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Ordering Trees by Their Wiener Indices *

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Abstract

The set of trees with n vertices is denoted by $\mathcal{T}_n$. In this paper, we consider the problem of ordering trees in $\mathcal{T}_n$ by their Wiener indices. Some order relations of trees in $\mathcal{T}_n$ are obtained. Based on the order relations, the trees in $\mathcal{T}_n$ with the first up to fifteenth smallest Wiener indices are determined.

1 Introduction

The Wiener index is one of the oldest topological indices of molecular structures. It was put forward by the physico-chemist Harold Wiener [1] in 1947. The Wiener index of a connected graph G is defined as the sum of distances between all pairs of vertices in G:

$$W = W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v). \tag{1}$$

where $V(G)$ is the vertex set of G, and $d_G(u, v)$ is the distance between vertices u and v of G.

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As summarized by Dobrynin and Gutman et al. in [2], the Wiener index belongs to the molecular structure descriptor that are nowadays extensively used in theoretical chemistry for the design of so-called quantitative structure-property relations (QSPR) and quantitative structure-activity relations (QSAR), where under 'property' are meant the physico-chemical properties and under 'activity', the pharmacological and biological activities of the respective chemical compounds.

There are two groups of closely related problems which have attracted the attention of researchers for a long time:

(a) how Wiener index depends on the structure of a graph;

(b) how Wiener index can be efficiently calculated, especially without the aid of a computer(by so-called 'paper-and-pencil' methods).

The greatest progress in solving the above problems was made for trees and hexagonal systems (see two recent surveys by Dorbrynin et al [2] and Gutman et al [3]).

For chemical applications, it may be especially interesting to identify the graph with maximum and minimum Wiener indices. Entringer et al [4] proved that among all trees of a given vertex number n, the Wiener index is maximized by the path P_n and minimized by the star S_n. For connected graphs with n vertices and m edges, the bound on the Wiener index was obtained by Šoltés [5]. And for the trees with n vertices and a fixed maximum vertex degree, Liu et al. [6] showed that the dendrimer on n vertices is the unique graph reaching the mimimum Wiener index. The same result was later obtained by Fisçhermann et al. [7] independently. In [7], they also characterized the trees which maximize the Wiener index among all trees of given order that have only vertices of two different degrees. In addition, for trees with n vertices and fixed pendent vertices, the upper bound on their Wiener indices was obtained by Shi [8]. The bound was later obtained independently by Entringer [9]. And the lower bound was obtained by Burns and Entringer [10]. A sharp upper bound on Wiener index of a graph depending on the vertex number and the independence number was given by Dankelmann [11]. As a corollary he obtained the maximum average distance of a graph with given vertices and matching number.

It is natural to consider not only the trees with the maximum and minimum Wiener indeces, but also the order of trees by Wiener indices. Ordering trees by their Wiener indices maybe help us to understand the relationship between the structures of trees and their Wiener indices. It was pointed out as above that the problem how $W(T)$ depends on the structure of T has attracted the attention of researchers for a long time. In this paper, by applying the edge-growing transformation and moving pendent edges, we obtain some order relations in the trees with n vertices and with one, two and three nonpendent edges, respectively. Based on the order relations, the trees with n vertices and with the first up to fifteenth smallest Wiener Indices are determined.

2 Preliminaries

Throughout the paper, we always denote by $\mathcal{T}_n$ the set of trees on n vertices.

Theorem 2.1 *[1] Let T be a tree and e its edge. Let $n_1(e)$ and $n_2(e) = n - n_1(e)$ be the numbers of vertices of the two components of $T - e$. Then*

$$W(T) = \sum_{e \in E(T)} n_1(e) n_2(e). \tag{2}$$

Entringer et al. [4] were the first to formulate the following result. Note, however, that the results equivalent to Theorem 2.2 were stated already by Bonchev and Trinajstić [12] but not in a theorematic form. In 1997, Gutman et al. [13] gave the following theorem.

Theorem 2.2 *[13] (a) If T is an n-vertex tree, then for all integers $n \geq 1$,*

$$W(S_n) \leq W(T) \leq W(P_n).$$

(b) If, in addition, T differs from S_n and P_n, then for all integers $n \geq 5$,

$$W(S_n) < W(T) < W(P_n).$$

A maximal subtree of a tree T containing a vertex v as an end vertex will be called a *branch* of T at v. The *weight* of a branch B, denoted by $bw(B)$, is the number of edges in it. The *centroid* of a tree T, denoted by $C(T)$, is the set of vertices of T for which the maximum branch weight at $v \in C(T)$ is minimized. The graph $S(n, m)$, $3 \leq m \leq n-1$, is the tree of order n with just one centroid vertex, say v, and each of the m branches of T at v is a path of length $\lfloor \frac{n-1}{m} \rfloor$ or $\lceil \frac{n-1}{m} \rceil$. The *treedumbbell* $D(n, a, b)$ consists of the path P_{n-a-b} together with a independent vertices adjacent to one pendent vertex of P_{n-a-b} and b independent vertices adjacent to the other pendent vertex.

Theorem 2.3 *[8, 9, 10] If T is a tree of order n with k pendent vertices, $2 \leq k \leq n$, then $W(S(n,k)) \leq W(T) \leq W(D(n, \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil))$. The lower bound is realized if and only if $T = S(n,k)$ and the upper if and only if $T = D(n, \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil)$.*

The following transformation was put forward by Xu [14] to study the spectral radius of trees. It can be applied for ordering trees by Wiener indices.

Definition 2.4 *[14] Let T be a tree in $\mathcal{T}_n$, and $n \geq 3$. And let $e = uv$ be a nonpendent edge of T, and let T_1 and T_2 be the two components of $T - e$. $u \in T_1$, $v \in T_2$, T_0 is the graph obtained from T in the following way.*

(1) Contract the edge $e = uv$.

(2) Add a pendent edge to the vertex $u(= v)$.

The procedures (1) and (2) are called the edge-growing transformation of T(on edge e), or e.g.t of T(on edge e) for short(see Fig. 1). If T is transformed into T_0 by one step of e.g.t of T, this transformation is denoted by $T \to T_0$.

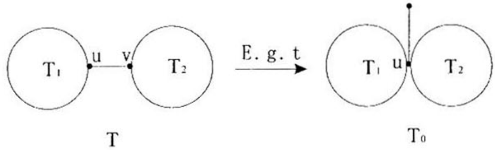

Figure 1: The edge-growing transformation of a tree T.

