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 vertex sets and the total number of the independent edgesets of the graph $G$, respectively. Let $\mathcal{T}_{n,d}$ denote the set of trees on $n$ vertices and diameter $d$. Li, Zhao and Gutman \cite{LiZhaoGutman} have determined the unique tree in $\mathcal{T}_{n,d}$ with maximal $\sigma$-value. Pan, Xu, Yang and Zhou \cite{PanXuYangZhou} have recently determined the unique tree in $\mathcal{T}_{n,d}$ 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 $\mathcal{T}_{n,d}$ ($3 \leq d \leq n - 4$) are characterized.

1. Introduction

Given a molecular graph $G$, the \textit{Merrifield-Simmons index} $\sigma = \sigma(G)$ and the \textit{Hosoya index} $z = z(G)$ are defined as the number of subsets of $V(G)$ in which no
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 vertex sets of the graph and the total number of the independent edge sets 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 Hosoya index, resp.) and the star $S_n$ has the maximal Merrifield-Simmons index (or the minimal Hosoya index, resp.). Li, Zhao and Gutman [14] have recently determined the unique tree in $T_{n,d}$ with maximal Merrifield-Simmons index. Pan, Xu, Yang and Zhou [17] have recently determined the unique tree in $T_{n,d}$ 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 $T_{n,d}$ ($3 \leq d \leq n - 3$), 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 $T_{n,d}$ 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 $diam(G)$, 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 $\mathcal{T}_{n,d} = \{ T : T $ is a tree with order $n$ 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 $G_1, G_2, \ldots, G_\omega$ 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

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

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

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

\[
\sigma(G_{s,t}) = \sigma(G_{s,t} - v) + \sigma \left( G_{s,t} - N_{G_{s,t}}[v] \right)
\]
\[
= \sigma \left( G_{s,t} - v - u \right) + \sigma \left( G_{s,t} - v - N_{G_{s,t}}[u] \right)
\]
\[
+ \sigma \left( G - N_{G_{s,t}}[v] - u \right) + \sigma \left( G_{s,t} - N_{G_{s,t}}[v] - N_{G_{s,t} - N_{G_{s,t}}[v]}[u] \right)
\]
\[
= 2^{s+t} \sigma(G - v - u) + 2^{s} \sigma(G - v - N_G[u])
\]
\[
+ 2^t \sigma(G - u - N_G[v]) + \sigma \left( G - N_G[v] - N_G[u] \right),
\]
\[ z(G_{s,t}) = z(G_{s,t} - v) + \sum_{v' \in N_{G_{s,t}}(v)} z(G_{s,t} - v - v') \]
\[ = z(G_{s,t} - v - u) + \sum_{v' \in N_{G_{s,t}}(v)} \sum_{u' \in N_{G_{s,t} - v - u}(u)} z(G_{s,t} - v - u - v' - u') \]
\[ + \sum_{v' \in N_{G_{s,t}}(v)} z(G_{s,t} - v - u - v') + \sum_{v' \in N_{G_{s,t} - v}(u)} z(G_{s,t} - v - u - u') \]
\[ = (1 + s + t + st) z(G - v - u) + (1 + t) \sum_{v' \in N_{G}(v)} z(G - v - u - v') \]
\[ + (1 + s) \sum_{u' \in N_{G - v}(u)} z(G - v - u - u') \]
\[ + \sum_{v' \in N_{G}(v) - u} \sum_{u' \in N_{G - v}(u)} z(G - v - u - v' - u'). \]

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

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

Therefore

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

\[
\begin{align*}
\sigma(HvT_l) &= \sigma(H - v)\sigma(T_l - v) + \sigma(H - N_H[v])\sigma(T_l - N_{T_l}[v]) \\
&= \sigma(H - v)\sigma(T_l - v) + \sigma(H - N_H[v])\sigma(T_l - v) \\
&= \sigma(H - N_H[v])\sigma(T_l) + [\sigma(H - v) - \sigma(H - N_H[v])]\sigma(T_l - v) \\
&\leq \sigma(H - N_H[v])\sigma(K_{1,l-1}) + [\sigma(H - v) - \sigma(H - N_H[v])]\sigma(K_{1,l-1} - v) \\
&= \sigma(HvK_{1,l-1});
\end{align*}
\]

