On the extremal Wiener polarity index of trees with a given diameter

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Abstract

The Wiener polarity index $W_p(G)$ of a graph $G = (V, E)$ is the number of unordered pairs of vertices $\{u, v\}$ of $G$ such that the distance $d_G(u, v)$ between $u$ and $v$ is 3. In this paper, we characterize the extremal trees with respect to the index among all trees of order $n$ and diameter $k$.

1 Introduction

Let $G = (V, E)$ be a connected (molecular) graph. The distance between two vertices $u$ and $v$ in $G$, denoted by $d_G(u, v)$, is the length of a shortest path between $u$ and $v$ in $G$. The Wiener polarity index of $G$, denoted by $W_P(G)$, is defined by

$$W_P(G) = |\{\{u, v\}|d_G(u, v) = 3, u, v \in V\}|$$

which is the number of unordered pairs of vertices $\{u, v\}$ of $G$ such that $d_G(u, v) = 3$.

In organic compounds, this number is the number of pairs of carbon atoms which are separated by three carbon-carbon bonds. The name ”Wiener polarity index” for the quantity defined in the equation above is introduced by Harold Wiener [1] for acyclic molecules in a slightly different manner. In the same paper, Wiener also introduced another index for acyclic molecules, called Wiener index, and now it is popular in chemical and mathematical literatures. The reader is referred to the review [2] for further details on the Wiener index, as well to the recent papers [3–10]. However,

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it seems that less attention has been paid for the Wiener polarity index \( W_P(G) \). In [11], \( W_P(G) \) was used to demonstrate quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons. Hosoya [12] found a physico-chemical interpretation of \( W_P(G) \). Very recently, Du, Li and Shi [13] described a linear time algorithm APT for computing the index of trees, and characterized the trees maximizing the index among all trees of given order.

In this paper, we will characterize the extremal trees with respect to the index among all trees of order \( n \) and diameter \( k \).

2 The minimal Wiener polarity index among all trees of order \( n \) and diameter \( k \)

In this section, we will characterize the minimal tree with respect to the Wiener polarity index among all trees of order \( n \) and diameter \( k \). Since \( W_p(G) = 0 \) for any graph \( G \) with diameter \( k \leq 2 \), we assume \( k \geq 3 \) in the following. First, we give some formulas for computing the Wiener polarity index of trees, where (ii) is direct by the definition.

**Lemma 1.** Let \( T = (V, E) \) be a tree. Then

\[
\begin{align*}
(i)([13]) & \quad W_p(T) = \sum_{uv \in E} (d_T(u) - 1)(d_T(v) - 1); \\
(ii) & \quad W_p(T) = \frac{1}{2} \sum_{u \in V} |D_3(T; u)|
\end{align*}
\]

where \( d_T(v) \) is the degree of \( v \) in \( T \) and \( D_3(T; u) = \{ x \in V | d_T(x, u) = 3 \} \).

The following lemma shows that the Wiener polarity index of a tree \( T \) with diameter \( k \geq 3 \) increases at least one whenever a new vertex is added to \( T \).

**Lemma 2.** Let \( T \) be a tree with order \( n \) and diameter \( k \geq 3 \). \( T' \) is a tree with order \( n + 1 \) obtained by adding a pendant edge \( xy \) to \( T \) such that the diameter of \( T' \) is also \( k \), where \( x \in T \) and \( y \notin T \). Then

\[
W_p(T') \geq W_p(T) + 1
\]

with equality if and only if one of the vertices adjacent to \( x \) has degree 2 and the others are pendant vertices.

**Proof.** Let \( x_1, x_2, \ldots, x_r \) be all vertices adjacent to \( x \) in \( T \). Then at least one of them has degree greater than 1 since the diameter of \( T \) is \( k \geq 3 \). By Lemma 1, we
have

\[ W(T') - W(T) = \sum_{uv \in E(T')} (d_{T'}(u) - 1)(d_{T'}(v) - 1) - \sum_{uv \in E(T)} (d_T(u) - 1)(d_T(v) - 1) \]

\[ = \sum_{i=1}^r (d_T(x_i) - 1) \geq 1 \]

with equality if and only if one of \( d_T(x_1), d_T(x_2), \ldots, d_T(x_r) \) is 2 and the others are 1.

\[ \square \]

Figure 1. The tree \( T(r, t) \), where \( r + t = n - k - 1 \).