Theorem 2.5 *Let T be a tree in $\mathcal{T}_n$ with at least one nonpendent edge, and $n \geq 3$. If T can be transformed into T_0 by carrying out one step of edge-growing transformation, then $W(T_0) < W(T)$.*

Proof. Let $e' = uv$ be a nonpendent edge of T, T_1 and T_2 the two components of $T - e'$. Let T_0 be the graph obtained from T by contracting edge e' and adding a new edge e'' to the vertex u in T. Without loss of generality, let $|V(T_1)| \geq |V(T_2)| \geq 2$, we have

$$\begin{aligned} W(T) &= \sum_{e\in E(T)} n_1(e)n_2(e) = \sum_{e\in E(T)\setminus\{e'\}} n_1(e)n_2(e) + |V(T_1)||V(T_2)| \\ W(T_0) &= \sum_{e\in E(T_0)\setminus\{e''\}} n_1(e)n_2(e) + |V(T_1)| + |V(T_2)| - 1 \\ &= \sum_{e\in E(T)\setminus\{e'\}} n_1(e)n_2(e) + |V(T_1)| + |V(T_2)| - 1 \end{aligned}$$

Thus,

$$\begin{aligned} W(T) &= W(T_0) + |V(T_1)||V(T_2)| - |V(T_1)| - |V(T_2)| + 1 \\ &= W(T_0) + (|V(T_1)| - 1)(|V(T_2)| - 1) \\ &> W(T_0) \end{aligned}$$ □

One can see easily by Theorem 2.5 that, for any tree T in $\mathcal{T}_n$ with a nonpendent edge, T can be transformed into the star S_n by carrying out e.g.t repeatedly. So, one can make a conclusion that $W(S_n) < W(T)$. $\mathcal{T}_n$ can be partitioned as some subsets by the numbers of nonpendent edges of trees in the following way. Let $\mathcal{T}_n^i = \{T \mid T \in \mathcal{T}_n$, and there exist exactly i nonpendent edge in $T\}$. Then $\mathcal{T}_n = \cup_{i=0}^{n-3}\mathcal{T}_n^i$. Obviously, the sets $\mathcal{T}_n^0$ and $\mathcal{T}_n^{n-3}$ contain only the star S_n and the path P_n, respectively. For any tree $T \in \mathcal{T}_n^i$, $i = 1, 2, \cdots, n-3$, one can transform T into S_n by carrying out exactly i steps of e.g.t to T repeatedly. At the same time, we notice that the sets $\mathcal{T}_n^1$ and $\mathcal{T}_n^2$ contain the following two kinds of trees as shown in Fig. 2, say $T_{i,j}^1$ $(= D(n,i,j))$ and $T_{r,s,t}^2$, respectively, where $i + j = n - 2$, and $1 \leq i, j \leq n-3$ for $T_{i,j}^1$, and $r + s + t = n - 3$, $r, t \geq 1$, $s \geq 0$ for $T_{r,s,t}^2$, respectively.

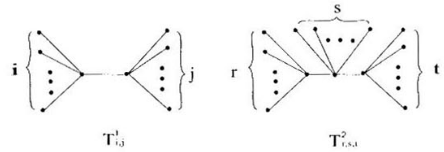

Figure 2: Trees in $\mathcal{T}_n^1$ and $\mathcal{T}_n^2$.

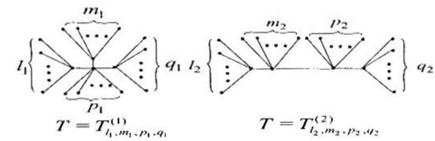

Figure 3: Trees in $\mathcal{T}_n^3$.

Also $\mathcal{T}_n^3$ contains only the two types of trees $T^{(1)}_{l_1,m_1,p_1,q_1}$ and $T^{(2)}_{l_2,m_2,p_2,q_2}$ as shown in Fig. 3, where $l_1 + m_1 + p_1 + q_1 = n - 4$, $p_1 \geq 0$, $q_1, l_1, m_1 \geq 1$ and $l_2 + m_2 + p_2 + q_2 = n - 4$, $l_2, q_2 \geq 1$, $p_2, m_2 \geq 0$.

Now we calculate the Wiener indices of the above trees by formula (2) as follows:

$$\begin{aligned}
W(T^1_{i,j}) &= (n-1)(n-2) + (i+1)(j+1). && (3)\\
W(T^2_{r,s,t}) &= (n-1)(n-3) + (r+1)(n-r-1) + (t+1)(n-t-1) && (4)\\
W(T^{(1)}_{l_1,m_1,p_1,q_1}) &= (l_1+1)(n-l_1-1) + (m_1+1)(n-m_1-1) \\
&\quad +(q_1+1)(n-q_1-1) + (n-1)(n-4) && (5)\\
W(T^{(2)}_{l_2,m_2,p_2,q_2}) &= (l_2+1)(n-l_2-1) + (l_2+m_2+2)(n-l_2-m_2-2) \\
&\quad +(q_2+1)(n-q_2-1) + (n-1)(n-4) && (6)
\end{aligned}$$

The following result was given by Barefoot[15] but not in a theorematic form.

Theorem 2.6 [*15*] *Suppose that ab is an edge of the tree T, A and B are the components of $T - ab$ containing a and b, respectively, and that S is the set of end vertices adjacent to a and different from b . Define the tree $T' = T - \{as|s \in S\} + \{bs|s \in S\}$ (Shown in Fig. 4). Then*

$$W(T') = W(T) + |S|(|V(A)| - |V(B)| - |S|).$$

Now we extend the result to general case.

