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Orderings a Class of Unicyclic Graphs with Respect to Hosoya and Merrifield-Simmons Index

(Tertib Kelas Graf Unisiklik Indeks Hosoya dan Merrifield-Simmons)

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ABSTRACT

Hosoya and Merrifield-Simmons index were the two valuable topological indices in chemical graph theory. The Hosoya and Merrifield-Simmons index of the class of unicyclic graphs G(k) were investigated, according to the distance between u and v on C_m, their orderings with respect to these two topological indices were obtained.

Keywords: Hosoya index; Merrifield-Simmons index; ordering; unicyclic graph

ABSTRAK

Indeks Hosoya dan Merrifield - Simmons adalah dua indeks topologi penting dalam teori graf kimia. Indeks Hosoya dan Merrifield - Simmons daripada kelas graf unisiklik G(k) dikaji mengikut jarak antara u dan v ke atas C_m, tertib mereka mengikut kedua-dua indeks topologi diperoleh.

Kata kunci: Graf unisiklik; indeks Hosoya; indeks Merrifield-Simmons; tertib

INTRODUCTION

The Hosoya index of a graph was introduced by Hosoya in 1971 and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures, denoted by $\mu(G)$, $\mu(G)$ is equal to the total number of matchings of G. The Merrifield-Simmons index was first introduced by Prodinger and Tichy in 1982 and this index is called Fibonacci number of a graph there, denoted by $\sigma(G)$, $\sigma(G)$ is equal to the total number of the independent sets of G. The Merrifield-Simmons index is one of most popular topological indices in chemistry, which was extensively studied in a monograph (Merrifield & Simmons 1989). Merrifield and Simmons showed the correlation between this index and boiling points. For detailed information on the chemical applications, please refer to Gutman and Polansky 1986, Merrifield and Simmons 1989 and Trinajstic 1992). Several papers deal with the characterization of the extremal graphs with respect to these two indices in several given graph classes. Usually, acyclic graphs, unicyclic graphs and trees are of major interest (Wagner et al. 2007; Yali et al. 2008; Zheng et al. 2008; Ziwen et al. 2011). In this paper, we determined a class of unicyclic graphs $G(k)$ and also obtain the ordering of Hosoya index and Merrifield-Simmons index on the unicyclic graphs.

Let $G = (V, E)$ be a graph with the vertex set $V(G)$ and edge set $E(G)$. If $W \subseteq V(G)$, we denote by $G - W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. If $W = \{v\}$ and $E' = \{uv\}$, we write $G - v$ and $G - uv$ instead of $G - \{v\}$ and $G - \{uv\}$, respectively, $N_G(v)$ denotes the set of vertices in G which are adjacent to the vertex v and let $N_G[v] = \{v\} \cup N_G(v)$. We denote by P_n and C_n the path and the cycle on n vertices, respectively. We denote the sequence of Fibonacci numbers by f_n, i.e. $f_0 = 0$, $f_1 = 1$ and $f_{n+1} = f_n + f_{n-1}$, for $n \geq 1$. f_n is extended to negative values of n via Bennet's formula $f_n = \frac{1}{\sqrt{5}}\left(\phi^n - (-\phi)^{-n}\right)$, where $\phi = \frac{1+\sqrt{5}}{2}$. Analogously, the Lucas numbers are denoted by l_n, i.e. $l_0 = 2$, $l_1 = 1$, $l_{n+1} = l_n + l_{n-1}$ and $l_n = \phi^n + (-\phi)^{-n})$, for $n \geq 1$. Therefore, for $n \geq 1$, we have $f_{n-1} + f_{n+1} = l_n$ and $l_{n-1} + l_{n+1} = 5f_n$. Other undefined notation may refer to Bondy and Murty 1976 and Ser et al. 2014.

$G(k)$ represents a class of unicyclic graphs consisting of a ring of C_m and two n order road P_n, two contact among the two road and C_m, respectively, for u and v and $d(u, v) = k$ (Figure 1).