\[
\begin{align*}
z(HvT_l) &= z(H - v)z(T_l - v) + \sum_{w \in N_H(v)} z(H - v - w)z(T_l) \\
&\quad + \sum_{w \in N_{T_l}(v)} z(H - v)z(T_l - v - w) \\
&= z(H - v)z(T_l - v) + \sum_{w \in N_H(v)} z(H - v - w)z(T_l) \\
&\quad + z(H - v)[z(T_l) - z(T_l - v)] \\
&= z(H - v)z(T_l) + \sum_{w \in N_H(v)} z(H - v - w)z(T_l) \\
&\geq z(H - v)z(K_{1,l-1}) + \sum_{w \in N_H(v)} z(H - v - w)z(K_{1,l-1}) \\
&= z(HvK_{1,l-1}).
\end{align*}
\]
Therefore the lemma holds.

3. Main Results

In this section, we will give the first ⌊\frac{d}{2}⌋ + 1 Merrifield-Simmons indices and the last ⌊\frac{d}{2}⌋ + 1 Hosoya indices of trees in the set \( \mathcal{T}_{n,d} \) \((3 \leq d \leq n - 3)\).

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 \( P_{d+1} = v_0v_1 \cdots v_{d-1}v_d \) by attaching \( p_i \) pendant vertices to \( v_i \), \( 1 \leq i \leq d - 1 \), respectively, where \( n = d + 1 + \sum_{i=1}^{d-1} p_i, \; p_i \geq 0, \; i = 1, 2, \cdots, d - 1 \). Denote \( W_{n,d,i} = T_{n,d}(0, \cdots, 0, n - d - 1, 0, \cdots, 0) \) and \( T_{n,d,i,j} = T_{n,d}(0, \cdots, 0, n - d - 2, 0, \cdots, 0, 1, 0, \cdots, 0) \). Then \( W_{n,d,i} = W_{n,d,d-i} \) and \( T_{n,d,i,j} = T_{n,d,d-i,d-j} \).

Let \( X_{n,d,i} \) \((2 \leq i \leq d-2)\) 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 \( Y_{n,d,i} \) \((2 \leq i \leq d-2)\) 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 \( \mathcal{F}_{n,d}^0 = \{ W_{n,d,i} : 1 \leq i \leq d - 1 \} \), \( \mathcal{F}_{n,d}^* = \{ X_{n,d,i} : 2 \leq i \leq d - 2 \} \), \( \mathcal{F}_{n,d}' = \{ Y_{n,d,i} : 2 \leq i \leq d - 2 \} \) and \( \mathcal{F}_{n,d}'' = \{ T_{n,d,i,j} : 1 \leq i < j \leq d - 1 \} \).

![Figure 1](image-url)

Let \( F_n \) be the \( n \)th Fibonacci number, i.e., \( F_0 = F_1 = 1, \; F_n = F_{n-1} + F_{n-2}, \; n \geq 2 \). 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 $z(W_{n,d,i}) = F_{d+1} + (n-d-1)F_i F_{d-i}$, where $1 \leq i \leq d$;

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

(iv) $\sigma(T_{n,d,i,i+1}) = 2^{n-d-2}F_{i+1}F_{d-i+2} + 2F_i F_{d-i}$, $z(T_{n,d,i,i+1}) = F_i F_{d-i+1} + F_{d-i+1}[(n-d-1)F_i + F_{i-1}]$, $\sigma(T_{n,d,i,i+2}) = 2^{n-d-2}F_{i+1}(F_{d-i+2} + F_{d-i}) + F_i F_{d-i+1}$, $z(T_{n,d,i,i+2}) = (F_{d-i} + F_{d-i-2})[(n-d-1)F_i + F_{i-1}] + F_i F_{d-i}$, $\sigma(T_{n,d,i,j}) = 2^{n-d-2}F_{i+1}(F_{d-i+1} + F_{j-i}F_{d-j+1}) + F_i(F_{d-i} + F_{j-i}F_{d-j+i})$ and $z(T_{n,d,i,j}) = [(n-d-1)F_i + F_{i-1}](F_{d-i} + F_{j-i}F_{d-j}) + F_i(F_{d-i-1} + F_{j-i-2}F_{d-j})$ for $j-i \geq 3$. In particular, $\sigma(T_{n,4,1,3}) = 9 \cdot 2^{n-5} + 5$, $z(T_{n,4,1,3}) = 4n - 13$, $\sigma(T_{n,1,d-1}) = 2^{n-d-1}(F_d + 2F_{d-2}) + F_{d-1} + 2F_{d-3}$ and $z(T_{n,1,d-1}) = (n-d+2)F_{d-2} + (2n-2d-1)F_{d-3}$ 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 $F_{d+2} = F_{i+1}F_{d-i+1} + F_i F_{d-i}$. By Lemma 3.1, we have