Theorem 2.7 *Let T be a tree in $\mathcal{T}_n$, and $P_{t+1} = v_0 v_1 v_2 \cdots v_t$ a path in T. Let T_i, $i = 0, 1, 2, \cdots, t$, be the component of $T - E(P_{t+1})$ containing v_i with $|V(T_i)| = n_i$, and let*

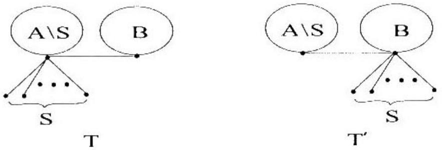

Figure 4: Trees in Theorem 2.6

$u_1, u_2, \cdots, u_s$ be pendent vertices of T, which is adjacent to v_t. Let $T^* = T - \sum_{j=1}^{s} v_t v_j + \sum_{j=1}^{s} v_0 v_j$. Then

$$W(T^*) - W(T) = s[\sum_{i=0}^{t}(2i-t)n_i - st].$$

Proof. Let $e_i = v_{i-1}v_i, i = 1, 2, \cdots, t$, and let $n_1(T-e_i)$ and $n_2(T-e_i) = n - n_1(e_i)$ denote the numbers of vertices in the components of $T - e_i$, containing v_{i-1} and v_i, respectively. For an edge $e \in E(T)\backslash E(P_{t+1})$, it is not difficult to see that $n_1(T-e)n_2(T-e) = n_1(T^*-e)n_2(T^*-e)$. So

$$\begin{aligned}
& W(T^*) - W(T) \\
= & \sum_{e_i \in E(P_i)} n_1(T^*-e_i)n_2(T^*-e_i) - \sum_{e_i \in E(P_i)} n_1(T-e_i)n_2(T-e_i) \\
= & \sum_{e_i \in E(P_i)} [(n_1(T-e_i)+s)(n_2(T-e_i)-s) - n_1(T-e_i)n_2(T-e_i)] \\
= & \sum_{e_i \in E(P_i)} (sn_2(T-e_i) - sn_1(T-e_i) - s^2) = s[t(n_t - n_0 - s) - \sum_{i=1}^{t-1}(t-2i)n_i] \\
= & s[\sum_{i=0}^{t}(2i-t)n_i - st]. \qquad \square
\end{aligned}$$

Corollary 2.8 *Let T be a tree in $\mathcal{T}_n$, and $e = v_0v_1 \in E(T)$. Let T_i, $i = 0, 1$, be the component of $T - e$ containing v_i with $|V(T_i)| = n_i$. and let $u_1, u_2, \cdots, u_s$ be pendent vertices of T, which is adjacent to v_1. Then*

$$W(T + \sum_{j=1}^{s}(-v_1u_j + v_0u_j)) - W(T) = s(n_1 - n_0 - s).$$

The above corollary is equivalent to Theorem 2.6.

Corollary 2.9 *Let T be a tree in $\mathcal{T}_n$, and $P_3 = v_0v_1v_2$ a path in T. Let T_i, $i = 0, 1, 2$, be the component of $T - E(P_3)$ containing v_i with $|V(T_i)| = n_i$, and let $u_1, u_2, \cdots, u_s$ be pendent vertices of T, which is adjacent to v_2. Then*

$$W(T + \sum_{j=1}^{s}(-v_2u_j + v_0u_j)) - W(T) = 2s(n_2 - n_0 - s).$$

Corollary 2.10 *Let T be a tree in $\mathcal{T}_n$, and $P_4 = v_0v_1v_2v_3$ a path in T. Let T_i, $i = 0,1,2,3$, be the component of $T-E(P_4)$ containing v_i with $|V(T_i)| = n_i$, and let $u_1, u_2, \cdots, u_s$ be pendent vertices of T, which is adjacent to v_3. Then*

$$W(T+\sum_{j=1}^{s}(-v_3u_j+v_0u_j)) - W(T) = s[3(n_3-n_0-s)-n_1+n_2].$$

3 Some order relations of trees in $\mathcal{T}_n$ by their Wiener indices.

At first, we give the order of trees with one nonpendent edge by their Wiener indices.

Theorem 3.1 *The order of trees in T_n^1 by their Wiener indices is as follows:*

$$W(T^1_{1,n-3}) < W(T^1_{2,n-4}) < \cdots < W(T^1_{\lfloor\frac{n-2}{2}\rfloor,\lceil\frac{n-2}{2}\rceil}).$$

Proof. Let $T \in T_n^1$, and let $e = v_0v_1$ be the nonpendent edge of T, with $d(v_0) = n_0+1$ and $d(v_1) = n_1+1$. Let u be a pendent vertex of T adjacent to v_1. By Corollary 2.8, we have $W(T-v_1u+v_0u) - W(T) = n_1 - n_0 - 1$. So, when $n_0 \geq n_1$, $W(T-v_1u+v_0u) < W(T)$. Obviously, we get the result. □

For the trees with two nonpendent edges, by Corollaries 2.8 and 2.9, we can get some order relations if the degree of a nonpendent vertex is fixed.

Theorem 3.2 *When $0 \leq s \leq n-5$,*

$$W(T^2_{1,s,n-4-s}) < W(T^2_{2,s,n-5-s}) < \cdots < W(T^2_{\lfloor\frac{n-3-s}{2}\rfloor,s,\lceil\frac{n-3-s}{2}\rceil}).$$

Theorem 3.3 *When $1 \leq t \leq \lfloor\frac{n}{2}\rfloor - 2$,*

$$W(T^2_{1,n-4-t,t}) < W(T^2_{2,n-5-t,t}) < \cdots < W(T^2_{t+1,n-4-2t,t}) = W(T^2_{n-3-t,0,t})$$
$$< \cdots < W(T^2_{\lfloor\frac{n}{2}\rfloor-1,\lceil\frac{n}{2}\rceil-2-t,t}) = W(T^2_{\lceil\frac{n}{2}\rceil-1,\lfloor\frac{n}{2}\rfloor-2-t,t}).$$

Proof Let $f(r) := W(T^2_{r,n-3-r-t,t}) = (n-3)(n-1)+(r+1)(n-r-1)+(t+1)(n-t-1) = (n-3)(n-1)+(t+1)(n-t-1)-(r-\frac{n-2}{2})^2+n-1+(\frac{n-2}{2})^2$. So $f(r)$ is an increasing function when $r \in [1, \frac{n-2}{2}]$, and a decreasing function when $r \in [\frac{n-2}{2}, n-3-t]$.
For a given t, $f(r)$ only depends on the value of $(r-\frac{n-2}{2})^2$. By calculating $(r-\frac{n-2}{2})^2$ for different r, we can get the equalities in the theorem. □

By Theorem 3.2, we have known the order of trees with some integer s. Then we want to know the order relation on trees with different s. So, we can first order the trees with larger s. And by Theorem 3.3, $W(T^2_{r,n-3-r-t,t}) = W(T^2_{n-2-r,r-t-1,t})$. It means that the Wiener index of each tree with larger s equals to that of a tree with smaller s. Therefore, we only need to consider the order of trees with larger s, and then we insert the corresponding trees with smaller s to get the order relation of all the trees with two nonpendent edges.

