J Math Chem (2010) 47:11–20
DOI 10.1007/s10910-009-9526-4

ORIGINAL PAPER

Ordering trees with given pendent vertices with respect to Merrifield-Simmons indices and Hosoya indices

Xuezheng Lv · Yan Yan · Aimei Yu · Jingjing Zhang

Received: 10 December 2008 / Accepted: 21 January 2009 / Published online: 13 February 2009
© Springer Science+Business Media, LLC 2009

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, we order a kind of trees with given number of pendent vertices with respect to Merrifield-Simmons indices and Hosoya indices.

Keywords Trees · Merrifield-Simmons indices · Hosoya indices · Pendent vertices

1 Introduction

Let G be a graph on n vertices. Two vertices of G are said to be independent if they are not adjacent in G. A k-independent set of G is a set of k mutually independent vertices. Denote by $i(G, k)$ the number of the k-independent sets of G. For convenience, we regard the empty vertex set as an independent set. Then $i(G, 0) = 1$ for any graph G. The Merrifield-Simmons index of G, denoted by $i(G)$, is defined as $i(G) = \sum_{k=0}^{n} i(G, k)$. Similarly, 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. Denote by $z(G, k)$ the number of the k-matchings of G. For convenience, we regard

X. Lv (✉) · Y. Yan · J. Zhang
Department of Mathematics, Renmin University of China, Beijing 100872, China
e-mail: xzlv@ruc.edu.cn

Y. Yan
e-mail: yyruc@sina.com

A. Yu
Department of Mathematics, Beijing Jiaotong University, Beijing 100044, China
e-mail: yuaimeimath@yeah.net

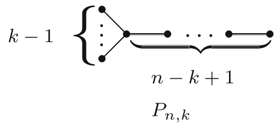

Fig. 1

the empty edge set as a matching. Then $z(G, 0) = 1$ for any graph G. The Hosoya index of G, denoted by $z(G)$, is defined as $z(G) = \sum_{k=0}^{[\frac{n}{2}]} z(G, k)$.

The Merrifield-Simmons index was introduced in 1982 by Prodinger and Tichy [18]. The Merrifield-Simmons index is one of the most popular topological indices in chemistry, which was extensively studied in a monograph [16]. Now there have been many papers studying the Merrifield-Simmons index (see [1,8,13–15,17,20,22–25]). The Hosoya index of a graph was introduced by Hosoya in 1971 [11] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures [16,19]. Since then, many authors have investigated the Hosoya index (e.g., see [3–10,12,15,19,23–25]). For n-vertex trees, 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 [9,18]).

Let $\mathcal{T}_{n,k}$ be the set of all trees with n vertices and k pendent vertices. Recently, Yu and Lv [21] showed that $P_{n,k}$ (as shown in Fig.1) is the tree with maximal Merrifield-Simmons indices and minimal Hosoya indices in $\mathcal{T}_{n,k}$. In [20], Wang etc. also characterized the trees with the first and second largest Merrifield-Simmons indices in $\mathcal{T}_{n,k}$. In this article, we order two kinds of the trees in $\mathcal{T}_{n,k}$ with respect to Merrifield-Simmons indices and Hosoya indices, respectively.

In order to state our results, we introduce some notation and terminology. Other undefined notation may refer to [2]. 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 $G - \{v\}$ and $G - \{xy\}$, 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.

2 Some Lemmas

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

Lemma 2.1 *Let G be a graph and uv be an edge of G. Then*

(1) $i(G) = i(G - uv) - i(G - (N_G[u] \cup N_G[v]))$,
(2) (see [9]) $z(G) = z(G - uv) + z(G - \{u, v\})$.

Lemma 2.2 (see [9]) *Let v be a vertex of G. Then*

(1) $i(G) = i(G - v) + i(G - N_G[v])$,

(2) $z(G) = z(G - v) + \sum_{u} z(G - \{u, v\})$, *where the summation extends over all vertices adjacent to* v.

In particular, when v is a pendent vertex of G and u is the unique vertex adjacent to v, we have $i(G) = i(G - v) + i(G - \{u, v\})$ and $z(G) = z(G - v) + z(G - \{u, v\})$. For example, if $G \cong P_n$, we get $i(P_n) = i(P_{n-1}) + i(P_{n-2})$ and $z(P_n) = z(P_{n-1}) + z(P_{n-2})$.

