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Research Article

The Merrifield-Simmons Index and Hosoya Index of $C(n, k, \lambda)$ Graphs

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The Merrifield-Simmons index $i(G)$ of a graph G is defined as the number of subsets of the vertex set, in which any two vertices are nonadjacent, that is, the number of independent vertex sets of G The Hosoya index $z(G)$ of a graph G is defined as the total number of independent edge subsets, that is, the total number of its matchings. By $C(n, k, \lambda)$ we denote the set of graphs with n vertices, k cycles, the length of every cycle is λ, and all the edges not on the cycles are pendant edges which are attached to the same vertex. In this paper, we investigate the Merrifield-Simmons index $i(G)$ and the Hosoya index $z(G)$ for a graph G in $C(n, k, \lambda)$.

1. Introduction

Let $G = (V(G), E(G))$ denote a graph whose set of vertices and set of edges are $V(G)$ and $E(G)$, respectively. For any $v \in V(G)$, we denote the neighbors of v as $N_G(v)$, and $[v] = N_G(v) \cup \{v\}$. By n, we denote the number of vertices of G. All graphs considered here are both finite and simple. We denote, respectively, by S_n, P_n, and C_n the star, path, and cycle with n vertices. For other graph-theoretical terminology and notation, we refer to [1]. By $C(n, k, \lambda)$ we denote the set of graphs with n vertices, k cycles, the length of every cycle is λ and all the edges not on the cycles are pendant edges which are attached to the same vertex, where $n_1 = n - [(\lambda - 1)k + 1] \geq 0$ and the vertex v denotes the central vertex of the graphs, as shown in Figure 1. The Merrifield-Simmons index $i(G)$ of a graph G is defined as the number of subsets of the vertex set, in which any two vertices are nonadjacent, that is, the number of independent vertex sets of G. The Hosoya index $z(G)$ of a graph G is defined as the total

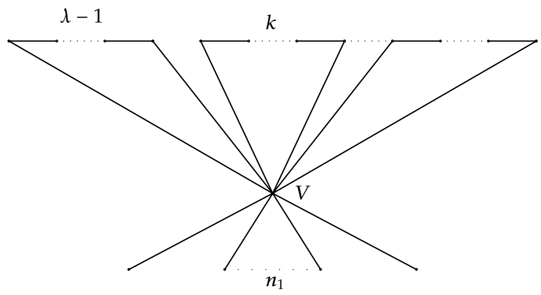

Figure 1: $C(n, k, \lambda)$ graphs.

number of independent edge subsets, that is, the total number of its matchings. In particular, the Merrifield-Simmons index, and Hosoya index of the empty graph are 1.

The Merrifield-Simmons index was introduced by Merrifield and Simmons [2] in 1989, and the Hosoya index was introduced by Hosoya [3] in 1971. They are one of the topological indices whose mathematical properties turned out to be applicable to several questions of molecular chemistry. For example, the connections with physicochemical properties such as boiling point, entropy or heat of vaporization are well studied.

Several papers deal with the Merrifield-Simmons index and Hosoya index in several given graph classes. Usually, trees, unicyclic graphs, and certain structures involving pentagonal and hexagonal cycles are of major interest [4–12].

In this paper, we investigate the Merrifield-Simmons index $i(G)$ and the Hosoya index $z(G)$ for a graph G in $C(n, k, \lambda)$.

2. Some Lemmas

In this section, we gather notations which are used throughout this paper and give some necessary lemmas which will be used to prove our main results.

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. By $\lfloor x \rfloor$ denote the smallest positive integer not less than x. By $f(n)$ we denote the nth Fibonacci number, where $n \in \mathbb{N}$, $f(n) + f(n+1) = f(n+2)$ with initial conditions $f(0) = 0$ and $f(1) = 1$.

The following lemma is obvious.

Lemma 2.1. *Let $n \in N$.*

(i) *If $n \geq 6$, then $f(n) \leq 2^{n-3}$.*

(ii) *If $n \geq 2$, then $f(n) \geq n/2$.*

We will make use of the following two well-known lemmas on the Merrifield-Simmons index and Hosoya index.