From formula (4), we find when $n > 11$,
$W(T^2_{r_1,n-5,t_1}) < W(T^2_{r_2,n-6,t_2}) < W(T^2_{r_3,n-7,t_3}) < (T^2_{r_4,n-8,t_4})$, where $r_i + t_i + 1 = r_{i+1} + t_{i+1}$, $i = 1,2,3$. In fact, we will show that when s is more than some integer, $W(T^2_{r,s,t})$ will decrease with s increasing.

Lemma 3.4 *For any $r, r', s, t, t' \in Z^+$, s.t. $r + s + t = r' + s + 1 + t' = n - 3$ and $s \geq \lfloor n - 4 - \sqrt{2n-6} \rfloor + 1$, $W(T^2_{r',s+1,t'}) < W(T^2_{r,s,t})$*

Proof. Since $W(T^2_{r',s+1,t'}) \leq W(T^2_{\lceil\frac{n-4-s}{2}\rceil,s+1,\lfloor\frac{n-4-s}{2}\rfloor})$ and $W(T^2_{n-4-s,s,1}) \leq W(T^2_{r,s,t})$ by theorem 2.9, we only need to show $W(T^2_{\lceil\frac{n-4-s}{2}\rceil,s+1,\lfloor\frac{n-4-s}{2}\rfloor}) < W(T^2_{n-4-s,s,1})$. By formula (4),

$$\begin{aligned}
& W(T^2_{\lceil\frac{n-4-s}{2}\rceil,s+1,\lfloor\frac{n-4-s}{2}\rfloor}) \\
= \ & (n-1)(n-3) + (\lfloor\frac{n-4-s}{2}\rfloor + 1)(n - \lfloor\frac{n-4-s}{2}\rfloor - 1) \\
& + (\lceil\frac{n-4-s}{2}\rceil + 1)(n - \lceil\frac{n-4-s}{2}\rceil - 1) \\
= \ & (n-1)(n-3) + (s+4)n - (s+3)^2 - 1 + 2\lfloor\frac{n-4-s}{2}\rfloor\lceil\frac{n-4-s}{2}\rceil. \\
& W(T^2_{n-4-s,s,1}) \\
= \ & (n-1)(n-3) + (s+3)(n-s-3) + 2(n-2) \\
= \ & (n-1)(n-3) + (s+5)n - (s+3)^2 - 4.
\end{aligned}$$

So, $W(T^2_{n-4-s,s,1}) - W(T^2_{\lceil\frac{n-4-s}{2}\rceil,s+1,\lfloor\frac{n-4-s}{2}\rfloor}) = n - 2\lfloor\frac{n-4-s}{2}\rfloor\lceil\frac{n-4-s}{2}\rceil - 3 \geq n - \frac{(n-4-s)^2}{2} - 3$. Thus, when $s \geq \lceil n - 4 - \sqrt{2(n-3)}\rceil$, we have $W(T^2_{\lceil\frac{n-4-s}{2}\rceil,s+1,\lfloor\frac{n-4-s}{2}\rfloor}) \leq W(T^2_{n-4-s,s,1})$, and equality holds iff $s = n-4-\sqrt{2(n-3)}$ is an integer. So, if $s \geq \lfloor n-4-\sqrt{2n-6}\rfloor + 1$, we have $W(T^2_{\lceil\frac{n-4-s}{2}\rceil,s+1,\lfloor\frac{n-4-s}{2}\rfloor}) < W(T^2_{n-4-s,s,1})$. The proof is completed. □

Theorem 3.5 *Trees in T^2_n can be ordered by*

$$\begin{aligned}
& W(T^2_{1,n-5,1}) < W(T^2_{2,n-6,1}) = W(T^2_{n-4,0,1}) < W(T^2_{3,n-7,1}) = W(T^2_{n-5,1,1}) < W(T^2_{2,n-7,2}) < \\
& W(T^2_{4,n-8,1}) = W(T^2_{n-6,2,1}) < W(T^2_{3,n-8,2}) = W(T^2_{n-5,0,2}) < W(T^2_{5,n-9,1}) = W(T^2_{n-7,3,1}) < \\
& \cdots < W(T^2_{n-5-s,s+1,1}) = W(T^2_{s+3,n-7-s,1}) < W(T^2_{n-6-s,s+1,2}) = W(T^2_{s+3,n-8-s,2}) < \cdots < \\
& W(T^2_{\lceil\frac{n-s}{2}\rceil-2,s+1,\lfloor\frac{n-s}{2}\rfloor-2}) < W(T^2_{n-4-s,s,1}) = W(T^2_{s+1,n-6-s,1}) < W(T),
\end{aligned} \tag{7}$$

where $s \geq \lfloor n - 4 - \sqrt{2n-6}\rfloor + 1$ and T is any tree in T^2_n which is different from any other tree in the inequality (7). And when $n - s$ is odd, $W(T^2_{\lceil\frac{n-s}{2}\rceil-2,s+1,\lfloor\frac{n-s}{2}\rfloor-2}) = W(T^2_{n-\lceil\frac{n-s}{2}\rceil,0,\lfloor\frac{n-s}{2}\rfloor-2})$.

Proof. By Lemma 3.4 and Theorem 3.3, one can easily get $W(T^2_{1,n-5,1}) < W(T^2_{2,n-6,1}) = W(T^2_{n-4,0,1}) < W(T^2_{3,n-7,1}) = W(T^2_{n-5,1,1}) < W(T^2_{2,n-7,2}) < W(T^2_{4,n-8,1}) = W(T^2_{n-6,2,1}) < W(T^2_{3,n-8,2}) = W(T^2_{n-5,0,2}) < W(T^2_{5,n-9,1}) = W(T^2_{n-7,3,1}) < \cdots < W(T^2_{n-5-s,s+1,1}) = W(T^2_{s+3,n-7-s,1}) < W(T^2_{n-6-s,s+1,2}) = W(T^2_{s+3,n-8-s,2}) < \cdots < W(T^2_{\lceil\frac{n-s}{2}\rceil-2,s+1,\lfloor\frac{n-s}{2}\rfloor-2}) < W(T^2_{n-4-s,s,1}) = W(T^2_{s+1,n-6-s,1})$. And when $n-s$ is odd, $W(T^2_{\lceil\frac{n-s}{2}\rceil-2,s+1,\lfloor\frac{n-s}{2}\rfloor-2}) = W(T^2_{n-\lceil\frac{n-s}{2}\rceil,0,\lfloor\frac{n-s}{2}\rfloor-2})$.

