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The trees on $n \geq 9$ vertices with the first to seventeenth greatest Wiener indices are chemical trees[1]

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Abstract

The Wiener index W is the sum of distances between all pairs of vertices of a connected graph. An order relation of trees is obtained with regard to the Wiener index. Based on this order relation, we determine the trees on $n \geq 9$ vertices with the first to seventeenth greatest Wiener indices, and they are chemical trees.

1 Introduction

The Wiener index is a graph invariant based on distances in a graph. It is denoted by $W(G)$ and defined as the sum of distances between all pairs of vertices in a connected graph G:

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

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

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The Wiener index is much studied in the chemical literature, since Harold Wiener [1], in 1947, was the first to consider it. Wiener's original definition was slightly different, yet equivalent to (1). The definition of the Wiener index, such as in Eq. (1), was first given by Hosoya [2].

Starting from the middle of the 1970s, the Wiener index gained much popularity and, since then, new results related to it are constantly being reported. For a review, historical details and further bibliography on the chemical applications of the Wiener index see [5,6,7,11,12,13]. Results on the Wiener index of trees and hexagonal systems were summarized in [3,4,8,9,10]. Specifically, the trees with maximum or minimum Wiener index were determined. Of course, ordering trees by their Wiener indices is interesting and valuable. Gutman et al. [16] gave a partial order among the starlike trees and the trees with the first up to fifteenth smallest Wiener indices among trees of order n are determined by Guo and Dong [14]. In this paper we obtain some order relations for trees, using the formula for calculating the Wiener index based on branching vertices, and determine the trees of order n with the first to seventeenth greatest Wiener indices, all of these trees are chemical trees.

There are many methods for computing the Wiener index of a tree. The following Lemma 1 gives a formula discovered by Doyle and Graver [15], which is suitable for calculating the Wiener index of trees with few branching points.

Recall that a vertex u of a tree T is said to be a branching point of T if $d_T(u) \geq 3$. Furthermore, u is said to be a out-branching point if at most one of the components of $T - u$ is not a path; otherwise, u is a in-branching point of T.

Note that any tree which is not a path has a out-branching point.

Lemma 1.([15]) Let T be a tree of order n, $u_1, u_2, \cdots, u_k$ be all the branching points of T, $d_T(u_i) = m_i$ $(i = 1, 2, \ldots, k)$, $T_{i1}, T_{i2}, \ldots, T_{im_i}$ be the components of $T - u_i$, and $n(T_{ij}) = n_{ij}$ $(j = 1, 2, \cdots, m_i; i = 1, 2, \ldots, k)$. Then

$$W(T) = C_{n+1}^3 - \sum_{i=1}^{k} \sum_{1 \leq p < q < r \leq m_i} n_{ip}\, n_{iq}\, n_{ir} \tag{2}$$

where $n_{i1} + n_{i2} + \cdots + n_{im_i} = n - 1$,$i = 1, 2, \ldots, k$ and $C_{n+1}^3 = \begin{pmatrix} n+1 \\ 3 \end{pmatrix}$.

2 Comparison of the Wiener indices of starlike trees of order n

Let $T(n; n_1, n_2, \ldots, n_m)$ denote the starlike tree of order n obtaining by inserting $n_1 - 1, n_2 - 1, \ldots, n_m - 1$ vertices into m edges of the star S_{m+1} of order $m+1$ respectively, where $n_1+n_2+\cdots+n_m=n-1$.

Note that any tree with only one branching point is a starlike tree, and the starlike tree $T(n;n_1,n_2,\ldots,n_m)$ has a branching point with degree m. By Eq. (2) of Lemma 1, we have

$$\begin{aligned} W(T(n;n_1,n_2,\ldots,n_m)) &= C_{n+1}^3 - \sum_{1\le i<j<k\le m} n_i n_j n_k \\ &= C_{n+1}^3 - f(n_1,n_2,\ldots,n_m) \end{aligned} \tag{3}$$

Here, the function $f(x_1,x_2,\ldots,x_n)$ is defined as follows:

$$f(x_1,x_2,\ldots,x_n)=\sum_{1\le i<j<k\le n} x_i\,x_j\,x_k$$

where $x_1,x_2,\ldots,x_n$ are non-negative integers, $n\ge 3$.