Let \( T(r, t) \) be the tree with order \( n \) and diameter \( k \geq 3 \) depicted in Figure 1, where \( r \geq t \geq 0 \) and \( r + t = n - k - 1 \). Then \( T(r, t) \) can be obtained from a path \( P_{k+1} = v_0v_1 \cdots v_k \) of length \( k \) by adding \( r + t \) pendant edges. If \( k > 3 \), then \( d(v_2) = 2 \) and from Lemma 2, we have

\[ W_p(T(r, t)) = W_p(P_{k+1}) + r + t = k - 2 + n - k - 1 = n - 3 \]

Note that any tree \( T \) different from the path \( P_{k+1} \) with order \( n \) and diameter \( k \) can be obtained from \( P_{k+1} \) by adding pendant edges step by step. When \( k = 3 \), it is easy to show that \( W_p(T) \geq n - 3 \) with equality if and only if \( T = T(n - 1, 0) \). When \( k > 3 \), we can ensure that the equality holds at each step for adding pendant edges. So, we can give the minimal Wiener polarity index of all trees with order \( n \) and diameter \( k > 2 \), and characterize the extremal tree by Lemma 2.

**Theorem 3.** Let \( T \) be a tree with order \( n \) and diameter \( k \). Then

\[ W_p(T) \geq n - 3 \]

with equality if and only if \( T = T(r, t) \) for \( k > 3 \) and \( T(n - 4, 0) \) for \( k = 3 \).

### 3 The maximal Wiener polarity index among all trees of order \( n \) and diameter \( k \)

In this section, we will determine the maximal Wiener polarity index among all trees of order \( n \) and diameter \( k \), and characterize the extremal tree. Note that the
trees with the maximal Wiener polarity index among all trees of order $n$ and diameter $k = 3, 4$ were characterized in [13], we only consider $k \geq 5$ in the following.

To characterize the trees with the maximal Wiener polarity index, an operation on trees is introduced in [13]. Let $T$ be a tree with order $n$ and diameter $k \geq 4$, $P_L(T) = v_0v_1v_2v_3v_4 \cdots v_k$ is a longest path of $T$. Then $T \odot v_0$ is the tree obtained from $T$ by deleting the edge $v_0v_1$ and adding a new edge $v_0v_3$ depicted in Figure 2.

**Lemma 4**([13]). Let $T$ be a tree with a longest path $P_L(T) = v_0v_1v_2v_3v_4 \cdots v_k$, and $k \geq 4$. Then

(i) $W_p(T) < W_p(T \odot v_0)$ for $k \geq 5$;

(ii) $W_p(T) \leq W_p(T \odot v_0)$ for $k = 4$.

In the following, we will show that there is a capillary tree $T'$ such that $W_p(T) \leq W_p(T')$ for any tree $T$ with diameter $k \geq 5$. 

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**Figure 2.** An operation on a tree $T$.

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**Figure 3.** A tree $T$ with order $n$ and diameter $k$.

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**Figure 4.** The tree $T_1 = T \odot U_1$. 

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(I) Let $T$ be a tree with a longest path $P_L(T) = v_0v_1v_2v_3v_4\cdots v_k$ and $k \geq 5$, depicted in Figure 3. If $U_1 = \{x|x \in V(T) - \{v_0, v_k\}, d_T(x, v_k) = k$ or $d_T(x, v_0) = k\} = \{x_1, x_2, \cdots, x_r\} \neq \emptyset$, then $T_1 = T \circ U_1 = (((T \circ x_1) \circ x_2)\cdots) \circ x_r$, depicted in Figure 4. By repeating Lemma 4, we have $W_p(T) < W_p(T_1)$ and $\text{diam}(T_1) = k$, where $\text{diam}(T_1)$ denotes the diameter of $T_1$.