\[
\sigma(W_{n,d,i}) - \sigma(X_{n,d,i}) &= (2^{n-d-3} + 1)F_{i+1}F_{d-i+1} - F_{d+2} \\
&= 2^{n-d-3}F_{i+1}F_{d-i+1} - F_i F_{d-i} > 0,
\]

\[
z(W_{n,d,i}) - z(X_{n,d,i}) &= -F_{d+1} - (n-d-4)F_i F_{d-i} < 0,
\]

\[
\sigma(X_{n,d,i}) - \sigma(Y_{n,d,i}) &= (2^{n-d-3} - 1)(3F_{i+1}F_{d-i+1} - 2F_{d+2}) \\
&= (2^{n-d-3} - 1)(F_{i+1}F_{d-i+1} - 2F_i F_{d-i}) \\
&= (2^{n-d-3} - 1)(2F_{i-2}F_{d-i-2} - F_{i-2}F_{d-i-2}) \geq 0,
\]

\[
z(X_{n,d,i}) - z(Y_{n,d,i}) &= -(n-d-3)F_{d+1} + (2n-2d-6)F_i F_{d-i} \\
&= (n-d-3)(F_{i-2}F_{d-i-2} - F_{i-1}F_{d-i-1}) \leq 0.
\]

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

\[
\begin{align*}
\sigma(W_n,4,1) - \sigma(T_n,4,1,3) &= (5 \cdot 2^{n-4} + 3) - (9 \cdot 2^{n-5} + 5) = 2^{n-5} - 2 > 0, \\
\sigma(T_n,4,1,3) - \sigma(W_n,4,2) &= (9 \cdot 2^{n-5} + 5) - (9 \cdot 2^{n-5} + 4) = 1 > 0; \\
z(W_n,4,1) - z(T_n,4,1,3) &= 3n - 7 - (4n - 13) = 6 - n < 0, \\
z(T_n,4,1,3) - z(W_n,4,2) &= 4n - 13 - (4n - 12) = -1 < 0,
\end{align*}
\]

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

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

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

\[
F_0F_n > F_2F_{n-2} > F_4F_{n-4} > \cdots > F_{2s}F_{2s+r} > F_{2s-1}F_{2s+r+1} > F_{2s-3}F_{2s+r+3} > \cdots > F_3F_{n-3} > F_1F_{n-1};
\]
(ii) For \( r \in \{2, 3\} \), we have

\[
F_0F_n > F_2F_{n-2} > F_4F_{n-4} > \cdots > F_{2s}F_{2s+r} > F_{2s+1}F_{2s+r-1}
\]
\[
> F_{2s-1}F_{2s+r+1} > \cdots > F_3F_{n-3} > F_1F_{n-1}.
\]

By Lemmas 3.1 and 3.5, we have

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

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

\[
\sigma(W_{n,d,1}) > \sigma(W_{n,d,3}) > \sigma(W_{n,d,5}) > \cdots > \sigma(W_{n,d,2k-1}) > \sigma(W_{n,d,2k})
\]
\[
> \sigma(W_{n,d,2k-2}) > \cdots > \sigma(W_{n,d,2});
\]
\[
z(W_{n,d,1}) < z(W_{n,d,3}) < z(W_{n,d,5}) < \cdots < z(W_{n,d,2k-1}) < z(W_{n,d,2k})
\]
\[
< z(W_{n,d,2k-2}) < \cdots < z(W_{n,d,2});
\]

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

\[
\sigma(W_{n,d,1}) > \sigma(W_{n,d,3}) > \sigma(W_{n,d,5}) > \cdots > \sigma(W_{n,d,2k-1}) > \sigma(W_{n,d,2k-2})
\]
\[
> \sigma(W_{n,d,2k-4}) > \cdots > \sigma(W_{n,d,2});
\]
\[
z(W_{n,d,1}) < z(W_{n,d,3}) < z(W_{n,d,5}) < \cdots < z(W_{n,d,2k-1}) < z(W_{n,d,2k-2})
\]
\[
< z(W_{n,d,2k-4}) < \cdots < z(W_{n,d,2});
\]

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

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

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

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

**Lemma 3.8.** Let \( T \in \mathcal{T}_{n,d}' \setminus \{T_{n,d,1,d-1}\} \), \( 5 \leq d \leq n - 3 \). Then

\[
\sigma(T) < \sigma(T_{n,d,1,d-1}) \quad \text{(or } z(T) > z(T_{n,d,1,d-1}), \text{ resp.)}.
\]
Proof. First we show that

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

for \( 1 \leq i < j \leq d - 2 \).

