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On the Ordering of Trees by the Two Indices

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Abstract. The Merrifield-Simmons index of a graph is defined as the total number of the independent sets of the graph and the Hosoya index of a graph is defined as the total number of the matchings of the graph. In this paper, among all the trees with n vertices and k pendent vertices, we determine the trees with the first $[n-k+1/2]$ largest Merrifield-Simmons index and the trees with the first $[n-k+1/2]$ smallest Hosoya index .

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1. Introduction

The Merrifield-Simmons index was introduced in 1982 by Prodinger and Tichy in [3]. The Merrifield-Simmons index is one of the most popular topological indices in chemistry, which was extensively studied in a monograph [12]. Now there have been many papers studying the Merrifield-Simmons index (see [1,8,9,11–16]). The Hosoya index of a graph was introduced by Hosoya in 1971 [4] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures [15]. Since then, many authors have investigated the Hosoya index (e.g., see [3–8,12,11,15]). For trees with n-vertex, it has been shown that the path P_n has the minimal Merrifield-Simmons index and maximal Hosoya index, and the star S_n has the maximal Merrifield-Simmons index and minimal Hosoya index (see [8,14]).

Let G be a graph. If $uv=e$ is an edge of G, by the definition of $m(G,k)$, then $m(G,k)=m(G-e,k)+m(G-u-v,k-1)$. Let n,k be two integers. Denote $\mathscr{T}_{n,k}$ by trees with n vertices and k pendent vertices. Let $P_{n,k}$ denote the graph obtained by identifying one end-vertex of P_{n-k+1} with the center of S_k. Let H_l $(l \le n-l-k+1)$ denote the graph obtained by identifying v_{l+1} of $P_{n-k+2}=v_1v_2\cdots v_{n-k+2}$ with the center of S_{k-1}. F_m is obtained by identifying one end-vertex of P_{n-k} with the center of S_{m+1} and the other with the center of S_{k-m+1}.

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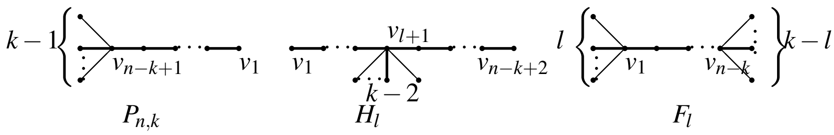

Figure 1. Graphs $P_{n,k}$, H_l and F_l.

2. Preliminaries

For $3 \leq k \leq n-2$, we define the following families of graphs

$$\mathscr{H}_{n,k} = \{H_l | 2 \leq l \leq [(n-k+1)/2]-1\}, \quad \mathscr{F}_{n,k} = \{F_l | 2 \leq l \leq [k/2]\}$$

Yu and Lv [5] proved that $P_{n,k}$ is the tree in $\mathscr{T}_{n,k}$ with maximum Merrifield-Simmons index and minimum Hosoya index. Lv,Yan,Yu and Zhang [7] ordered two kinds trees in $\mathscr{T}_{n,k}$ by Merrifield-Simmons index and Hosoya index. In this paper, we will characterize trees such that $\sigma(H_2) \leq \sigma(T) \leq \sigma(P_{n,k}), z(P_{n,k}) \leq z(T) \leq z(H_2)$ and $E(P_{n,k}) \leq E(T) \leq E(H_4)$ in $\mathscr{T}_{n,k}$. Thus the results in this paper extend those of [5,7].

In order to state our results, we introduce some notation and terminology. Other undefined notation we refer to [1]. 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 $E' = xy$, we write $G-v$ and $G-xy$ instead of $G-W$ and $G-E'$, respectively. In the paper, we always denote by P_n the path on n vertices and by $[x]$ the largest integer no more than x, denote by $N_G(v)$ the set of vertices adjacent with v.

Lemma 2.1. [7,8] *Let G be a graph, $v \in V(G)$. Then*

(1) $\sigma(G) = \sigma(G-v) + \sigma(G-N_G(v))$.
(2) $z(G) = z(G-v) + \sum_u z(G-\{u,v\})$, *where Σ goes over adjacency vertex of u.*

Lemma 2.2. [7,8] *Let G be a graph, $uv = e \in E(G)$. Then*

(1) $\sigma(G) = \sigma(G-e) - \sigma(G-\{N_G(u) \cup N_G(v)\})$.
(2) $z(G) = z(G-e) + z(G-\{u,v\})$.

