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On the Merrifield-Simmons Indices and Hosoya indices of Trees with a Prescribed Diameter

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Abstract

The Merrifield-Simmons index $\sigma = \sigma(G)$ and the Hosoya index $z = z(G)$ of a (molecular) graph G are defined as the total number of the independent vertexsets and the total number of the independent edgesets of the graph G, respectively. Let $\mathscr{T}_{n,d}$ denote the set of trees on n vertices and diameter d. Li, Zhao and Gutman [MATCH Commun. Math. Comput. Chem. 54(2005) 389-402] have determined the unique tree in $\mathscr{T}_{n,d}$ with maximal σ-value. Pan, Xu, Yang and Zhou [MATCH Commun. Math. Comput. Chem., to appear] have recently determined the unique tree in $\mathscr{T}_{n,d}$ with minimal z-value. In this paper, the first $\lfloor \frac{d}{2} \rfloor + 1$ Merrifield-Simmons indices and the last $\lfloor \frac{d}{2} \rfloor + 1$ Hosoya indices of trees in the set $\mathscr{T}_{n,d}$ $(3 \leq d \leq n-4)$ are characterized.

1. Introduction

Given a molecular graph G, the *Merrifield-Simmons index* $\sigma = \sigma(G)$ and the *Hosoya index* $z = z(G)$ are defined as the number of subsets of $V(G)$ in which no

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two vertices are adjacent and the number of subsets of $E(G)$ in which no edges are incident, respectively, i.e., in graph-theoretical terminology, the total number of the independent vertexsets of the graph and the total number of the independent edgesets of the graph G.

The Hosoya index of a graph was introduced by Hosoya in 1971 [9] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures ([16, 18]). In [16], Merrifield and Simmons developed a topological approach to structural chemistry. The cardinality of the topological space in their theory turns out to be equal to $\sigma(G)$ of the respective molecular graph G. In [6], Gutman first uses “Merrifield-Simmons index” to name the quantity. Since then, many authors have investigated the Hosoya index and Merrifield-Simmons index (e.g., see [2]-[8], [11], [14], [17], [19]-[23]). An important direction is to determine the graphs with maximal or minimal Merrifield-Simmons indices (or Hosoya indices, resp.) in a given class of graphs. It has been shown in [7, 12] that the path P_n has the minimal Merrifield-Simmons index (or the maximal Hosoys index, resp.) and the star S_n has the maximal Merrifield-Simmons index (or the minimal Hosoys index, resp.). Li, Zhao and Gutman [14] have recently determined the unique tree in $\mathscr{T}_{n,d}$ with maximal Merrifield-Simmons index. Pan, Xu, Yang and Zhou [17] have recently determined the unique tree in $\mathscr{T}_{n,d}$ with minimal Hosoya index.

In this paper, we will give the first $\lfloor \frac{d}{2} \rfloor + 1$ Merrifield-Simmons indices and the last $\lfloor \frac{d}{2} \rfloor + 1$ Hosoya indices of trees in the set $\mathscr{T}_{n,d}$ $(3 \leq d \leq n-3)$, respectively. Moreover, for $d = n-2$, the first $\lfloor \frac{d}{2} \rfloor$ Merrifield-Simmons indices and the last $\lfloor \frac{d}{2} \rfloor$ Hosoya indices of trees in the set $\mathscr{T}_{n,d}$ are also given, respectively.

In order to discuss our results, we first introduced some terminologies and notations of graphs. For other undefined notations, the reader is referred to [1]. We only consider finite, undirected and simple graphs. For a vertex x of a graph G, we denote the neighborhood and the degree of x by $N_G(x)$ and $d_G(x)$, respectively. A *pendant vertex* is a vertex of degree 1. Denote $N_G[x] = N_G(x) \cup \{x\}$. For two vertices x and y $(x \neq y)$, the distance between x and y is the number of edges in a shortest path joining x and y. The diameter of a graph, denoted by $\mathrm{diam}(G)$, is the maximum distance between any two vertices of G. We will use $G - x$ or $G - xy$ to denote the graph that arises from G by deleting the vertex $x \in V(G)$ or the edge $xy \in E(G)$. Similarly, $G + xy$ is a graph that arises from G by adding an edge $xy \notin E(G)$, where $x,\ y \in V(G)$.

A tree is a connected acyclic graph. Let T be a tree of order n with diameter d. If $d = 2$, then $T \cong K_{1,n-1}$, a path of order n; and if $d = n-1$, then $T \cong P_n$, a star of order n. Therefore, in the following, we assume that $3 \leq d \leq n-2$. Let $\mathscr{T}_{n,d} = \{T : T \text{ is a tree with order } n \text{ and diameter } d,\ 3 \leq d \leq n-2\}$.

2. Preliminaries

We first give some lemmas that will be used in the proof of our results.

Lemma 2.1 (see [7]). *Let G be a graph and uv be an edge of G. Then*

(i) $\sigma(G) = \sigma(G - uv) - \sigma\left(G - (N_G[u] \cup N_G[v])\right);$

(ii) $z(G) = z(G - uv) + z(G - \{u, v\}).$

Lemma 2.2 (see [7]). *Let v be a vertex of G. Then*

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

(ii) $z(G) = z(G - v) + \sum_{u \in N_G(v)} z(G - \{u, v\}).$

From Lemma 2.2, if v is a vertex of G, then $\sigma(G) > \sigma(G - v)$. Moreover, if G is a graph with at least one edge, then $z(G) > z(G - v)$.