Now we will show $W(T^2_{n-4-s,s,1}) = W(T^2_{s+1,n-6-s,1}) < W(T)$. We let $T = T^2_{r',s',t'}$, $r' \geq t'$, and distinguish the following three cases.

Case 1. $t' = 1$.

Since T is different from the trees in the inequality (7), $s > s' > n-6-s$. By Theorem 3.3, $W(T) > W(T^2_{n-4-s,s,1})$.

Case 2. $t' > 1$ and $s' \leq \lceil\frac{n}{2}\rceil - 2 - t'$.

By Theorem 3.2, we have $W(T) > W(T^2_{n-4-s',s',1})$. $s' \leq \lceil\frac{n}{2}\rceil - 2 - t' \leq \lceil\frac{n}{2}\rceil - 4 \leq \lceil n-4-\sqrt{2n-6}\rceil \leq s$. And by Theorem 3.3, we have $W(T^2_{n-4-s',s',1}) \geq W(T^2_{n-4-s,s,1})$. Thus, $W(T) > W(T^2_{n-4-s,s,1})$.

Case 3. $t' > 1$ and $s' \geq \lfloor\frac{n}{2}\rfloor - 2 - t'$.

By Theorem3.3, $W(T^2_{r',s',t'}) = W(T^2_{n-2-r',r'-t'-1,t'})$. Thus $r'-t'-1 = (n-3-s'-t') - t'-1 \leq (n-3-(\lfloor\frac{n}{2}\rfloor-2-t')-t')-t'-1 = \lceil\frac{n}{2}\rceil-2-t'$, since $s' > \lfloor\frac{n}{2}\rfloor-2-t'$. Similar to case 2, we can get $W(T^2_{n-2-r',r'-t'-1,t'}) > W(T^2_{n-4-s,s,1})$. So, $W(T) > W(T^2_{n-4-s,s,1})$.

The proof is completed. □

Lemma 3.6 *When $n \geq 9$, let $T \in \{T^{(1)}_{l,m,p,q} | l+m+p+q = n-4\} \backslash \{T^{(1)}_{1,1,n-7,1}, T^{(1)}_{2,1,n-8,1}, T^{(1)}_{3,1,n-9,1}\}$, then $W(T^{(1)}_{1,1,n-7,1}) < W(T^{(1)}_{2,1,n-8,1}) < W(T^{(1)}_{3,1,n-9,1}) < W(T)$.*

Proof. $W(T^{(1)}_{1,1,n-7,1}) = (n-1)(n-4) + 6n - 12$.
$W(T^{(1)}_{2,1,n-8,1}) = (n-1)(n-4) + 7n - 17$.
$W(T^{(1)}_{3,1,n-9,1}) = (n-1)(n-4) + 8n - 24$.

So, $W(T^{(1)}_{1,1,n-7,1}) < W(T^{(1)}_{2,1,n-8,1}) < W(T^{(1)}_{3,1,n-9,1})$.

Now we will show $W(T^{(1)}_{3,1,n-9,1}) < W(T)$. Let $T = T^{(1)}_{l,m,p,q}$, $l \geq m \geq q$. We distinguish the following three cases.

Case 1. $l = 2$. Then $T = T^{(1)}_{2,2,n-9,1}$ or $T = T^{(1)}_{2,2,n-10,2}$.

$W(T^{(1)}_{2,2,n-9,1}) = (n-1)(n-4) + 8n - 22 > W(T^{(1)}_{3,1,n-9,1})$

$W(T^{(1)}_{2,2,n-10,2}) = (n-1)(n-4) + 9n - 27 > W(T^{(1)}_{3,1,n-9,1})$

Case 2. $l = 3$. Then $m \geq 2$, $q \geq 1$.

By Corollary 2.8, $W(T^{(1)}_{3,m,p,q}) = W(T^{(1)}_{3,1,n-9,1}) + (m-1)(n-m-3) + (q-1)(n-q-3)$. Since $m-1 \geq 1$, $n-m-3 > 0$, $q-1 \geq 0$, $n-q-3 > 0$, $W(T^{(1)}_{l,m,p,q}) > W(T^{(1)}_{1,3,n-9,1})$.

Case 3. $l \geq 4$. Then $m \geq 1$, $q \geq 1$.

$W(T^{(1)}_{l,m,p,q}) = W(T^{(1)}_{3,1,n-9,1}) + (l-3)(n-l-5) + (m-1)(n-m-3) + (q-1)(n-q-3)$. Since $l-3 \geq 1$, $n-l-5 \geq 1$, $m-1 \geq 0, n-m-3 \geq 0$, $q-1 \geq 0, n-q-3 \geq 0$, $W(T^{(1)}_{l,m,p,q}) > W(T)$. □

Compare formulae (5),(6), we easily get $W(T^{(1)}_{l_1,m_1,p_1,q_1}) = W(T^{(2)}_{l_2,m_2,p_2,q_2})$, when $l_1 = l_2,\ m_1 = l_2 + m_2 + 1,\ q_1 = q_2$.

And the equality (6) can be written as the following symmetrically:
$W(T^{(2)}_{l_2,m_2,p_2,q_2}) = (l_2+1)(n-l_2-1) + (p_2+q_2+2)(n-p_2-q_2-2) + (q_2+1)(n-q_2-1)$.
So, similarly, $W(T^{(1)}_{l_1,m_1,p_1,q_1}) = W(T^{(2)}_{l_2,m_2,p_2,q_2})$, when $l_1 = l_2,\ m_1 = p_2 + q_2 + 1,\ q_1 = q_2$.

Lemma 3.7 *When $p > l$, we have $W(T^{(2)}_{l,m,p,q}) = W(T^{(1)}_{l,l+m+1,p-l-1,q})$.*
When $m > q$, we have $W(T^{(2)}_{l,m,p,q}) = W(T^{(1)}_{l,p+q+1,m-q-1,q})$.