Especially, if v is a pendent vertex G and u is the unique adjacency vertex of v, then

$$\sigma(G) = \sigma(G-v) - \sigma(G-\{u,v\}), z(G) = z(G-v) - z(G-\{u,v\}).$$

Lemma 2.3. [8] *Let $G_1, G_2, \cdots, G_k$ be k components of G. Then*

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

Lemma 2.4. [7,13] *Let $A_l = \sigma(P_l)\sigma(P_{n-l}), z(B_l) = z(P_l)z(P_{n-l})$, where $1 \leq l \leq [n/2]$. Then*

(1) $A_1 > A_3 > \cdots > A_{[\frac{n}{2}]} > \cdots > A_4 > A_2$,
(2) $B_2 > B_4 > \cdots > B_{[\frac{n}{2}]} > \cdots > B_3 > B_1$.

In [5], Yu and Lv defined two kinds of *operations* to $T \in \mathscr{T}_{n,k}$ and compared their Merrifield-Simmons indices and Hosoya indices .

Let $P = v_0 v_1 \cdots v_k (k \geq 1)$ be a path in T. Denote $s(T)$ by the number of vertices with $d(v) > 2$ of T, by $p(T)$ we denote the number of path with the length greater than 1 of T.

Lemma 2.5. [5] *Let $T, T' \in \mathscr{T}_{n,k}$. If T' is obtained from T by* Operation *I, then*

$$\sigma(T') > \sigma(T), z(T') < z(T).$$

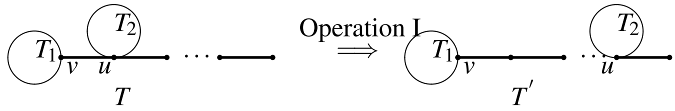

Figure 2. Operation I.

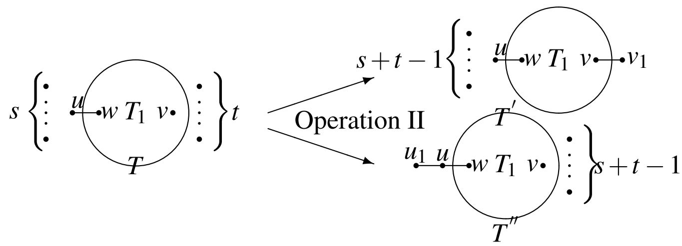

Figure 3. Operation II.

Lemma 2.6. [5] *Let* $T, T^{'} \in \mathscr{T}_{n,k}$*. If* $T^{'}$, $T^{''}$ *are obtained from* T *by* Operation *II, then*

(1) *either* $\sigma(T^{'}) > \sigma(T)$ *or* $\sigma(T^{''}) > \sigma(T)$.
(2) *either* $z(T^{'}) < z(T)$ *or* $z(T^{''}) < z(T)$.

Lemma 2.7. [5] *Let* $G \neq P_1$ *be a connected graph with* $v \in V(G)$*.* $P(n,k,G,v)$ *means the graph that* v_k *of* $P = v_1 v_2 \cdots v_n$ *is identified with* v*. If* $n = 4m+i$, $i \in \{1,2,3,4\}$, $m \geq 0$, *then*

(1) $\sigma(P(n,2,G,v)) > \sigma(P(n,4,G,v)) > \cdots > \sigma(P(n,2m+2l,G,v)) > \sigma(P(n,2m+1,G,v)) > \cdots > \sigma(P(n,3,G,v)) > \sigma(P(n,1,G,v))$.
(2) $z(P(n,2,G,v)) < z(P(n,4,G,v)) < \cdots < z(P(n,2m+2l,G,v)) < z(P(n,2m+1,G,v)) < \cdots < z(P(n,3,G,v)) < z(P(n,1,G,v))$, *where* $l = \lfloor (i-1)/2 \rfloor$.