Lemma 2.3 (see [7]). *If $G_1, G_2, \cdots, G_\omega$ are the components of a graph G, then*

(i) $\sigma(G) = \prod_{j=1}^{\omega} \sigma(G_j);$

(ii) $z(G) = \prod_{j=1}^{\omega} z(G_j).$

Lemma 2.4. *Let G be a graph and $v, u \in V(G)$. Suppose that $G_{s,t}$ be a graph obtained from G by attaching s, t pendant vertices to v, u, respectively. Then either*

$$\sigma(G_{s+i,t-i}) > \sigma(G_{s,t}) \ \ (\text{or } z(G_{s+i,t-i}) < z(G_{s,t}), \text{ resp.}) \qquad \text{for } 1 \leq i \leq t;$$

or

$$\sigma(G_{s-i,t+i}) > \sigma(G_{s,t}) \ \ (\text{or } z(G_{s-i,t+i}) < z(G_{s,t}), \text{ resp.}) \qquad \text{for } 1 \leq i \leq s.$$

Proof. If $uv \notin E(G)$, then by Lemma 2.2 and Lemma 2.3, we have

$$\begin{aligned}
\sigma(G_{s,t}) &= \sigma(G_{s,t} - v) + \sigma\left(G_{s,t} - N_{G_{s,t}}[v]\right) \\
&= \sigma\left(G_{s,t} - v - u\right) + \sigma\left(G_{s,t} - v - N_{G_{s,t}-v}[u]\right) \\
&\quad + \sigma\left(G - N_{G_{s,t}}[v] - u\right) + \sigma\left(G_{s,t} - N_{G_{s,t}}[v] - N_{G_{s,t}-N_{G_{s,t}}[v]}[u]\right) \\
&= 2^{s+t}\sigma(G - v - u) + 2^{s}\sigma\left(G - v - N_G[u]\right) \\
&\quad + 2^{t}\sigma\left(G - u - N_G[v]\right) + \sigma\left(G - N_G[v] - N_G[u]\right),
\end{aligned}$$

$$
\begin{aligned}
z(G_{s,t}) &= z(G_{s,t}-v) + \sum_{v'\in N_{G_{s,t}}(v)} z(G_{s,t}-v-v') \\
&= z(G_{s,t}-v-u) + \sum_{v'\in N_{G_{s,t}}(v)} \sum_{u'\in N_{G_{s,t}-v-v'}(u)} z(G_{s,t}-v-u-v'-u') \\
&\quad + \sum_{v'\in N_{G_{s,t}}(v)} z(G_{s,t}-v-u-v') + \sum_{u'\in N_{G_{s,t}-v}(u)} z(G_{s,t}-v-u-u') \\
&= (1+s+t+st)z(G-v-u) + (1+t)\sum_{v'\in N_G(v)} z(G-v-u-v') \\
&\quad +(1+s)\sum_{u'\in N_{G-v}(u)} z(G-v-u-u') \\
&\quad + \sum_{v'\in N_G(v)} \sum_{u'\in N_{G-v}(u)} z(G-v-u-v'-u').
\end{aligned}
$$

If $uv \in E(G)$, then, by Lemma 2.2 and Lemma 2.3, we have

$$
\begin{aligned}
\sigma(G_{s,t}) &= \sigma(G_{s,t}-v) + \sigma(G_{s,t}-N_{G_{s,t}}[v]) \\
&= \sigma(G_{s,t}-v-u) + \sigma(G_{s,t}-v-N_{G_{s,t}-v}[u]) + \sigma(G_{s,t}-N_{G_{s,t}}[v]) \\
&= 2^{s+t}\sigma(G-v-u) + 2^{s}\sigma(G-v-N_G[u]) + 2^{t}\sigma(G-u-N_G[v]), \\
z(G_{s,t}) &= z(G_{s,t}-v) + \sum_{v'\in N_{G_{s,t}}(v)} z(G_{s,t}-v-v') \\
&= 2z(G_{s,t}-v-u) + \sum_{v'\in N_{G_{s,t}}(v)-u} \sum_{u'\in N_{G_{s,t}-v-v'}(u)} z(G_{s,t}-v-u-v'-u') \\
&\quad + \sum_{v'\in N_{G_{s,t}}(v)-u} z(G_{s,t}-v-u-v') + \sum_{u'\in N_{G_{s,t}-v}(u)} z(G_{s,t}-v-u-u') \\
&= (2+s+t+st)z(G-v-u) + (1+t)\sum_{v'\in N_G(v)-u} z(G-v-u-v') \\
&\quad +(1+s)\sum_{u'\in N_{G-v}(u)} z(G-v-u-u') \\
&\quad + \sum_{v'\in N_G(v)-u} \sum_{u'\in N_{G-v}(u)} z(G-v-u-v'-u').
\end{aligned}
$$

Therefore

$$
\begin{aligned}
& 2\sigma(G_{s,t}) - \sigma(G_{s+i,t-i}) - \sigma(G_{s-i,t+i}) \\
= \ & (2^{i+1} - 2^{2i} - 1)\left[2^{s-i}\sigma(G-v-N_G[u]) + 2^{t-i}\cdot\sigma(G-u-N_G[v])\right] < 0, \\
& 2z(G_{s,t}) - z(G_{s+i,t-i}) - z(G_{s-i,t+i}) = 2i^2 z(G-v-u) > 0.
\end{aligned}
$$

