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On the Wiener Index of Trees with Fixed Diameter

Huiqing LIU[1,*] and Xiang-Feng PAN[2,†]

[1] *School of Mathematics and Computer Science, Hubei University, Wuhan 430062, China*

[2] *School of Mathematics and Computational Science, Anhui University, Hefei 230039, China*

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Abstract

The Wiener index of a (molecular) graph is defined as $W(G) = \sum_{u,v} d_G(u,v)$, where $d_G(u,v)$ is the distance between u and v in G and the sum goes over all the pairs of vertices. In this paper, we obtain the trees with minimum and second-minimum Wiener indices among all the trees with n vertices and diameter d, respectively.

1. Introductions

It is well known that a topological index is a map from the set of chemical compounds represented by molecular graphs to the set of real numbers. There are

*Partially supported by NNSFC (No. 10571105, 10671081); email: hql_2008@163.com

†Partially supported by the Doctors and Masters Group Foundation of Anhui University and NNSFC (No.10626053); email: xfpan@ustc.edu

more than hundred topological indices available in the literature (see [11]-[14]). Many topological indices are closely correlated with some physico-chemical characteristics of the underlying compounds. In 1947, Harold Wiener introduced the first chemical index, now call the Wiener index, and published a series of papers [15]-[18] to show that there are excellent correlations between the Wiener index of the molecular graph of an organic compound and a variety of physical and chemical indices of molecular compound. The vast majority of chemical applications of the Wiener index deal with acyclic organic molecules; for reviews see [4, 5, 6, 8]. The molecular graphs of these are trees (see [7]).

The Wiener index of a graph G, defined in [15], is

$$W(G) = \sum_{u,v} d_G(u,v),$$

where $d_G(u,v)$ is the distance between u and v in G and the sum goes over all the pairs of vertices.

Recently, finding the graphs with minimum or maximum topological indices attracted the attention of a few researchers and many results are achieved (see [1, 3, 4, 9, 19, 20]). In this paper, the minimum and second-minimum Wiener indices of trees in the set $\mathscr{T}_{n,d}$ $(3 \le d \le n-3)$ are characterized.

All graphs considered here are finite and simple. Undefined terminology and notation may refer to [2]. 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 $(x \ne y)$, the distance between x and y is the number of edges in a shortest path joining x and y. The diameter of a graph G, denoted by $\mathrm{diam}(G)$, is the maximum distance between any two vertices of G. The distance of a vertex $x \in V(G)$, denoted by $D_G(v)$, is the sum of distances between x and all other 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 $d = n-1$, then $T \cong P_n$, a path of order n; and if $d = 2$, then $T \cong K_{1,n-1}$, a star of order n. Therefore, in the following, we assume that $3 \le d \le n-2$. Let $\mathscr{T}_{n,d} = \{T : T$ is a tree with order n and diameter d, $3 \le d \le n-2\}$.

2. Lemmas

First we give some lemmas which are used in the proof of our results.

Lemma 2.1 [10]. *Let H, X, Y be three connected, pairwise disjoint graphs. Suppose that u, v are two vertices of H, v' is a vertex of X, u' is a vertex of Y. Let G be the graph obtained from H, X, Y by identifying v with v' and u with u', respectively. Let G_1^* be the graph obtained from H, X, Y by identifying vertices v, v', u', and let G_2^* be the graph obtained from H, X, Y by identifying vertices u, v', u'. Then*

$$W(G_1^*) < W(G) \qquad \text{or} \qquad W(G_2^*) < W(G).$$

By Lemma 2.1, we have the following result.

Corollary 2.1. *Let G be a graph and $v, u \in V(G)$. Suppose that $G_{s,t}$ be the graph obtained from G by attaching s, t pendant vertices to v, u, respectively (see Fig. 1). Then*

$$W(G_{s-i,t+i}) < W(G_{s,t}) \quad \text{for} \quad 1 \le i \le s$$

or

$$W(G_{s+i,t-i}) < W(G_{s,t}) \quad \text{for} \quad 1 \le i \le t.$$

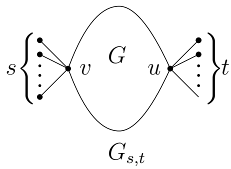

Fig. 1

Let H_1, H_2 be two connected graphs with $V(H_1) \cap V(H_2) = \{v\}$. Let $H_1 v H_2$ be a graph defined by $V(G) = V(H_1) \cup V(H_2)$, $V(H_1) \cap V(H_2) = \{v\}$ and $E(G) = E(H_1) \cup E(H_2)$. By the definition of the Wiener index, we have the following result.