Lemma 2.8. [7]

(1) *If* $k \geq 4$, $n-k \geq 5$, *then*

$$\sigma(H_3) > \sigma(H_5) > \cdots > \sigma(H_{[\frac{n-k+1}{2}]}) > \cdots > \sigma(H_6)$$
$$> \sigma(H_4) > \sigma(H_2) \geq \sigma(F_2) > \sigma(F_3) > \cdots > \sigma(F_{[\frac{k}{2}]}).$$

(2) *If* $k \geq 5$, $n-k \geq 5$, *then*

$$z(H_3) < z(H_5) < \cdots < z(H_{[\frac{n-k+1}{2}]}) < \cdots < z(H_6)$$
$$< z(H_4) < z(H_2) \leq z(F_2) < z(F_3) < \cdots < z(F_{[\frac{k}{2}]}).$$

(3) *If* $k = 4$, $n-k \geq 7$, *then*

$$z(H_3) < z(H_5) < \cdots < z(H_{[\frac{n-k+1}{2}]}) < \cdots < z(H_6) < z(H_4) \leq z(F_2) < z(H_2).$$

Lemma 2.9. [5] *Let* $T \in \mathscr{T}_{n,k}$*. Then*

(1) $\sigma(T) \leq 2^{k-1} f_{n-k+1} + f_{n-k}$ *with equality if and only if* $T \cong P_{n,k}$.
(2) $z(T) \geq k f_{n-k} + f_{n-k-1}$ *with equality if and only if* $T \cong P_{n,k}$.

3. Main results and proofs

Lemma 3.1. (1) *If $k \geq 4$, $n-k \geq 5$, then $\sigma(H_2) = \sigma(F_2)$ if and only if $k = 4$ and $n-k = 5$.*

(2) *If $k \geq 5$, $n-k \geq 5$, then $z(H_2) = z(F_2)$ if and only if $k = 5$ and $n-k = 5$.*

Proof. By calculation, we have

$$\sigma(H_2) - \sigma(F_2) = (2^{k-2} - 3)\sigma(P_{n-k-5}) - \sigma(P_{n-k-6})$$

$$z(F_2) - z(H_2) = (k-4)z(P_{n-k-4}) - z(P_{n-k-5})$$

Then, the result follows from Lemma 2.6. ∎

Lemma 3.2. *Let $T \in \mathscr{T}_{n,k}$, If $s(T) \geq 2$, then ,*

$$\sigma(T) \leq \sigma(F_2), z(T) \geq z(F_2).$$

Proof. Applying Operation *I* and *II* to T repeatly we get the graph T' such that $s(T') = 2$. Then repeatly using Operation I to T' we get the graph T'' such that $T'' \cong F_l$. From lemmas 2.5, 2.6, 2.8 follows. ∎

The graphs $E_{n,k}$ and $E^1_{n,k}$ shown in Figure 4 will be used in the following paper.

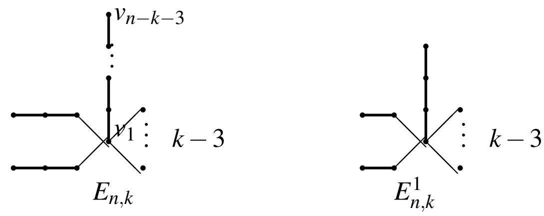

Figure 4. Graphs $E_{n,k}$ and $E^1_{n,k}$.

Lemma 3.3. *Let $T \in \mathscr{T}_{n,k}$, If $s(T) = 1$, $T \notin \{P_{n,k}\} \cup \mathscr{H}_{n,k} \cup \mathscr{F}_{n,k}$, then*

(1) *$\sigma(T) \leq \sigma(E^1_{n,k})$ and $z(T) \geq z(E^1_{n,k})$ for $n = k+5$.*

(2) *$\sigma(T) \leq \sigma(E_{n,k})$ and $z(T) \geq z(E_{n,k})$ for $n > k+5$.*

Proof. From the condition of the lemma we have $p(T) \geq 3$. Repeatly applying Operation I to T' we get that $s(T') = 1$ and $p(T') = 3$. Thus the lemma follows from Lemmas 2.5, 2.6 and 2.7. ∎

Lemma 3.4. *Let $k \geq 4$.*

(1) *If $n = k+5$, then $\sigma(E^1_{n,k}) \leq \sigma(H_2)$ and $z(H_2) \leq z(E^1_{n,k})$.*

(2) *If $n > k+5$, then $\sigma(E_{n,k}) \leq \sigma(H_2)$ and $z(H_2) \leq z(E_{n,k})$.*