By above result, we just need to order the trees in $\{T^{(1)}_{l_1,m_1,p_1,q_1} | l_1+m_1+p_1+q_1 = n-5\}$ and compare them to the trees in $\{T^{(2)}_{l_2,m_2,p_2,q_2} | l_2 \geq p_2,\ q_2 \geq m_2\}$ to get the order of T^3_n.

Theorem 3.8 *Let $n \geq 17$ and $T \in T^3_n \backslash \{T^{(1)}_{1,1,n-7,1}, T^{(1)}_{1,1,n-8,2}, T^{(2)}_{1,n-6,0,1}, T^{(1)}_{1,1,n-9,3}, T^{(2)}_{1,n-7,1,1}\}$, then*
$W(T^{(1)}_{1,1,n-7,1}) < W(T^{(1)}_{2,1,n-8,1}) = W(T^{(2)}_{1,n-6,0,1}) < W(T^{(1)}_{3,1,n-9,1}) = W(T^{(2)}_{1,n-7,1,1}) < W(T)$.

Proof. By formulae (6) and Lemma 3.6, we can get
$W(T^{(1)}_{1,1,n-7,1}) < W(T^{(1)}_{2,1,n-8,1}) = W(T^{(2)}_{1,n-6,0,1}) < W(T^{(1)}_{3,1,n-9,1}) = W(T^{(2)}_{1,n-7,1,1})$.

If $T = T^{(1)}_{l,m,p,q}$, by Lemma 3.6, $W(T^{(1)}_{3,1,n-9,1}) < W(T)$.

If $T = T^{(2)}_{l,m,p,q}$, and $p > l$ or $m > q$, without loss of generation, we suppose $p > l$, then $W(T^{(2)}_{l,m,p,q}) = W(T^{(1)}_{l,l+m+1,p-l-1,q}) > W(T^{(1)}_{3,1,n-9,1})$.

If $T = T^{(2)}_{l,m,p,q}$, $l \geq p$, and $q \geq m$, without loss of generation, we suppose $l+p \geq q+m$. If $l+p \geq q+m \geq 3$, since $n \geq 17$, then $l+p \geq 7$. By Corollary 2.9 and Lemma 3.7, $W(T^{(2)}_{l,m,p,q}) = W(T^{(2)}_{1,m,,l+p-1,q}) + 2(l-1)(p+q) = W(T^{(1)}_{1,m+2,l+p-3,q}) + 2(l-1)(p+q)$. Since $m+2+q \geq 5$, $l+p-3 \geq 4$, $T^{(1)}_{1,m+2,l+p-3,q} \neq T^{(1)}_{1,1,n-7,1}, T^{(1)}_{2,1,n-8,1}$ and $T^{(1)}_{3,1,n-9,1}$. By Lemma 3.6, we have $W(T^{(1)}_{1,m+2,l+p-3,q}) > W(T^{(1)}_{3,1,n-9,1})$. Therefore, $W(T^{(2)}_{l,m,p,q}) > W(T^{(1)}_{3,1,n-9,1})$. If $q+m \leq 2$, then $l+p \geq 11$ and $l \geq 6$. By formula (6), it is easy to verify that $W(T^{(2)}_{l,m,p,q}) > W(T^{(2)}_{1,n-7,1,1}) = W(T^{(1)}_{3,1,n-9,1})$. □

4 The first fourteen trees in $\mathcal{T}_n$ with Smaller Wiener indices.

Theorem 4.1 *Let $T \in T_n \backslash \{S_n, T^1_{n-3,1}, T^1_{n-4,2}, T^1_{n-5,3}, T^1_{n-6,4}, T^2_{1,n-5,1}, T^2_{2,n-6,1}, T^2_{2,n-7,2}, T^2_{3,n-7,1}, T^2_{n-4,0,1}, T^2_{1,n-5,1}, T^{(1)}_{1,1,n-7,1}, T^{(1)}_{2,1,n-8,1}, T^{(2)}_{1,n-6,0,1}\}$, $n \geq 24$, then*

$$W(S_n) < W(T^1_{n-3,1}) < W(T^1_{n-4,2}) < W(T^2_{1,n-5,1}) < W(T^1_{n-5,3}) < W(T^2_{2,n-6,1})$$

$$= W(T^2_{n-4,0,1}) < W(T^{(1)}_{1,1,n-7,1}) < W(T^1_{n-6,4}) < W(T^2_{3,n-7,1}) = W(T^2_{n-5,1,1})$$

$$< W(T^2_{2,n-7,2}) < W(T^{(1)}_{2,1,n-8,1}) = W(T^{(2)}_{1,n-6,0,1}) < W(S(n,n-5)) < W(T).$$

Proof. $W(S_n) = (n-1)^2 = (n-2)(n-1) + n - 1$,
$W(T^1_{n-3,1}) = (n-2)(n-1) + 2(n-2)$,
$W(T^1_{n-4,2}) = (n-2)(n-1) + 3(n-3)$,
$W(T^2_{1,n-5,1}) = (n-3)(n-1) + 4(n-2) = (n-2)(n-1) + 3n - 7$,
$W(T^1_{n-5,3}) = (n-2)(n-1) + 4(n-4)$,
$W(T^2_{2,n-6,1}) = W(T^2_{n-4,0,1}) = (n-1)(n-3) + 5n - 13 = (n-2)(n-1) + 4n - 12$,
$W(T^{(1)}_{1,1,n-7,1}) = (n-1)(n-4) + 6(n-2) = (n-1)(n-2) + 4n - 10$,
$W(T^1_{n-6,4}) = (n-1)(n-3) + 6n - 26 = (n-1)(n-2) + 5n - 25$,
$W(T^2_{3,n-7,1}) = W(T^2_{n-5,1,1}) = (n-1)(n-3) + 6n - 20 = (n-2)(n-1) + 5n - 19$,
$W(T^2_{2,n-7,2}) = (n-1)(n-3) + 6n - 18 = (n-2)(n-1) + 5n - 17$,
$W(T^{(1)}_{1,2,n-8,1}) = W(T^{(2)}_{n-6,0,1,1}) = (n-1)(n-3) + 6n - 16 = (n-2)(n-1) + 5n - 15$,
$W(S(n, n-5)) = (n-1)(n-3) + 6n - 14$.
So, when $n \geq 24$, $W(S_n) < W(T^1_{n-3,1}) < W(T^1_{n-4,2}) < W(T^2_{1,n-5,1}) < W(T^1_{n-5,3}) < W(T^2_{2,n-6,1})$
$= W(T^2_{n-4,0,1}) < W(T^{(1)}_{1,1,n-7,1}) < W(T^1_{n-6,4}) < W(T^2_{3,n-7,1}) = W(T^2_{1,n-5,1}) < W(T^2_{2,n-7,2})$
$< W(T^{(1)}_{1,2,n-8,1}) = W(T^{(2)}_{1,n-6,0,1}) < W(S(n, n-5))$.