Lemma 2.3 (see [9]) *If* $G_1, G_2, \cdots, G_t$ *are the components of a graph* G, *we have*

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

Lemma 2.4 (see [13]) *Let* $A_l = i(P_l)i(P_{n-l})$, *then for* $1 \leq l \leq [\frac{n}{2}]$, $A_1 > A_3 > \cdots > A_{[\frac{n}{2}]} > \cdots > A_4 > A_2$.

We proved a similar result of Lemma 2.4 for Hosoya indices.

Lemma 2.5 *Let* $B_l = z(P_l)z(P_{n-l})$, *then for* $1 \leq l \leq [\frac{n}{2}]$, $B_1 < B_3 < \cdots < B_{[\frac{n}{2}]} < \cdots < B_4 < B_2$.

Proof By Lemma 2.1(2), we have

$$\begin{aligned}
B_l &= z(P_l)z(P_{n-l}) \\
&= z(P_n) - z(P_{l-1})z(P_{n-l-1}) \\
&= z(P_n) - [z(P_{n-2}) - z(P_{l-2})z(P_{n-l-2})] \\
&= z(P_n) - z(P_{n-2}) + [z(P_{n-4}) - z(P_{l-3})z(P_{n-l-3})] \\
&= z(P_n) - z(P_{n-2}) + z(P_{n-4}) + \cdots + (-1)^{l-1}z(P_{n-(2l-2)}) + (-1)^{l}z(P_{n-2l}).
\end{aligned}$$

It is easy to see

$$\begin{aligned}
B_{l+1} - B_l &= (-1)^{l+1}z(P_{n-2l-2}), \\
B_{l+2} - B_l &= (-1)^{l+1}z(P_{n-2l-2}) + (-1)^{l+2}z(P_{n-2l-4}) \\
&= (-1)^{l+1}[z(P_{n-2l-2}) - z(P_{n-2l-4})].
\end{aligned}$$

Then if $l \equiv 0(mod2)$, for $2 \leq l \leq \left[\frac{n}{2}\right] - 1$, $B_{l+1} - B_l < 0$, and for $2 \leq l \leq \left[\frac{n}{2}\right] - 2$, $B_{l+2} - B_l < 0$. If $l \equiv 1(mod2)$, for $2 \leq l \leq [\frac{n}{2}] - 1$, $B_{l+1} - B_l > 0$, and for $2 \leq l \leq \left[\frac{n}{2}\right] - 2$, $B_{l+2} - B_l > 0$. Therefore, $B_1 < B_3 < \cdots < B_{[\frac{n}{2}]} < \cdots < B_4 < B_2$. □

In [21], Yu and Lv defined two kinds of operations of $T \in \mathcal{T}_{n,k}$ and showed that these two kinds of operations make the Merrifield-Simmons indices of the trees increase strictly and the Hosoya indices of the trees decrease strictly. We first introduce the two operations.

Let $P = v_0v_1 \ldots v_k$ $(k \geq 1)$ be a path of a tree T. If $d_T(v_0) \geq 3$, $d_T(v_k) = 1$ and $d_T(v_i) = 2$ $(0 < i < k)$, we call P a pendant path of T with root v_0 and particularly when $k = 1$, we call P a pendant edge. For $T \in \mathcal{T}_{n,k}$, let $s(T)$ be the number of

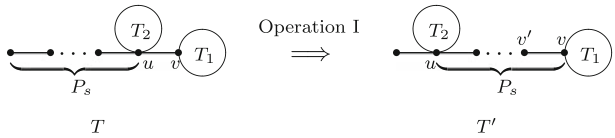

Fig. 2

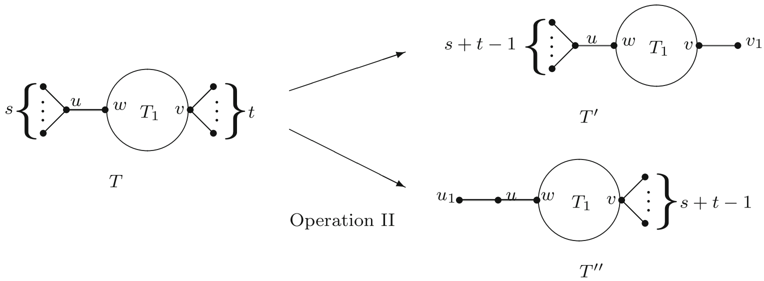

Fig. 3

vertices in T with degree more than 2 and $p(T)$ the number of pendent paths in T with length more than 1.