Thus, if $\sigma(G_{s,t}) - \sigma(G_{s-i,t+i}) \geq 0$ (or $z(G_{s,t}) - z(G_{s-i,t+i}) \leq 0$, resp.), then

$$\sigma(G_{s,t}) - \sigma(G_{s+i,t-i}) < -[\sigma(G_{s,t}) - \sigma(G_{s-i,t+i})] \leq 0$$

(or $z(G_{s,t}) - z(G_{s+i,t-i}) > -[z(G_{s,t}) - z(G_{s-i,t+i})] \geq 0$, resp.). Hence the lemma holds. ■

Let $H_1,\ H_2$ be two connected graphs with $V(H_1) \cap V(H_2) = \{v\}$. Let H_1vH_2 be a graph defined by $V(G) = V(H_1) \cup V(H_2)$, $V(H_1) \cap V(H_2) = \{v\}$ and $E(G) = E(H_1) \cup E(H_2)$.

Lemma 2.5. *Let H be a connected graph and T_l be a tree of order l with $V(H) \cap V(T_l) = \{v\}$. Then*

$$\sigma(HvT_l) \leq \sigma(HvK_{1,l-1}) \text{ (or } z(HvT_l) \geq z(HvK_{1,l-1}) \text{, resp.)}$$

and equality holds if and only if $HvT_l \cong HvK_{1,l-1}$, where v is identified with the center of the star $K_{1,l-1}$ in $HvK_{1,l-1}$.

Proof. Note that $\sigma(T_l) \leq \sigma(K_{1,l-1})$, $\sigma(T_l - v) \leq \sigma(K_{1,l-1} - v)$, $\sigma(H - v) > \sigma(H - N_H[v])$ and $z(T_l) \geq z(K_{1,l-1})$. By Lemmas 2.2 and 2.3, we have

$$\begin{aligned}
\sigma(HvT_l) &= \sigma(H-v)\sigma(T_l-v) + \sigma(H-N_H[v])\sigma(T_l - N_{T_l}[v]) \\
&= \sigma(H-v)\sigma(T_l-v) + \sigma(H-N_H[v])[\sigma(T_l) - \sigma(T_l - v)] \\
&= \sigma(H-N_H[v])\sigma(T_l) + [\sigma(H-v) - \sigma(H-N_H[v])]\sigma(T_l - v) \\
&\leq \sigma(H-N_H[v])\sigma(K_{1,l-1}) + [\sigma(H-v) - \sigma(H-N_H[v])]\sigma(K_{1,l-1} - v) \\
&= \sigma(HvK_{1,l-1}); \\
z(HvT_l) &= z(H-v)z(T_l-v) + \sum_{w \in N_H(v)} z(H-v-w)z(T_l) \\
&\quad + \sum_{u \in N_{T_l}(v)} z(H-v)z(T_l - v - u) \\
&= z(H-v)z(T_l-v) + \sum_{w \in N_H(v)} z(H-v-w)z(T_l) \\
&\quad + z(H-v)[z(T_l) - z(T_l - v)] \\
&= z(H-v)z(T_l) + \sum_{w \in N_H(v)} z(H-v-w)z(T_l) \\
&\geq z(H-v)z(K_{1,l-1}) + \sum_{w \in N_H(v)} z(H-v-w)z(K_{1,l-1}) \\
&= z(HvK_{1,l-1}).
\end{aligned}$$

Therefore the lemma holds. ■

3. Main Results

In this section, we will give the first $\lfloor \frac{d}{2} \rfloor + 1$ Merrifield-Simmons indices and the last $\lfloor \frac{d}{2} \rfloor + 1$ Hosoya indices of trees in the set $\mathscr{T}_{n,d}$ $(3 \le d \le n-3)$.

In order to formulate our results, we need to define some trees (see Figure 1) as follows.

Let $T_{n,d}(p_1, \cdots, p_{d-1})$ be a tree of order n created from a path $P_{d+1} = v_0 v_1 \ldots v_{d-1} v_d$ by attaching p_i pendant vertices to v_i, $1 \le i \le d-1$, respectively, where $n = d+1+\sum_{i=1}^{d-1} p_i$, $p_i \ge 0$, $i = 1, 2, \cdots, d-1$. Denote $W_{n,d,i} = T_{n,d}(\underbrace{0, \cdots, 0}_{i-1}, n-d-1, 0, \cdots, 0)$ and $T_{n,d,i,j} = T_{n,d}(\underbrace{0, \cdots, 0}_{i-1}, n-d-2, \underbrace{0, \cdots, 0}_{j-i-1}, 1, 0, \cdots, 0)$. Then $W_{n,d,i} = W_{n,d,d-i}$ and $T_{n,d,i,j} = T_{n,d,d-i,d-j}$.

Let $X_{n,d,i}$ $(2 \le i \le d-2)$ be a graph obtained from $W_{n-1,d,i}$ by attaching a pendant vertex to one pendant vertex of $W_{n-1,d,i}$, except for v_0, v_d. Then $X_{n,d,i} = X_{n,d,d-i}$.