If $T \in T^1_n$, then by Theorem 3.1, when $n \geq 24$, $W(T) \geq W(T^1_{n-7,5}) = (n-1)(n-3) + 7n - 37 > W(S(n, n-5))$.

If $T \in T^2_n$, $W(T^2_{1,n-8,4}) = (n-1)(n-3) + 7n - 29$. Then $W(S(n, n-5)) < W(T^2_{1,n-8,4}) \leq W(T)$ by Theorem 3.5.

If $T \in T^3_n$, $W(T^{(1)}_{3,1,n-9,1}) = (n-1)(n-3) + 7n - 23 > W(S(n, n-5))$, and so, by Lemma 3.8, $W(T) \geq W(T^{(1)}_{3,1,n-9,1}) > W(S(n, n-5))$.

If $T \in T^4_n$, by Theorem 2.3, $W(T) > W(S(n, n-5))$.

If $T \in T^i_n$, where $i \geq 5$, we can transform T to some tree in T^4_n by carrying out $i-4$ steps e.g.t. Therefore, by Theorem 2.5 and Theorem 2.3, $W(S(n, n-5)) < W(T)$.

The proof is completed. □

Meanwhile, for $9 \leq n \leq 23$, we can list the trees with the first, $\cdots$, up to the 15^{th} smallest number of Wiener indices as follows.

(1) when $n = 9$,

$W(S_9) < W(T^1_{6,1}) < W(T^1_{5,2}) < W(T^1_{4,3}) = W(T^2_{1,4,1}) < W(T^2_{2,3,1}) = W(T^2_{5,0,1}) < W(T^2_{3,2,1}) = W(T^2_{4,1,1}) = W(T^{(1)}_{1,1,2,1}) < W(T^2_{2,2,2}) < W(T^{(1)}_{1,1,1,2}) = W(T^{(2)}_{3,0,1,1}) < W(S(9,4))$.

(2) when $n = 10$,

$W(S_{10}) < W(T^1_{7,1}) < W(T^1_{6,2}) < W(T^2_{1,5,1}) < W(T^1_{5,3}) < W(T^1_{4,4}) < W(T^2_{2,4,1}) = W(T^2_{6,0,1}) < W(T^{(1)}_{1,1,3,1}) = W(T^2_{5,1,1}) = W(T^2_{3,3,1}) < W(T^2_{4,2,1}) < W(T^2_{2,3,2}) < W(T^{(1)}_{1,1,2,2}) = W(T^{(2)}_{4,0,1,1}) < W(S(10,5))$.

(3) when $n = 11$,

$W(S_{11}) < W(T^1_{8,1}) < W(T^1_{7,2}) < W(T^2_{1,6,1}) < W(T^1_{6,3}) < W(T^1_{5,4}) < W(T^2_{2,5,1}) = W(T^2_{7,0,1}) < W(T^{(1)}_{1,1,4,1}) < W(T^2_{3,4,1}) = W(T^2_{6,1,1}) < W(T^2_{4,3,1}) = W(T^2_{5,2,1}) = W(T^2_{2,4,2}) < W(T^{(1)}_{1,1,3,2}) = W(T^{(2)}_{5,0,1,1}) < W(S(11,6))$.

(4) when $n = 12$,

$W(S_{12}) < W(T^1_{9,1}) < W(T^1_{8,2}) < W(T^2_{1,7,1}) < W(T^1_{7,3}) < W(T^1_{6,4}) < W(T^2_{2,6,1}) = W(T^2_{8,0,1}) = W(T^1_{5,5}) < W(T^{(1)}_{1,1,5,1}) < W(T^2_{3,5,1}) = W(T^2_{7,1,1}) < W(T^2_{2,5,2}) < W(T^2_{4,4,1}) = W(T^2_{6,2,1}) < W(T^{(1)}_{1,1,4,2}) = W(T^{(2)}_{6,0,1,1}) < W(S(12,7))$.

(5) when $n = 13$,

$W(S_{13}) < W(T^1_{10,1}) < W(T^1_{9,2}) < W(T^2_{1,8,1}) < W(T^1_{8,3}) < W(T^1_{2,7,1}) = W(T^2_{9,0,1}) = W(T^2_{7,4}) < W(T^{(1)}_{1,1,6,1}) = W(T^1_{6,5}) < W(T^2_{3,6,1}) = W(T^2_{8,1,1}) < W(T^2_{2,6,2}) < W(T^2_{4,5,1}) = W(T^2_{7,2,1}) = W(T^{(1)}_{1,1,5,2}) = W(T^{(2)}_{7,0,1,1}) < W(S(13,8))$...

(6) when $n = 14$,

$W(S_{14}) < W(T^1_{11,1}) < W(T^1_{10,2}) < W(T^2_{1,9,1}) < W(T^1_{9,3}) < W(T^2_{2,8,1}) = W(T^2_{10,0,1}) < W(T^1_{8,4}) < W(T^{(1)}_{1,1,7,1}) < W(T^1_{7,5}) < W(T^1_{6,6}) < W(T^2_{3,7,1}) = W(T^2_{9,1,1}) < W(T^2_{2,7,2}) < W(T^{(1)}_{1,1,6,2})$
$= W(T^{(2)}_{8,0,1,1}) < W(T^2_{4,6,1}) = W(T^2_{8,2,1}) < W(S(14,9))$.