If $T \ncong P_{n,k}$ and $p(T) \geq 1$, then T can be seen as the tree as shown in Fig. 2, where P_s $(s \geq 3)$ is the pendent path of T with s vertices and root u, T_1 and T_2 are two subtrees of T with vertices v and u as roots, respectively, and $T_1, T_2 \ncong P_1$. If T' is obtained from T by replacing P_s with a pendent edge and replacing the edge uv with a path P_s, we say that T' is obtained from T by *Operation I* (as shown in Fig. 2). It is easy to see that $T' \in \mathcal{T}_{n,k}$.

Lemma 2.6 ([21]) *If T' is obtained from T by Operation I, then $i(T') > i(T)$ and $z(T') < z(T)$.*

If $s(T) \geq 2$ and $p(T) = 0$, then we always can find two pendent vertices u_1 and v_1 of T such that $d(u_1, v_1) = \max\{d(u, v) : u, v \in V(T)\}$. Let $u_1u, v_1v \in E(T)$, assume $N_T(u) = \{u_1, u_2, \ldots, u_s, w\}$ $(s \geq 2)$, $N_T(v) = \{v_1, v_2, \ldots, v_t, w'\}$ $(t \geq 2)$, where $u_1, u_2, \ldots, u_s, v_1, v_2, \ldots, v_t$ are pendent vertices of T. If $T' = T - \{vv_2, \ldots, vv_t\} + \{uv_2, \ldots, uv_t\}$ and $T'' = T - \{uu_2, \ldots, uu_s\} + \{vu_2, \ldots, vu_s\}$, we say that T' and T'' are obtained from T by *Operation II* (see Fig. 3), respectively. It is easy to see that $T', T'' \in \mathcal{T}_{n,k}$.

Lemma 2.7 ([21]) *If T' and T'' are obtained from T by Operation II, then*

(1) *either $i(T') > i(T)$ or $i(T'') > i(T)$;*
(2) *either $z(T') < z(T)$ or $z(T'') < z(T)$.*

3 Main results

Suppose H_l and F_m are the trees shown in Fig. 4. By symmetry, we may assume $l \leq n - l - k + 1$ and $m \leq k - m$, which means we can assume $2 \leq l \leq [\frac{n-k+1}{2}]$ and

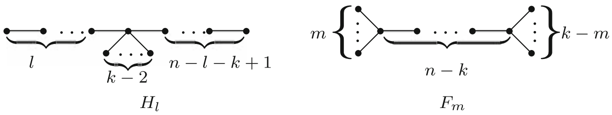

Fig. 4

$2 \leq m \leq \left[\frac{k}{2}\right]$. For $3 \leq k \leq n-2$, we denote

$$\mathcal{H}_{n,k} = \left\{ H_l \mid 2 \leq l \leq \left[\frac{n-k+1}{2}\right] - 1 \right\}$$

and

$$\mathcal{F}_{n,k} = \left\{ F_m \mid 2 \leq m \leq \left[\frac{k}{2}\right] \right\}.$$

Recall the definition of $s(T)$ and $p(T)$, it is easy to see that $P_{n,k}$ is the unique tree in $\mathcal{T}_{n,k}$ with $s(T) = 1$, $p(T) = 1$, $\mathcal{H}_{n,k}$ is the set of all trees in $\mathcal{T}_{n,k}$ with $s(T) = 1$, $p(T) = 2$ and $\mathcal{F}_{n,k}$ is the set of all trees in $\mathcal{T}_{n,k}$ with $s(T) = 2$, $p(T) = 0$.

By Lemmas 2.6 and 2.7, we can prove the following result.

