

Erratum to ‘The trees on $n \geq 9$ vertices with the first to seventeenth greatest Wiener indices are chemical trees’^{*}

Muhuo Liu^{1,2}, Bolian Liu², Qian Li¹

¹ Department of Applied Mathematics, South China Agricultural University,
Guangzhou, P. R. China, 510642

² School of Mathematic Science, South China Normal University,
Guangzhou, P. R. China, 510631

(Received April 22, 2009)

Abstract: Deng once determined the trees on $n \geq 9$ vertices with the first to seventeenth greatest Wiener indices [H. Y. Deng, The trees on $n \geq 9$ vertices with the first to seventeenth greatest Wiener indices are chemical trees, MATCH Comm. Math. Comput. Chem. 57(2007) 393-402]. Unfortunately, some mistakes are found in Deng’s paper. This paper will present a correct order of the first to fifteenth greatest Wiener indices for trees on $n \geq 28$.

1 Introduction

Throughout this paper, we only concern with connected, undirected simple graphs. Let $N(u)$ be the first neighbor vertex set of u , then $d(u) = |N(u)|$ is called the degree of u . As usual, P_n and S_n denote the path and star of order n , respectively.

The *distance* $d_G(u, v)$ between the vertices u and v of the graph G is equal to the length of (number of edges in) the shortest path that connects u and v . There are two important

^{*}The first author is supported by the fund of South China Agricultural University (No. 4900-k08225); The second author is the corresponding author who is supported by NNSF of China (No. 10771080) and SRFDP of China (No. 20070574006). E-mail address: liubl@scau.edu.cn

graph-based structure-descriptors, called Wiener index and hyper-Wiener index, based on distances in a graph. The *Wiener index* $W(G)$ is denoted by [1]

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

and the *hyper-Wiener index* $WW(G)$ is defined as [2]

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)^2.$$

The Wiener index and hyper-Wiener index are much studied in the chemical literatures because of their important applications in chemistry. Recently, the Wiener index and hyper-Wiener index gained much popularity. More and more mathematicians and chemists became interested in them and devoted themselves to the study. The mathematical properties of Wiener index and hyper-Wiener index with their applications in chemistry can be referred to [3-10] and the references cited therein.

We now introduce some more key notations. Recall that a vertex u of a tree T is called a *branching point* of T if $d(u) \geq 3$. Furthermore, u is said to be an *out-branching point* if at most one of the components of $T - u$ is not a path; otherwise, u is an *in-branching point* of T .

Let $T(n; n_1, n_2, \dots, n_m)$ denote the starlike tree of order n obtained by inserting $n_1 - 1, \dots, n_m - 1$ vertices into m edges of the star S_{m+1} of order $m + 1$ respectively, where $n_1 + \dots + n_m = n - 1$. Note that any tree with only one branching point is a starlike tree.

If T is a tree of order n with exactly two branching points u_1 and u_2 , with $d(u_1) = r$ and $d(u_2) = t$. The orders of $r - 1$ components, which are paths, of $T - u_1$ are p_1, \dots, p_{r-1} , the order of the component which is not a path of $T - u_1$ is $p_r = n - p_1 - \dots - p_{r-1} - 1$. The orders of $t - 1$ components, which are paths, of $T - u_2$ are q_1, \dots, q_{t-1} , the order of the component which is not a path of $T - u_2$ is $q_t = n - q_1 - \dots - q_{t-1} - 1$. We denote this tree by $T(n; p_1, \dots, p_{r-1}; q_1, \dots, q_{t-1})$, where $r \leq t, p_1 \geq \dots \geq p_{r-1}$ and $q_1 \geq \dots \geq q_{t-1}$.

Gutman first obtained the trees on n vertices with the smallest and greatest hyper-Wiener index (i.e., the star and path) in [11]. Very recently, the trees with the seven smallest and the fifteen greatest hyper-Wiener indices were determined in [12], respectively. Also, among all connected graphs of order n ($n > 2k$), the first up to $(k + 1)$ -th smallest Wiener indices and the first up to $(k + 1)$ -th smallest hyper-Wiener indices are

determined in [13], respectively. Gutman et al. also considered the similar order of Wiener index among the starlike trees in [14]. After then, the first up to fifteenth smallest Wiener indices among trees of order n were identified in [15]. Recently, Deng considered the order of greatest Wiener indices among trees and he once obtained

Theorem A [16] Suppose $n \geq 9$ and T is a tree of order n . Then, $W(T(n; n - 3, 1, 1)) > W(T(n; n - 4, 2, 1)) > W(T(n; 1, 1; 1, 1)) > W(T(n; n - 5, 3, 1)) > W(T(n; n - 4, 1, 1, 1)) \geq W(T(n; 1, 1; 2, 1)) > W(T(n; n - 6, 4, 1)) > W(T(n; n - 5, 2, 2)) > W(T(n; 1, 1; 3, 1)) > W(T(n; 2, 1; 2, 1)) > W(T(n; 1, 1; 1, 1, 1)) > W(T(n; n - 7, 5, 1)) > W(T(n; 1, 1; 4, 1)) > W(T(n; n - 5, 2, 1, 1)) \geq W(T(n; 1, 1; 2, 2)) \geq W(T(n; 2, 1; 3, 1)) > W(T_D) \geq W(T)$, where T_D is shown in Fig. 1.

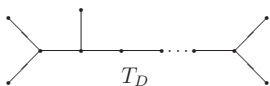


Fig. 1. The tree T_D .

Unfortunately, as the following example shown, Theorem A is not correct. In the sequel, $\binom{n+1}{3}$ is written as C_{n+1}^3 .