Proof. Here we only prove (2). By Lemmas 2.1, 2.2, we get

$$\sigma(E_{n,k}) = 25 \cdot 2^{k-3}\sigma(P_{n-k-4}) + 9\sigma(P_{n-k-5}),$$

$$\sigma(H_2) = (18 \cdot 2^{k-3} + 4)\sigma(P_{n-k-4}) + (12 \cdot 2^{k-3} + 2)\sigma(P_{n-k-5}).$$

$$\sigma(H_2) - \sigma(E_{n,k}) = (5 \cdot 2^{k-3} - 3)\sigma(P_{n-k-5}) + (-7 \cdot 2^{k-3} + 4)\sigma(P_{n-k-6}).$$

So, when $n > k+5$, $\sigma(H_2)-\sigma(E_{n,k}) > 0$. Similarly,

$$z(E_{n,k}) = (9k-6)z(P_{n-k-4}) + 9z(P_{n-k-5}),$$
$$z(H_2) = (6k+1)z(P_{n-k-4}) + 4kz(P_{n-k-5}),$$
$$z(E_{n,k}) - z(H_2) = (-k+2)z(P_{n-k-5}) + (3k-7)z(P_{n-k-6}).$$

So, for $n > k+5$, $z(E_{n,k}) - z(H_2) > 0$. ∎

Theorem 3.1. *Let $T \in \mathscr{T}_{n,k}$.*

(1) *If $k > 4$, $n-k \geq 5$ or $k \geq 4$, $n-k > 5$, then $\sigma(H_2) \leq \sigma(T) \leq \sigma(P_{n,k})$ if and only if $T \in T \in \{H_l\} \cup \{P_{n,k}\}(l \geq 2)$.*
(2) *If $k \geq 5$, $n-k > 5$ or $k > 5$, $n-k \geq 5$, then $z(P_{n,k}) \leq z(T) \leq z(H_2)$ if and only if $T \in \{H_l\} \cup \{P_{n,k}\}(l \geq 2)$.*
(3) *If $k = 4, n-k \geq 7$, then $z(P_{n,k}) \leq z(T) \leq z(F_2)$ if and only if $T \in \{H_l\} \cup \{P_{n,k}\} \cup \{F_2\}(l \geq 3)$.*

Proof. Here we only prove (1). From Lemma 2.8, it is easy to obtain the sufficiency. Next we show the necessity by contradiction. Let $T \in \mathscr{T}_{n,k}$. For $T \notin \{H_l\} \cup \{P_{n,k}\}, l \geq 2$, if $s(T) \geq 2$, by Lemmas 2.8, 3.1, 3.2, 3.3 and Corollary 3.1, $\sigma(T) \leq \sigma(F_2) < \sigma(H_2)$. For $s(T) = 1$, by Lemmas 3.1, 3.3, 3.4, $\sigma(T) < \sigma(H_2)$. So, the theorem holds. ∎

Corollary 3.1.

(1) *If $k \geq 4, n-k \geq 7$, then the trees in $\mathscr{T}_{n,k}$ with the first $[(n-k+1)/2]$ largest Merrifield-Simmons index are*

$$P_{n,k}, H_3, H_5, \cdots, H_{[(n-k+1)/2]}, \cdots, H_6, H_4, H_2.$$

If $k = 4, n-k = 5$, then the trees in $\mathscr{T}_{n,k}$ with the first $[(n-k+1)/2]$ largest Merrifield-Simmons index are

$$P_{n,k}, H_3, H_5, \cdots, H_{[(n-k+1)/2]}, \cdots, H_6, H_4, H_2 = F_2.$$

(2) *If $k \geq 5, n-k > 5$ or $k > 5, n-k \geq 5$, then the trees in $\mathscr{T}_{n,k}$ with the first $[(n-k+1)/2]$ smallest Hosoya index are*

$$P_{n,k}, H_3, H_5, \cdots, H_{[(n-k+1)/2]}, \cdots, H_6, H_4, H_2.$$

If $k = 5, n-k = 5$, then the trees in $\mathscr{T}_{n,k}$ with the first $[n-k+1/2]$ smallest Hosoya index are

$$P_{n,k}, H_3, H_5, \cdots, H_{[(n-k+1)/2]}, \cdots, H_6, H_4, H_2 = F_2.$$

(3) *If $k = 4, n-k \geq 7$, then the trees in $\mathscr{T}_{n,k}$ with the first $[n-k+1/2]$ smallest Hosoya index are*

$$P_{n,k}, H_3, H_5, \cdots, H_{[(n-k+1)/2]}, \cdots, H_6, H_4, F_2.$$

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