METHODS

According to the definitions of the Merrifield-Simmons index and Hosoya index, we immediately get the following results.

Lemma 1 Let G be a simple graph and $v \in V(G)$, $uv \in E(G)$ (Prodinger & Tichy 1982) then

(i) $\mu(G) = \mu(G - uv) + \mu(G - u - v)$;

(ii) $\mu(G) = \mu(G - v) + \sum_{x \in N_G(v)} \mu\left(G - \{v, x\}\right)$.

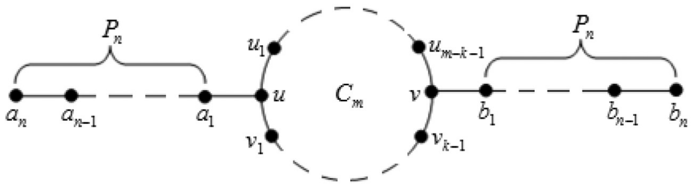

FIGURE 1. Unicyclic graph *G(k)*

Lemma 2 Let G be a simple graph and $u, v \in V(G)$, $uv \in E(G)$ (Prodinger & Tichy 1982) then

(i) $\sigma(G) = \sigma(G - v) + \sigma(G - N_G[v])$;

(ii) $\sigma(G) = \sigma(G) = \sigma(G - uv) - \sigma(G - (N_G[u] \cup N_G[v]))$.

Lemma 3 If $G_1, G_2, \ldots, G_k$ are the components of a graph G (Prodinger & Tichy 1982) we have

(i) $\mu(G) = \prod_{i=1}^{k} \mu(G_i)$;

(ii) $\sigma(G) = \prod_{i=1}^{k} \sigma(G_i)$.

Lemma 4 $\mu(P_n) = f_{n+1}$ and $\sigma(P_n) = f_{n+2}$ for any $n \in$ N (Prodinger & Tichy 1982).

Lemma 5 $\mu(C_n) = f_{n+1} + f_{n-1}$ and $\sigma(C_n) = f_{n+1} + f_{n-1}$ for any $n \geq 3$ (Prodinger & Tichy 1982).

Lemma 6 For any $m \geq n$, we have $f_m f_n = \frac{1}{5}(l_{m+n} - (-1)^n l_{m-n})$ (Wagner 2007).

RESULTS AND DISCUSSION

Theorem 1 Let $G(k)$ be the graph shown in Figure 1, where $1 \leq k \leq \left\lfloor \frac{m}{2} \right\rfloor$, then

$$\mu(G(1)) > \mu(G(3)) > \ldots > \mu(G(\left\lfloor \frac{m}{2} \right\rfloor)) > \ldots > \mu(G(4)) > \mu(G(2)).$$

Proof. By Lemma 1(i). Lemma 3. Lemma 4 and Lemma 5, we have $\mu(G(k)) = \mu(G(k) - ua_1) + \mu(G(k) - u - a_1)$

$= \mu(G(k)) = ua_1 - vb_1) + \mu(G(k) - ua_1 - v - b_1) + \mu(G(k) - u - a_1 - vb_1) + \mu(G(k) - u - a_1 - v - b_1)$

$= (f_{m+1} + f_{m-1}) \cdot f_{n+1}^2 + 2f_n f_{n+1} f_m + f_n^2 f_k f_{m-k}$

Analogously, we have

$$\mu(G(k+1)) = (f_{m+1} + f_{m-1}) \cdot f_{n+1}^2 + 2f_n f_{n+1} f_m + f_n^2 f_{k+1} f_{m-k-1}$$

$$\mu(G(k+2)) = (f_{m+1} + f_{m-1}) \cdot f_{n+1}^2 + 2f_n f_{n+1} f_m + f_n^2 f_{k+2} f_{m-k-2}$$