Example 1.1. By an elementary computation (or the application of Lemma 2.4), it follows that $W(T(n; 1, 1; n - 6, 1)) = C_{n+1}^3 - 5n + 27$ and $W(T_D) = C_{n+1}^3 - 5n + 21$. Thus, $W(T(n; 1, 1; n - 6, 1)) > W(T_D)$, a contradiction to Theorem A.

Thus, we give a correct order of the greatest Wiener indices of trees in this paper, namely

Theorem 1.1 Suppose $n \geq 28$ and T is a tree of order n . Then, $W(P_n) > W(T(n; n - 3, 1, 1)) > W(T(n; n - 4, 2, 1)) > W(T(n; 1, 1; 1, 1)) > W(T(n; n - 5, 3, 1)) > W(T(n; n - 4, 1, 1, 1)) = W(T(n; 1, 1; 2, 1)) > W(T(n; n - 6, 4, 1)) > W(T(n; n - 5, 2, 2)) > W(T(n; 1, 1; n - 5, 1)) = W(T(n; 1, 1; 3, 1)) > W(T(n; 2, 1; 2, 1)) > W(T(n; 1, 1; 1, 1, 1)) > W(T(n; n - 7, 5, 1)) > W(T(n; 1, 1; n - 6, 1)) = W(T(n; 1, 1; 4, 1)) > W(T(n; n - 5, 2, 1, 1)) = W(T(n; 1, 1; 2, 2)) = W(T(n; 2, 1; 3, 1)) > W(T_D) > W(T)$.

Remark. By comparing with Theorem A and Theorem 1.1, two trees, say $T(n; 1, 1; n - 5, 1)$ and $T(n; 1, 1; n - 6, 1)$, are left out in [16].

2 The proof of Theorem 1.1

Given a simple and undirected graph $G = (V, E)$. Let $G - u$ (resp. $G - uv$) denote the graph obtained from G by deleting the vertex $u \in V(G)$ (resp. the edge $uv \in E(G)$). Similarly, $G + uv$ is a graph yielded from G by adding an edge $uv \notin E(G)$, where $u, v \in V(G)$.



Fig. 2. The graphs $G_{k,l}$ and $G_{k-1,l+1}$.

Suppose v is a vertex of graph G . As shown in Fig. 2, let $G_{k,l}$ ($l \geq k \geq 1$) be the graph obtained from G by attaching two new paths $P: v(= v_0)v_1v_2 \cdots v_k$ and $Q: v(= u_0)u_1u_2 \cdots u_l$ of length k and l , respectively, at v , where v_1, v_2, \dots, v_k and u_1, u_2, \dots, u_l are distinct new vertices. Let $G_{k-1,l+1} = G_{k,l} - v_{k-1}v_k + u_lv_k$.

Lemma 2.1 *Suppose G is a connected graph on $n \geq 2$ vertices, or an isolated vertex. If $l \geq k \geq 1$, then $W(G_{k,l}) \leq W(G_{k-1,l+1})$, the equality holds if and only if G is an isolated vertex.*

Proof. It is easy to see that

$$W(G_{k-1,l+1}) - W(G_{k,l}) = \sum_{w \in V(G_{k-1,l+1})} d_{G_{k-1,l+1}}(w, v_k) - \sum_{w \in V(G_{k,l})} d_{G_{k,l}}(w, v_k). \quad (1)$$

Let $V_1 = V(G) \setminus \{v\}$, then $V(G_{k,l}) \setminus V_1 = V(G_{k-1,l+1}) \setminus V_1$. Let $V_2 = V(G_{k,l}) \setminus V_1$. Clearly,

$$\sum_{w \in V(G_{k,l})} d_{G_{k,l}}(w, v_k) = \sum_{w \in V_1} d_{G_{k,l}}(w, v_k) + \sum_{w \in V_2} d_{G_{k,l}}(w, v_k). \quad (2)$$

$$\sum_{w \in V(G_{k-1,l+1})} d_{G_{k-1,l+1}}(w, v_k) = \sum_{w \in V_1} d_{G_{k-1,l+1}}(w, v_k) + \sum_{w \in V_2} d_{G_{k-1,l+1}}(w, v_k). \quad (3)$$

Note that the subgraph of $G_{k,l}$ induced by V_2 is a path of length $k+l$, which is isomorphic to the subgraph of $G_{k-1,l+1}$ induced by V_2 , thus

$$\sum_{w \in V_2} d_{G_{k,l}}(w, v_k) = \sum_{w \in V_2} d_{G_{k-1,l+1}}(w, v_k). \quad (4)$$

Therefore, by combining equalities (1)-(4), we have

$$\begin{aligned}
 W(G_{k-1,l+1}) - W(G_{k,l}) &= \sum_{w \in V_1} d_{G_{k-1,l+1}}(w, v_k) - \sum_{w \in V_1} d_{G_{k,l}}(w, v_k) \\
 &= \sum_{w \in V_1} (d_{G_{k-1,l+1}}(w, v_k) - d_{G_{k,l}}(w, v_k)). \tag{5}
 \end{aligned}$$

If G is an isolated vertex, then $V_1 = \emptyset$. By equality (5), it follows that $W(G_{k-1,l+1}) = W(G_{k,l})$. If G is not an isolated vertex, since $l \geq k$, then $d_{G_{k-1,l+1}}(w, v_k) > d_{G_{k,l}}(w, v_k)$ holds for every $w \in V_1$. Thus, the result follows from equality (5). ■



Fig. 3. The graphs $M_{t,t+s}$ and $M_{t+1,t+s}$.