Lemma 2.2. *Let $G = (V(G), E(G))$ be a graph.*

(i) *If $G_1, G_2, \ldots, G_m$ are the components of the graph G, then $i(G) = \prod_{i=1}^{m} i(G_i)$ (see [10, Lemma 1]).*

(ii) *If $x \in V(G)$, then $i(G) = i(G - \{x\}) + i(G - [x])$ (see [10, Lemma 1]).*

(iii) *$i(S_n) = 2^{n-1} + 1$; $i(P_n) = f(n+2)$ for any $n \in \mathbb{N}$; $i(C_n) = f(n-1) + f(n+1)$ for any $n \geq 3$ (see [13]).*

Lemma 2.3. *Let $G = (V(G), E(G))$ be a graph.*

(i) *If $G_1, G_2, \ldots, G_m$ are the components of the graph G, then $z(G) = \prod_{i=1}^{m} z(G_i)$ (see [10, Lemma 1]).*

(ii) *If $e = xy \in E(G)$, then $z(G) = z(G - \{e\}) + z(G - \{x, y\})$ (see [14]).*

(iii) *If $x \in V(G)$, then $z(G) = z(G - \{x\}) + \sum_{y \in N_G(x)} z(G - \{x, y\})$ (see [10, Lemma 1]).*

(iv) *$z(S_n) = n$; $z(P_n) = f(n+1)$ for any $n \in \mathbb{N}$; $z(C_n) = f(n-1) + f(n+1)$ for any $n \geq 3$ (see [14]).*

3. The Merrifield-Simmons Index of $C(n, k, \lambda)$

In this section, we will give the Merrifield-Simmons index of $C(n, k, \lambda)$ and their order.

Theorem 3.1. *Let $1 \leq k \leq \lfloor (n-1)/(\lambda-1) \rfloor$, $\lambda \geq 3$. Then*

$$i(C(n, k, \lambda)) = 2^{[n-(\lambda-1)k-1]} f(\lambda+1)^k + f(\lambda-1)^k. \tag{3.1}$$

Proof. By Lemma 2.2 and an elementary calculating, we have

$$\begin{aligned} i(C(n, k, \lambda)) &= i(G - \{v\}) + i(G - [v]) = i(P_1)^{[n-(\lambda-1)k-1]} [i(P_{\lambda-1})]^k + [i(P_{\lambda-3})]^k \\ &= 2^{[n-(\lambda-1)k-1]} f(\lambda+1)^k + f(\lambda-1)^k. \end{aligned} \tag{3.2}$$

□

Theorem 3.2. *Let $3 \leq \lambda \leq \lfloor (n-1)/k_0 \rfloor + 1$, $k_0 \geq 1$, $n \geq 5$. Then $i(C(n, k_0, \lambda+1)) < i(C(n, k_0, \lambda))$.*

Proof. Let $3 \leq \lambda \leq \lfloor (n-1)/k_0 \rfloor + 1$. We have

$$\begin{aligned} \Delta_1 &= i(C(n, k_0, \lambda+1)) - i(C(n, k_0, \lambda)) \\ &= 2^{(n-\lambda k_0-1)} f(\lambda+2)^{k_0} + f(\lambda)^{k_0} - 2^{[n-k_0(\lambda-1)-1]} f(\lambda+1)^{k_0} - f(\lambda-1)^{k_0} \\ &= 2^{(n-\lambda k_0-1)} \left[f(\lambda+2)^{k_0} - 2^{k_0} f(\lambda+1)^{k_0} \right] + \left[f(\lambda)^{k_0} - f(\lambda-1)^{k_0} \right]. \end{aligned} \tag{3.3}$$

Obviously, $2^{(n-\lambda k_0-1)} \geq 1$ by $z(C(n, k_0, \lambda+1))$ be exist. Again by $f(\lambda+2) < 2f(\lambda+1)$, we have

$$2^{(n-\lambda k_0-1)} \left[f(\lambda+2)^{k_0} - 2^{k_0} f(\lambda+1)^{k_0} \right] \leq f(\lambda+2)^{k_0} - 2^{k_0} f(\lambda+1)^{k_0}. \tag{3.4}$$

