increasing the Hosoya index and decreasing the Merrifield-Simmons index

For convenience, we introduce two transformations in this section, which increase the Hosoya index and decrease the Merrifield-Simmons index.

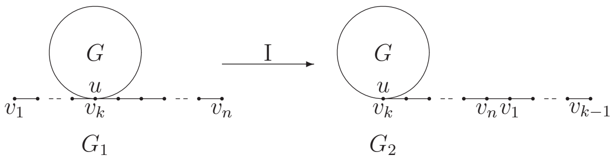

Figure 1. Transformation I.

Transformation I. Let $G \neq P_1$ be a connected graph and choose $u \in V(G)$. G_1 denotes the graph that results from identifying u with the vertex v_k of a simple path $v_1v_2\cdots v_n$, $1<k<n$; G_2 is obtained from G_1 by deleting $v_{k-1}v_k$ and adding v_1v_n (see Figure 1).

Lemma 2.1([17]). Let G_1 and G_2 be the graphs in Figure 1. Then
(i)$Z(G_1) < Z(G_2)$;
(ii)$i(G_1) > i(G_2)$.

Remark. Repeating Transformation I, any tree T attached on the cycle C_r in an unicyclic graph G with girth r can be changed into a path as showed in Figure 2. And the Hosoya index increase and the Merrifield-Simmons index decrease.

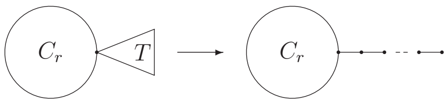

Figure 2. A tree T attached on the cycle C_r can be changed into a path.

Transformation II. Let $P = uu_1u_2 \cdots u_tv$ be a path in G and $G \neq P$, the degrees of $u_1, \cdots, u_t$ in G are 2. G_1 denotes the graph that results from identifying u with the vertex v_k of a simple path $v_1v_2 \cdots v_k$ and identifying v with the vertex v_{k+1} of a simple path $v_{k+1}v_{k+2} \cdots v_n$, $1 < k < n-1$; G_2 is obtained from G_1 by deleting $v_{k-1}v_k$ and adding v_1v_n, G_3 is obtained from G_1 by deleting $v_{k+1}v_{k+2}$ and adding v_1v_n (see Figure 3).

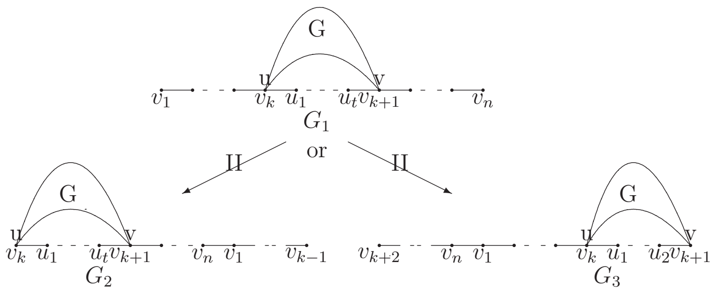

Figure 3. Transformation II.

Lemma 2.2. Let G_1, G_2 and G_3 be the graphs in Figure 3. Then
(i) $Z(G_1) < Z(G_2)$ or $Z(G_1) < Z(G_3)$;
(ii) $i(G_1) > i(G_2)$ or $i(G_1) > i(G_3)$.

Proof. (i) Let $X = N_G(u) - \{u_1\}$ and $Y = N_G(v) - \{u_t\}$.