It is easy to see

$$\mu(G(k)) - \mu(G(k+1)) = f_{n+1}^2 \cdot (f_k f_{m-k} - f_{k+1} f_{m-k-1})$$

$$\mu(G(k)) - \mu(G(k+2)) = f_n^2 \cdot (f_k f_{m-k} - f_{k+2} f_{m-k-2})$$

By Lemma 6, we have

$$f_k f_{m-k} - f_{k+1} f_{m-k-1} = \frac{1}{5}(-1)^{k+1}(l_{m-2k} + l_{m-2k-2}) = (-1)^{k+1} f_{m-2k-1}$$

$$f_k f_{m-k} - f_{k+2} f_{m-k-2} = \frac{1}{5}(-1)^{k+1}(l_{m-2k} - l_{m-2k-4}) = (-1)^{k+1} f_{m-2k-2}$$

Hence, we have

$$\mu(G(k)) - \mu(G(k+1)) = (-1)^{k+1} \; f_n^2 \cdot f_{m-2k-1}$$

and

$$\mu(G(k)) - \mu(G(k+2)) = (-1)^{k+1} \; f_n^2 \cdot f_{m-2k-2}.$$

Then if $k \equiv 0 (\mathrm{mod}\ 2)$, $\mu(G(k)) < \mu(G(k+1))$, and $\mu(G(k)) < \mu(G(k+2))$; if $k = 1 (\mathrm{mod}\ 2)$, $\mu(G(k+1))$, and $\mu(G(k)) > \mu(G(k+2))$.

Therefore,

$$\mu(G(1)) > \mu(G(3)) > \ldots > \mu(G(\left\lfloor \frac{m}{2} \right\rfloor)) > \ldots > \mu(G(4)) > \mu(G(2)).$$

This completes the proof of Theorem 1.

Theorem 2 Let $G(k)$ be the graph shown in Figure 1, where $1 \leq k \leq \left\lfloor \frac{m}{2} \right\rfloor$, then

$$\sigma(G(1) < \sigma(G(3)) < \ldots < \sigma(G(\left\lfloor \frac{m}{2} \right\rfloor)) < \ldots < \sigma(G(4)) < \sigma(G(2)).$$

Proof. By Lemma 2(i). Lemma 3. Lemma 4 and Lemma 5, we have $\sigma(G(k)) = \sigma(G(k) - u) + \sigma(G(k) - N_{G(k)}[u])$

$= \sigma(G(k) - u - v) + \sigma(G(k) - u - N_{G(k)-u}[v]) + \sigma(G(k) - N_{G(k)}[u] - v) + \sigma(G(k) - N_{G(k)}[u] - N_{G(k) - N_{G(k)}[u]}[v])$

$= f_{n+2}^2 f_{k+1} + f_{m-k+1} + 2f_{n+2} f_{n+1} f_k f_{m-k} + f_{n+1}^2 f_{k-1} f_{m-k-1}$

Analogously, we have

$$\sigma(G(k+1)) = f_{n+2}^2 f_{k+2} f_{m-k} + 2f_{n+2} f_{n+1} f_{k+1} f_{m-k-1} + f_{n+1}^2 f_k f_{m-k-2}$$

$$\sigma(G(k+2)) = f_{n+2}^2 f_{k+3} f_{m-k-1} + 2f_{n+2} f_{n+1} f_{k+2} f_{m-k-2} + f_{n+1}^2 f_{k+1} f_{m-k-3}$$

It is easy to see

$$\begin{aligned}\sigma(G(k+1)) - \sigma(G(k+1)) = {} & f_{n+2}^2.(f_{k+1} f_{m-k+1} - f_{k+2} f_{m-k}) \\ & +2f_{n+1} f_{n+2}.(f_k f_{m-k} - f_{k+1} f_{m-k-1}) \\ & +f_{n+1}^2.(f_{k-1} f_{m-k-1} - f_k f_{m-k-2})\end{aligned}$$

and

$$\begin{aligned}\sigma(G(k)) - \sigma(G(k+2)) = {} & f_{n+2}^2.(f_{k+1} f_{m-k+1} - f_{k+3} f_{m-k-1}) \\ & +2f_{n+1} f_{n+2}.(f_k f_{m-k} - f_{k+2} f_{m-k-2}) \\ & +f_{n+1}^2.(f_{k-1} f_{m-k-1} - f_{k+1} f_{m-k-3})\end{aligned}$$