Thus

$$
\begin{aligned}
\Delta_1 &\le f(\lambda+2)^{k_0} - 2^{k_0} f(\lambda+1)^{k_0} + f(\lambda)^{k_0} - f(\lambda-1)^{k_0} \\
&= \left[f(\lambda+1)+f(\lambda)\right]^{k_0} - 2^{k_0} f(\lambda+1)^{k_0} + \left[f(\lambda)^{k_0} - f(\lambda-1)^{k_0}\right] \\
&= \left[f(\lambda+1)^{k_0} + k_0 f(\lambda+1)^{k_0-1} f(\lambda) + \cdots + f(\lambda)^{k_0}\right] \\
&\quad - 2^{k_0} f(\lambda+1)^{k_0} + \left[f(\lambda)^{k_0} - f(\lambda-1)^{k_0}\right] \\
&< \left[\left(2^{k_0}-1\right) f(\lambda+1)^{k_0} + f(\lambda)^{k_0}\right] - 2^{k_0} f(\lambda+1)^{k_0} + \left[f(\lambda)^{k_0} - f(\lambda-1)^{k_0}\right] \\
&= -f(\lambda+1)^{k_0} + 2 f(\lambda)^{k_0} - f(\lambda-1)^{k_0} \\
&= -\left[f(\lambda)+f(\lambda-1)\right]^{k_0} + 2 f(\lambda)^{k_0} - f(\lambda-1)^{k_0} \\
&< -\left[f(\lambda)^{k_0} + \left(2^{k_0}-1\right) f(\lambda-1)^{k_0}\right] + 2 f(\lambda)^{k_0} - f(\lambda-1)^{k_0} \\
&= -2^{k_0} f(\lambda-1)^{k_0} + f(\lambda)^{k_0} \quad (\text{by} f(\lambda) < 2 f(\lambda-1)) \\
&= -\left[(2 f(\lambda-1))^{k_0} - f(\lambda)^{k_0}\right] < 0.
\end{aligned}
\tag{3.5}
$$

By Theorem 3.2, we obtain the order of the Merrifield-Simmons index of $C(n, k_0, \lambda)$. □

Corollary 3.3. *Let $3 \le \lambda \le \lfloor (n-1)/k_0 \rfloor + 1$, $k_0 \ge 1$, $n \ge 5$. Then $i(C(n,k_0,3)) > i(C(n,k_0,4)) > i(C(n,k_0,5)) > \cdots$, and $C(n,k_0,3)$ has the largest Merrifield-Simmons index among the graphs in $C(n,k_0,\lambda)$.*

Theorem 3.4. *Let $1 \le k \le \lfloor (n-1)/(\lambda_0 - 1) \rfloor$, $\lambda_0 \ge 3$, $n \ge 3$. Then $i(C(n,k+1,\lambda_0)) < i(C(n,k,\lambda_0))$.*

Proof. Let $k \ge 1$, $n \ge 3$. If $\lambda_0 = 3$, then

$$
\begin{aligned}
\Delta_2 &= i(C(n,k+1,3)) - i(C(n,k,3)) \\
&= 2^{[n-2(k+1)-1]} f(4)^{k+1} + f(2)^{k+1} - 2^{[n-2k-1]} f(4)^k - f(2)^k \\
&= 2^{n-1}\left(\frac{3}{4}\right)^{k+1} - 2^{n-1}\left(\frac{3}{4}\right)^{k} = -2^{n-1}\left(\frac{3}{4}\right)^{k} \cdot \frac{1}{4} < 0.
\end{aligned}
\tag{3.6}
$$

If $\lambda_0 = 4$, then

$$
\begin{aligned}
\Delta_3 = i(C(n,k+1,4)) - i(C(n,k,4)) &= 2^{[n-3(k+1)-1]} f(5)^{k+1} + f(3)^{k+1} \\
&\quad - 2^{[n-3k-1]} f(5)^k - f(3)^k = 2^{n-3k-4} 5^k (-3) + 2^k \le -3 \cdot 5^k + 2^k < 0.
\end{aligned}
\tag{3.7}
$$

If $\lambda_0 \geq 5$, then

$$\begin{aligned}
\Delta_4 &= i(C(n,k+1,\lambda_0)) - i(C(n,k,\lambda_0)) \\
&= 2^{[n-(\lambda_0-1)(k+1)-1]} f(\lambda_0+1)^{k+1} + f(\lambda_0-1)^{k+1} \\
&\quad - 2^{[n-(\lambda_0-1)k-1]} f(\lambda_0+1)^{k} - f(\lambda_0-1)^{k} \\
&= 2^{[n-(\lambda_0-1)(k+1)-1]} f(\lambda_0+1)^{k}\left[f(\lambda_0+1) - 2^{\lambda_0-1}\right] \\
&\quad + f(\lambda_0-1)^{k+1} - f(\lambda_0-1)^{k}.
\end{aligned} \tag{3.8}$$

Obviously, $2^{[n-(\lambda_0-1)(k+1)-1]} \geq 1$ by $z(C(n,k+1,\lambda_0))$ exists. Again by Lemma 2.1(i), we have

$$f(\lambda_0+1) - 2^{\lambda_0-1} \leq -f(\lambda_0+1) \leq 0. \tag{3.9}$$

Thus

$$\begin{aligned}
\Delta_4 &\leq f(\lambda_0+1)^{k}\left[f(\lambda_0+1) - 2^{\lambda_0-1}\right] + f(\lambda_0-1)^{k+1} - f(\lambda_0-1)^{k} \\
&\leq f(\lambda_0+1)^{k}\left[-f(\lambda_0+1)\right] + f(\lambda_0-1)^{k+1} - f(\lambda_0-1)^{k} \\
&= -\left[f(\lambda_0+1)^{k+1} - f(\lambda_0-1)^{k+1}\right] - f(\lambda_0-1)^{k} < 0.
\end{aligned} \tag{3.10}$$