Lemma 3.1 *Let T be a tree in $\mathcal{T}_{n,k}$. If $T \notin \{P_{n,k}\} \cup \mathcal{H}_{n,k} \cup \mathcal{F}_{n,k}$, there must be a tree $T' \in \mathcal{H}_{n,k} \cup \mathcal{F}_{n,k}$ such that $i(T') > i(T)$ and $z(T') < z(T)$.*

Proof If $s(T) \geq 3$, repeatedly using Operation I and II, we can get a tree T' from T such that $T' \in \mathcal{F}_{n,k}$, $i(P_{n,k}) > i(T') > i(T)$ and $z(P_{n,k}) < z(T'') < z(T)$.

If $s(T) = 1$ and $p(T) > 2$, repeatedly using Operation I, we can get a tree $T'' \in \mathcal{H}_{n,k}$ such that $i(P_{n,k}) > i(T') > i(T)$ and $z(P_{n,k}) < z(T') < z(T)$.

If $s(T) = 2$ and $p(T) \geq 1$, similarly we can get a tree $T' \in \mathcal{F}_{n,k}$ from T by Operation I with $i(P_{n,k}) > i(T') > i(T)$, $z(P_{n,k}) < z(T') < z(T)$. This completes the proof. □

It has been known $P_{n,k}$ has the largest Merrifield-Simmons index and least Hosoya index in $\mathcal{T}_{n,k}$. Now we focused on the trees in $\mathcal{H}_{n,k} \cup \mathcal{F}_{n,k}$. We first order the trees in $\mathcal{H}_{n,k}$ with respect to Merrifield-Simmons indices and Hosoya indices. In [13], Li and Zhao give the following result.

Lemma 3.2 (see [13]) $i(H_3) > i(H_5) > \cdots > i\left(H_{\left[\frac{n-k+1}{2}\right]}\right) > \cdots > i(H_6) > i(H_4) > i(H_2)$.

We order the trees in $\mathcal{H}_{n,k}$ with respect to Hosoya indices.

Lemma 3.3 $z(H_3) < z(H_5) < \cdots < z\left(H_{\left[\frac{n-k+1}{2}\right]}\right) < \cdots < z(H_6) < z(H_4) < z(H_2)$.

Proof Denote $n' = n - k + 1$, then

$$\begin{aligned} z(H_l) &= z(P_l)[(k-1)z(P_{n'-l}) + z(P_{n'-l-1})] + z(P_{l-1})z(P_{n'-l}) \\ &= (k-2)z(P_l)z(P_{n'-l}) + z(P_{n'+1}) \end{aligned}$$

Let $B_l = z(P_l)z(P_{n'-l})$. Since $k \geq 3$ and $n' = n - k + 1$, $z(H_i) < z(H_j)$ if and only if $B_i < B_j$ for any $2 \leq i, j \leq [\frac{n-k+1}{2}]$. By Lemma 2.5, we know $B_3 < \cdots < B_{[\frac{n}{2}]} < \cdots < B_4 < B_2$. So $z(H_3) < z(H_5) < \cdots < z\left(H_{\left[\frac{n-k+1}{2}\right]}\right) < \cdots < z(H_6) < z(H_4) < z(H_2)$. □

Then we order the trees in $\mathcal{F}_{n,k}$ with respect to Merrifield-Simmons indices and Hosoya indices.

Lemma 3.4 *$i(F_2) > i(F_3) > \cdots > i\left(F_{\left[\frac{k}{2}\right]}\right)$, and $z(F_2) < z(F_3) < \cdots z\left(F_{\left[\frac{k}{2}\right]}\right)$.*

Proof Since $3 \leq k \leq n-2$, we know $n - k \geq 2$. If $n - k \geq 4$, by Lemmas 2.1, 2.2 and 2.3, we have

$$\begin{aligned} i(F_m) &= 2^m[2^{k-m}i(P_{n-k-2}) + i(P_{n-k-3})] + [2^{k-m}i(P_{n-k-3}) + i(P_{n-k-4})] \\ &= 2^k i(P_{n-k-2}) + i(P_{n-k-4}) + [2^m + 2^{k-m}]i(P_{n-k-3}) \\ z(F_m) &= (m+1)[(k-m+1)z(P_{n-k-2}) + z(P_{n-k-3})] \\ &\quad +(k-m+1)z(P_{n-k-3}) + z(P_{n-k-4}) \\ &= (m+1)(k-m+1)z(P_{n-k-2}) + (k+2)z(P_{n-k-3}) + z(P_{n-k-4}) \end{aligned}$$

If $n - k = 2$, similarly we have $i(F_m) = 2^k + [2^m + 2^{k-m}]$, $z(F_m) = (m+1)(k-m+1) + 1$. And if $n - k = 3$, we have $i(F_m) = 2^{k+1} + 1 + [2^m + 2^{k-m}]$, $z(F_m) = (m+1)(k-m+1) + k + 2$.