Note that $f(x_1,x_2,\ldots,x_n)$ is symmetric, i.e.,

$$f(x_1,x_2,\ldots,x_n)=f(x_{i_1},x_{i_2},\ldots,x_{i_n})$$

for any permutation $x_{i_1},x_{i_2},\ldots,x_{i_n}$ of $x_1,x_2,\ldots,x_n$.

Lemma 2. If $x_i\ge x_j\ge 1$, $1\le i\le n$, $1\le j\le n$, $i\ne j$. Then

$$f(x_1,\ldots,x_i,\ldots,x_j,\ldots,x_n)>f(x_1,\ldots,x_i+1,\ldots,x_j-1,\ldots,x_n).$$

Proof. Without loss of the generality, suppose that $i=1$ and $j=n$.

$$\begin{aligned} & f(x_1,x_2,\ldots,x_n)-f(x_1+1,x_2,\ldots,x_n-1) \\ = & \sum_{1\le i<j<k\le n} x_ix_jx_k - \sum_{1<i<j<k<n} x_ix_jx_k - \sum_{1<j<k<n}(x_1+1)x_jx_k \\ & - \sum_{1<i<j<n} x_ix_j(x_n-1) - \sum_{1<j<n}(x_1+1)x_j(x_n-1) \\ = & -\sum_{1<j<k<n} x_jx_k + \sum_{1<i<j<n} x_ix_j + \sum_{1<j<n}(x_1x_n-(x_1+1)(x_n-1))x_j \\ = & (x_1+1-x_n)\sum_{1<j<n} x_j > 0. \end{aligned}$$

So, $f(x_1,x_2,\ldots,x_n)>f(x_1+1,x_2,\ldots,x_n-1)$.

From Lemma 2 and Eq. (3), the following result is immediate.

Theorem 3. If $n_1\ge n_2\ge\cdots\ge n_m\ge 1$, then
(i) $W(T(n;n_1+1,n_2,\ldots,n_m-1)>W(T(n;n_1,n_2,\ldots,n_m)$;
(ii) $W(T(n;\ldots,n_i+1,\ldots,n_j-1,\ldots)>W(T(n;\ldots,n_i,\ldots,n_j,\ldots)$.

And, the tree with maximum Wiener index among the starlike trees with order n and a branching point of degree m is $T(n;n-m,1,\ldots,1)$; the tree with maximum Wiener index among the starlike trees of order n is $T(n; n-3, 1, 1)$.

We write $T_1 \succeq T_2$ ($T_1 \succ T_2$) if $W(T_1) \geq W(T_2)$ ($W(T_1) > W(T_2)$) for two trees T_1 and T_2. Using Theorem 3, some relations for ordering the starlike trees of order n and a branching point of degree m are obtained as follows:

(i) $m = 3$.

$T(n; n-3, 1, 1) \succ T(n; n-4, 2, 1) \succ T(n; n-5, 3, 1) \succ T(n; n-6, 4, 1) \succ T(n; n-5, 2, 2) \succ T(n; n-7, 5, 1) \succ T(n; n-8, 6, 1) \succ T(n; n-6, 3, 2) \succ T(n; n-9, 7, 1) \succ T(n; n-10, 8, 1) \succ T(n; n-7, 4, 2) \succ T(n; n-11, 9, 1) \succ T(n; n-7, 3, 3) \succ T(n; n-12, 10, 1) \succ T(n; n-8, 5, 2) \succ \cdots$.

(ii) $m = 4$.

$T(n; n-4, 1, 1, 1) \succ T(n; n-5, 2, 1, 1) \succ T(n; n-6, 3, 1, 1) \succ T(n; n-6, 2, 2, 1) \succ T(n; n-7, 4, 1, 1) \succ T(n; n-7, 3, 2, 1) \succ T(n; n-7, 2, 2, 2) \succ \cdots$.

(iii) $m = 5$.

$T(n; n-5, 1, 1, 1, 1) \succ T(n; n-6, 2, 1, 1, 1) \succ T(n; n-7, 3, 1, 1, 1) \succ T(n; n-7, 2, 2, 1, 1) \succ \cdots$.