Suppose v_1 is a vertex of graph G , and v_2, \dots, v_{t+s}, u_0 are distinct new vertices (not in G). Let G' be the graph obtained from G by attaching a new path $P: v_1 v_2 \cdots v_{t+s}$. Let $M_{t,t+s} = G' + v_t u_0$ and $M_{t+i,t+s} = G' + v_{t+i} u_0$, where $1 \leq i \leq s$. For instance, $M_{t,t+s}$ and $M_{t+1,t+s}$ are depicted in Fig. 3.

Lemma 2.2 *Suppose G is a connected graph on $n \geq 2$ vertices, or an isolated vertex. If $t \geq s \geq 1$, then $W(M_{t,t+s}) \leq W(M_{t+1,t+s})$. Moreover, the equality holds if and only if $t = s$ and G is an isolated vertex.*

Proof. For convenience, sometimes we write $M_{t,t+s}$ as M , and $M_{t+1,t+s}$ as M' in the proof of this lemma. Let $V_1 = V(G) \setminus \{v_1\}$, then $V(M_{t,t+s}) \setminus V_1 = V(M_{t+1,t+s}) \setminus V_1$. Let $V_2 = V(M_{t,t+s}) \setminus V_1$. Thus,

$$\begin{aligned}
 W(M_{t+1,t+s}) - W(M_{t,t+s}) &= \sum_{w \in V(M')} d_{M'}(w, u_0) - \sum_{w \in V(M)} d_M(w, u_0) \\
 &= \sum_{w \in V_1} (d_{M'}(w, u_0) - d_M(w, u_0)) + \sum_{w \in V_2} d_{M'}(w, u_0) - \sum_{w \in V_2} d_M(w, u_0). \tag{6}
 \end{aligned}$$

Note that $d_{M'}(w, u_0) > d_M(w, u_0)$ holds for every $w \in V_1$, and

$$\sum_{w \in V_2} d_{M'}(w, u_0) - \sum_{w \in V_2} d_M(w, u_0) = t + 1 - (s + 1) = t - s \geq 0.$$

Thus, the result follows by equality (6). ■

From Lemma 2.2, it immediately follows that

Proposition 2.1 *Suppose G is a connected graph on $n \geq 2$ vertices, or an isolated vertex.*

If $t \geq s \geq 1$, then $W(M_{t,t+s}) \leq W(M_{t+i,t+s})$, where $1 \leq i \leq s$.

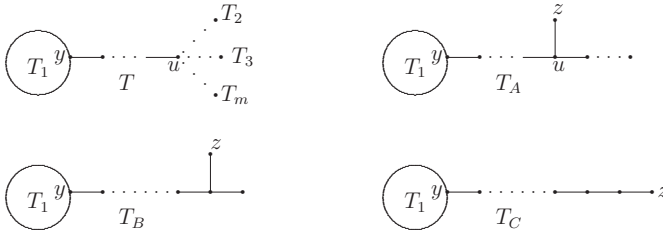


Fig. 4. The trees T , T_A , T_B and T_C .

For convenience, we introduce a transfer operation: $T \rightarrow T_A \rightarrow T_B \rightarrow T_C$, as shown in Fig. 4, where T is a tree of order n , u is an out-branching point of T , $d(u) = m$, and all the components T_1, T_2, \dots, T_m of $T - u$ except T_1 are paths.

Lemma 2.3 [12,16] *Let u be an out-branching point of a tree T of order n , $d(u) = m$ ($m \geq 3$), and let all components T_1, T_2, \dots, T_m of $T - u$ except T_1 be paths. Then,*

$$W(T) \leq W(T_A) \leq W(T_B) < W(T_C),$$

and $W(T) = W(T_A)$ (or $W(T_B)$) if and only if $T = T_A$ (or T_B).

Proof. By Lemma 2.1, it is easy to see that $W(T) \leq W(T_A)$ with the equality holding if and only if $T = T_A$. Moreover, Lemma 2.1 implies that $W(T_B) < W(T_C)$. Next we shall prove that $W(T_A) \leq W(T_B)$ with the equality holding if and only if $T_A = T_B$.

Let T_u denote the component of $T_A - y$, which contains u . Set $V_1 = V(T_u) \cup \{y\}$. Then, $V(T_A) \setminus V_1 = V(T_B) \setminus V_1$. Let $V_2 = V(T_A) \setminus V_1$. It is easy to see that

$$\begin{aligned} & \sum_{\{w,v\} \subseteq V(T_B)} d_{T_B}(w, v) - \sum_{\{w,v\} \subseteq V(T_A)} d_{T_A}(w, v) \\ &= \sum_{w \in V(T_B)} d_{T_B}(w, z) - \sum_{w \in V(T_A)} d_{T_A}(w, z) \\ &= \sum_{w \in V_1} d_{T_B}(w, z) - \sum_{w \in V_1} d_{T_A}(w, z) + \sum_{w \in V_2} (d_{T_B}(w, z) - d_{T_A}(w, z)). \end{aligned} \tag{7}$$

Note that $\sum_{w \in V_1} d_{T_B}(w, z) \geq \sum_{w \in V_1} d_{T_A}(w, z)$, and $d_{T_B}(w, z) \geq d_{T_A}(w, z)$ holds for every $w \in V_2$, then the conclusion follows from equality (7). ■

Lemma 2.4 [16,17] *Let T be a tree of order n , u_1, u_2, \dots, u_k be the all branching points of T , $d(u_i) = m_i$ ($i = 1, 2, \dots, k$), $T_{i1}, T_{i2}, \dots, T_{im_i}$ be the components of $T - u_i$, and the order of T_{ij} is equal to n_{ij} ($j = 1, 2, \dots, m_i; i = 1, 2, \dots, k$). Then,*

$$W(T) = C_{n+1}^3 - \sum_{i=1}^k \sum_{1 \leq p < q < r \leq m_i} n_{ip}n_{iq}n_{ir},$$

where $n_{i1} + n_{i2} + \dots + n_{im_i} = n - 1$, $i = 1, 2, \dots, k$.