Let $Y_{n,d,i}$ $(2 \le i \le d-2)$ be a graph obtained from $W_{d+2,d,i}$ by attaching $n-d-2$ pendant vertices to one pendant vertex of $W_{d+2,d,i}$, except for v_0, v_d. Then $Y_{n,d,i} = Y_{n,d,d-i}$.

Denote $\mathscr{T}^0_{n,d} = \{W_{n,d,i} \ : \ 1 \le i \le d-1\}$, $\mathscr{T}^*_{n,d} = \{X_{n,d,i} \ : \ 2 \le i \le d-2\}$, $\mathscr{T}'_{n,d} = \{Y_{n,d,i} \ : \ 2 \le i \le d-2\}$ and $\mathscr{T}''_{n,d} = \{T_{n,d,i,j} \ : \ 1 \le i < j \le d-1\}$.

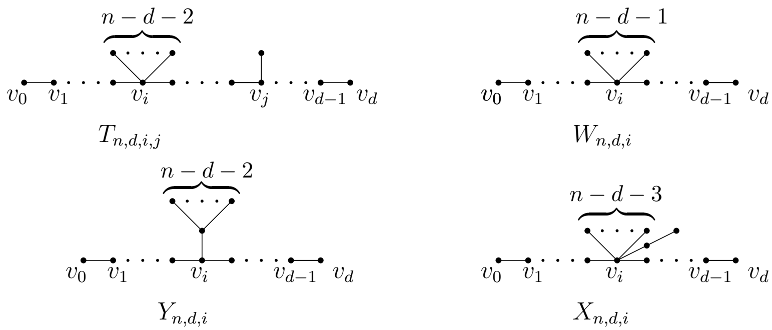

Figure 1

Let F_n be the nth Fibonacci number, i.e., $F_0 = F_1 = 1$, $F_n = F_{n-1} + F_{n-2}$, $n \ge 2$. Note that $\sigma(P_n) = F_{n+1}$, $z(P_n) = F_n$.

By Lemmas 2.1-2.3, we have the following results.

Lemma 3.1. *Let $W_{n,d,i}$, $X_{n,d,i}$, $Y_{n,d,i}$ be the graphs shown in Figure 1. Then*

(i) $\sigma(W_{n,d,i}) = F_{d+2} + (2^{n-d-1} - 1)F_{i+1}F_{d-i+1}$ *and* $z(W_{n,d,i}) = F_{d+1} + (n-d-1)F_iF_{d-i}$, *where* $1 \leq i \leq d-1$;

(ii) $\sigma(X_{n,d,i}) = 2F_{d+2} + (3 \cdot 2^{n-d-3} - 2)F_{i+1}F_{d-i+1}$ *and* $z(X_{n,d,i}) = 2F_{d+1} + (2n-2d-5)F_iF_{d-i}$, *where* $2 \leq i \leq d-2$;

(iii) $\sigma(Y_{n,d,i}) = 2^{n-d-2}F_{d+2} + F_{i+1}F_{d-i+1}$ *and* $z(Y_{n,d,i}) = (n-d-1)F_{d+1} + F_iF_{d-i}$, *where* $2 \leq i \leq d-2$;

(iv) $\sigma(T_{n,d,i,i+1}) = 2^{n-d-2}F_{i+1}F_{d-i+2} + 2F_iF_{d-i}$, $z(T_{n,d,i,i+1}) = F_iF_{d-i-1} + F_{d-i+1}[(n-d-1)F_i + F_{i-1}]$, $\sigma(T_{n,d,i,i+2}) = 2^{n-d-2}F_{i+1}(F_{d-i+2} + F_{d-i}) + F_iF_{d-i+1}$, $z(T_{n,d,i,i+2}) = (F_{d-i} + F_{d-i-2})[(n-d-1)F_i + F_{i-1}] + F_iF_{d-i}$, $\sigma(T_{n,d,i,j}) = 2^{n-d-2}F_{i+1}(F_{d-i+1} + F_{j-i}F_{d-j+1}) + F_i(F_{d-i} + F_{j-i-1}F_{d-j+1})$ *and* $z(T_{n,d,i,j}) = [(n-d-1)F_i + F_{i-1}](F_{d-i} + F_{j-i-1}F_{d-j}) + F_i(F_{d-i-1} + F_{j-i-2}F_{d-j})$ *for* $j - i \geq 3$. *In particular,* $\sigma(T_{n,4,1,3}) = 9 \cdot 2^{n-5} + 5$, $z(T_{n,4,1,3}) = 4n - 13$, $\sigma(T_{n,d,1,d-1}) = 2^{n-d-1}(F_d + 2F_{d-2}) + F_{d-1} + 2F_{d-3}$ *and* $z(T_{n,d,1,d-1}) = (n-d+2)F_{d-2} + (2n-2d-1)F_{d-3}$ *for* $d \geq 5$.

Lemma 3.2. *Let $W_{n,d,i}$, $X_{n,d,i}$, $Y_{n,d,i}$ be the graphs shown in Figure 1. Then*

(i) $\sigma(W_{n,d,i}) > \sigma(X_{n,d,i})$ *and* $z(W_{n,d,i}) < z(X_{n,d,i})$ *for* $2 \leq i \leq d-2$ *and* $3 \leq d \leq n-3$;

(ii) $\sigma(X_{n,d,i}) \geq \sigma(Y_{n,d,i})$ *and* $z(X_{n,d,i}) \leq z(Y_{n,d,i})$ *for* $2 \leq i \leq d-2$ *and* $4 \leq d \leq n-3$.