(II) Let $T_2 = T_1 - \{v_0, v_k\}$. If $\text{diam}(T_2) = k - 2 \geq 5$, we take $T_2' = T_2 \circ U_2$, depicted in Figure 5, where $U_2 = \{x|x \in V(T_2) - N(v_2) \cup N(v_{k-2}), d_T(x, v_{k-1}) = k - 2$ or $d_T(x, v_1) = k - 2\}$, $N(v_0)$ and $N(v_k)$ are the neighborhoods of $v_2$ and $v_{k-2}$, respectively. $T_3$ is obtained from $T_1$ by replacing the subtree $T_2$ with $T_2'$. If $U_2 \neq \emptyset$, then $W_p(T_2) < W_p(T_2')$ by Lemma 4 and $W_p(T_3) - W_p(T_1) = W(T_2') - W_p(T_2) > 0$. So, $W_p(T_1) < W_p(T_3)$, and $\text{diam}(T_3) = k$.

(III) Let $T_4$ be the subtree of $T_3$ depicted in Figure 5. If $\text{diam}(T_4) = k - 4 \geq 5$, continuing the operation on $T_4$ as on $T_2$ in (II), there is a tree with order $n$ and diameter $k$ such that its Wiener polarity index is greater than $W_p(T_3)$. In this way, we can get that

(i) If $k$ is odd, then there is a capillary tree like $T_6$ (depicted in Figure 6) such that $W_p(T) < W_p(T_6)$, where $x_1 + x_2 + \cdots + x_{k-3} = n - k - 1$.

(ii) If $k$ is even, there is a tree $T_5$ (depicted in Figure 6) such that $W_p(T) < W_p(T_5)$. Let $T_7$ be the subtree of $T_5$ depicted in Figure 6, and $U_3 = \{x|x \in V(T_7) - N(v_{k-1}) \cup N(v_{k+1}), d_T(x, v_k) = 2\}$. $T_5'$ is the tree obtained from $T_5$ by deleting all pendent edges in $T_5$ which are incident to $x$ and adding new edges $xv_{k+1}$ for all $x \in U_3$. If $U_3 \neq \emptyset$, 

\[ ... 

\[ 

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{The tree $T_3$.}
\end{figure}
then

\[ W_p(T'_5) - W_p(T_5) = (|U_3| \times (d(v_3) - 1) + |U_3| \times (d(v_{k+2}) - 1)) - |U_3| \times (d(v_3) - 1) \]

\[ = |U_3| \times (d(v_{k+2}) - 1) > 0 \]

i.e., \( W_p(T_5) < W_p(T'_5) \). Here, \( T'_5 \) is also a capillary tree like \( T_6 \).

\[ T_6 = CT_n(x_1, x_2, \cdots, x_{k-3}) \]

Figure 6. The trees \( T_5 \) and \( T_6 \).

Therefore, we have shown that

**Lemma 5.** If \( T \) is a tree with order \( n \) and diameter \( k \geq 5 \), then there is a capillary tree \( T' = CT_n(x_1, x_2, \cdots, x_{k-3}) \) such that \( W_p(T) \leq W_p(T') \) with equality only if \( T \) is also a capillary tree like \( T_6 \).

Now, we only need to find the tree with maximal Wiener polarity index among all capillary trees \( CT_n(x_1, x_2, \cdots, x_{k-3}) \), where \( x_1 + x_2 + \cdots + x_{k-3} = n - k - 1 \).

**Lemma 6.** Let \( T = CT_n(x_1, x_2, \cdots, x_{k-3}) \) be a capillary tree depicted in Figure 6, where \( x_1 + x_2 + \cdots + x_{k-3} = n - k - 1 \).

(i) If there exit \( i \) and \( j \) such that \( 1 \leq i < j < n - k - 1 \), and

\[ x_i > 0, x_{i+1} = \cdots = x_j = 0, x_{j+1} > 0 \]

then \( W_p(T) < W_p(T') \), where \( T' \) is also a capillary tree obtained from \( T \) by deleting edges \( v_{i+1}v_{i+2} \) and \( v_{j+1}v_{j+2} \) and adding edges \( v_{i+1}v_{j+2} \) and \( v_{k}v_{i+2} \);  

(ii) If there exit \( i \) and \( j \) such that \( 1 \leq i < j \leq n - k - 1 \), \( j - i + 1 \geq 4 \) and

\[ x_1 = \cdots = x_{i-1} = 0, x_i > 0, x_{i+1} > 0, \cdots, x_j > 0, x_{j+1} = \cdots = x_{k-3} = 0 \]

i.e, \( T = CT_n(0, \cdots, 0, x_i, x_{i+2}, \cdots, x_j, 0, \cdots, 0) \), then \( W_p(T) < W_p(T'') \), where \( T'' = CT_n(0, \cdots, 0, 0, x_{i+1}, x_{i+2} + x_{i+1}, x_{i+3}, \cdots, x_j, 0, \cdots, 0) \), i.e., \( T'' \) is also a capillary tree
obtained from $T$ by deleting $x_i$ pendant edges attached to $v_{i+1}$ and adding $x_i$ pendant edges to $v_{i+2}$.