And

$W(T(n; n-4, 1, 1, 1)) = C_{n+1}^3 - 3n + 11$
$W(T(n; n-5, 2, 1, 1)) = C_{n+1}^3 - 5n + 23$
$W(T(n; n-6, 3, 1, 1)) = C_{n+1}^3 - 7n + 32$
$W(T(n; n-6, 2, 2, 1)) = C_{n+1}^3 - 8n + 36$
$W(T(n; n-7, 4, 1, 1)) = C_{n+1}^3 - 9n + 59$
$W(T(n; n-7, 3, 2, 1)) = C_{n+1}^3 - 11n + 71$
$W(T(n; n-7, 2, 2, 2)) = C_{n+1}^3 - 12n + 76$
$W(T(n; n-5, 1, 1, 1, 1)) = C_{n+1}^3 - 6n + 26$
$W(T(n; n-6, 2, 1, 1, 1)) = C_{n+1}^3 - 9n + 47$
$W(T(n; n-7, 3, 1, 1, 1)) = C_{n+1}^3 - 12n + 74$
$W(T(n; n-7, 2, 2, 1, 1)) = C_{n+1}^3 - 13n + 79$
$W(T(n; n-6, 1, 1, 1, 1, 1)) = C_{n+1}^3 - 10n + 50$
$W(T(n; n-7, 2, 1, 1, 1, 1)) = C_{n+1}^3 - 14n + 82$.

Then, the ordering of the starlike trees of order n is:

$$\begin{aligned}
&T(n; n-3, 1, 1) \succ T(n; n-4, 2, 1) \succ T(n; n-5, 3, 1) \succ T(n; n-4, 1, 1, 1) \\
&\succ T(n; n-6, 4, 1) \succ T(n; n-5, 2, 2) \succ T(n; n-7, 5, 1) \succ T(n; n-5, 2, 1, 1) \\
&\succ T(n; n-8, 6, 1) \succ T(n; n-6, 3, 2) \succeq T(n; n-5, 1, 1, 1, 1) \succ T(n; n-9, 7, 1) \\
&\succ T(n; n-6, 3, 1, 1) \succ T(n; n-10, 8, 1) \succ T(n; n-7, 4, 2) \succ T(n; n-6, 2, 2, 1) \\
&\succ T(n; n-11, 9, 1) \succ T(n; n-7, 3, 3) \succ T(n; n-7, 4, 1, 1) \succ T(n; n-6, 2, 1, 1, 1) \\
&\succ T(n; n-12, 10, 1) \succ T(n; n-8, 5, 2) \cdots .
\end{aligned} \tag{4}$$

3 Trees of order n with the first to seventeenth greatest Wiener indices

For convenience, we introduce a transfer operation: $T \to T_A \to T_B \to T_C$, as shown in Figure 1, where T is a tree of order n, u is an out-branching point of T, $d_T(u) = m$, and all the components $T_1, T_2, \ldots, T_m$ of $T - u$ except T_1 are paths.

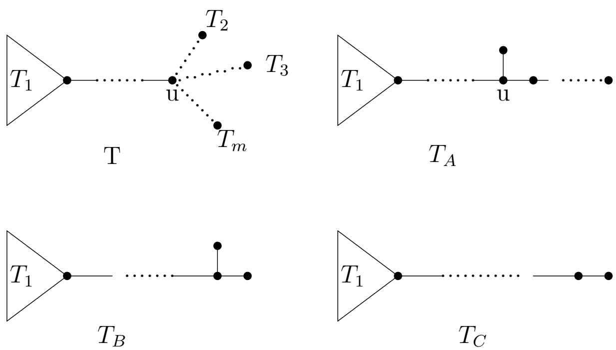

Figure 1.

Lemma 4. Let u be an out-branching point of a tree of order n, $d_T(u) = m$, and let all components $T_1, T_2, \ldots, T_m$ of $T - u$ except T_1 be paths. Then

$$W(T) \le W(T_A) \le W(T_B) < W(T_C)$$

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

Proof. Let $u_1, u_2, \ldots, u_k$ and u be all the branching points. Then $u_1, u_2, \ldots, u_k$ are in T_1 since $T_2, \ldots, T_m$ are paths. Suppose that $d_T(u_i) = m_i$ and $T_{i1}, T_{i2}, \ldots, T_{im_i}$ are all the components of $T - u_i$, $n(T_{ij}) = n_{ij}$, $j = 1, 2, \ldots, m_i$, $i = 1, 2, \ldots, k$; $n(T_t) = n_t$, $t = 1, 2, \ldots, m$.