Suppose $f(m) = 2^m + 2^{k-m}$ and $g(m) = (m+1)(k-m+1)$, then from the above we know that for $2 \leq i, j \leq \left[\frac{k}{2}\right]$,

$$i(F_i) > i(F_j) \text{ if and only if } f(i) > f(j),$$

and

$$z(F_i) < z(F_j) \text{ if and only if } g(i) < g(j).$$

It is easy to see that $f'(m) = \ln 2[2^m - 2^{k-m}] \leq 0$ since $m \leq \left[\frac{k}{2}\right]$ and the equality holds only if $m = \frac{k}{2}$. So if $m \leq \left[\frac{k}{2}\right]$, then $f(m)$ is a strictly decreasing function. Thus $i(F_2) > i(F_3) > \cdots > i\left(F_{\left[\frac{k}{2}\right]}\right)$. Also we have $g'(m) = k - 2m \geq 0$ and the equality holds only if $m = \frac{k}{2}$. So if $m \leq \left[\frac{k}{2}\right]$, $g(m)$ is a strictly increasing function. Thus $z(F_2) < z(F_3) < \cdots z\left(F_{\left[\frac{k}{2}\right]}\right)$. □

From Lemmas 3.2, 3.3 and 3.4, we can order the trees in $\mathcal{H}_{n,k} \cup \mathcal{F}_{n,k}$ by Merrifield-Simmons indices and Hosoya indices, respectively.

Theorem 3.1 (1) *If* $k \geq 4$ *and* $n-k \geq 5$*, then*

$$i\left(F_{\left[\frac{k}{2}\right]}\right) < \cdots < i(F_3) < i(F_2) \leq i(H_2) < i(H_4) < \cdots$$
$$< i\left(H_{\left[\frac{n-k+1}{2}\right]}\right) < \cdots < i(H_5) < i(H_3);$$

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

$$z\left(F_{\left[\frac{k}{2}\right]}\right) > \cdots > z(F_3) > z(F_2) \geq z(H_2) > z(H_4) > \cdots$$
$$z\left(H_{\left[\frac{n-k+1}{2}\right]}\right) > \cdots > z(H_5) > z(H_3);$$

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

$$z(H_2) > z(F_2) \geq z(H_4) > \cdots z\left(H_{\left[\frac{n-k+1}{2}\right]}\right) > \cdots > z(H_5) > z(H_3).$$

Proof (1) By Lemmas 3.2 and 3.4, we only need to show that $i(F_2) < i(H_2)$ if $k \geq 4$ and $n-k \geq 5$. Since

$$\begin{aligned}
i(H_2) - i(F_2) &= 3 \times 2^{k-2} i(P_{n-k-1}) + 2i(P_{n-k-2}) - 4[2^{k-2} i(P_{n-k-2}) \\
&\quad + i(P_{n-k-3})] - [2^{k-2} i(P_{n-k-3}) + i(P_{n-k-4})] \\
&= (3 \times 2^{k-2} - 4) i(P_{n-k-3}) - 2^{k-2} i(P_{n-k-1}) + 2i(P_{n-k-2}) \\
&\quad - i(P_{n-k-4}) \\
&= (2^{k-1} - 4) i(P_{n-k-3}) - 2^{k-2} i(P_{n-k-2}) + 2i(P_{n-k-2}) \\
&\quad - i(P_{n-k-4}) \\
&= (2^{k-2} - 4) i(P_{n-k-3}) - 2^{k-2} i(P_{n-k-4}) + 2i(P_{n-k-2}) \\
&\quad - i(P_{n-k-4}) \\
&= 2^{k-2} i(P_{n-k-5}) - 4i(P_{n-k-3}) + 2i(P_{n-k-2}) - i(P_{n-k-4}) \\
&= 2^{k-2} i(P_{n-k-5}) - 2i(P_{n-k-3}) + i(P_{n-k-4}) \\
&= (2^{k-2} - 1) i(P_{n-k-5}) - i(P_{n-k-3}) \\
&= (2^{k-2} - 3) i(P_{n-k-5}) - i(P_{n-k-6}),
\end{aligned}$$

then if $k \geq 4$ and $n-k \geq 5$, $i(F_2) \leq i(H_2)$.