If \( j - i \geq 3 \), then

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

if \( j = i + 1 \), then

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

if \( j = i + 2 \), then

\[
\begin{align*}
\sigma(T_{n,d,i,d-1}) - \sigma(T_{n,d,i,i+2}) &= F_i(F_{d-i} + 2F_{d-i-2}) - F_iF_{d-i+1} = F_iF_{d-i-4} > 0, \\
z(T_{n,d,i,d-1}) - z(T_{n,d,i,i+2}) &= F_i(F_{d-i-1} + F_{d-i-3} - F_{d-i}) = -F_iF_{d-i-4} < 0.
\end{align*}
\]

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

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

and hence the lemma holds.

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

\[ \sigma(T) < \sigma(T_{n,d,1,d-1}) \text{ (or } z(T) > z(T_{n,d,1,d-1}), \text{ resp.)}. \]

**Proof.** Let \( P_{d+1} = v_0v_1 \ldots v_{d-1}v_d \) 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 \( T^1 = T_{n,d}(p_1, \ldots, p_{d-1}) \) 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 \( H = P_{d+1} \cup \bigcup_{1 \leq k \leq d-1, k \neq i} T_{p_k} \). Then \( T = Hv_{1}T_{p_i} \). By Lemma 2.5, we have

\[ \sigma(HvT_{p_i}) \leq \sigma(HvK_{1,p_{i-1}}) \text{ (or } z(HvT_{p_i}) \geq z(HvK_{1,p_{i-1}}), \text{ resp.)}. \]

Thus \( \sigma(T) \leq \sigma(T_{n,d}(p_1, \ldots, p_{d-1})) \) (or \( \sigma(T) \leq \sigma(T_{n,d}(p_1, \ldots, p_{d-1})), \text{ resp.)}. \)

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

\[ \sigma(T_{n,d}(p_1, \ldots, p_k, \ldots, p_l, \ldots, p_m)) < \sigma(T_{n,d}(p_1, \ldots, p_k + p_l, \ldots, 0, \ldots, p_{d-1})) \]

or \( \sigma(T_{n,d}(p_1, \ldots, p_k, \ldots, p_l, \ldots, p_m)) < \sigma(T_{n,d}(p_1, \ldots, 0, \ldots, p_k + p_l, \ldots, p_{d-1})) \). Thus there is a tree \( T^2 \cong T_{n,d,i,j} \) such that \( \sigma(T^1) < \sigma(T^2) \) (or \( z(T^1) > z(T^2), \text{ resp.)}. \) 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 $T \notin \mathcal{T}_{n,d}^0$. 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 $\sigma(T) \leq \sigma(T^3) \leq \sigma(X_{n,d,i}) < \sigma(X_{n,d,3}) < \sigma(T_{n,d,1,d-1})$ (or $z(T) \geq z(T^3) \geq z(X_{n,d,i}) \geq z(X_{n,d,3}) \geq z(T_{n,d,1,d-1})$, resp.) or $\sigma(T) \leq \sigma(T^3) \leq \sigma(Y_{n,d,i}) < \sigma(Y_{n,d,3}) < \sigma(T_{n,d,1,d-1})$ (or $z(T) \geq z(T^3) \geq z(Y_{n,d,i}) \geq z(Y_{n,d,3}) \geq z(T_{n,d,1,d-1})$, 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 $\left\lfloor \frac{d}{2} \right\rfloor + 1$ Merrifield-Simmons indices (or the last $\left\lceil \frac{d}{2} \right\rceil + 1$ Hosoya indices, resp.) of trees in the set $\mathcal{T}_{n,d}$ with $5 \leq d = 4k + r \leq n - 3$, $0 \leq r \leq 3$ are as follows:

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

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**References**