$$A = Z(G - \{u, u_1, \cdots, u_t, v\})$$

$$B = \sum_{y \in Y} Z(G - \{u, u_1, \cdots, u_t, v, y\})$$

$$C = \sum_{x \in X} Z(G - \{u, u_1, \cdots, u_t, v, x\})$$

$$D = \sum_{x \in X} \sum_{y \in Y} Z(G - \{u, u_1, \cdots, u_t, v, y\})$$

$$\begin{aligned}
Z(G_1) &= Z(G_1 - \{u\}) + \sum_{x \in X} Z(G_1 - \{u, x\}) + Z(G_1 - \{u, u_1\}) \\
&\quad + Z(G_1 - \{u, v_{k-1}\}) \\
&= Z(G_1 - \{u, v\}) + \sum_{y \in Y} Z(G_1 - \{u, v, y\}) + Z(G_1 - \{u, v, u_t\}) \\
&\quad + Z(G_1 - \{u, v, v_{k+2}\}) + \sum_{x \in X} Z(G_1 - \{u, x, v\}) \\
&\quad + \sum_{x \in X} \sum_{y \in Y} Z(G_1 - \{u, x, v, y\}) + \sum_{x \in X} Z(G_1 - \{u, x, v, u_t\}) \\
&\quad + \sum_{x \in X} Z(G_1 - \{u, x, v, v_{k+2}\}) + Z(G_1 - \{u, u_1, v\}) \\
&\quad + \sum_{y \in Y} Z(G_1 - \{u, u_1, v, y\}) + Z(G_1 - \{u, u_1, v, u_t\}) \\
&\quad + Z(G_1 - \{u, u_1, v, v_{k+2}\}) + Z(G_1 - \{u, v_{k-1}, v\}) \\
&\quad + \sum_{y \in Y} Z(G_1 - \{u, v_{k-1}, v, y\}) + Z(G_1 - \{u, v_{k-1}, v, u_t\}) \\
&\quad + Z(G_1 - \{u, v_{k-1}, v, v_{k+2}\}) \\
&= Af(k)f(n-k)f(t+1) + Bf(k)f(n-k)f(t+1) \\
&\quad + Af(k)f(n-k)f(t) + Af(k)f(n-k-1)f(t+1) \\
&\quad + Cf(k)f(n-k)f(t+1) + Df(k)f(n-k)f(t+1) \\
&\quad + Cf(k)f(n-k)f(t) + Cf(k)f(n-k-1)f(t+1) \\
&\quad + Af(k)f(n-k)f(t) + Bf(k)f(n-k)f(t) \\
&\quad + Af(k)f(n-k)f(t-1) + Af(k)f(n-k-1)f(t) \\
&\quad + Af(k-1)f(n-k)f(t+1) + Bf(k-1)f(n-k)f(t+1) \\
&\quad + Af(k-1)f(n-k)f(t) + Af(k-1)f(n-k-1)f(t+1) \\
&= A[f(k)f(n-k)f(t+1) + f(k)f(n-k)f(t) \\
&\quad + f(k)f(n-k-1)f(t+1) + f(k)f(n-k)f(t) \\
&\quad + f(k)f(n-k)f(t-1) + f(k)f(n-k-1)f(t) \\
&\quad + f(k-1)f(n-k)f(t+1) + f(k-1)f(n-k)f(t) \\
&\quad + f(k-1)f(n-k-1)f(t+1)] + B[f(k)f(n-k)f(t+1) \\
&\quad + f(k)f(n-k)f(t) + f(k-1)f(n-k)f(t+1)] \\
&\quad + C[f(k)f(n-k)f(t+1) + f(k)f(n-k)f(t) \\
&\quad + f(k)f(n-k-1)f(t+1)] + Df(k)f(n-k)f(t+1) \\
&= A[f(k+1)f(n-k+1)f(t+1) + f(k+1)f(n-k)f(t) \\
&\quad + f(k)f(n-k+1)f(t) + f(k)f(n-k)f(t-1)] \\
&\quad + B[f(k+1)f(n-k)f(t+1) + f(k)f(n-k)f(t)] \\
&\quad + C[f(k)f(n-k+1)f(t+1) + f(k)f(n-k)f(t)] \\
&\quad + Df(k)f(n-k)f(t+1)
\end{aligned}$$

$$\begin{aligned}
Z(G_2) &= Z(G_2-\{u\})+\sum_{x\in X} Z(G_2-\{u,x\})+Z(G_2-\{u,u_1\})\\
&= Z(G_2-\{u,v\})+\sum_{y\in Y} Z(G_2-\{u,v,y\})+Z(G_2-\{u,v,u_t\})\\
&\quad +Z(G_2-\{u,v,v_{k+2}\})+\sum_{x\in X} Z(G_2-\{u,x,v\})\\
&\quad +\sum_{x\in X}\sum_{y\in Y} Z(G_2-\{u,x,v,y\})+\sum_{x\in X} Z(G_2-\{u,x,v,u_t\})\\
&\quad +\sum_{x\in X} Z(G_2-\{u,x,v,v_{k+2}\})+Z(G_2-\{u,u_1,v\})\\
&\quad +\sum_{y\in Y} Z(G_2-\{u,u_1,v,y\})+Z(G_2-\{u,u_1,v,u_t\})\\
&\quad +Z(G_2-\{u,u_1,v,v_{k+2}\})\\
&= Af(n-1)f(t+1)+Bf(n-1)f(t+1)+Af(n-1)f(t)\\
&\quad +Af(n-2)f(t+1)+Cf(n-1)f(t+1)+Df(n-1)f(t+1)\\
&\quad +Cf(n-1)f(t)+Cf(n-2)f(t+1)+Af(n-1)f(t)\\
&\quad +Bf(n-1)f(t)+Af(n-1)f(t-1)+Af(n-2)f(t)\\
&= A[f(n-1)f(t+1)+f(n-1)f(t)+f(n-2)f(t+1)\\
&\quad +f(n-1)f(t)+f(n-1)f(t-1)+f(n-2)f(t)]\\
&\quad +B[f(n-1)f(t+1)+f(n-1)f(t)]\\
&\quad +C[f(n-1)f(t+1)+f(n-1)f(t)+f(n-2)f(t+1)]\\
&\quad +Df(n-1)f(t+1)\\
&= A[f(n)f(t+1)+f(n+1)f(t)+f(n-1)f(t-1)]\\
&\quad +B[f(n-1)f(t+1)+f(n-1)f(t)]\\
&\quad +C[f(n)f(t+1)+f(n-1)f(t)]\\
&\quad +Df(n-1)f(t+1)
\end{aligned}$$