By Lemma 1, we have that

$$\begin{aligned} W(T) &= C_{n+1}^3 - \sum_{i=1}^{k} \sum_{1 \le p < q < r \le m_i} n_{ip} n_{iq} n_{ir} - \sum_{1 \le i < j < k \le m} n_i n_j n_k \\ &= W_0 - f(n_1, n_2, \ldots, n_m) \end{aligned}$$

where $W_0 = C_{n+1}^3 - \sum_{i=1}^{k} \sum_{1 \le p < q < r \le m_i} n_{ip} n_{iq} n_{ir}$.

Without loss of generality, we can assume that $n_2 \ge n_3 \ge \cdots \ge n_m \ge 1$.

From Lemma 2, we have

$$\begin{aligned} &f(n_1, n_2, n_3, \ldots, n_{m-1}, n_m) > f(n_1, n_2 + 1, n_3, \ldots, n_{m-1}, n_m - 1) > \cdots \\ &> f(n_1, n_2 + n_m - 1, n_3, \ldots, n_{m-1}, 1) > f(n_1, n_2 + n_m, n_3, \ldots, n_{m-1}, 0) > \cdots \\ &> f(n_1, n_2 + n_3 + \ldots + n_m - 1, 1, 0, \ldots, 0). \end{aligned}$$

So, $W(T) \leq W(T_A)$ with the equality if and only if $T = T_A$ since $W(T_A) = W_0 - f(n_1, n_2 + n_3 + \cdots + n_m - 1, 1, 0, \ldots, 0)$.

Also, $W(T_A) \leq W(T_B)$ with equality if and only if $T_B = T_A$ since $W(T_A) = W_0 - n_1(n_2 + n_3 + \cdots + n_m - 1) = W_0 - n_1(n - 2 - n_1) \leq W_0 - (n-3)$.

Finally, $W(T_B) < W_0 = W(T_C)$.

Remark. From Lemma 4, the Wiener index increases after the transfer operations: $T \to T_A \to T_B \to T_C$. Repeating the above operations, any tree T with an out-branching point must be changed into a tree T_B in which any out-branching point u has degree 3 and the components of $T_B - u$, except one, have only one vertex; Also, T can be changed into a tree T_C with fewer branching points than T. So the path P_n has the greatest Wiener index among the trees of order n.

If a tree has exactly two branching points, then both branching points must be out-branching points. From Lemma 4 the following result is immediate.

Theorem 5. Let T be a tree of order n with exactly two branching points, then $W(T) \leq W(T(n;1,1;1,1)$ with equality if and only if $T = T(n;1,1;1,1)$, where $T(n;1,1;1,1)$ is shown in Figure 2.

Now, we consider the ordering of trees with exactly two branching points. Let T be a tree of order n with exactly two branching points u_1 and u_2, $d_T(u_1) = r$, $d_T(u_2) = t$. The orders of $r-1$ components, which are paths, of $T - u_1$ are $p_1, \ldots, p_{r-1}$, the order of the component which is not a path of $T - u_1$ is $p_r = n - (p_1 + \cdots + p_{r-1}) - 1$. The orders of $t-1$ components, which are paths, of $T - u_2$ are $q_1, \ldots, q_{t-1}$, the order of the component which is not a path of $T - u_2$ is $q_t = n - (q_1 + \cdots + q_{t-1}) - 1$. We denote this tree by $T(n; p_1, \ldots, p_{r-1}; q_1, \ldots, q_{t-1})$, where $r \leq t$, $p_1 \geq p_2 \geq \cdots \geq p_{r-1}$ and $q_1 \geq q_2 \geq \cdots \geq q_{t-1}$. By Lemma 1, we have

$$\begin{aligned} W(T(n; p_1, \ldots, p_{r-1}; q_1, \ldots, q_{t-1})) &= C_{n+1}^3 - \sum_{1 \leq i < j < k \leq r} p_i p_j p_k - \sum_{1 \leq i < j < k \leq t} q_i q_j q_k \\ &= C_{n+1}^3 - f(p_1, p_2, \ldots, p_r) - f(q_1, q_2, \ldots, q_t). \qquad (5) \end{aligned}$$