By Theorem 3.4, we obtain the order of the Merrifield-Simmons index of $C(n,k,\lambda_0)$. □

Corollary 3.5. *Let $1 \leq k \leq \lfloor (n-1)/(\lambda_0-1) \rfloor$, $n \geq 3$. Then $i(C(n,1,\lambda_0)) > i(C(n,2,\lambda_0)) > i(C(n,3,\lambda_0)) > \cdots$, and $C(n,1,\lambda_0)$ has the largest Merrifield-Simmons index of among the graphs in $C(n,k,\lambda_0)$.*

4. The Hosoya Index of $C(n,k,\lambda)$

In this section, we will give the Hosoya index of $C(n,k,\lambda)$ and their order.

Theorem 4.1. *Let $1 \leq k \leq \lfloor (n-1)/(\lambda-1) \rfloor$ and $\lambda \geq 3$. Then*

$$z(C(n,k,\lambda)) = [n-(\lambda-1)k] f(\lambda)^{k} + 2k f(\lambda-1) f(\lambda)^{k-1}. \tag{4.1}$$

Proof. For all $1 \leq k \leq \lfloor (n-1)/(\lambda-1) \rfloor$ and $\lambda \geq 3$, according to Lemma 2.3, we have the following:

$$\begin{aligned}
z(C(n,k,\lambda)) &= z(G-\{v\}) + \sum_{x \in N_G(v)} z(G-\{x,v\}) \\
&= [z(P_{\lambda-1})]^k + [n-(\lambda-1)k-1][z(P_{\lambda-1})]^k + 2k[z(P_{\lambda-2}), z(P_{\lambda-1})]^{k-1} \\
&= f(\lambda)^k + [n-(\lambda-1)k-1]f(\lambda)^k + 2kf(\lambda-1)f(\lambda)^{k-1} \\
&= [n-(\lambda-1)k]f(\lambda)^k + 2kf(\lambda-1)f(\lambda)^{k-1}.
\end{aligned} \tag{4.2}$$

□

Theorem 4.2. *Let* $3 \leq \lambda \leq \lfloor (n-1)/k_0 \rfloor + 1$, $k_0 \geq 1$ *and* $n \geq 5$. *Then* $z(C(n,k_0,\lambda)) < z(C(n,k_0,\lambda+1))$.

Proof. Let $3 \leq \lambda \leq \lfloor (n-1)/k_0 \rfloor + 1$, $k_0 \geq 1$ and $n \geq 5$. We have

$$\begin{aligned}
\Delta_5 &= z(C(n,k_0,\lambda+1)) - z(C(n,k_0,\lambda)) \\
&= (n-\lambda k_0)f(\lambda+1)^{k_0} + 2k_0 f(\lambda)f(\lambda+1)^{k_0-1} \\
&\quad - (n-\lambda k_0 + k_0)f(\lambda)^{k_0} - 2k_0 f(\lambda-1)f(\lambda)^{k_0-1} \\
&= (n-\lambda k_0)\left[f(\lambda+1)^{k_0} - f(\lambda)^{k_0}\right] + 2k_0 f(\lambda)f(\lambda+1)^{k_0-1} \\
&\quad - k_0 f(\lambda)^{k_0} - 2k_0 f(\lambda-1)f(\lambda)^{k_0-1}.
\end{aligned} \tag{4.3}$$

Obviously, $(n-\lambda k_0) \geq 1$ by $z(C(n,k_0,\lambda+1))$ exists. We have

$$\begin{aligned}
&(n-\lambda k_0)\left[f(\lambda+1)^{k_0} - f(\lambda)^{k_0}\right] \\
&\qquad \geq f(\lambda+1)^{k_0} - f(\lambda)^{k_0} \\
&\qquad = \left[f(\lambda) + f(\lambda-1)\right]^{k_0-1} - f(\lambda)^{k_0} \\
&\qquad \geq f(\lambda)^{k_0} + k_0 f(\lambda)^{k_0-1} f(\lambda-1) - f(\lambda)^{k_0} \\
&\qquad = k_0 f(\lambda)^{k_0-1} f(\lambda-1), \\
&2k_0 f(\lambda)f(\lambda+1)^{k_0-1} \\
&\qquad = 2k_0 f(\lambda)\left[f(\lambda) + f(\lambda-1)\right]^{k_0-1} \geq 2k_0 f(\lambda)\left[f(\lambda)^{k_0-1} + (k_0-1)f(\lambda)^{k_0-2} f(\lambda-1)\right] \\
&\qquad = 2k_0 f(\lambda)^{k_0} + 2k_0(k_0-1)f(\lambda)^{k_0-1} f(\lambda-1).
\end{aligned} \tag{4.4}$$