$$\begin{aligned}
Z(G_3) &= Z(G_3-\{u\})+\sum_{x\in X} Z(G_3-\{u,x\})\\
&\quad +Z(G_3-\{u,u_1\})+Z(G_3-\{u,v_{k-1}\})\\
&= Z(G_3-\{u,v\})+\sum_{y\in Y} Z(G_3-\{u,v,y\})+Z(G_3-\{u,v,u_t\})\\
&\quad +\sum_{x\in X} Z(G_3-\{u,x,v\})+\sum_{x\in X}\sum_{y\in Y} Z(G_3-\{u,x,v,y\})\\
&\quad +\sum_{x\in X} Z(G_3-\{u,x,v,u_t\})+Z(G_3-\{u,u_1,v\})\\
&\quad +\sum_{y\in Y} Z(G_3-\{u,u_1,v,y\})+Z(G_3-\{u,u_1,v,u_t\})\\
&\quad +Z(G_3-\{u,v_{k-1},v\})+\sum_{y\in Y} Z(G_3-\{u,v_{k-1},v,y\})\\
&\quad +Z(G_3-\{u,v_{k-1},v,u_t\})
\end{aligned}$$

$$
\begin{aligned}
&= Af(n-1)f(t+1)+Bf(n-1)f(t+1)+Af(n-1)f(t)\\
&\quad +Cf(n-1)f(t+1)+Df(n-1)f(t+1)+Cf(n-1)f(t)\\
&\quad +Af(n-1)f(t)+Bf(n-1)f(t)+Af(n-1)f(t-1)\\
&\quad +Af(n-2)f(t+1)+Bf(n-2)f(t+1)+Af(n-2)f(t)\\
&= A[f(n-1)f(t+1)+f(n-1)f(t)+f(n-1)f(t)\\
&\quad +f(n-1)f(t-1)+f(n-2)f(t+1)+f(n-2)f(t)]\\
&\quad +B[f(n-1)f(t+1)+f(n-1)f(t)+f(n-2)f(t+1)]\\
&\quad +C[f(n-1)f(t+1)+f(n-1)f(t)]\\
&\quad +Df(n-1)f(t+1)\\
&= A[f(n)f(t+1)+f(n+1)f(t)+f(n-1)f(t-1)]\\
&\quad +B[f(n)f(t+1)+f(n-1)f(t)]\\
&\quad +C[f(n-1)f(t+1)+f(n-1)f(t)]\\
&\quad +Df(n-1)f(t+1)
\end{aligned}
$$

If $B \leq C$, then by Lemma 1.1

$$
\begin{aligned}
\Delta_1 = {} & Z(G_2)-Z(G_1)\\
= {} & A[(f(n)-f(k+1)f(n-k+1))f(t+1)+(f(n+1)-f(k+1)f(n-k)\\
& -f(k)f(n-k+1))f(t)+(f(n-1)-f(k)f(n-k))f(t-1)]\\
& +B[(f(n-1)-f(k+1)f(n-k))f(t+1)+(f(n-1)-f(k)f(n-k))f(t)]\\
& +C[(f(n)-f(k)f(n-k+1))f(t+1)+(f(n-1)-f(k)f(n-k))f(t)]\\
& +D[f(n-1)-f(k)f(n-k)]f(t+1)\\
\\
= {} & A[-f(k-1)f(n-k-1)f(t+1)+f(k-1)f(n-k-1)f(t)\\
& +f(k-1)f(n-k-1)f(t-1)]\\
& +B[-f(k-1)f(n-k-2)f(t+1)+f(k-1)f(n-k-1))f(t)]\\
& +C[f(k-1)f(n-k)f(t+1)+f(k-1)f(n-k-1)f(t)]\\
& +Df(k-1)f(n-k-1)f(t+1)\\
= {} & B[-f(k-1)f(n-k-2)f(t+1)+f(k-1)f(n-k-1))f(t)]\\
& +C[f(k-1)f(n-k)f(t+1)+f(k-1)f(n-k-1)f(t)]\\
& +Df(k-1)f(n-k-1)f(t+1)>0
\end{aligned}
$$