Lemma 2.2. *Let H be a connected graph and T_l be a tree of order l with $V(H) \cap V(T_l) = \{v\}$. Then*

$$W(HvT_l) \ge W(HvK_{1,l-1})$$

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 $HvK_{1,l-1}$.

Lemma 2.3 [4]. *Let G be a graph of order n, v a pendant vertex of G and u the vertex adjacent to v. Then*

$$W(G) = W(G-v) + D_{G-v}(u) + n - 1.$$

Proof. By the definition of the Wiener index, we have

$$\begin{aligned} W(G) &= \sum_{x,y \in V(G)-v} d_G(x,y) + \sum_{x \in V(G)} d_G(x,v) \\ &= W(G-v) + D_{G-v}(u) + n - 1. \end{aligned}$$

■

Lemma 2.4. *Let G be a non-trivial connected graph and let $v \in V(G)$. Suppose that two paths $P = vv_1v_2\cdots v_k$, $Q = vu_1u_2\cdots u_m$ of lengths k, m $(k \geq m \geq 1)$ are attached to G by their ends vertices at v, respectively, to form $G^*_{k,m}$. Then*

$$W(G^*_{k,m}) < W(G^*_{k+1,m-1}).$$

Proof. By Lemma 2,3, we have

$$\begin{aligned} W(G^*_{k,m}) &= W(G^*_{k,m-1}) + D_{G^*_{k,m-1}}(u_{m-1}) + |G^*_{k,m}| - 1; \\ W(G^*_{k+1,m-1}) &= W(G^*_{k,m-1}) + D_{G^*_{k,m-1}}(v_k) + |G^*_{k+1,m-1}| - 1. \end{aligned}$$

Therefore $W(G^*_{k,m}) - W(G^*_{k+1,m-1}) = D_{G^*_{k,m-1}}(u_{m-1}) - D_{G^*_{k,m-1}}(v_k) < 0$. ■

Lemma 2.5. *Let $P = v_0v_1\cdots v_d$ be a path of order $d+1$. Then*

$$D_P(v_j) = \frac{2j^2 - 2dj + d^2 + d}{2}$$

for $1 \leq j \leq d-1$. Moreover, if $1 \leq i < j \leq d/2$, then $D_P(v_i) > D_P(v_j)$, and if $d/2 \leq i < j \leq d-1$, then $D_P(v_i) < D_P(v_j)$.

Proof. By the definition of the function D, we have

$$D_P(v_j) = (1 + 2 + \cdots + j) + (1 + 2 + \cdots + (d-j)) = \frac{2j^2 - 2dj + d^2 + d}{2}.$$

Thus the result holds. ■

3. Conclusions

In this section, we will give the minimum and the second minimum Wiener index in the set $\mathscr{T}_{n,d}$ $(3 \leq d \leq n-2)$. In order to formulate our results, we need to define some trees (see Fig. 2) as follows.

Let $T_{n,d}(p_1, \ldots, p_{d-1})$ be a tree of order n created from a path $P_{d+1} = v_0v_1 \ldots v_{d-1}v_d$ by attaching p_i pendant vertices to v_i, $1 \leq i \leq d-1$, respectively, where $n = d+1+\sum_{i=1}^{d-1} p_i$, $p_i \geq 0$, $i = 1, 2, \ldots, d-1$. Denote $T_{n,d,i} = T_{n,d}(\underbrace{0, \ldots, 0}_{i-1}, n-d-1, 0, \ldots, 0)$ and $Z_{n,d,i,j} = T_{n,d}(\underbrace{0, \ldots, 0}_{i-1}, n-d-2, \underbrace{0, \ldots, 0}_{j-i-1}, 1, 0, \ldots, 0)$. Then $T_{n,d,i} = T_{n,d,d-i}$.