Proof. Note that $F_{d+2} = F_{i+1}F_{d-i+1} + F_iF_{d-i}$. By Lemma 3.1, we have

$$\begin{aligned}
\sigma(W_{n,d,i}) - \sigma(X_{n,d,i}) &= (2^{n-d-3} + 1)F_{i+1}F_{d-i+1} - F_{d+2} \\
&= 2^{n-d-3}F_{i+1}F_{d-i+1} - F_iF_{d-i} > 0, \\
z(W_{n,d,i}) - z(X_{n,d,i}) &= -F_{d+1} - (n-d-4)F_iF_{d-i} < 0, \\
\sigma(X_{n,d,i}) - \sigma(Y_{n,d,i}) &= (2^{n-d-3} - 1)(3F_{i+1}F_{d-i+1} - 2F_{d+2}) \\
&= (2^{n-d-3} - 1)(F_{i+1}F_{d-i+1} - 2F_iF_{d-i}) \\
&= (2^{n-d-3} - 1)(2F_{i-1}F_{d-i-1} - F_{i-2}F_{d-i-2}) \geq 0, \\
z(X_{n,d,i}) - z(Y_{n,d,i}) &= -(n-d-3)F_{d+1} + (2n-2d-6)F_iF_{d-i} \\
&= (n-d-3)(F_{i-2}F_{d-i-2} - F_{i-1}F_{d-i-1}) \leq 0.
\end{aligned}$$

Thus the lemma holds. ■

Theorem 3.3. *(i)* $\sigma(W_{n,3,1}) > \sigma(T_{n,3,1,2})$ *and* $z(W_{n,3,1}) < z(T_{n,3,1,2})$ *for* $n \geq 5$;

(ii) $\sigma(W_{n,4,1}) > \sigma(T_{n,4,1,3}) > \sigma(W_{n,4,2})$ *and* $z(W_{n,4,1}) < z(T_{n,4,1,3}) < z(W_{n,4,2})$ *for* $n \geq 7$.

Proof. (i) follows by Lemma 2.4.

(ii) Note that

$$\begin{aligned}
\sigma(W_{n,4,1}) - \sigma(T_{n,4,1,3}) &= (5 \cdot 2^{n-4} + 3) - (9 \cdot 2^{n-5} + 5) = 2^{n-5} - 2 > 0, \\
\sigma(T_{n,4,1,3}) - \sigma(W_{n,4,2}) &= (9 \cdot 2^{n-5} + 5) - (9 \cdot 2^{n-5} + 4) = 1 > 0; \\
z(W_{n,4,1}) - z(T_{n,4,1,3}) &= 3n - 7 - (4n - 13) = 6 - n < 0, \\
z(T_{n,4,1,3}) - z(W_{n,4,2}) &= 4n - 13 - (4n - 12) = -1 < 0,
\end{aligned}$$

and hence the results holds. ■

Lemma 3.4. *Suppose that* $5 \leq d \leq n-3$. *Then*

(i) $\sigma(T_{n,d,1,d-1}) > \sigma(X_{n,d,3})$ *and* $z(T_{n,d,1,d-1}) < z(X_{n,d,3})$*;*

(ii) $\sigma(W_{n,d,2}) > \sigma(T_{n,d,1,d-1})$ *and* $z(W_{n,d,2}) < z(T_{n,d,1,d-1})$.

Proof. Note that $F_{d+2} = F_{i+1}F_{d-i+1} + F_iF_{d-i}$. By Lemma 3.1, we have

$$\begin{aligned}
\sigma(T_{n,d,1,d-1}) - \sigma(X_{n,d,3}) &= 2^{n-d-3}(4F_d + 8F_{d-2} - 15F_{d-2}) + F_{d-1} + 2F_{d-3} - 6F_{d-3} \\
&= 2^{n-d-3}(4F_{d-3} + F_{d-2}) + F_{d-4} - 2F_{d-3} > 0, \\
\sigma(W_{n,d,2}) - \sigma(T_{n,d,1,d-1}) &= 2^{n-d-1}(3F_{d-1} - F_d - 2F_{d-2}) + 2F_{d-2} - F_{d-1} - 2F_{d-3} \\
&= 2^{n-d-1}F_{d-5} + F_{d-4} - 2F_{d-3} > 0, \\
z(T_{n,d,1,d-1}) - z(X_{n,d,3}) &= (n-d+2)F_{d-2} + (2n-2d-1)F_{d-3} \\
&\quad -3(2n-2d-5)F_{d-3} - 2F_{d+1} \\
&= (n-d-4)(F_{d-4} - (3n-3d-6)F_{d-3}) < 0, \\
z(W_{n,d,2}) - z(T_{n,d,1,d-1}) &= F_{d+1} + 2(n-d-1)F_{d-2} \\
&\quad -(n-d+2)F_{d-2} - (2n-2d-1)F_{d-3} \\
&= (n-d-1)F_{d-4} - (n-d-2)F_{d-3} < 0.
\end{aligned}$$

Thus the lemma holds. ■

Lemma 3.5 [15, 13]. *Let* $n = 4s + r$, *where* n, s *and* r *are integers with* $0 \leq r \leq 3$.