By Lemma 2.4, we have

$$W(P_n) = C_{n+1}^3,$$

$$W(T(n; n - 3, 1, 1)) = C_{n+1}^3 - n + 3,$$

$$W(T(n; n - 4, 2, 1)) = C_{n+1}^3 - 2n + 8,$$

$$W(T(n; 1, 1; 1, 1)) = C_{n+1}^3 - 2n + 6,$$

$$W(T(n; n - 5, 3, 1)) = C_{n+1}^3 - 3n + 15,$$

$$W(T(n; n - 4, 1, 1, 1)) = W(T(n; 1, 1; 2, 1)) = C_{n+1}^3 - 3n + 11,$$

$$W(T(n; n - 6, 4, 1)) = C_{n+1}^3 - 4n + 24,$$

$$W(T(n; n - 5, 2, 2)) = C_{n+1}^3 - 4n + 20,$$

$$W(T(n; 1, 1; n - 5, 1)) = W(T(n; 1, 1; 3, 1)) = C_{n+1}^3 - 4n + 18,$$

$$W(T(n; 2, 1; 2, 1)) = C_{n+1}^3 - 4n + 16,$$

$$W(T(n; 1, 1; 1, 1, 1)) = C_{n+1}^3 - 4n + 14,$$

$$W(T(n; n - 7, 5, 1)) = C_{n+1}^3 - 5n + 35,$$

$$W(T(n; 1, 1; n - 6, 1)) = W(T(n; 1, 1; 4, 1)) = C_{n+1}^3 - 5n + 27,$$

$$W(T(n; n - 5, 2, 1, 1)) = W(T(n; 2, 1; 3, 1)) = W(T(n; 1, 1; 2, 2)) = C_{n+1}^3 - 5n + 23,$$

$$W(T_D) = C_{n+1}^3 - 5n + 21.$$

Thus, we have

Lemma 2.5 *If $n \geq 28$, then $W(P_n) > W(T(n; n - 3, 1, 1)) > W(T(n; n - 4, 2, 1)) > W(T(n; 1, 1; 1, 1)) > W(T(n; n - 5, 3, 1)) > W(T(n; n - 4, 1, 1, 1)) = W(T(n; 1, 1; 2, 1)) > W(T(n; n - 6, 4, 1)) > W(T(n; n - 5, 2, 2)) > W(T(n; 1, 1; n - 5, 1)) = W(T(n; 1, 1; 3, 1)) > W(T(n; 2, 1; 2, 1)) > W(T(n; 1, 1; 1, 1, 1)) > W(T(n; n - 7, 5, 1)) > W(T(n; 1, 1; n - 6, 1)) = W(T(n; 1, 1; 4, 1)) > W(T(n; n - 5, 2, 1, 1)) = W(T(n; 2, 1; 3, 1)) = W(T(n; 1, 1; 2, 2)) > W(T_D)$.*

By Lemma 2.4, it also follows that

$$W(T(n; 2, 1; 1, 1, 1)) = C_{n+1}^3 - 5n + 19,$$

$$W(T(n; 1, 1; n - 6, 2)) = W(T(n; n - 6, 3, 1, 1)) = W(T(n; 1, 1; 3, 2)) = C_{n+1}^3 - 7n + 39,$$

$$W(T(n; n - 6, 1; 1, 1, 1)) = C_{n+1}^3 - 7n + 35,$$

$$W(T(n; n - 7, 1; 1, 1, 1)) = C_{n+1}^3 - 8n + 46,$$

$$W(T(n; 1, 1; n - 7, 2)) = C_{n+1}^3 - 9n + 59,$$

$$W(T(n; n - 8, 6, 1)) = C_{n+1}^3 - 6n + 48,$$

$$W(T(n; 1, 1; n - 7, 1)) = W(T(n; 1, 1; 5, 1)) = C_{n+1}^3 - 6n + 38,$$

$$W(T(n; n - 6, 3, 2)) = C_{n+1}^3 - 6n + 36,$$

$$W(T(n; 2, 1; n - 6, 1)) = W(T(n; 2, 1; 4, 1)) = C_{n+1}^3 - 6n + 32,$$

$$W(T(n; 3, 1; 3, 1)) = C_{n+1}^3 - 6n + 30,$$

$$W(T(n; 2, 1; 2, 2)) = C_{n+1}^3 - 6n + 28,$$

$$W(T(n; n - 5, 1, 1, 1, 1)) = W(T(n; 1, 1; 2, 1, 1)) = C_{n+1}^3 - 6n + 26.$$

The next lemma can be obtained directly from the above equalities.

