Research Article

A Note on the Minimum Wiener Polarity Index of Trees with a Given Number of Vertices and Segments or Branching Vertices

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Received 4 July 2020; Revised 2 January 2021; Accepted 11 January 2021; Published 23 January 2021

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The Wiener polarity index of a graph $G$, usually denoted by $W_p(G)$, is defined as the number of unordered pairs of those vertices of $G$ that are at distance 3. A vertex of a tree with degree at least 3 is called a branching vertex. A segment of a tree $T$ is a nontrivial path $S$ whose end-vertices have degrees different from 2 in $T$ and every other vertex (if exists) of $S$ has degree 2 in $T$. In this note, the best possible sharp lower bounds on the Wiener polarity index $W_p$ are derived for the trees of fixed order and with a given number of branching vertices or segments, and all the trees attaining this lower bound are characterized.

1. Introduction

A topological index is a numerical quantity calculated from a graph, which remains unchanged under graph isomorphism [1]. Topological indices have attracted much attention in recent years, as many of them provide a good correlation between the molecular structure of a chemical compound and its properties. Examples for calculating the topological indices of particular graphs can be found in [2–4].

The Wiener polarity index $W_p$ is one of the oldest topological indices, which was proposed in 1947 by the chemist Harold Wiener [5], for predicting the boiling points of paraffins. The index $W_p$ for a graph $G$ is defined as the number of unordered pairs of those vertices of $G$ that are at distance 3. In the previous decade, $W_p$ has attracted much attention from researchers; for example, see the surveys [6, 7], papers [8–25], and related references therein.

Before moving further, let us recall some definitions and notations first. All the graphs considered in this note are simple and finite. Let $G$ be a graph with the vertex set $V(G)$ and the set of edges $E(G)$. The degree of a vertex $u \in V(G)$ is denoted by $d_u(G)$ (or simply by $d_u$ if the graph under consideration is clear). The number of vertices in a graph is known as its order. A graph of order $n$ is called an $n$-vertex graph. A vertex of degree 1 is called a pendant vertex, while a vertex of degree greater than 2 is known as a branching vertex. Let $N_G(u)$ (or $N(u)$) be the set of all those vertices of $G$ that are adjacent to the vertex $u \in V(G)$. As usual, we denote by $P_n$ and $S_n$ the path and the star graph of order $n$, respectively. A segment $S$ of a tree $T$ is a nontrivial path (that is, a path of length at least 1) in $T$ with the property that both the end-vertices of $S$ have degrees different from 2 in $T$ and every other vertex (if exists) of $S$ has degree 2. A tree $ST$ is called starlike tree (or generalized star) if it contains exactly one branching vertex (we call it the central vertex of $ST$). A path $P = v_0, v_1, \ldots, v_k$ in a tree $T$ is called a pendant path (internal path, respectively) of length $k$, if one of the two vertices $v_0, v_k$ is pendant and the other is branching (both the vertices $v_0$ and $v_k$ are branching, respectively) and $d_{v_i} = 2$ if $1 \leq i \leq k - 1$. The notation and terminology of (chemical) graph theory that are not defined in this note can be found in [1, 26–28].

By using the definition of the Wiener polarity index, Lukovits and Linert [29] demonstrated the quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons. Considerable work has been...
done, however, on characterizing the trees that maximize or minimize $W_p$ under various additional conditions: for example, with given order [15], degree sequence [30, 31], diameter [32], and pendant vertices [33, 34]. Shafique and Ali [35] gave some structural properties of the trees of fixed order and with a given number of segments or branching vertices having maximum/minimum $W_p$ value. Here, in this note, we are specifically interested in extending the results obtained in the paper [35].

Du et al. [15] showed that $W_p$ of a tree $T$ can be written as

$$W_p(T) = \sum_{uv \in E(T)} (d_u - 1)(d_v - 1),$$

(1)

where $uv$ is the edge connecting the vertices $u, v \in V(T)$. Here, it is important to note that $W_p$ coincides with reduced second Zagreb index [35–37], for the case of trees.

For fixed integers $n$ and $s$, denote by $ST_{n,s}$ and $T_{n,b}$ the classes of all $n$-vertex trees with $s$ segments and $b$ branching vertices, respectively, where $1 \leq s \leq n - 1$ and $1 \leq b \leq (n/2) - 1$. In this note, we characterize all the trees attaining minimum $W_p$ value from each of the two classes $ST_{n,s}$ and $T_{n,b}$ and hence provide the solution of a problem, left open in [35], concerning the minimum $W_p$ value. Let $T'$ be a tree obtained from a tree $T$ after applying a transformation such that $V(T) = V(T')$. Throughout this note, whenever we consider such trees, by $d_i$ and $N(v)$ we mean the degree and set of neighbors, respectively, of the vertex $v \in V(T) = V(T')$ in $T$.