(i) For $r \in \{0, 1\}$, *we have*

$$\begin{aligned}
F_0F_n &> F_2F_{n-2} > F_4F_{n-4} > \cdots > F_{2s}F_{2s+r} > F_{2s-1}F_{2s+r+1} \\
&> F_{2s-3}F_{2s+r+3} > \cdots > F_3F_{n-3} > F_1F_{n-1};
\end{aligned}$$

(ii) For $r \in \{2,3\}$, *we have*

$$\begin{aligned} F_0F_n &> F_2F_{n-2} > F_4F_{n-4} > \cdots > F_{2s}F_{2s+r} > F_{2s+1}F_{2s+r-1} \\ &> F_{2s-1}F_{2s+r+1} > \cdots > F_3F_{n-3} > F_1F_{n-1}. \end{aligned}$$

By Lemmas 3.1 and 3.5, we have

Lemma 3.6. *Let* $d = 4k + r$, *where* k *and* r *are integers with* $0 \le r \le 3$.

(i) For $r \in \{0,1\}$, *we have*

$$\begin{aligned} \sigma(W_{n,d,1}) &> \sigma(W_{n,d,3}) > \sigma(W_{n,d,5}) > \cdots > \sigma(W_{n,d,2k-1}) > \sigma(W_{n,d,2k}) \\ &> \sigma(W_{n,d,2k-2}) > \cdots > \sigma(W_{n,d,2}); \\ z(W_{n,d,1}) &< z(W_{n,d,3}) < z(W_{n,d,5}) < \cdots < z(W_{n,d,2k-1}) < z(W_{n,d,2k}) \\ &< z(W_{n,d,2k-2}) < \cdots < z(W_{n,d,2}); \end{aligned}$$

(ii) For $r \in \{2,3\}$, *we have*

$$\begin{aligned} \sigma(W_{n,d,1}) &> \sigma(W_{n,d,3}) > \sigma(W_{n,d,5}) > \cdots > \sigma(W_{n,d,2k-1}) > \sigma(W_{n,d,2k-2}) \\ &> \sigma(W_{n,d,2k-4}) > \cdots > \sigma(W_{n,d,2}); \\ z(W_{n,d,1}) &< z(W_{n,d,3}) < z(W_{n,d,5}) < \cdots < z(W_{n,d,2k-1}) < z(W_{n,d,2k-2}) \\ &< z(W_{n,d,2k-4}) < \cdots < z(W_{n,d,2}). \end{aligned}$$

Note that the analogous inequalities hold for $X_{n,d,i}$ and $Y_{n,d,i}$, and hence $\sigma(T) \le \sigma(X_{n,d,3})$ (or $z(T) \ge z(X_{n,d,3})$, resp.) for $T \in \mathscr{T}^*_{n,d}$; and $\sigma(T) \le \sigma(Y_{n,d,3})$ (or $z(T) \ge z(Y_{n,d,3})$, resp.) for $T \in \mathscr{T}'_{n,d}$.

Corollary 3.7. *The first* $\lfloor \frac{d}{2} \rfloor$ *Merrifield-Simmons indices (or the last* $\lfloor \frac{d}{2} \rfloor$ *Hosoya indices, resp.) of trees in the set* $\mathscr{T}_{n,d}$ *with* $d = n-2 = 4k+r$, $0 \le r \le 3$ *are as follows:*

$$\begin{gathered} W_{n,d,1}, W_{n,d,3}, \ldots, W_{n,d,2k-1}, W_{n,d,2k}, W_{n,d,2k-2}, \ldots, W_{n,d,2},\ \textit{when } r \in \{0,1\}; \\ W_{n,d,1}, W_{n,d,3}, \ldots, W_{n,d,2k-1}, W_{n,d,2k-2}, W_{n,d,2k-4}, \ldots, W_{n,d,2},\ \textit{when } r \in \{2,3\}. \end{gathered}$$

Note that $\mathscr{T}_{n,n-2}$ contains no other trees than the above listed.

Lemma 3.8. *Let* $T \in \mathscr{T}''_{n,d} \setminus \{T_{n,d,1,d-1}\}$, $5 \le d \le n-3$. *Then*

$$\sigma(T) < \sigma(T_{n,d,1,d-1}) \ (\textit{or } z(T) > z(T_{n,d,1,d-1}),\ \textit{resp.}).$$

Proof. First we show that

$$\sigma(T_{n,d,i,d-1}) > \sigma(T_{n,d,i,j}) \text{ (or } z(T_{n,d,i,d-1}) < z(T_{n,d,i,j}), \text{ resp.)}$$

for $1 \le i < j \le d-2$.