Lemma 2.6 *If $n \geq 28$, then (1) $W(T_D) > W(T(n; 2, 1; 1, 1, 1)) > W(T(n; 1, 1; n - 6, 2)) = W(T(n; n - 6, 3, 1, 1)) = W(T(n; 1, 1; 3, 2)) > W(T(n; n - 6, 1; 1, 1, 1)) > W(T(n; n - 7, 1; 1, 1, 1)) > W(T(n; 1, 1; n - 7, 2));$ (2) $W(T_D) > W(T(n; n - 8, 6, 1)) > W(T(n; 1, 1; n - 7, 1)) = W(T(n; 1, 1; 5, 1)) > W(T(n; n - 6, 3, 2)) > W(T(n; 2, 1; n - 6, 1)) = W(T(n; 2, 1; 4, 1)) > W(T(n; 3, 1; 3, 1)) > W(T(n; 2, 1; 2, 2)) > W(T(n; n - 5, 1, 1, 1, 1)) = W(T(n; 1, 1; 2, 1, 1)).$*

Lemma 2.7 *If $n \geq 28$ and T is a tree with exactly one branching point of degree $m \geq 5$, then $W(T) \leq W(T(n; n - 5, 1, 1, 1, 1)) < W(T_D)$.*

Proof. By hypothesis, $T = T(n; n_1, n_2, \dots, n_m)$. Without loss of generality, assume $n_1 \geq n_2 \geq \dots \geq n_m$. We prove the lemma by induction on m .

If $m = 5$, by Lemma 2.1 and Lemma 2.6 it follows that $W(T) = W(T(n; n_1, n_2, n_3, n_4, n_5)) \leq W(T(n; n_1 + n_5 - 1, n_2, n_3, n_4, 1)) \leq W(T(n; n_1 + n_4 + n_5 - 2, n_2, n_3, 1, 1)) \leq W(T(n; n_1 + n_3 + n_4 + n_5 - 3, n_2, 1, 1, 1)) \leq W(T(n; n - 5, 1, 1, 1, 1)) < W(T_D)$. Thus, this lemma holds for $m = 5$.

If $m \geq 6$, by Lemma 2.1, Lemma 2.6 and the induction hypothesis it follows that $W(T) = W(T(n; n_1, n_2, \dots, n_m)) < W(T(n; n_1 + n_m, n_2, \dots, n_{m-1})) \leq W(T(n; n - 5, 1, 1, 1, 1)) < W(T_D)$.

This completes the proof of this lemma. ■

Lemma 2.8 *Suppose $n \geq 28$, and T is a tree with only one branching point. If $T \notin \{T(n; n-3, 1, 1), T(n; n-4, 2, 1), T(n; n-5, 3, 1), T(n; n-4, 1, 1, 1), T(n; n-6, 4, 1), T(n; n-5, 2, 2), T(n; n-7, 5, 1), T(n; n-5, 2, 1, 1)\}$, then $W(T) < W(T_D)$.*

Proof. Suppose the degree of the unique branching point is m , then $T = T(n; n_1, \dots, n_m)$. Without loss of generality, assume $n_1 \geq \dots \geq n_m$. If $m \geq 5$, then the conclusion follows from Lemma 2.7. We consider the next two cases.

Case 1. $m = 3$.

If $n_3 \geq 2$, since $T \neq T(n; n-5, 2, 2)$, then $n_1 \geq n_2 \geq 3$. By Lemma 2.1 and Lemma 2.6 it follows that $W(T(n; n_1, n_2, n_3)) \leq W(T(n; n_1 + n_3 - 2, n_2, 2)) \leq W(T(n; n-6, 3, 2)) < W(T_D)$.

If $n_3 = 1$, since $T \notin \{T(n; n-3, 1, 1), T(n; n-4, 2, 1), T(n; n-5, 3, 1), T(n; n-6, 4, 1), T(n; n-7, 5, 1)\}$, then $n_1 \geq n_2 \geq 6$. By Lemma 2.1 and Lemma 2.6 it follows that $W(T) \leq W(T(n; n-8, 6, 1)) < W(T_D)$.

Case 2. $m = 4$. Since $T \neq T(n; n-4, 1, 1, 1)$, then $n_2 \geq 2$. Two subcases occur.

Subcase 1. $n_3 \geq 2$. Note that $n_1 \geq 3$ (by $n \geq 28$) and $n_2 \geq n_3 \geq 2$, by Lemma 2.1 and Lemma 2.6 it follows that $W(T(n; n_1, n_2, n_3, n_4)) \leq W(T(n; n_1 + n_4 - 1, n_2, n_3, 1)) < W(T(n; n_1 + n_4 - 1, n_2 + n_3 - 1, 1, 1)) \leq W(T(n; n-6, 3, 1, 1)) < W(T_D)$.

Subcase 2. $n_3 = 1$. Then, $n_4 = 1$. Since $T \neq T(n; n-5, 2, 1, 1)$, then $n_1 \geq n_2 \geq 3$, by Lemma 2.1 and Lemma 2.6 it follows that $W(T) = W(T(n; n_1, n_2, 1, 1)) \leq W(T(n; n-6, 3, 1, 1)) < W(T_D)$.

This completes the proof of this lemma. ■

Lemma 2.9 *Suppose $n \geq 28$, and $T = T(n; p_1, \dots, p_{r-1}; q_1, \dots, q_{t-1})$. If $t \geq 5$, then $W(T) < W(T(n; n-5, 1, 1, 1, 1)) < W(T_D)$.*

Proof. By Lemma 2.3, Lemmas 2.6-2.7 it follows that $W(T) < W(T(n; q_1, \dots, q_{t-1}, n - q_1 - \dots - q_{t-1} - 1)) \leq W(T(n; n-5, 1, 1, 1, 1)) < W(T_D)$. ■

Lemma 2.10 *Suppose $n \geq 28$, and $T = T(n; p_1, \dots, p_{r-1}; q_1, \dots, q_{t-1})$. If $t = r = 4$, then $W(T) < W(T_D)$.*

Proof. By hypothesis, $T = T(n; p_1, p_2, p_3; q_1, q_2, q_3)$. Without loss of generality, suppose that $q_1 + q_2 + q_3 \geq p_1 + p_2 + p_3$. We consider the next cases.