2. Sharp Lower Bound on Wiener Polarity Index for $n$-Vertex Trees with a Fixed Number of Segments

Note that $ST_{n,1}$ consists of only the path graph $P_n$, and $ST_{n,2}$ is empty. Thus, we proceed in this note with the assumption $3 \leq s \leq n - 1$. Denote by $ST_{n,s}' \subset ST_{n,s}$ the starlike tree with $s - 1$ pendant paths of length $1$ (see Figure 1). Let $ST_{n,s}^* \subset ST_{n,s}$ be the class of all $n$-vertex trees with exactly one internal path and $s - 1$ pendant paths of length $1$. For the tree(s) having the minimum Wiener Polarity index among all the members of the class $ST_{n,s}$, we firstly prove some lemmas.

**Lemma 1.** Let $n$ and $s$ be positive integers such that $3 \leq s \leq n - 1$. If $T \in ST_{n,s}$ is a tree such that $W_p(T)$ is minimum among all the trees of $ST_{n,s}$, then $T$ contains at most one pendant path of length greater than $1$.

**Proof.** Suppose, contrarily, that $P = v_0, v_1, \ldots, v_L$ and $P' = v_0', v_1', \ldots, v_L'$ ($L \geq 2$) are two pendant paths in $T$, where $d_{v_0} = d_{v_0}' = 1$ and $d_{v_i}, d_{v_i}' \geq 2$ (note that the vertices $v_i$ and $v_i'$ may coincide). If $T'' = T - \{v_{s-1}v_{s-2} + v_{s-2}v_0\}$, then $T'' \in ST_{n,s}$, and we have

$$W_p(T) - W_p(T'') = d_{v_s} - 2 > 0,$$

(2)

a contradiction to the choice of $T$.

Lemma 1 ensures that the trees $ST_{n,3}'$ and $ST_{n,4}'$ have the minimum $W_p$ value in the classes $ST_{n,3}$ and $ST_{n,4}$, respectively. Also, it is obvious that the star graph $S_n$ gives the minimum $W_p$ value (that is, 0) in the class $ST_{n,n-1}^*$. Therefore, we proceed with the assumption $5 \leq s \leq n - 2$. Denote by $ST_{n,s} \subset ST_{n,s}$ the subclass consisting of all starlike trees. Moreover, by Lemma 1, $ST_{n,s}'$ attains the minimum $W_p$ value in the class $ST_{n,s}$. Now, we consider the class $ST_{n,s} \setminus ST_{n,s}'$, where $5 \leq s \leq n - 2$. □

**Lemma 2.** Let $n$ and $s$ be positive integers such that $5 \leq s \leq n - 2$. If $T \in ST_{n,s} \setminus ST_{n,s}'$ is a tree having minimum $W_p$ value among all the members of $ST_{n,s} \setminus ST_{n,s}'$, then each pendant path of $T$ is of length $1$.

**Proof.** We contrarily assume that there is a pendant path $P = v_0, v_1, \ldots, v_s$ of length $s \geq 2$ in $T$, where $d_{v_0} = 1$ and $d_{v_s} \geq 3$. Let $v \in V(T)$ be a branching vertex different from $v_s$ and let $u$ be the neighbor of $v_s$ lying on the $v_s - v$ path. Note that $d_{v_s} \geq 2$ and that $u$ may coincide with $v$. Let $T'' = T - \{v_0, v_s, v_1, \ldots, v_s, v_1, u\}$, then it can be observed that $T'' \in ST_{n,s} \setminus ST_{n,s}'$, and we have $W_p(T) - W_p(T'') = (d_{v_s} - 1)(d_{v_s} - 2) > 0$, a contradiction to the choice of $T$. □

**Theorem 1.** Let $n$ and $s$ be positive integers such that $3 \leq s \leq n - 2$. If $T \in ST_{n,s}$, then

$$W_p(T) \geq n - 3,$$

(3)

and the equality sign in (3) holds if and only if either $T \equiv S_n^*$ (see Figure 1) or $T \in ST_{n,s}'$. □

**Proof.** If $T \in ST_{n,s}$ contains more than one pendant path of length at least 2, then by the proof of Lemma 1, there exists a tree $T'$ having at most one pendant path of length at least 2 such that $W_p(T) > W_p(T')$. Thus, it is enough to prove the result when $T \in ST_{n,s}$ contains at most one pendant path of length at least 2. In the remaining proof, we assume that $T \in ST_{n,s}$ has at most one pendant path of length at least 2.