If $j - i \ge 3$, then

$$\begin{aligned}
& \sigma(T_{n,d,i,d-1}) - \sigma(T_{n,d,i,j}) \\
= \; & 2^{n-d-2}F_{i+1}(F_{d-i+1} + F_2F_{d-i-1}) - 2^{n-d-2}F_{i+1}(F_{d-i+1} + F_{j-i}F_{d-j+1}) \\
& +F_i(F_{d-i} + 2F_{d-i-2}) - F_i(F_{d-i} + F_{j-i-1}F_{d-j+1}) \\
= \; & 2^{n-d-2}F_{i+1}(F_2F_{d-i-1} - F_{j-i}F_{d-j+1}) + F_i(F_2F_{d-i-2} - F_{j-i-1}F_{d-j+1}) > 0, \\
& z(T_{n,d,i,d-1}) - z(T_{n,d,i,j}) \\
= \; & [(n-d-1)F_i + F_{i-1}](F_{d-i} + F_{d-i-2} - F_{d-i} - F_{j-i-1}F_{d-j}) \\
& +F_i(F_{d-i-1} + F_{d-i-3} - F_{d-i-1} - F_{j-i-2}F_{d-j}) \\
= \; & [(n-d-1)F_i + F_{i-1}](F_1F_{d-i-2} - F_{j-i-1}F_{d-j}) + F_i(F_1F_{d-i-3} - F_{j-i-2}F_{d-j}) \\
< \; & 0;
\end{aligned}$$

if $j = i+1$, then

$$\begin{aligned}
& \sigma(T_{n,d,i,d-1}) - \sigma(T_{n,d,i,i+1}) \\
= \; & 2^{n-d-2}F_{i+1}(F_{d-i+1} + 2F_{d-i-1}) - 2^{n-d-2}F_{i+1}(F_{d-i+1} + F_{d-i}) \\
& +F_i(F_{d-i} + 2F_{d-i-2}) - 2F_iF_{d-i} \\
= \; & 2^{n-d-2}F_{i+1}(2F_{d-i-1} - F_{d-i}) + F_i(2F_{d-i-2} - F_{d-i}) \\
= \; & 2^{n-d-2}F_{i+1}F_{d-i-3} - F_iF_{d-i-3} > 0, \\
& z(T_{n,d,i,d-1}) - z(T_{n,d,i,i+1}) \\
= \; & [(n-d-1)F_i + F_{i-1}](F_{d-i} + F_{d-i-2} - F_{d-i+1}) + F_iF_{d-i-3} \\
= \; & -[(n-d-2)F_i + F_{i-1}]F_{d-i-3} < 0;
\end{aligned}$$

if $j = i+2$, then

$$\sigma(T_{n,d,i,d-1}) - \sigma(T_{n,d,i,i+2}) = F_i(F_{d-i} + F_2F_{d-i-2}) - F_iF_{d-i+1} = F_iF_{d-i-4} > 0,$$
$$z(T_{n,d,i,d-1}) - z(T_{n,d,i,i+2}) = F_i(F_{d-i-1} + F_{d-i-3} - F_{d-i}) = -F_iF_{d-i-4} < 0.$$

Next we show that

$$\sigma(T_{n,d,1,d-1}) > \sigma(T_{n,d,i,d-1}) \text{ and } z(T_{n,d,1,d-1}) < z(T_{n,d,i,d-1})$$

for $2 \leq i \leq d-2$. Note that

$$\begin{aligned}
& \sigma(T_{n,d,1,d-1}) - \sigma(T_{n,d,i,d-1}) \\
= \ & \sigma(W_{n-1,d,1}) + F_2\sigma(W_{n-3,d-2,1}) - \sigma(W_{n-1,d,i}) - F_2\sigma(W_{n-3,d-2,i}) \\
= \ & [\sigma(W_{n-1,d,1}) - \sigma(W_{n-1,d,i})] + F_2[\sigma(W_{n-3,d-2,1}) - \sigma(W_{n-3,d-2,i})] > 0, \\
& z(T_{n,d,1,d-1}) - z(T_{n,d,i,d-1}) \\
= \ & z(W_{n-1,d,1}) + z(W_{n-3,d-2,1}) - z(W_{n-1,d,i}) - z(W_{n-3,d-2,i}) \\
= \ & [z(W_{n-1,d,1}) - z(W_{n-1,d,i})] + [z(W_{n-3,d-2,1}) - z(W_{n-3,d-2,i})] < 0,
\end{aligned}$$

and hence the lemma holds. ■

Lemma 3.9. *Let $T \in \mathscr{T}_{n,d} \setminus (\mathscr{T}^0_{n,d} \cup \{T_{n,d,1,d-1}\})$ with $5 \leq d \leq n-3$. Then*

$$\sigma(T) < \sigma(T_{n,d,1,d-1}) \ (\textit{or } z(T) > z(T_{n,d,1,d-1}), \textit{ resp.}).$$

Proof. Let $P_{d+1} = v_0v_1 \dots v_{d-1}v_d$ be a path of length d of T with $d(v_0) = d(v_d) = 1$. Let $V_d = \{v_i : d(v_i) \geq 3, 1 \leq i \leq d-1\}$. Since $n \geq d+3$, $V_d \neq \emptyset$. We consider two cases.

Case 1. $|V_d| \geq 2$.

In this case, let $v_k \in V_d$, and let T_{p_i} be a subtree of $T - E(P_{d+1})$ which containing v_i, $1 \leq i \leq d-1$ and $|V(T_{p_i})| = p_i$. Let $t = |\{p_i \ : \ p_i > 0\}|$.