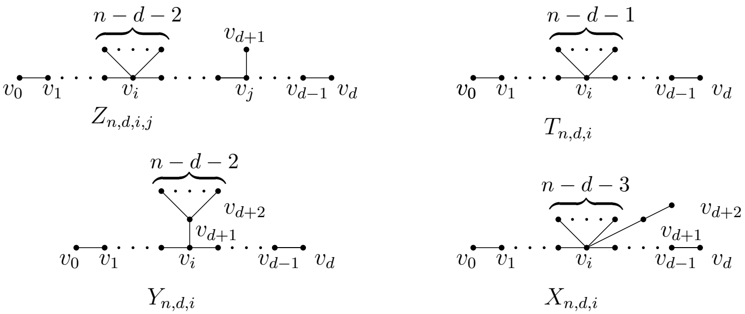

Fig. 2

For $2 \leq i \leq d-2$, let $X_{n,d,i}$ be a graph obtained from $T_{n-1,d,i}$ by attaching a pendant vertex to one pendant vertex of $T_{n,d,i}$, except for v_0, v_d, and let $Y_{n,d,i}$ be a graph obtained from $T_{d+2,d,i}$ by attaching $n-d-2$ pendant vertices to one pendant vertex of $T_{d+2,d,i}$, except for v_0, v_d. Then $X_{n,d,i} = X_{n,d,d-i}$ and $Y_{n,d,i} = Y_{n,d,d-i}$.

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

Lemma 3.1. *For any $1 \leq j < i \leq \lfloor \frac{d}{2} \rfloor$, we have $W(T_{n,d,i}) < W(T_{n,d,j})$. Therefore, for any tree $T \in \mathscr{T}^0_{n,d}$, $W(T) \geq W(T_{n,d,\lfloor \frac{d}{2} \rfloor})$ with equality if and only if $T \cong T_{n,d,\lfloor \frac{d}{2} \rfloor}$.*

Proof. We only need to prove the case $j = i-1$. Take $v = v_i$ and take two paths $P = v_0v_1 \cdots v_i$, $Q = v_iv_{i+1} \cdots v_d$ in Lemma 2.4, we obtain the desired result. ■

Note that the analogous inequality hold for $X_{n,d,i}$ and $Y_{n,d,i}$, and hence $W(T) \geq W(X_{n,d,\lfloor \frac{d}{2} \rfloor})$ for $T \in \mathscr{T}^*_{n,d}$; and $W(T) \geq W(Y_{n,d,\lfloor \frac{d}{2} \rfloor})$ for $T \in \mathscr{T}'_{n,d}$.

By Lemma 3.1, we have the following result.

Corollary 3.2. *The last $\lfloor \frac{d}{2} \rfloor$ Wiener indices of trees in the set $\mathscr{T}_{n,d}$ with $d = n-2$ are as follows:*

$$T_{n,d,\lfloor \frac{d}{2} \rfloor},\ T_{n,d,\lfloor \frac{d}{2} \rfloor -1},\ \ldots\ ,\ T_{n,d,2},\ T_{n,d,1}.$$

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

Lemma 3.3. *Suppose that $3 \leq d \leq n-3$. Then*
(i) $W(Z_{n,d,\lfloor \frac{d}{2} \rfloor, \lfloor \frac{d}{2} \rfloor +1}) < W(X_{n,d,\lfloor \frac{d}{2} \rfloor}) \leq W(Y_{n,d,\lfloor \frac{d}{2} \rfloor})$;
(ii) for d is odd, $W(Z_{n,d,\lfloor \frac{d}{2} \rfloor, \lfloor \frac{d}{2} \rfloor +1}) < W(T_{n,d,\lfloor \frac{d}{2} \rfloor -1})$;
(iii) for d is even, $W(Z_{n,d,\lfloor \frac{d}{2} \rfloor, \lfloor \frac{d}{2} \rfloor +1}) = W(T_{n,d,\lfloor \frac{d}{2} \rfloor -1})$.