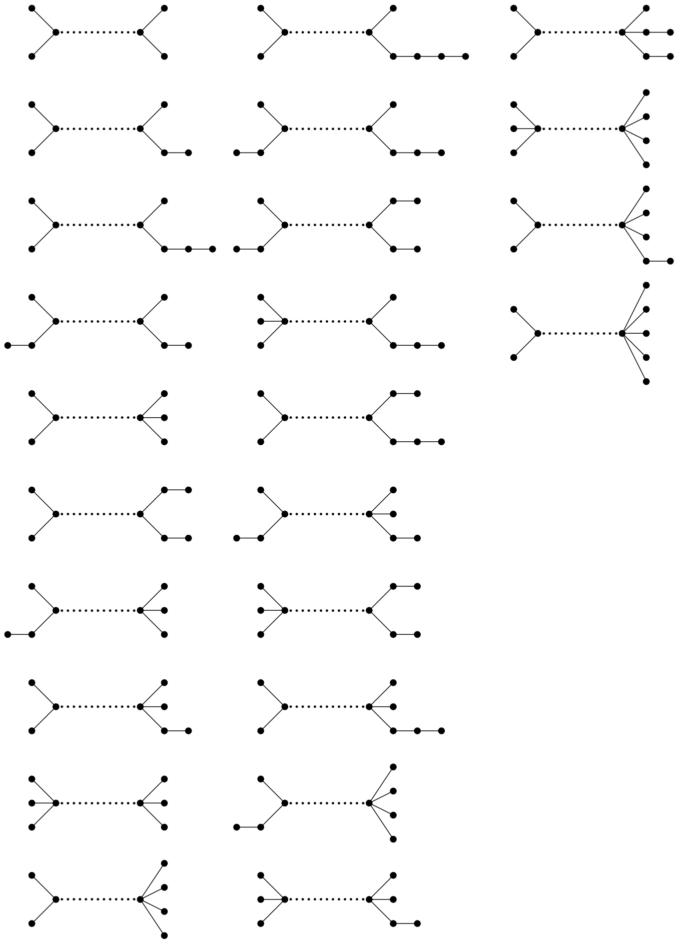

Figure 2.

If $p_1+\cdots+p_{r-1}+q_1+\cdots+q_{t-1} \geq 8$, then $W(T(n; p_1, \ldots, p_{r-1}; q_1, \ldots, q_{t-1})) \leq W(T(n; 1, 1; 5, 1)) = C_{n+1}^3 - 6n + 38$ by the transfer operation $T \to T_A \to T_B$.

For $p_1+\cdots+p_{r-1}+q_1+\cdots+q_{t-1} \leq 7$, the trees $T(n; p_1, \ldots, p_{r-1}; q_1, \ldots, q_{t-1})$ are shown in Figure 2. From Lemma 4 and Equation (4), the ordering of these trees is:

$$\begin{aligned}
&T(n;1,1;1,1) \succ T(n;1,1;2,1) \succ T(n;1,1;3,1) \succ T(n;2,1;2,1) \succ \\
&T(n;1,1;1,1,1) \succ T(n;1,1;4,1) \succ T(n;1,1;2,2) \succeq T(n;2,1;3,1) \succ \\
&T(n;2,1;1,1,1) \succ T(n;2,1;2,2) \succ T(n;1,1;2,1,1) \succ T(n;3,1;1,1,1) \succ \\
&T(n;1,1,1;1,1,1) \succ T(n;1,1;3,2) \succ T(n;2,1;2,1,1) \succeq T(n;2,2;1,1,1) \succ \\
&T(n;1,1;1,1,1,1) \succ T(n;1,1;3,1,1) \succ T(n;2,1;1,1,1,1) \succeq \\
&T(n;1,1,1;2,1,1) \succ T(n;1,1;2,2,1) \succ T(n;1,1,1;1,1,1,1) \succ \\
&T(n;1,1;2,1,1,1) \succ T(n;1,1;1,1,1,1,1) \succ \cdots .
\end{aligned} \tag{6}$$

For the trees with at least three branching points, we have the following two results.