(7) when $n = 15$,

$W(S_{15}) < W(T^1_{12,1}) < W(T^1_{11,2}) < W(T^2_{1,10,1}) < W(T^1_{10,3}) < W(T^2_{2,9,1}) = W(T^2_{11,0,1}) < W(T^1_{9,4}) < W(T^{(1)}_{1,1,8,1}) < W(T^1_{8,5}) < W(T^1_{7,6}) = W(T^2_{3,8,1}) = W(T^2_{10,1,1}) < W(T^2_{2,8,2}) < W(T^{(1)}_{1,1,7,2}) = W(T^{(2)}_{9,0,1,1}) = W(T^2_{4,7,1}) = W(T^2_{9,2,1}) < W(S(15,10))$.

(8) when $n = 16$,

$W(S_{16}) < W(T^1_{13,1}) < W(T^1_{12,2}) < W(T^2_{1,11,1}) < W(T^1_{11,3}) < W(T^2_{2,10,1}) = W(T^2_{12,0,1}) < W(T^{(1)}_{1,1,9,1}) < W(T^1_{10,4}) < W(T^1_{9,5}) < W(T^2_{3,9,1}) = W(T^2_{11,1,1}) < W(T^1_{8,6}) = W(T^2_{2,9,2}) < W(T^{(1)}_{1,1,8,2}) = W(T^{(2)}_{10,0,1,1}) < W(S(16,11))$.

(9) when $n = 17$,

$W(S_{17}) < W(T^1_{14,1}) < W(T^1_{13,2}) < W(T^1_{1,12,1}) < W(T^1_{12,3}) < W(T^2_{2,11,1}) = W(T^2_{13,0,1}) < W(T^{(1)}_{1,1,10,1}) < W(T^1_{11,4}) < W(T^1_{10,5}) = W(T^2_{3,10,1}) = W(T^2_{12,1,1}) < W(T^2_{2,10,2}) < W(T^{(1)}_{1,1,9,2}) = W(T^{(2)}_{11,0,1,1}) = W(T^1_{9,6}) < W(S(17,12))$.

(10) when $n = 18$,

$W(S_{18}) < W(T^1_{15,1}) < W(T^1_{14,2}) < W(T^1_{1,13,1}) < W(T^1_{13,3}) < W(T^2_{2,12,1}) = W(T^2_{14,0,1}) < W(T^{(1)}_{1,1,11,1}) < W(T^1_{12,4}) < W(T^2_{3,11,1}) = W(T^2_{13,1,1}) < W(T^1_{11,5}) < W(T^2_{2,11,2}) < W(T^{(1)}_{1,1,10,2})$
$= W(T^{(2)}_{12,0,1,1}) < W(T^1_{10,6}) = W(S(18,13))$.

(11) when $n = 19$,

$W(S_{19}) < W(T^1_{16,1}) < W(T^1_{15,2}) < W(T^1_{1,14,1}) < W(T^1_{14,3}) < W(T^2_{2,13,1}) = W(T^2_{15,0,1}) < W(T^{(1)}_{1,1,12,1}) < W(T^1_{13,4}) < W(T^2_{3,12,1}) = W(T^2_{14,1,1}) < W(T^1_{12,5}) < W(T^2_{2,12,2}) < W(T^{(1)}_{1,1,11,2})$
$= W(T^{(2)}_{12,0,1,1}) < W(S(19,14))$.

(12) when $n = 20$,

$W(S_{20}) < W(T^1_{17,1}) < W(T^1_{16,2}) < W(T^1_{1,15,1}) < W(T^1_{15,3}) < W(T^2_{2,14,1}) = W(T^2_{16,0,1}) < W(T^{(1)}_{1,1,13,1}) < W(T^1_{14,4}) < W(T^2_{3,13,1}) = W(T^2_{15,1,1}) < W(T^1_{2,13,2}) < W(T^1_{13,5}) < W(T^{(1)}_{1,1,12,2}) = W(T^{(2)}_{13,0,1,1}) < W(S(20,15))$.

(13) when $n = 21$,

$W(S_{21}) < W(T^1_{18,1}) < W(T^1_{17,2}) < W(T^2_{1,16,1}) < W(T^1_{16,3}) < W(T^2_{2,15,1}) = W(T^2_{17,0,1}) < W(T^{(1)}_{1,1,14,1}) < W(T^1_{15,4}) < W(T^2_{3,14,1}) = W(T^2_{16,1,1}) < W(T^1_{2,14,2}) < W(T^{(1)}_{1,1,13,2}) =$

$W(T^{(2)}_{14,0,1,1}) = W(T^1_{14,5}) < W(S(21,16))$.

(14) when $n = 22$,

$W(S_{22}) < W(T^1_{19,1}) < W(T^1_{18,2}) < W(T^1_{1,17,1}) < W(T^1_{17,3}) < W(T^2_{2,16,1}) = W(T^2_{18,0,1}) < W(T^{(1)}_{1,1,15,1}) < W(T^1_{16,4}) < W(T^2_{3,15,1}) = W(T^2_{17,1,1}) < W(T^1_{2,15,2}) < W(T^{(1)}_{1,1,14,2}) = W(T^{(2)}_{15,0,1,1}) < W(T^1_{15,5}) < W(S(22,17))$.

(15) when $n = 23$,

$W(S_{23}) < W(T^1_{20,1}) < W(T^1_{19,2}) < W(T^1_{1,18,1}) < W(T^1_{18,3}) < W(T^2_{2,17,1}) = W(T^2_{19,0,1}) < W(T^{(1)}_{1,1,16,1}) < W(T^1_{17,4}) < W(T^2_{3,16,1}) = W(T^2_{18,1,1}) < W(T^1_{2,16,2}) < W(T^{(1)}_{1,1,15,2}) = W(T^{(2)}_{16,0,1,1}) < W(T^1_{16,5}) = W(S(23,18))$.

Discussion. In the previous works on Wiener index, many researchers focused on determining the trees with the maximum and minimum Wiener indices. This topic can be naturally extended to ordering trees by Wiener indices. It can determine not only the trees with the maximum and minimum Wiener indices but also the trees with the second, the third, up to some kth smallest Wiener indices. In the above, by introducing some tree transformations, we obtain some order relations of several classes of trees, furthermore the trees with n vertices and with the first up to fifteenth smallest Wiener indices are determined. Because Wiener indices of molecular structures are closely related to physical and chemical properties such as boiling point etc., the above results would be useful in understanding the relationship between some molecular structures and their physical and chemical properties according to Wiener indices, and in determining molecular structures with some given properties and Wiener indices.

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