Proof. By Lemma 2.3, we have

$$\begin{aligned}
W(Z_{n,d,\lfloor \frac{d}{2} \rfloor, \lfloor \frac{d}{2} \rfloor +1}) &= W(T_{n-1,d,\lfloor \frac{d}{2} \rfloor}) + D_{T_{n-1,d,\lfloor \frac{d}{2} \rfloor}}(v_{\lfloor \frac{d}{2} \rfloor +1}) + n - 1, \\
&= W(T_{n-1,d,\lfloor \frac{d}{2} \rfloor}) + D_{P_{d+1}}(v_{\lfloor \frac{d}{2} \rfloor +1}) + 2(n-d-2) + n - 1, \\
W(X_{n,d,\lfloor \frac{d}{2} \rfloor}) &= W(T_{n-1,d,\lfloor \frac{d}{2} \rfloor}) + D_{T_{n-1,d,\lfloor \frac{d}{2} \rfloor}}(v_{d+1}) + n - 1, \\
&= W(T_{n-1,d,\lfloor \frac{d}{2} \rfloor}) + D_{P_{d+1}}(v_{\lfloor \frac{d}{2} \rfloor}) + d + 1 + 2(n-d-3) + n - 1.
\end{aligned}$$

Thus by Lemma 2.5, we have

$$\begin{aligned}
W(Z_{n,d,\lfloor \frac{d}{2} \rfloor, \lfloor \frac{d}{2} \rfloor +1}) - W(X_{n,d,\lfloor \frac{d}{2} \rfloor}) &= D_{P_{d+1}}(v_{\lfloor \frac{d}{2} \rfloor +1}) - D_{P_{d+1}}(v_{\lfloor \frac{d}{2} \rfloor}) - d + 1 \\
&= 2\lfloor \frac{d}{2} \rfloor + 2 - 2d \\
&\leq 2 - d < 0.
\end{aligned}$$

Note that $X_{d+3,d,\lfloor \frac{d}{2} \rfloor} \cong Y_{d+3,d,\lfloor \frac{d}{2} \rfloor}$, and hence by Lemmas 2.3 and 2.5, we have

$$\begin{aligned}
W(X_{n,d,\lfloor \frac{d}{2} \rfloor}) - W(Y_{n,d,\lfloor \frac{d}{2} \rfloor}) &= W(X_{n-1,d,\lfloor \frac{d}{2} \rfloor}) - W(Y_{n-1,d,\lfloor \frac{d}{2} \rfloor}) - d + 1 \\
&< W(X_{n-1,d,\lfloor \frac{d}{2} \rfloor}) - W(Y_{n-1,d,\lfloor \frac{d}{2} \rfloor}) \\
&< \cdots\cdots \\
&< W(X_{d+3,d,\lfloor \frac{d}{2} \rfloor}) - W(Y_{d+3,d,\lfloor \frac{d}{2} \rfloor}) = 0.
\end{aligned}$$

Thus (i) holds.

By Lemma 2.5, $D_{P_{d+1}}(v_{\lfloor\frac{d}{2}\rfloor+1}) \le D_{P_{d+1}}(v_{\lfloor\frac{d}{2}\rfloor-1})$. Thus by Lemma 2.3,

$$\begin{aligned}
& W(Z_{n,d,\lfloor\frac{d}{2}\rfloor,\lfloor\frac{d}{2}\rfloor+1}) - W(T_{n,d,\lfloor\frac{d}{2}\rfloor-1}) \\
= \; & W(T_{n-1,d,\lfloor\frac{d}{2}\rfloor}) + D_{P_{d+1}}(v_{\lfloor\frac{d}{2}\rfloor+1}) - W(T_{n-1,d,\lfloor\frac{d}{2}\rfloor-1}) - D_{P_{d+1}}(v_{\lfloor\frac{d}{2}\rfloor-1}) + n - d - 2 \\
\le \; & W(T_{n-1,d,\lfloor\frac{d}{2}\rfloor}) - W(T_{n-1,d,\lfloor\frac{d}{2}\rfloor-1}) + n - d - 2 \\
= \; & D_{T_{n-2,d-1,\lfloor\frac{d}{2}\rfloor-1}}(v_0) - D_{T_{n-2,d-1,\lfloor\frac{d}{2}\rfloor-1}}(v_{d-1}) + n - d - 2 \\
= \; & (n-d-2)(2\lfloor\frac{d}{2}\rfloor - d). \qquad (*)
\end{aligned}$$