Case 1. $q_1 + q_2 + q_3 \geq 5$. By Lemma 2.1 we have $W(T) < W(T(n; q_1, q_2, q_3, n - q_1 - q_2 - q_3 - 1)) \leq W(T(n; q_1 + q_3 - 1, q_2, 1, n - q_1 - q_2 - q_3 - 1)) \leq W(T(n; q_1 + q_2 + q_3 - 2, 1, 1, n - q_1 - q_2 - q_3 - 1))$. Note that $q_1 + q_2 + q_3 - 2 \geq 3$ and $n - q_1 - q_2 - q_3 - 1 > p_1 + p_2 + p_3 \geq 3$, then $W(T(n; q_1 + q_2 + q_3 - 2, 1, 1, n - q_1 - q_2 - q_3 - 1)) \leq W(T(n; n - 6, 3, 1, 1)) < W(T_D)$ follows from Lemma 2.1 and Lemma 2.6.

Case 2. $q_1 + q_2 + q_3 = 4$. This implies that $T = T(n; p_1, p_2, p_3; 2, 1, 1)$. By Lemma 2.3 and Lemma 2.6 it follows that $W(T) = W(T(n; p_1, p_2, p_3; 2, 1, 1)) < W(T(n; 1, 1; 2, 1, 1)) < W(T_D)$.

Case 3. $q_1 + q_2 + q_3 = 3$. Then, $p_1 + p_2 + p_3 = 3$. By Lemma 2.1 and Lemma 2.6 it follows that $W(T) = W(T(n; 1, 1, 1; 1, 1, 1)) < W(T(n; 2, 1; 1, 1, 1)) < W(T_D)$. ■

Lemma 2.11 *Suppose $n \geq 28$, and $T = T(n; p_1, \dots, p_{r-1}; q_1, \dots, q_{t-1})$ with $t = 4, r = 3$. If $T \neq T(n; 1, 1; 1, 1, 1)$, then $W(T) < W(T_D)$.*

Proof. By hypothesis, $T = T(n; p_1, p_2; q_1, q_2, q_3)$. Two cases occur as follows.

Case 1. $q_1 + q_2 + q_3 \geq 5$. By Lemma 2.1, we have $W(T) < W(T(n; q_1, q_2, q_3, n - q_1 - q_2 - q_3 - 1)) \leq W(T(n; q_1 + q_3 - 1, q_2, 1, n - q_1 - q_2 - q_3 - 1)) \leq W(T(n; q_1 + q_2 + q_3 - 2, 1, 1, n - q_1 - q_2 - q_3 - 1))$. Note that $n - q_1 - q_2 - q_3 - 1 \geq p_1 + p_2 + 1 \geq 3$ and $q_1 + q_2 + q_3 - 2 \geq 3$, by Lemma 2.1 and Lemma 2.6 it follows that $W(T(n; q_1 + q_2 + q_3 - 2, 1, 1, n - q_1 - q_2 - q_3 - 1)) \leq W(T(n; n - 6, 3, 1, 1)) < W(T_D)$.

Case 2. $q_1 + q_2 + q_3 = 4$. This implies that $T = T(n; p_1, p_2; 2, 1, 1)$. By Lemma 2.3 and Lemma 2.6 it follows that $W(T(n; p_1, p_2; 2, 1, 1)) \leq W(T(n; 1, 1; 2, 1, 1)) < W(T_D)$.

Case 3. $q_1 + q_2 + q_3 = 3$. Since $T \neq T(n; 1, 1; 1, 1, 1)$, then $3 \leq p_1 + p_2 \leq n - 5$. We divide the proof into four subcases.

Subcase 1. $3 \leq p_1 + p_2 \leq 6$. By Lemma 2.1, it follows that $W(T) \leq W(T(n; p_2 + p_1 - 1, 1; 1, 1, 1))$. Recall that $n \geq 28$, by Propositions 2.1 and Lemma 2.6 we have $W(T(n; p_2 + p_1 - 1, 1; 1, 1, 1)) \leq W(T(n; 2, 1; 1, 1, 1)) < W(T_D)$.

Subcase 2. $7 \leq p_1 + p_2 \leq n - 7$. This implies that $n - p_1 - p_2 - 1 \geq 6$. By Lemma 2.1 and Lemma 2.6 it follows that $W(T) < W(T(n; p_1, p_2, n - p_1 - p_2 - 1)) \leq W(T(n; p_2 + p_1 - 1, 1, n - p_1 - p_2 - 1)) \leq W(T(n; n - 8, 6, 1)) < W(T_D)$.

Subcase 3. $p_1 + p_2 = n - 6$. By Lemma 2.1 and Lemma 2.6 it follows that $W(T) \leq W(T(n; n - 7, 1; 1, 1, 1)) < W(T_D)$.

Subcase 4. $p_1 + p_2 = n - 5$. By Lemma 2.1 and Lemma 2.6 it follows that $W(T) \leq W(T(n; n - 6, 1; 1, 1, 1)) < W(T_D)$.