By Lemma 6, we have

$$f_{k+1} f_{m-k+1} - f_{k+2} f_{m-k} = \frac{1}{5}(-1)^{k+2}(l_{m-2k} + l_{m-2k-2}) = (-1)^{k+2} f_{m-2k-1}$$

$$f_k f_{m-k} - f_{k+1} f_{m-k-1} = \frac{1}{5}(-1)^{k+1}(l_{m-2k} + l_{m-2k-2}) = (-1)^{k+1} f_{m-2k-1}$$

$$f_{k-1} f_{m-k-1} - f_k f_{m-k-2} = \frac{1}{5}(-1)^{k}(l_{m-2k} + l_{m-2k-2}) = (-1)^{k} f_{m-2k-1}$$

$$f_{k+1} f_{m-k+1} - f_{k+3} f_{m-k-1} = \frac{1}{5}(-1)^{k+2}(l_{m-2k} - l_{m-2k-4}) = (-1)^{k+2} f_{m-2k-2}$$

$$f_k f_{m-k} - f_{k+2} f_{m-k-2} = \frac{1}{5}(-1)^{k+1}(l_{m-2k} + l_{m-2k-4}) = (-1)^{k+1} f_{m-2k-2}$$

$$f_{k-1} f_{m-k-1} - f_{k+1} f_{m-k-3} = \frac{1}{5}(-1)^{k}(l_{m-2k} + l_{m-2k-4}) = (-1)^{k} f_{m-2k-2}$$

Hence, we have

$$\begin{aligned}\sigma(G(k)) - \sigma(G(k+1)) &= (-1)^{k+2} f_{n+2}^2 f_{m-2k-1} + (-1)^{k+1}. \\ &\quad 2f_{n+1} f_{n+2} f_{m-2k-1} + (-1)^k f_{n+1}^2 f_{m-2k-1} \\ &= (-1)^k f_{m-2k-1}.(f_{n+2}^2 - 2f_{n+1} f_{n+2} + f_{n+1}^2) \\ &= (-1)^k f_{m-2k-1}.(f_{n+2} - f_{n+1})^2 \\ &= (-1)^k f_n^2 f_{m-2k-1}.\end{aligned}$$

and

$$\begin{aligned}\sigma(G(k)) - \sigma(G(k+2)) &= (-1)^{k+2} f_{n+2}^2 f_{m-2k-2} + (-1)^{k+1}. \\ &\quad 2f_{n+1} f_{n+2} f_{m-2k-2} + (-1)^k f_{n+1}^2 f_{m-2k-1} \\ &= (-1)^k f_{m-2k-2}.(f_{n+2}^2 - 2f_{n+1} f_{n+2} + f_{n+1}^2) \\ &= (-1)^k f_{m-2k-2}.(f_{n+2} - f_{n+1})^2 \\ &= (-1)^k f_n^2 f_{m-2k-2}.\end{aligned}$$

Then if $k \equiv 0 (\mathrm{mod}\ 2)$, $\sigma(G(k)) > \sigma(G(k+1))$ and $\sigma(G(k)) > \sigma(G(k+2))$; if $k \equiv 1 (\mathrm{mod}\ 2)$, $\sigma(G(k)) < \sigma(G(k+1))$, and $\sigma(G(k)) < \sigma(G(k+2))$.

Therefore,

$$\sigma(G(1)) < \sigma(G(3)) < \ldots < \sigma(G(\left\lfloor \frac{m}{2} \right\rfloor)) < \ldots < \sigma(G(4)) < \sigma(G(2)).$$

Conclusion

This completes the proof of Theorem 2.

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