Hence (ii) and (iii) hold by $(*)$. ■

Lemma 3.4. *Let* $T \in \mathscr{T}''_{n,d} \setminus \{Z_{n,d,\lfloor\frac{d}{2}\rfloor,\lfloor\frac{d}{2}\rfloor+1}\}$, $3 \le d \le n-3$. *Then*

$$W(T) > W(Z_{n,d,\lfloor\frac{d}{2}\rfloor,\lfloor\frac{d}{2}\rfloor+1}).$$

Proof. Denote $T = Z_{n,d,i,j}$. Let $P = v_0v_1\ldots v_{d-1}v_d$ be a path of length d in T with $d(v_0) = d(v_d) = 1$, and let v_{d+1} be a pendant vertex of T adjacent to v_j. We choose T such that $W(T)$ is as small as possible. We first show the following facts.

Fact 1. $i \le \lfloor\frac{d}{2}\rfloor$.

Proof of Fact 1. Assume that $i > \lfloor\frac{d}{2}\rfloor$. Then $j > \lfloor\frac{d}{2}\rfloor+1$. Note that $Z_{n,d,i,j} - v_0 \cong Z_{n,d,i-1,j-1} - v_d \cong Z_{n-1,d-1,i-1,j-1}$. Thus by Lemma 2.3,

$$\begin{aligned}
W(Z_{n,d,i,j}) - W(Z_{n,d,i-1,j-1}) &= D_{Z_{n-1,d-1,i-1,j-1}}(v_0) - D_{Z_{n-1,d-1,i-1,j-1}}(v_{d-1}) \\
&= (n-d-2)(2i-d-1) + (2j-d-1) > 0,
\end{aligned}$$

a contradiction with our choice. ■

Fact 2. $W(Z_{n,d,i,j}) \ge W(Z_{n,d,i,\lfloor\frac{d}{2}\rfloor+1})$.

Proof of Fact 2. Note that $Z_{n,d,i,j} - v_{d+1} \cong T_{n-1,d,i}$. If $j > \lfloor\frac{d}{2}\rfloor + 1$, then by Lemmas 2.3 and 2.5,

$$\begin{aligned}
W(Z_{n,d,i,j}) - W(Z_{n,d,i,\lfloor\frac{d}{2}\rfloor+1}) &= D_{T_{n-1,d,i}}(v_j) - D_{T_{n-1,d,i}}(v_{\lfloor\frac{d}{2}\rfloor+1}) \\
&> D_P(v_j) - D_P(v_{\lfloor\frac{d}{2}\rfloor+1}) > 0.
\end{aligned}$$

■

Fact 3. $W(Z_{n,d,i,\lfloor\frac{d}{2}\rfloor+1}) > W(Z_{n,d,\lfloor\frac{d}{2}\rfloor,\lfloor\frac{d}{2}\rfloor+1})$.

Proof of Fact 3. Note that $Z_{n,d,i,j} - v_{d+1} \cong T_{n-1,d,i}$. If $i < \lfloor\frac{d}{2}\rfloor$, then by Lemmas 2.3 and 3.1,

$$\begin{aligned}
& W(Z_{n,d,i,\lfloor\frac{d}{2}\rfloor+1}) - W(Z_{n,d,\lfloor\frac{d}{2}\rfloor,\lfloor\frac{d}{2}\rfloor+1}) \\
= & \Big(W(T_{n-1,d,i}) - W(T_{n-1,d,\lfloor\frac{d}{2}\rfloor})\Big) + \Big(D_{T_{n-1,d,i}}(v_{\lfloor\frac{d}{2}\rfloor+1}) - D_{T_{n-1,d,\lfloor\frac{d}{2}\rfloor}}(v_{\lfloor\frac{d}{2}\rfloor+1})\Big) \\
> & D_{T_{n-1,d,i}}(v_{\lfloor\frac{d}{2}\rfloor+1}) - D_{T_{n-1,d,\lfloor\frac{d}{2}\rfloor}}(v_{\lfloor\frac{d}{2}\rfloor+1}) > 0.
\end{aligned}$$