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

$$\begin{aligned}
z(F_2) - z(H_2) &= 3 \times (k-1)z(P_{n-k-2}) + (k+2)z(P_{n-k-3}) + z(P_{n-k-4}) \\
&\quad -2(k-2)z(P_{n-k-1}) - z(P_{n-k+2}) \\
&= 3kz(P_{n-k-2}) - 3z(P_{n-k-2}) + (k+2)z(P_{n-k-3}) + z(P_{n-k-4}) \\
&\quad -2kz(P_{n-k-1}) + 4z(P_{n-k-1}) - [3z(P_{n-k-1}) + 2z(P_{n-k-2})] \\
&= 3kz(P_{n-k-2}) - 3z(P_{n-k-2}) + (k+2)z(P_{n-k-3}) + z(P_{n-k-4}) \\
&\quad -2kz(P_{n-k-1}) + z(P_{n-k-1}) - 2z(P_{n-k-2}) \\
&= kz(P_{n-k-1}) - 4z(P_{n-k-2}) + 3z(P_{n-k-3}) + z(P_{n-k-4}) \\
&\quad - 2kz(P_{n-k-3}) \\
&= kz(P_{n-k-4}) - 3z(P_{n-k-4}) - z(P_{n-k-3}) \\
&= (k-4)z(P_{n-k-4}) - z(P_{n-k-5}) \geq 0.
\end{aligned}$$

Together with Lemmas 3.3 and 3.4, we can finish the proof.

(3) From the proof of (2), we know if $k = 4$ and $n-k \geq 7$, $z(H_2) > z(F_2)$. But then

$$\begin{aligned}
z(F_2) - z(H_4) &= 9z(P_{n-6}) + 6z(P_{n-7}) + z(P_{n-8}) - 10z(P_{n-7}) - z(P_{n-2}) \\
&= 5z(P_{n-5}) + 5z(P_{n-6}) - 10z(P_{n-7}) - [3z(P_{n-5}) + 2z(P_{n-6})] \\
&= 2z(P_{n-5}) + 3z(P_{n-6}) - 10z(P_{n-7}) \\
&= 5z(P_{n-6}) - 8z(P_{n-7}) = 5z(P_{n-8}) - 3z(P_{n-7}) \\
&= 2z(P_{n-8}) - 3z(P_{n-9}) = 2z(P_{n-10}) - z(P_{n-9}) \geq 0.
\end{aligned}$$

Together with Lemmas 3.3 and 3.4, we can finish the proof. □

Recall the definition of $\mathcal{H}_{n,k}$ and $\mathcal{F}_{n,k}$. It is easy to see that: if $k = 3$, $\mathcal{F}_{n,k} = \emptyset$; if $n-k \leq 2$, $\mathcal{H}_{n,k} = \emptyset$; if $k = 3$ and $n-k = 2$, $\mathcal{F}_{n,k} = \mathcal{H}_{n,k} = \emptyset$. Note that if T is the tree with the second largest Merrifield-Simmons index or the second least Hosoya index in $\mathcal{T}_{n,k}$, then $T \in \mathcal{H}_{n,k}$ or $\mathcal{F}_{n,k}$. So it follows that:

(1) if $k = 3$, $T \in \mathcal{H}_{n,k}$;
(2) if $n-k \leq 2$, $T \in \mathcal{F}_{n,k}$;
(3) if $k = 3$ and $n-k = 2$, T does not exist.

Then by Lemma 3.1, we can get the following two results.

Corollary 3.1 *Let T be the tree with the second largest Merrifield-Simmons index in $\mathcal{T}_{n,k}$ $(3 \leq k \leq n-2)$, then*

$$T \cong \begin{cases} H_3, \ if \ n-k \geq 5; \\ H_2, \ if \ k = 3 \ and \ 3 \leq n-k \leq 4 \ or \ k \geq 4 \ and \ n-k = 4; \\ F_2, \ if \ k \geq 4 \ and \ 2 \leq n-k \leq 3. \end{cases}$$

Proof By Lemma 3.2, if $k = 3$ and $n-k \geq 5$, $T \cong H_3$; if $k = 3$ and $3 \leq n-k \leq 4$, $T \cong H_2$ (since H_l $(l \geq 3)$ does not exist if $n-k \leq 4$).