If $B > C$, then by Lemma 1.1

$$
\begin{aligned}
\Delta_2 = {} & z(G_3)-z(G_1)\\
= {} & A[(f(n)-f(k+1)f(n-k+1))f(t+1)+(f(n+1)\\
& -f(k+1)f(n-k)-f(k)f(n-k+1))f(t)+(f(n-1)\\
& -f(k)f(n-k))f(t-1)]+B[(f(n)-f(k+1)f(n-k))f(t+1)\\
& +(f(n-1)-f(k)f(n-k))f(t)]\\
& +C[(f(n-1)-f(k)f(n-k+1))f(t+1)\\
& +(f(n-1)-f(k)f(n-k))f(t)]\\
& +D[f(n-1)-f(k)f(n-k)]f(t+1)\\
= {} & B[f(k)f(n-k-1)f(t+1)+f(k-1)f(n-k-1))f(t)]\\
& +C[-f(k-2)f(n-k-1)f(t+1)+f(k-1)f(n-k-1)f(t)]\\
& +Df(k-1)f(n-k-1)f(t+1)>0
\end{aligned}
$$

(ii) Let

$$A' = i(G - \{u, u_1, \cdots, u_t, v\})$$

$$B' = i(G - \{u, u_1, \cdots, u_t\} \cup N_G[v])$$

$$C' = i(G - \{u_1, \cdots, u_t, v\} \cup N_G[u])$$

$$D' = i(G - N_G[u] \cup N_G[v])$$

$$\begin{aligned} i(G_1) &= i(G_1 - \{u\}) + i(G_1 - N_G[u]) \\ &= i(G_1 - \{u, v\}) + i(G_1 - \{u\} \cup N_{G_1}[v]) \\ &\quad + i(G_1 - \{v\} \cup N_{G_1}[u]) + i(G_1 - N_{G_1}[u] \cup N_{G_1}[v]) \\ &= A' f(k+1) f(n-k+1) f(t+2) + B' f(k+1) f(n-k) f(t+1) \\ &\quad + C' f(k) f(n-k+1) f(t+1) + D' f(k) f(n-k) f(t) \end{aligned}$$

$$\begin{aligned} i(G_2) &= i(G_2 - \{u\}) + i(G_2 - N_G[u]) \\ &= i(G_2 - \{u, v\}) + i(G_2 - \{u\} \cup N_{G_2}[v]) \\ &\quad + i(G_2 - \{v\} \cup N_{G_2}[u]) + i(G_2 - N_{G_2}[u] \cup N_{G_2}[v]) \\ &= A' f(n) f(t+2) + B' f(n-1) f(t+1) \\ &\quad + C' f(n) f(t+1) + D' f(n-1) f(t) \end{aligned}$$

$$\begin{aligned} i(G_3) &= i(G_3 - \{u\}) + i(G_3 - N_G[u]) \\ &= i(G_3 - \{u, v\}) + i(G_3 - \{u\} \cup N_{G_3}[v]) \\ &\quad + i(G_3 - \{v\} \cup N_{G_3}[u]) + i(G_3 - N_{G_3}[u] \cup N_{G_3}[v]) \\ &= A' f(n) f(t+2) + B' f(n) f(t+1) \\ &\quad + C' f(n-1) f(t+1) + D' f(n-1) f(t) \end{aligned}$$

If $B > C$, then $A' > B' > C' > D'$. By Lemma 1.1, we have

$$\begin{aligned} \Delta'_1 &= i(G_1) - i(G_2) \\ &= A'[f(k+1) f(n-k+1) - f(n)] f(t+2) \\ &\quad + B'[f(k+1) f(n-k) - f(n-1)] f(t+1) \\ &\quad + C'[f(k) f(n-k+1) - f(n)] f(t+1) \\ &\quad + D'[f(k) f(n-k) - f(n-1)] f(t) \\ &= A' f(k-1) f(n-k-1) f(t+2) \\ &\quad + B' f(k-1) f(n-k-2) f(t+1) \\ &\quad - C' f(k-1) f(n-k) f(t+1) \\ &\quad - D' f(k-1) f(n-k-1) f(t) \\ &> C'[f(k-1) f(n-k-1) f(t+2) + f(k-1) f(n-k-2) f(t+1) \\ &\quad - f(k-1) f(n-k) f(t+1) - f(k-1) f(n-k-1) f(t)] \\ &= 0 \end{aligned}$$

If $B' \leq C'$, then $A' > C' \geq B' > D'$. By Lemma 1.1, we have

$$\begin{aligned}
\Delta_2' &= i(G_1) - i(G_3) \\
&= A'[f(k+1)f(n-k+1) - f(n)]f(t+2) \\
&\quad +B'[f(k+1)f(n-k) - f(n)]f(t+1) \\
&\quad +C'[f(k)f(n-k+1) - f(n-1)]f(t+1) \\
&\quad +D'[f(k)f(n-k) - f(n-1)]f(t) \\
&= A'f(k-1)f(n-k-1)f(t+2) \\
&\quad -B'f(k)f(n-k-1)f(t+1) \\
&\quad +C'f(k-2)f(n-k-1)f(t+1) \\
&\quad -D'f(k-1)f(n-k-1)f(t) \\
&> B'[f(k-1)f(n-k-1)f(t+2) - f(k)f(n-k-1)f(t+1) \\
&\quad +f(k-2)f(n-k-1)f(t+1) - f(k-1)f(n-k-1)f(t)] \\
&= 0
\end{aligned}$$

The proof is completed.