By combining the above arguments, the result follows. ■

Lemma 2.12 *Suppose $n \geq 28$, and $T = T(n; p_1, \dots, p_{r-1}; q_1, \dots, q_{t-1})$ with $t = 3$, $r = 3$. If $T \notin \{T(n; 1, 1; 1, 1), T(n; 1, 1; 2, 1), T(n; 1, 1; n-5, 1), T(n; 1, 1; 3, 1), T(n; 2, 1; 2, 1), T(n; 1, 1; n-6, 1), T(n; 1, 1; 4, 1), T(n; 2, 1; 3, 1), T(n; 1, 1; 2, 2)\}$, then $W(T) < W(T_D)$.*

Proof. By hypothesis, $T = T(n; p_1, p_2; q_1, q_2)$. Without loss of generality, suppose $q_1 + q_2 \geq p_1 + p_2$. Since $T \notin \{T(n; 1, 1; 1, 1), T(n; 1, 1; 2, 1), T(n; 2, 1; 2, 1)\}$, then $4 \leq q_1 + q_2 \leq n - 4$. We consider the next cases.

Case 1. $q_1 + q_2 = 4$. Since $T \neq T(n; 1, 1; 3, 1)$ and $T \neq T(n; 1, 1; 2, 2)$, then $3 \leq p_1 + p_2 \leq 4$. Two subcases occur as follows.

Subcase 1. $p_1 + p_2 = 3$. Since $T \neq T(n; 2, 1; 3, 1)$, then $T = T(n; 2, 1; 2, 2)$. By Lemma 2.6, $W(T(n; 2, 1; 2, 2)) < W(T_D)$.

Subcase 2. $p_1 + p_2 = 4$. By Lemma 2.1 and Lemma 2.6, we have $W(T) \leq W(T(n; p_1, p_2; 3, 1)) \leq W(T(n; 3, 1; 3, 1)) < W(T_D)$.

Case 2. $q_1 + q_2 = 5$. Two subcases occur as follows.

Subcase 1. $q_1 = 3$, $q_2 = 2$. By Lemma 2.3 and Lemma 2.6, we have $W(T) = W(T(n; p_1, p_2; 3, 2)) \leq W(T(n; 1, 1; 3, 2)) < W(T_D)$.

Subcase 2. $q_1 = 4$, $q_2 = 1$. Since $T \neq T(n; 1, 1; 4, 1)$, then $3 \leq p_1 + p_2 \leq 5$. By Lemma 2.1, Proposition 2.1 and Lemma 2.6, we have $W(T) = W(T(n; p_1, p_2; 4, 1)) \leq W(T(n; p_1 + p_2 - 1, 1; 4, 1)) \leq W(T(n; 2, 1; 4, 1)) < W(T_D)$.

Case 3. $q_1 + q_2 = 6$. By Lemma 2.1, Lemma 2.3 and Lemma 2.6, it follows that $W(T) \leq W(T(n; p_1, p_2; 5, 1)) \leq W(T(n; 1, 1; 5, 1)) < W(T_D)$.

Case 4. $7 \leq q_1 + q_2 \leq n - 7$. Then, $n - q_1 - q_2 - 1 \geq 6$. By Lemma 2.1 and Lemma 2.6 it follows that $W(T) < W(T(n; q_1, q_2, n - q_1 - q_2 - 1)) \leq W(T(n; q_1 + q_2 - 1, 1, n - q_1 - q_2 - 1)) \leq W(T(n; n - 8, 6, 1)) < W(T_D)$.

Case 5. $q_1 + q_2 = n - 6$. By Lemma 2.1, Lemma 2.3 and Lemma 2.6 it follows that $W(T) \leq W(T(n; p_1, p_2; n - 7, 1)) \leq W(T(n; 1, 1; n - 7, 1)) < W(T_D)$.

Case 6. $q_1 + q_2 = n - 5$. Two subcases occur as follows.

Subcase 1. $q_2 = 1$. Then, $q_1 = n - 6$. Since $T \neq T(n; 1, 1; n - 6, 1)$, then $T = T(n; 2, 1; n - 6, 1)$. By Lemma 2.6, we have $W(T) = W(T(n; 2, 1; n - 6, 1)) < W(T_D)$.

Subcase 2. $q_2 \geq 2$. By Lemma 2.1, Lemma 2.3 and Lemma 2.6 it follows that $W(T) \leq W(T(n; p_1, p_2; n - 7, 2)) \leq W(T(n; 1, 1; n - 7, 2)) < W(T_D)$.

Case 7. $q_1 + q_2 = n - 4$. This implies that $p_1 = p_2 = 1$. Since $T \neq T(n; 1, 1; n - 5, 1)$, then $q_1 \geq q_2 \geq 2$. By Lemma 2.1 and Lemma 2.6, we have $W(T) = W(T(n; 1, 1; q_1, q_2)) \leq W(T(n; 1, 1; n - 6, 2)) < W(T_D)$.

This completes the proof. ■

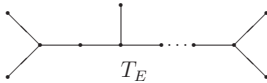


Fig. 5. The tree T_E .

Lemma 2.13 Suppose $n \geq 28$, and T is a tree of order n with exactly three branching points. If $T \neq T_D$, then $W(T) < W(T_D)$.

Proof. Let u_1, u_2, u_3 be the three branching points of T . Let u_1 be an in-branching point and u_2, u_3 be two out-branching points. Now suppose $d(u_1) = m, T_1, \dots, T_m$ be the components of $T - u_1$ and let them be paths except T_{m-1}, T_m , where the order of T_i is n_i for $1 \leq i \leq m$. By the definition of T it follows that $u_2 \in V(T_{m-1})$ and $u_3 \in V(T_m)$, which implies that $n_{m-1} \geq 3$ and $n_m \geq 3$. Without loss of generality, we suppose $n_{m-1} \geq n_m$. The next cases should be taken into account.