If $k \geq 4$ and $n-k=2$, then $T \cong F_2$ by Lemma 3.4. If $k \geq 4$ and $3 \leq n-k \leq 4$, by Lemma 3.2 and 3.4, we know $T \cong H_2$ or $T \cong F_2$. Note that

$$i(F_2) = \begin{cases} 3 \times 2^k + 2^{k-1} + 9, \text{ if } & n-k=4; \\ 2^{k+1} + 2^{k-2} + 5, \quad \text{if } & n-k=3. \end{cases}$$

$$i(H_2) = \begin{cases} 15 \times 2^{k-2} + 6, \text{ if } & n-k=4; \\ 9 \times 2^{k-2} + 4, \quad \text{if } & n-k=3. \end{cases}$$

Thus we know $T \cong H_2$ if $k \geq 4$ and $n-k=4$; $T \cong F_2$ if $k \geq 4$ and $n-k=3$. If $k \geq 4$ and $n-k \geq 5$, by Theorem 3.1, we know $T \cong H_3$. Proof is completed. □

Corollary 3.2 *Let T be the tree with the second least Hosoya index in $\mathcal{T}_{n,k}$ ($3 \leq k \leq n-2$), then*

$$T \cong \begin{cases} H_3, & if\ n-k \geq 5; \\ H_2, & if\ k=3\ and\ 3 \leq n-k \leq 4\ or\ k>4\ and\ n-k=4; \\ H_2\ or\ F_2, & if\ k=4\ and\ n-k=4; \\ F_2, & if\ k>4\, and\ 2 \leq n-k \leq 3. \end{cases}$$

Proof By Lemma 3.3, we have if $k=3$ and $n-k \geq 5$, $T \cong H_3$; if $k=3$ and $3 \leq n-k \leq 4$, $T \cong H_2$.

If $k \geq 4$ and $n-k=2$, then $T \cong F_2$ by Lemma 3.4. If $k \geq 4$ and $3 \leq n-k \leq 4$, by Lemmas 3.3 and 3.4, we know $T \cong H_2$ or $T \cong F_2$. Since

$$z(F_2) = \begin{cases} 7k-3, \text{ if } n-k=4; \\ 4k-1, \text{ if } n-k=3. \end{cases}$$

$$z(H_2) = \begin{cases} 6k+1, \text{ if } n-k=4; \\ 4k, \qquad \text{if } n-k=3. \end{cases}$$

Thus we know $T \cong H_2$ or F_2 if $k=4$ and $n-k=4$; $T \cong H_2$ if $k>4$ and $n-k=4$; $T \cong F_2$ if $k \geq 4$ and $n-k=3$.

If $k \geq 4$ and $n-k \geq 5$, similarly we know $T \cong H_3$ or $T \cong F_2$. Since

$$\begin{aligned} z(F_2) &= 3[(k-1)z(P_{n-k-2}) + z(P_{n-k-3})] + (k-1)z(P_{n-k-3}) + z(P_{n-k-4}) \\ &= 3(k-1)z(P_{n-k-2}) + (k+2)z(P_{n-k-3}) + z(P_{n-k-4}) \\ z(H_3) &= z(P_3)[(k-1)z(P_{n-k-2}) + z(P_{n-k-3})] + z(P_2)z(P_{n-k-2}) \\ &= 3(k-1)z(P_{n-k-2}) + 3z(P_{n-k-3}) + 2z(P_{n-k-2}), \end{aligned}$$

then $z(T_2) - z(H_3) = (k-1)z(P_{n-k-3}) + z(P_{n-k-4}) - 2z(P_{n-k-2}) \geq 2z(P_{n-k-3}) - z(P_{n-k-2}) > 0$. So we have $z(H_3) < z(F_2)$ which means $T \cong H_3$. This completes the proof. □

Acknowledgements X. Lv was supported by National Natural Science Foundation of China (No. 10726065). A. Yu was partially supported by National Natural Science Foundation of China (No. 10671090).