3 The largest Hosoya index and the smallest Merrifield-Simmons index of unicyclic graphs

In this section, we give the largest Hosoya index and the smallest Merrifield-Simmons index of unicyclic graphs with order n and girth r, and characterize the extremal graphs.

Let $\mathcal{U}(n,r)$ denote the set of all unicyclic graphs with order n and girth r, $H_{n,r}$ the unicyclic graph that results from identifying one vertex u of C_r with the vertex v_0 of a simple path $v_0v_1v_2\cdots v_{n-r}$ of length $n-r$.

Theorem 3.1. Let $G \in \mathcal{U}(n,r)$. Then

(i) $Z(G) \leq Z(H_{n,r}) = f(n+1) + f(r-1)f(n-r+1)$ with the equality if and only if $G \cong H_{n,r}$,

(ii)([16]) $i(G) \geq i(H_{n,r}) = f(n+1) + f(r-1)f(n-r+2)$ with the equality if and only if $G \cong H_{n,r}$, and $G \cong C_n$ or $G \cong H_{n,3}$ for $r = 3$.

Proof. Let x,y and v_1 be the vertices adjacent to u in $H_{n,r}$. Then

$$\begin{aligned} Z(H_{n,r}) = &\ Z(H_{n,r} - \{u\}) + Z(H_{n,r} - \{u,x\}) + Z(H_{n,r} - \{u,y\}) \\ &+ Z(H_{n,r} - \{u,v_1\}) \\ = &\ f(r)f(n-r+1) + 2f(r-1)f(n-r+1) + f(r)f(n-r) \\ = &\ f(r)f(n-r+2) + 2f(r-1)f(n-r+1) \\ = &\ f(n+1) + f(r-1)f(n-r+1) \end{aligned}$$

$$\begin{aligned} i(H_{n,r}) = &\ i(H_{n,r} - \{u\}) + i(H_{n,r} - \{u,x,y,v_1\}) \\ = &\ f(r+1)f(n-r+2) + f(r-1)f(n-r+1) \\ = &\ f(r)f(n-r+2) + f(r-1)f(n-r+1) + f(r-1)f(n-r+2) \\ = &\ f(n+1) + f(r-1)f(n-r+2) \end{aligned}$$

$i(C_n) = i(H_{n,3}) = f(n+1) + f(n-1)$

Repeating transformation I on G, the graph G can be changed into G' that results from attaching some paths on some vertices of C_r. By Lemma 2.1, we have $Z(G') \geq Z(G)$ and $i(G') \leq i(G)$. Then, repeating transformation II on the graph G', G' can be changed into the graph $H_{n,r}$. By Lemma 2.2, we have $Z(H_{n,r}) \geq Z(G')$ with the equality if and only if $G' \cong H_{n,r}$; $i(H_{n,r}) \leq i(G')$ with the equality if and only if $G' \cong H_{n,r}$, and $G \cong C_n$ or $G \cong H_{n,3}$ for $r = 3$.

So the proof of theorem is completed.

Corollary 3.2. (i) C_n is the unique graph with the largest Hosoya index among all unicyclic graphs of order n;

(ii)([16]) C_n and $H_{n,3}$ are the graphs with the smallest Merrifield-Simmons index among all unicyclic graphs of order n.

Proof. For any $G \in \mathcal{U}(n,r)$, we have $Z(G) \leq Z(H_{n,r})$ and $i(G) \geq i(H_{n,r})$ from Theorem 3.1. By Lemma 1.1,

$Z(C_n) - Z(H_{n,r}) = f(n-1) - f(r-1)f(n-r+1) = f(r-2)f(n-r) \geq 0$

with the equality if and only if $n = r$;

$i(C_n) - i(H_{n,r}) = f(n-1) - f(r-1)f(n-r+2) = f(r-3)f(n-r) \geq 0$

with the equality if and only if $n = r$ or $r = 3$.

So, C_n is the unique graph with the largest Hosoya index among all unicyclic graphs of order n, C_n and $H_{n,3}$ are the graphs with the smallest Merrifield-Simmons index among all unicyclic graphs of order n.

4 Transformations decreasing the Hosoya index and increasing the Merrifield-Simmons index

For convenience, we introduce two transformations in this section, which decreasing the Hosoya index and increase the Merrifield-Simmons index.