Theorem 6. Let T be a tree of order n with exactly three branching points, then $W(T) \leq W(T_E)$ with equality if and only if $T = T_E$, where T_E is the tree of order n as shown in Figure 3.

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 out-branching points. By Lemma 4, we have

$$W(T) \leq W(T_D)$$

where T_D is the tree of order n with three branching points as shown in Figure 3 and u_1 is its unique in-branching point.

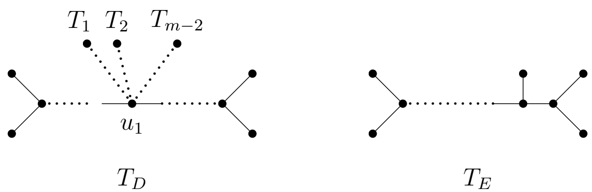

Figure 3.

Let $d_{T_D}(u) = m$, $T_1, T_2, \ldots, T_m$ be the components of $T_D - u_1$ and let they be paths except T_1, T_2, $n(T_i) = n_i$, $i = 1, 2, \ldots, m$. By Lemma 1,

$$
\begin{aligned}
W(G_1) &= C_{n+1}^3 - 2(n-3) - \sum_{1\le i<j<k\le m} n_i n_j n_k \\
&= C_{n+1}^3 - 2(n-3) - f(n_1, n_2, \ldots, n_m) \\
&\le C_{n+1}^3 - 2(n-3) - f(n_1, n_2, n-n_1-n_2-1, 0, \ldots, 0) \\
&= C_{n+1}^3 - 2(n-3) - n_1 n_2 (n-n_1-n_2-1) \\
&\le C_{n+1}^3 - 2(n-3) - 3n_2(n-4-n_2) \qquad (n_2 \text{ is given and } n_1 \ge 3) \\
&\le C_{n+1}^3 - 2(n-3) - 3(n-5) \quad (\text{since } n_2 \ge 3 \text{ and } n-4-n_2 \ge 1) \\
&= W(T_E)
\end{aligned}
$$

So, $W(T) \le W(T_E)$ and the equality holds if and only if $n - n_1 - n_2 - 1 = 1$ and $n_1 = 3$(or $n_2 = 3$), i.e, $T = T_E$.

Theorem 7. If T is a tree of order n with k branching points, $k \ge 3$, then $W(T) \le W(T_E)$.

Proof. We prove the theorem by induction on the number k of branching points.

It is true for $k = 3$ from Theorem 6.

Let $k \ge 4$ and T be a tree of order n with k branching points. Then T must have an out-branching point u, and by Lemma 4, $W(T) \le W(T_C)$, where T_C has $k-1$ branching points. $W(T_C) \le W(T_E)$ by the inductive hypothesis. So, $W(T) \le W(T_E)$.

Finally, we give the trees of order n with the first to seventeenth largest Wiener indices. They all are chemical trees. Since $W(T_E) = C_{n+1}^3 - 5n + 21$, $W(T(n; n-5, 2, 1, 1)) = C_{n+1}^3 - 5n + 35$ and $W(T(n; n-8, 6, 1)) = C_{n+1}^3 - 6n + 48$, $W(T(n; 2, 1; 3, 1)) = C_{n+1}^3 - 5n + 23$ and $W(T(n; 2, 1; 1, 1, 1)) = C_{n+1}^3 - 5n + 19$, from Eqs. (4) and (6), we have the ordering of trees with n vertices.

Theorem 8. Let $n \ge 9$. Then $T(n; n-3, 1, 1) \succ T(n; n-4, 2, 1) \succ T(n; 1, 1; 1, 1) \succ T(n; n-5, 3, 1) \succ T(n; n-4, 1, 1, 1) \succeq T(n; 1, 1; 2, 1) \succ T(n; n-6, 4, 1) \succ T(n; n-5, 2, 2) \succ T(n; 1, 1; 3, 1) \succ T(n; 2, 1; 2, 1) \succ T(n; 1, 1; 1, 1, 1) \succ T(n; n-7, 5, 1) \succ T(n; 1, 1; 4, 1) \succ T(n; n-5, 2, 1, 1) \succeq T(n; 1, 1; 2, 2) \succeq T(n; 2, 1; 3, 1) \succ T_E \cdots$.

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