References

1. A.F. Alameddine, Bounds on the Fibonacci number of a maximal outerplanar graph. Fibonacci Q. **36**, 206–210 (1998)
2. J.A. Bondy, U.S.R. Murty, *Graph Theory with Applications* (Macmillan, New York, 1976)
3. O. Chan, I. Gutman, T.K. Lam, R. Merris, Algebraic connections between topological indices. J. Chem. Inform. Comput. Sci. **38**, 62–65 (1998)
4. S.J. Cyvin, I. Gutman, Hosoya index of fused molecules. MATCH Commun. Math. Comput. Chem. **23**, 89–94 (1988)
5. S.J. Cyvin, I. Gutman, N. Kolakovic, Hosoya index of some polymers. MATCH Commun. Math. Comput. Chem. **24**, 105–117 (1989)
6. M. Fischermann, A. Hoffmann, D. Rautenbach, L. Szekely, L. Volkmann, Wiener index versus maximum degree in trees. Discret. Appl. Math. **122**, 127–137 (2002)
7. I. Gutman, On the Hosoya index of very large molecules. MATCH Commun. Math. Comput. Chem. **23**, 95–103 (1988)
8. I. Gutman, Extremal hexagonal chains. J. Math. Chem. **12**, 197–210 (1993)
9. I. Gutman, O.E. Polansky, *Mathematical Concepts in Organic Chemistry*. (Springer, Berlin, 1986)
10. I. Gutman, D. Vidović, B. Furtula, Coulson function and Hosoya index. Chem. Phys. Lett. **355**, 378–382 (2002)
11. H. Hosoya, Topological index, a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons. Bull. Chem. Soc. Jpn. **44**, 2332–2339 (1971)
12. Y.P. Hou, On acyclic systems with minimal Hosoya index. Discret. Appl. Math. **119**, 251–257 (2002)
13. X. Li, H. Zhao, On the Fibonacci Numbers of trees. Fibonacci Q. **44**, 32–38 (2006)
14. X.L. Li, H.X. Zhao, I. Gutman, On the Merrifield-Simmons index of trees. MATCH Commun. Math. Comput. Chem. **54**, 389–402 (2005)
15. X.Z. Lv, A.M. Yu, The Merrifield-Simmons indices and Hosoya indices of trees with a given maximum degree. MATCH Commun. Math. Comput. Chem. **56**, 605–616 (2006)
16. R.E. Merrifield, H.E. Simmons, *Topological Methods in Chemistry*. (Wiley, New York, 1989)
17. A.S. Pedersen, P.D. Vestergaard, The number of independent sets in unicyclic graphs. Discret. Appl. Math. **152**, 246–256 (2005)
18. H. Prodinger, R.F. Tichy, Fibonacci numbers of graphs. Fibonacci Q. **20**, 16–21 (1982)
19. L. Türker, Contemplation on the Hosoya indices. J. Mol. Struct. (Theochem) **623**, 75–77 (2003)
20. M. Wang, H. Hua, D. Wang, The first and second largest Merrifield-Simmons indices of trees with prescribed pendent vertices. J. Math. Chem. **43**(2), 727–736 (2008)
21. A.M. Yu, X.Z. Lv, The Merrifield-Simmons Indices and Hosoya Indices of trees with *k* pendent vertices. J. Math. Chem. **41**, 33–43 (2007)
22. A.M. Yu, F. Tian, A kind of graphs with minimal Hosoya indices and maximal Merrifield-Simmons indices. MATCH Commun. Math. Comput. Chem. **55**, 103–118 (2006)
23. L.Z. Zhang, The proof of Gutman's conjectures concerning extremal hexagonal chains. J. Sys. Sci. Math. Sci. **18**, 460–465 (1998)
24. L.Z. Zhang, F. Tian, Extremal hexagonal chains concerning largest eigenvalue. Sci. China (Ser. A) **44**, 1089–1097 (2001)
25. L.Z. Zhang, F. Tian, Extremal catacondensed benzenoids. J. Math. Chem. **34**, 111–122 (2003)
26. H.X. Zhao, X.L. Li, On the Fibonacci numbers of trees. Fibonacci Q. **44**, 32–38 (2006)