Transformation III. Let $G \in \mathcal{U}(n,r)$, $C_r = v_1v_2\cdots v_rv_1$ be the unique cycle of graph G. If there is one vertex v with degree more than 2 on the cycle C_r, uv be an edge of G, $N_G(u)$ is the neighborhood of u and $N_G(u) - \{v\} = \{w_1, w_2, \cdots, w_s\}$. Then $G' = G - \{uw_1, uw_2, \cdots, uw_s\} + \{vw_1, vw_2, \cdots, vw_s\}$, as shown in Figure 4.

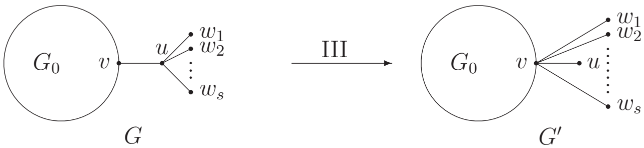

Figure 4. Transformation III.

Lemma 4.1. Let G' is obtained from G by transformation III, then
(i)$i(G') > i(G)$;
(ii) $Z(G') < Z(G)$.

Proof. (i) By the definition of independent sets we have

$$\begin{aligned} i(G) &= i(G-u) + i(G - N_G[u]) \\ &= 2^s i(G_0) + i(G_0 - v) \\ i(G') &= i(G-u) + i(G - N_G[u]) \\ &= i(G_0) + (2^{s+1} - 1) i(G_0 - v) \end{aligned}$$

where $G_0 = G - \{u, w_1, w_2, \cdots, w_s\}$.

Then

$$\begin{aligned} \Delta &= i(G') - i(G) \\ &= (2^s - 1)[2i(G_0 - v) - i(G_0)] \end{aligned}$$

$i(G) \le 2i(G-v)$ since $i(G) = i(G-u) + i(G-N_G[u])$ and $i(G-N_G[v]) \le i(G-v)$. So, $i(G') > i(G)$.

(ii) We have

$$\begin{aligned} Z(G) &= Z(G-uv) + Z(G-\{u,v\}) \\ &= (1+s)\cdot Z(G_0) + Z(G_0 - v) \\ Z(G') &= Z(G_0) + (s+1)\cdot Z(G_0 - v) \end{aligned}$$

and

$$\begin{aligned} \Delta &= Z(G') - Z(G) \\ &= s[Z(G_0 - v) - Z(G_0)] \end{aligned}$$

$Z(G') < Z(G)$ since $Z(G_0 - v) < Z(G_0)$.

So the proof is completed.

Transformation IV. Let G be an unicyclic graph in $\mathcal{U}(n,r)$, $C_r = v_1 v_2 \cdots v_r v_1$ be the unique cycle of G. If there are i and j such that $1 \le i < j \le r$ and $d_G(v_i) = s+2$, $d_G(v_j) = t+2$, $s,t \ge 1$. $N_G(v_i) = \{v_{i-1}, v_{i+1}, u_1, u_2, \cdots, u_s\}$, $N_G(v_j) = \{v_{j-1}, v_{j+1}, w_1, w_2, \cdots, w_t\}$. Then $G' = G - \{v_i u_1, v_i u_2, \cdots, v_i u_s\} + \{v_j u_1, v_j u_2, \cdots, v_j u_s\}$, $G'' = G - \{v_j w_1, v_j w_2, \cdots, v_j w_s\} + \{v_i w_1, v_i w_2, \cdots, v_i w_s\}$, as shown in Figure 5.

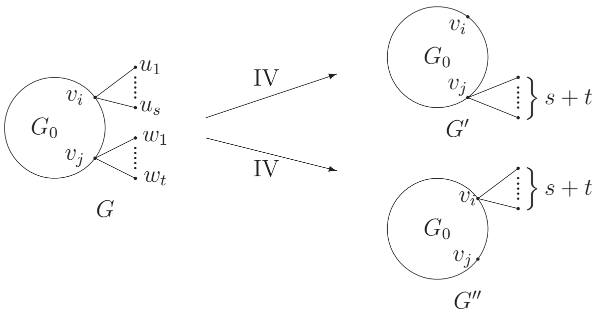

Figure 5. Transformation IV.

Lemma 4.2. Let G' and G'' is obtained from G by transformation IV, then

(i) $i(G') > i(G)$ or $i(G'') > i(G)$;

(ii) $Z(G') < Z(G)$ or $Z(G'') < Z(G)$.