Thus

$$\begin{aligned}\Delta_5 &\geq k_0 f(\lambda)^{k_0-1} f(\lambda-1) + 2k_0 f(\lambda)^{k_0} + 2k_0(k_0-1) f(\lambda)^{k_0-1} f(\lambda-1)\\ &\quad - k_0 f(\lambda)^{k_0} - 2k_0 f(\lambda-1) f(\lambda)^{k_0-1}\\ &= k_0 f(\lambda)^{k_0} + 2k_0\left(k_0 - \frac{3}{2}\right) f(\lambda)^{k_0-1} f(\lambda-1) > 0.\end{aligned} \tag{4.5}$$

By Theorem 4.2, we obtain the order of the Hosoya index of $C(n, k_0, \lambda)$. □

Corollary 4.3. *Let* $3 \leq \lambda \leq \lfloor (n-1)/k_0 \rfloor + 1$, $k_0 \geq 1$, $n \geq 5$. *Then* $z(C(n, k_0, 3)) < z(C(n, k_0, 4)) < z(C(n, k_0, 5)) < \cdots$, *and* $C(n, k_0, 3)$ *has the smallest Hosoya index among the graphs in* $C(n, k_0, \lambda)$.

Theorem 4.4. *Let* $1 \leq k \leq \lfloor (n-1)/(\lambda_0-1) \rfloor$, $\lambda_0 \geq 3$, $n \geq 3$. *Then* $z(C(n, k, \lambda_0)) < z(C(n, k+1, \lambda_0))$.

Proof. Let $k \geq 1$, $\lambda_0 \geq 3$, $n \geq 3$,

$$\begin{aligned}\Delta_6 &= z(C(n, k+1, \lambda_0)) - z(C(n, k, \lambda_0))\\ &= [n - (\lambda_0-1)(k+1)] f(\lambda_0)^{k+1} + 2(k+1) f(\lambda_0-1) f(\lambda_0)^k\\ &\quad - [n - (\lambda_0-1)k] f(\lambda_0)^k - 2k f(\lambda_0-1) f(\lambda_0)^{k-1}\\ &= \left[n - (\lambda_0-1)(k+1), f(\lambda_0)^{k+1} - f(\lambda_0)^k\right] - (\lambda_0-1) f(\lambda_0)^k\\ &\quad + 2k f(\lambda_0-1)\left[f(\lambda_0)^k - f(\lambda_0)^{k-1}\right] + 2 f(\lambda_0-1) f(\lambda_0)^k.\end{aligned} \tag{4.6}$$

Obviously, $n - (\lambda_0-1)(k+1) \geq 1$ by $z(C(n, k+1, \lambda_0))$ exists. We have

$$\begin{gathered}[n - (\lambda_0-1)(k+1)]\left[f(\lambda_0)^{k+1} - f(\lambda_0)^k\right] \geq 0,\\ 2k f(\lambda_0-1)\left[f(\lambda_0)^k - f(\lambda_0)^{k-1}\right] > 0.\end{gathered} \tag{4.7}$$

Thus

$$\begin{aligned}\Delta_6 &> 2 f(\lambda_0-1) f(\lambda_0)^k - (\lambda_0-1) f(\lambda_0)^k\\ &= f(\lambda_0)^k [2 f(\lambda_0-1) - (\lambda_0-1)] \geq 0 \quad (\text{by Lemma 2.1(ii)}).\end{aligned} \tag{4.8}$$

By Theorem 4.4, we obtain the order of the Hosoya index of $C(n, k, \lambda_0)$. □

Corollary 4.5. *Let* $1 \leq k \leq \lfloor (n-1)/(\lambda_0-1) \rfloor$, $\lambda_0 \geq 3$, $n \geq 3$. *Then* $z(C(n, 1, \lambda_0)) < z(C(n, 2, \lambda_0)) < z(C(n, 2, \lambda_0)) < \cdots$, *and* $C(n, 1, \lambda_0)$ *has the smallest Hosoya index of among the graphs in* $C(n, k, \lambda_0)$.

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