**Proof.** (i) $W_p(T') - W_p(T) = [(x_i + 1)(x_{j+1} + 1) + 1] - [(x_i + 1) + (x_{j+1} + 1)] = x_ix_j > 0$. So, $W_p(T) < W_p(T')$.

(ii) $W_p(T'') - W_p(T) = [1 + (x_{i+1} + 1)(x_i + x_{i+2} + 1) + (x_i + x_{i+2} + 1)(x_{i+3} + 1)] - [(x_i + 1)(x_{i+1} + 1) + (x_{i+1} + 1)(x_{i+2} + 1) + (x_{i+2} + 1)(x_{i+3} + 1)] = x_ix_{i+3} > 0$. So, $W_p(T) < W_p(T'')$.

**Theorem 7.** If $T$ is a tree with order $n$ and diameter $k \geq 5$, then

$$W_p(T) \leq \left\lfloor \frac{n-k-1}{2} \right\rfloor \left\lceil \frac{n-k-1}{2} \right\rceil + (2n - k - 4)$$

with equality if and only if $T$ is a capillary tree $CT_n(0, \ldots, 0, x_i, x_{i+1}, x_{i+2}, 0, \ldots, 0)$ such that where $1 \leq i \leq k - 5$, $x_i + x_{i+1} + x_{i+2} = n - k - 1$, $x_i \geq 0$, $x_{i+2} \geq 0$ and $x_{i+1} = \left\lfloor \frac{n-k-1}{2} \right\rfloor$ or $\left\lceil \frac{n-k-1}{2} \right\rceil$.

**Proof.** By Lemmas 5 and 6, there is a capillary tree $T^* = CT_n(0, \ldots, 0, x_i, x_{i+1}, x_{i+2}, 0, \ldots, 0)$ such that $W_p(T) \leq W_p(T^*)$, where $x_i + x_{i+1} + x_{i+2} = n - k - 1$, $x_i \geq 0$, $x_{i+2} \geq 0$ and $x_{i+1} > 0$ except $n = k + 1$. And

$$W_p(T^*) = (x_i + 1) + (x_i + 1)(x_{i+1} + 1) + (x_{i+1} + 1)(x_{i+2} + 1)$$

$$+ (x_{i+2} + 1) + (k - 6)$$

$$= x_ix_{i+1} + x_{i+1}x_{i+2} + 2(x_i + x_{i+1} + x_{i+2}) + k - 2$$

$$= x_{i+1}(x_i + x_{i+2}) + 2(n - k - 1) + k - 2$$

$$= x_{i+1}(n - k - 1 - x_{i+1}) + (2n - k - 4)$$

$$\leq \left\lfloor \frac{n-k-1}{2} \right\rceil (nk - 1 - \left\lceil \frac{n-k-1}{2} \right\rceil) + (2n - k - 4)$$

$$= \left\lfloor \frac{n-k-1}{2} \right\rceil \left\lceil \frac{n-k-1}{2} \right\rceil + (2n - k - 4)$$

with equality if and only if $x_{i+1} = \left\lfloor \frac{n-k-1}{2} \right\rceil$ or $\left\lceil \frac{n-k-1}{2} \right\rceil$, i.e., $T^*$ is a capillary tree $CT_n(0, \ldots, 0, x_i, x_{i+1}, x_{i+2}, 0, \ldots, 0)$ such that where $1 \leq i \leq k - 5$, $x_i + x_{i+1} + x_{i+2} = n - k - 1$, $x_i \geq 0$, $x_{i+2} \geq 0$ and $x_{i+1} = \left\lfloor \frac{n-k-1}{2} \right\rceil$ or $\left\lceil \frac{n-k-1}{2} \right\rceil$. 
References