■

By Facts 1, 2 and 3, the proof of the lemma is complete. ■

Lemma 3.5. *Let $T \in \mathscr{T}_{n,d} \setminus (\mathscr{T}^0_{n,d} \cup \{Z_{n,d,\lfloor\frac{d}{2}\rfloor,\lfloor\frac{d}{2}\rfloor+1}\})$ with $3 \le d \le n-3$. Then*

$$W(T) > W(Z_{n,d,\lfloor\frac{d}{2}\rfloor,\lfloor\frac{d}{2}\rfloor+1}).$$

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

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

In this case, we first obtain a tree $T_1 \cong T_{n,d}(p_1, \ldots, p_{d-1})$ such that $W(T) \ge W(T_1)$ and equality holds if and only if $T \cong T_1$ by Lemma 2.2.

Since $T \notin \mathscr{T}^0_{n,d}$, we have $p_i, p_j \ne 0$, $1 \le i < j \le d-1$. Thus by Corollary 2.1, we can obtain a tree $T_2 \cong Z_{n,d,i,j}$ such that $W(T_1) > W(T_2)$, and by Lemma 3.4, we have $W(T_2) > W(Z_{n,d,\lfloor\frac{d}{2}\rfloor,\lfloor\frac{d}{2}\rfloor+1})$. Therefore $W(T) \ge W(T_1) > W(T_2) > W(Z_{n,d,\lfloor\frac{d}{2}\rfloor,\lfloor\frac{d}{2}\rfloor+1})$.

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 $d(x_j) \ge 2$, $1 \le j \le r$, and $d(x_{r+1}) = \cdots = d(x_s) = 1$. Then $r \ge 1$ as $T \notin \mathscr{T}^0_{n,d}$. Let $T_i(x_j)$ be subtrees of $T - v_i$ which contain x_j, and $|V(T_i(x_j))| = s_j + 1$, $1 \le j \le r$. By Lemma 2.2, we can obtain a tree T_3 created from $T_{d+s+1,d,i}$ by attaching s_j pendant vertices to x_j, $1 \le j \le s$, respectively, such that $W(T) \ge W(T_3)$. By Corollary 2.1, we can obtained a tree $T_4 \in \mathscr{T}^*_{n,d} \cup \mathscr{T}'_{n,d}$ such that $W(T_3) \ge W(T_4)$. If $T_4 \in \mathscr{T}^*_{n,d}$, then, by Lemma 3.3, $W(T) \ge W(T_3) \ge W(T_4) \ge W(X_{n,d,\lfloor\frac{d}{2}\rfloor}) > W(Z_{n,d,\lfloor\frac{d}{2}\rfloor,\lfloor\frac{d}{2}\rfloor+1})$.

If $T_4 \in \mathscr{T}'_{n,d}$, then, by Lemma 3.3, $W(T) \geq W(T_3) \geq W(T_4) \geq W(Y_{n,d,\lfloor \frac{d}{2} \rfloor}) > W(Z_{n,d,\lfloor \frac{d}{2} \rfloor,\lfloor \frac{d}{2} \rfloor+1})$. ■

By Lemmas 3.1, 3.3 and 3.5, we have the following results.

Theorem 3.6. *(i) The minimum Wiener index of trees in the set $\mathscr{T}_{n,d}$ with $3 \leq d \leq n-2$ is $T_{n,d,\lfloor \frac{d}{2} \rfloor}$;*

(ii) For d is odd, the second-minimum Wiener index of trees in the set $\mathscr{T}_{n,d}$ with $3 \leq d \leq n-3$ is $Z_{n,d,\lfloor \frac{d}{2} \rfloor,\lfloor \frac{d}{2} \rfloor+1}$;

(iii) For d is even, the second-minimum Wiener index of trees in the set $\mathscr{T}_{n,d}$ with $3 \leq d \leq n-3$ is $T_{n,d,\lfloor \frac{d}{2} \rfloor-1}$ or $Z_{n,d,\lfloor \frac{d}{2} \rfloor,\lfloor \frac{d}{2} \rfloor+1}$.

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