Proof. Whether v_i, v_j are adjacent or not, we have

$$\begin{aligned}
i(G) &= i(G-v_i)+i(G-N_G[v_i]) \\
&= 2^{s+t}i(G_0-v_i-v_j)+2^t i(G_0-\{v_j\cup N_{G_0}[v_i]\}) \\
&\quad +2^s i(G_0-\{v_i\cup N_{G_0}[v_j]\})+i(G_0-\{N_{G_0}[v_j]\cup N_{G_0}[v_i]\}) \\
i(G') &= i(G-v)+i(G-N_G[v]) \\
&= 2^{s+t}[i(G_0-v_i-v_j)+i(G_0-\{v_j\cup N_{G_0}[v_i]\})] \\
&\quad +i(G_0-\{v_i\cup N_{G_0}[v_j]\})+i(G_0-\{N_{G_0}[v_j]\cup N_{G_0}[v_i]\}) \\
i(G'') &= i(G-v)+i(G-N_G[v]) \\
&= 2^{s+t}[i(G_0-v_i-v_j)+i(G_0-\{v_i\cup N_{G_0}[v_j]\})] \\
&\quad +i(G_0-\{v_j\cup N_{G_0}[v_i]\})+i(G_0-\{N_{G_0}[v_j]\cup N_{G_0}[v_i]\})
\end{aligned}$$

where $G_0 = G-\{u_1,u_2,\cdots,u_s,w_1,w_2,\cdots,w_t\}$.

$$\begin{aligned}
\Delta_1 &= i(G')-i(G) \\
&= (2^s-1)\cdot[2^t\cdot i(G_0-\{v_j\cup N_{G_0}[v_i]\})-i(G_0-\{v_i\cup N_{G_0}[v_j]\})] \\
\Delta_2 &= i(G'')-i(G) \\
&= (2^t-1)\cdot[2^s\cdot i(G_0-\{v_i\cup N_{G_0}[v_j]\})-i(G_0-\{v_j\cup N_{G_0}[v_i]\})]
\end{aligned}$$

If $i(G')\le i(G)$, then $i(G_0-\{v_i\cup N_{G_0}[v_j]\})\ge 2^t\cdot i(G_0-\{v_j\cup N_{G_0}[v_i]\})$. And

$$i(G'')-i(G)\ge(2^t-1)(2^{s+t}-1)i(G_0-\{v_j\cup N_{G_0}[v_i]\})>0$$

$$\begin{aligned}
Z(G) &= Z(G-uv)+Z(G-\{u,v\}) \\
&= Z(G_0)+sZ(G_0-v_i)+tZ(G_0-v_j)+stZ(G_0-v_i-v_j) \\
Z(G') &= Z(G-uv)+Z(G-\{u,v\}) \\
&= Z(G_0)+(s+t)Z(G_0-v_j) \\
Z(G'') &= Z(G-uv)+Z(G-\{u,v\}) \\
&= Z(G_0)+(s+t)Z(G_0-v_i)
\end{aligned}$$

$$\begin{aligned}
\Delta_1' &= Z(G)-Z(G') \\
&= s(Z(G_0-v_i)-Z(G_0-v_j)+tZ(G_0-v_i-v_j)) \\
\Delta_2' &= Z(G)-Z(G'') \\
&= t(Z(G_0-v_j)-Z(G_0-v_i)+sZ(G_0-v_i-v_j))
\end{aligned}$$

If $Z(G)\le Z(G')$, then $Z(G_0-v_j)\ge Z(G_0-v_i)+tZ(G_0-v_i-v_j)$. And

$$\begin{aligned}
\Delta_2' &= Z(G)-Z(G'') \\
&\ge t(Z(G_0-v_i)+tZ(G_0-v_i-v_j)-Z(G_0-v_i)+sZ(G_0-v_i-v_j)) \\
&= t(s+t)Z(G_0-v_i-v_j)>0
\end{aligned}$$

So the proof is completed.

5 The smallest Hosoya index and the largest Merrifield-Simmons index of unicyclic graphs

In this section, we characterize the unicyclic graphs with the smallest and the second smallest Hosoya index and the largest and the second largest Merrifield-Simmons index.

Let $\mathcal{U}(n,r)$ denote the set of all unicyclic graphs with order n and girth r and $F_{n,r}$ denote the unicyclic graph constructed by attaching $n-r$ leaves to one vertex on a cycle of length r.

Theorem 5.1. Let $G \in \mathcal{U}(n,r)$ be an arbitrary unicyclic graph with order n and girth r, then

(i) $i(G) \leq i(F_{n,r})$ with the equality if and only if $G \cong F_{n,k}$;

(ii) $Z(G) \geq Z(F_{n,k})$ with the equality if and only if $G \cong F_{n,k}$.

Proof. Repeating transformation III on G, the graph G can be changed into G', in which the edges not on the cycles C_r, are pendent edges. By Lemma 4.1, we have $i(G') \geq i(G)$ and $Z(G') \leq Z(G)$.

Next repeating transformation IV on the graph G', G' can be changed into a graph G'', in which the pendent edges are attached to the same vertex u of C_r, i.e., $G'' \cong F_{n,r}$. By Lemma 4.2, we have $i(F_{n,r}) \geq i(G')$ and $Z(F_{n,k}) \leq Z(G')$.