We first show that there is a tree $T^1 = T_{n,d}(p_1, \dots, p_{d-1})$ such that $\sigma(T) \leq \sigma(T^1)$ (or $z(T) \geq z(T^1)$, resp.) and equality holds if and only if $T \cong T^1$. Denote $H = P_{d+1} \cup \left(\bigcup\limits_{1 \leq k \leq d-1, k \neq i} T_{p_k} \right)$. Then $T = Hv_iT_{p_i}$. By Lemma 2.5, we have $\sigma(HvT_{p_i}) \leq \sigma(HvK_{1,p_i-1})$ (or $z(HvT_{p_i}) \geq z(HvK_{1,p_i-1})$, resp.). Thus $\sigma(T) \leq \sigma(T_{n,d}(p_1, \dots, p_{d-1}))$ (or $\sigma(T) \leq \sigma(T_{n,d}(p_1, \dots, p_{d-1}))$, resp.).

Since $T \notin \mathscr{T}^0_{n,d}$, we have $t \geq 2$. If $t = 2$, then $T \in \mathscr{T}''_{n,d}$. If $t > 3$, then we will show that there is a tree $T^2 \cong T_{n,d,i,j}$ such that $\sigma(T^1) < \sigma(T^2)$ (or $z(T^1) > z(T^2)$, resp.). Let $p_k, p_l, p_m \neq 0$, $1 \leq k < l < m \leq d-1$. By Lemma 2.4, we have eiher

$$\sigma(T_{n,d}(p_1, \dots, p_k, \dots, p_l, \cdots, p_{d-1})) < \sigma(T_{n,d}(p_1, \dots, p_k + p_l, \dots, 0, \cdots, p_{d-1}))$$

or $\sigma(T_{n,d}(p_1, \dots, p_k, \dots, p_l, \cdots, p_{d-1})) < \sigma(T_{n,d}(p_1, \dots, 0, \dots, p_k + p_l, \cdots, p_{d-1}))$. Thus there is a tree $T^2 \cong T_{n,d,i,j}$ such that $\sigma(T^1) < \sigma(T^2)$ (or $z(T^1) > z(T^2)$, resp.). Hence by Lemma 3.8, we have $\sigma(T) \leq \sigma(T^1) \leq \sigma(T^2) < \sigma(T_{n,d,1,d-1})$ (or $z(T) \geq z(T^1) \geq z(T^2) > z(T_{n,d,1,d-1})$, resp.).

Case 2. $|V_d| = 1$.

In this case, we let $v_i \in V_d$ and $N(v_i) \setminus \{v_{i-1}, v_{i+1}\} = \{x_1, \ldots, x_s\}$ with $d(x_j) \geq 2$, $1 \leq j \leq r$, and $d(x_{r+1}) = \cdots = d(x_s) = 1$. Then $r \geq 1$ as $T \notin \mathscr{T}^0_{n,d}$. Let $T_i(x_j)$ be subtrees of $T - v_i$ which contain x_j, and $|V(T_i(x_j))| = s_j + 1$, $1 \leq j \leq r$.

Let T^3 be a tree created from $T_{d+s+1,d,i}$ by attaching s_j pendant vertices to x_j, $1 \leq j \leq s$, respectively. Then, by Lemma 2.5, we have $\sigma(T) \leq \sigma(T^3)$ (or $z(T) \geq z(T^3)$, resp.).

By Lemma 2.4, we have either $\sigma(T^3) \leq \sigma(X_{n,d,i})$ (or $z(T^3) \geq z(X_{n,d,i})$, resp.) or $\sigma(T^3) \leq \sigma(Y_{n,d,i})$ (or $z(T^3) \geq z(Y_{n,d,i})$, resp.). Thus, by Lemmas 3.2, 3.4 and 3.6, either $\sigma(T) \leq \sigma(T^3) \leq \sigma(X_{n,d,i}) \leq \sigma(X_{n,d,3}) < \sigma(T_{n,d,1,d-1})$ (or $z(T) \geq z(T^3) \geq z(X_{n,d,i}) \geq z(X_{n,d,3}) > z(T_{n,d,1,d-1})$, resp.) or $\sigma(T) \leq \sigma(T^3) \leq \sigma(Y_{n,d,i}) \leq \sigma(Y_{n,d,3}) < \sigma(T_{n,d,1,d-1})$ (or $z(T) \geq z(T^3) \geq z(Y_{n,d,i}) \geq z(Y_{n,d,3}) > z(T_{n,d,1,d-1})$, resp.).

Therefore the proof of the lemma is complete. ∎

By Lemmas 3.2, 3.4, 3.6 and 3.9, we have the following result.

Theorem 3.10. *The first $\lfloor \frac{d}{2} \rfloor + 1$ Merrifield-Simmons indices (or the last $\lfloor \frac{d}{2} \rfloor + 1$ Hosoya indices, resp.) of trees in the set $\mathscr{T}_{n,d}$ with $5 \leq d = 4k + r \leq n - 3$, $0 \leq r \leq 3$ are as follows:*

$$W_{n,d,1}, W_{n,d,3}, \ldots, W_{n,d,2k-1}, W_{n,d,2k}, W_{n,d,2k-2}, \ldots, W_{n,d,2}, T_{n,d,1,d-1}, \text{ when } r \in \{0,1\};$$
$$W_{n,d,1}, W_{n,d,3}, \ldots, W_{n,d,2k-1}, W_{n,d,2k-2}, W_{n,d,2k-4}, \ldots, W_{n,d,2}, T_{n,d,1,d-1}, \text{ when } r \in \{2,3\}.$$

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