Case 1. $n_1 + n_2 + \dots + n_{m-2} \geq 2$. Note that $n_{m-1} \geq n_m \geq 3$, by Lemma 2.1 and Lemma 2.6 it follows that $W(T) < W(T(n; n_{m-1}, n_m, n_1 + \dots + n_{m-2})) \leq W(T(n; n - 6, 3, 2)) < W(T_D)$.

Case 2. $n_1 + n_2 + \dots + n_{m-2} = 1$. Then, $m = 3$ and $n_1 = 1$. Four subcases occur.

Subcase 1. $n_3 \geq 6$. Thus, $n_2 \geq 6$. By Lemma 2.1 and Lemma 2.6 it follows that $W(T) < W(T(n; n_2, n_3, 1)) \leq W(T(n; n - 8, 6, 1)) < W(T_D)$.

Subcase 2. $n_3 = 5$. Then, $n_2 = n - n_1 - n_3 - 1 = n - 7$. By Lemma 2.3 and Lemma 2.6 it follows that $W(T) < W(T(n; 1, 1; n - 7, 1)) < W(T_D)$.

Subcase 3. $n_3 = 4$. Then, $n_2 = n - n_1 - n_3 - 1 = n - 6$. By Lemma 2.3 it follows that $W(T) \leq W(T_E)$, where T_E is shown in Fig. 5. By Lemma 2.4, we have $W(T_E) = C_{n+1}^3 - 6n + 30$. Thus, $W(T_E) < W(T_D)$.

Subcase 4. $n_3 = 3$. Since $T \neq T_D$, by Lemma 2.3 it follows that $W(T) < W(T_D)$.

The result follows by combining the above arguments. ■

Lemma 2.14 Suppose $n \geq 28$, and T is a tree of order n with k branching points. If $k \geq 3$ and $T \neq T_D$, then $W(T) < W(T_D)$.

Proof. We prove the lemma by induction on k . By Lemma 2.13, it is true for $k = 3$.

Let $k \geq 4$, and T be a tree of order n with k branching points. Then T must have an out-branching point, and by Lemma 2.3, $W(T) < W(T_C)$, where T_C has $k - 1$ branching points. Thus, $W(T_C) \leq W(T_D)$ follows from the induction hypothesis and Lemma 2.13. This completes the proof. ■

The proof of Theorem 1.1. If T has exactly one branching point, then the result follows from Lemma 2.8. If T has exactly two branching points, by symmetry we may suppose that $T = T(n; p_1, \dots, p_{r-1}; q_1, \dots, q_{t-1})$, where $r \leq t$, $p_1 \geq \dots \geq p_{r-1}$ and $q_1 \geq \dots \geq q_{t-1}$. Then result follows from Lemmas 2.9-2.12. If T has exactly k ($k \geq 3$) branching points, then result follows from Lemmas 2.13-2.14.

By combining the above arguments, Theorem 1.1 follows. ■

Acknowledgements

The authors are grateful to Professor Hanyuan Deng for his valuable comments and suggestions, which led to an improvement of the original manuscript.

References

- [1] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17-20.
- [2] M. Randić, Novel molecular descriptor for structure-property studies, *Chem. Phys. Lett.* **211** (1993) 478-483.
- [3] D. E. Needham, I. C. Wei, P. G. Seybold, Molecular modeling of the physical properties of the alkanes, *J. Am. Chem. Soc.* **110** (1988) 4186-4194.
- [4] G. Rucker, C. Rucker, On the topological indices, boiling points, and cycloalkanes, *J. Chem. Inf. Comput. Sci.* **39** (1999) 788-802.
- [5] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta. Appl. Math.* **66** (2001) 211-249.

- [6] I. Gutman, Y. N. Yeh, S. L. Lee, J. C. Chen, Wiener numbers of dendrimers, *MATCH Comm. Math. Comput. Chem.* **30** (1994) 103-115.
- [7] B. C. Entringer, Distance in graphs: Trees, *J. Combin. Math. Combin. Comput.* **24** (1997) 65-84.
- [8] S. Klavžar, P. Zigert, I. Gutman, An algorithm for the calculation of the hyper-Wiener index of benzenoid hydrocarbons, *Comput. Chem.* **24** (2000) 229-233.
- [9] X. Li, A. F. Jalbout, Bond order weighted hyper-Wiener index, *J. Mol. Structure (Theochem)* **634** (2003) 121-125.
- [10] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, The hyper-Wiener index of graph operations, *Math. Appl.* **56** (2008) 1402-1407.
- [11] I. Gutman, A property of the Wiener number and its modifications, *Indian J. Chem.* **36A** (1997) 128-132.
- [12] M. H. Liu, B. L. Liu, Trees with the seven smallest and fifteen greatest hyper-Wiener indices, *MATCH Comm. Math. Comput. Chem.* **63** (2010) 151-170.
- [13] M. H. Liu, X. Z. Tan, The first to $(k + 1)$ -th smallest Wiener (hyper-Wiener) indices of connected graphs, *Kragujevac J. Math.* preprinted.
- [14] I. Gutman, J. Rada, O. Araujo, The Wiener index of starlike trees and a related partial order, *MATCH Comm. Math. Comput. Chem.* **42** (2000) 145-154.
- [15] X. Guo, H. Dong, Ordering trees by their Wiener indices, *J. Xiamen Univ. (Nat. Sci.)* **44** (2005) 297-298.
- [16] H. Y. Deng, The trees on $n \geq 9$ vertices with the first to seventeenth greatest Wiener indices are chemical trees, *MATCH Comm. Math. Comput. Chem.* **57** (2007) 393-402.
- [17] J. K. Doyle, J. E. Graver, Mean distance in a graph, *Discrete Math.* **7** (1977) 147-154.