The equalities hold if and only if no transformations III-IV on G, i.e., $G \cong F_{n,k}$.

So the proof of theorem is completed.

In the following, we give the smallest and the second smallest Hosoya index and the largest and the second largest Merrifield-Simmons index among all unicyclic graphs.

Lemma 5.2. Let $n \geq r > 3$. Then

(i)([16]) $i(F_{n,r}) = f(r-1) + 2^{n-r} f(r+1)$;

(ii) $Z(F_{n,r}) = f(r-1) + f(r+1) + (n-r)f(r)$;

(iii) $i(F_{n,r}) \leq i(F_{n,r-1})$ with the equality if and only if $n = k = 4$;

(iv) $Z(F_{n,r}) > Z(F_{n,r-1})$.

Proof. By deleting a leaf of $F_{n,r}$,

$$i(F_{n,r}) = i(F_{n-1,r}) + 2^{n-r-1}i(P_{r-1}) = i(F_{n-1,r}) + 2^{n-r-1}f(r+1)$$

$$Z(F_{n,r}) = i(F_{n-1,r}) + Z(P_{r-1}) = i(F_{n-1,r}) + f(r)$$

From the recursive relations, we can get (i) and (ii).

$$\begin{aligned} & i(F_{n,r-1}) - i(F_{n,r}) \\ = \; & f(r-2) + 2^{n-r+1}f(r) - f(r-1) - 2^{n-r}f(r+1) \\ = \; & 2^{n-r}f(r-2) - f(r-3) \geq 0 \end{aligned}$$

with the equality if and only if $n = k = 4$.

$$\begin{aligned} & Z(F_{n,r}) - Z(F_{n,r-1}) \\ = \; & f(r-1) + f(r+1) + (n-r)f(r) \\ & -[f(r-2) + f(r) + (n-r+1)f(r-1)] \\ = \; & f(r-3) + (n-r)f(r-2) > 0 \end{aligned}$$

The proof of Lemma 5.2 is completed.

From Theorem 5.1 and Lemma 5.2, Theorem 5.3 is immediate

Theorem 5.3. Let G be an arbitrary unicyclic graph with n vertices. Then

(i) $i(G) \leq 3 \times 2^{n-3} + 1$ with the equality if and only if G is a 4-cycle or $G \cong F_{n,3}$;

(ii) $Z(G) \geq 2n - 2$ with equality if and only if $G \cong F_{n,3}$.

Theorem 5.4. Let G be an arbitrary unicyclic graph with $n \geq 5$ vertices.

(i)([16])If $G \ncong F_{n,3}$ and C_4, then $i(G) \leq 5 \times 2^{n-4} + 2$ with the equality if and only if $G \cong F^1_{n,3}$, $F^1_{n,3}$ is obtained from a C_3 by attaching one leaf to one of its vertices and $n-4$ leaves to another of its vertices (see Figure 6);

(ii) If $G \ncong F_{n,3}$, then $Z(G) \geq 3n - 6$ with the equality if and only if $G \cong F^1_{n,3}$.

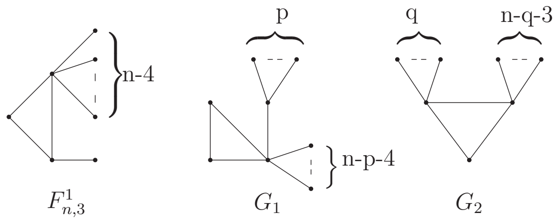

Figure 6. The graphs $F^1_{n,3}$, G_1 and G_2.

Proof. (i) It has been proved in [16].

(ii) Let $C_r = v_1v_2v_3\cdots v_rv_1$ be the unique cycle in G.

If $r \geq 4$, then $Z(G) \geq F_{n,4} = 3n-5 > 3n-6$ by Theorem 5.1 and Lemma 5.2.

If $r = 3$, since $G \ncong F_{n,3}$, G can be changed into G_1 or G_2 by the transformations III and IV, and $Z(G) \geq Z(G_1)$ or $Z(G_2)$ by Lemmas 4.1 and 4.2, where $1 \leq p \leq n-4$ and $1 \leq q \leq n-4$.

Let $g(p) = Z(G_1)$ and $h(q) = Z(G_2)$. $Z(G_1) = (p+1)Z(F_{n-p-1,3}) + 2$ and $g(p) = -2p^2 + (2n-6)p + (2n-2)$. $h(q) = -q^2 + (n-3)q + (2n-2)$ by computing immediately.

Note that $g(p) \geq \min\{g(1), g(n-4)\} = 4n-10 > 3n-6$ and $h(q) \geq \min\{h(1), h(n-4)\} = 3n-6$ with the equality if and only if $q = 1$ or $q = n-4$. So, $Z(G) \geq 3n-6$ with the equality if and only if $G \cong F^1_{n,3}$.

The proof is completed.

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