If either $T \equiv S_n^*$ or $T \in ST_{n,s}'$, then by elementary calculations, one has $W_p(T) = n - 3$. We apply induction on $s$ to prove the desired result. Note that if $s = 3$ or $4$, then by Lemma 1, it holds that $W_p(T) \geq n - 3$ with equality if and only if $T \equiv S_n^*$. Also, if $s = 5$, then by using Lemmas 1 and 2, we have $W_p(T) \geq n - 3$ with equality if and only if either $T \equiv S_n^*$ or $T \in ST_{n,s}'$. Next, suppose that $6 \leq s \leq n - 2$, and that the result holds for every $s'$ satisfying $3 \leq s' \leq s - 1$.

Let $P = u_1, u_2, \ldots, u_r$ be a longest path in $T$, where $r \geq 4$. Note that each of the two vertices $u_2$ and $u_{r-1}$ has exactly one nonpendent neighbor in $T$. Since $T$ contains at most one pendant path of length at least $2$, at least one of the two vertices $u_2$ and $u_{r-1}$ is branching. Without loss of generality, we assume that $u_2$ is branching. Let $N(u_2) = \{u_1, u_3, u_4, u_5, \ldots, u_t\}$ where $t \geq 1$ and $d_{u_i} = 1$ for every $i \in \{1, 2, \ldots, t\}$. Let

![Figure 1: The graph $S_n^*$](image)
$T' = T - \{u_1\}$. Note that $T' \in \mathbb{T}_{n-1,r-1}$ when $t \geq 2$, and $T' \in \mathbb{T}_{n-1,r+2}$ when $t = 1$. Hence, by using the inductive hypothesis, we have

$$W_p(T) = W_p(T') + (d_{w_1} - 1) \geq n - 4 + (d_{w_1} - 1) \quad (4)$$

If $t \geq 2$, then the equality $W_p(T) = n - 3$ holds if and only if $d_{w_1} = 2$ and either $T' \in \mathbb{ST}_{n-1,r-1}$ or $T' \equiv S_{n-1}^r$. If $t = 1$, then the equality $W_p(T) = n - 3$ holds if and only if $d_{w_1} = 2$ and $T' \equiv S_{n-1}^{r+1}$ (because in this case, the tree $T'$ contains a pendant path of length at least 2). Thus, we conclude that $W_p(T) \geq n - 3$ with equality if and only if $T \equiv S_n^r$ or $T \in \mathbb{ST}_{n,r}$. This completes the induction and hence the proof. \square

3. Sharp Lower Bound on Wiener Polarity Index for n-Vertex Trees with a Given Number of Branching Vertices

Recall that $\mathbb{T}_{n,b}$ is the class of all $n$-vertex trees with $b$ branching vertices, where $1 \leq b \leq (n/2) - 1$. For $b = 1$, the star graph $S_3$ attains the minimum $W_p$ value (see [36]). Thus, throughout this section, we assume $2 \leq b \leq (n/2) - 1$. Note that Lemma 3 may be proved in a fully analogous way to that of Lemma 2.

Lemma 3 (see [35]). Let $b$ and $n$ be positive integers such that $2 \leq b \leq (n/2) - 1$. If $T \in \mathbb{T}_{n,b}$ is a tree having minimum $W_p$ value among all the members of $\mathbb{T}_{n,b}$, then every pendant path of $T$ is of length 1.

Let $x_{ij}$ be the number of edges in a tree $T$ connecting the vertices of degrees $i$ and $j$.

Lemma 4. Let $b$ and $n$ be positive integers such that $2 \leq b \leq (n/2) - 1$. If $T \in \mathbb{T}_{n,b}$ is a tree having minimum $W_p$ value among all the members of $\mathbb{T}_{n,b}$ and $x_{i,1} \neq 0$ for some $i \geq 4$, then $T$ does not contain any pair of adjacent branching vertices.

Proof. Contrarily, suppose that $w, z \in V(T)$ is a pair of adjacent branching vertices and let $v \in V(T)$ be a pendant vertex adjacent to a vertex $u \in V(T)$ of degree at least 4. Note that $u$ may coincide with either of the vertices $w$ and $z$. If $T' = T - \{uv, wz\} + \{uw, vz\}$, then it can be observed that $T' \in \mathbb{T}_{n,b}$ and we have

$$W_p(T) - W_p(T') = \sum_{x \in N(u), x \neq v} (d_x - 1) + d_w d_z - 2d_w - 2d_z + 3,$$

which is positive because of the fact that the function $f(a, b) = ab - 2a - 2b + 3$ is strictly increasing in both $a$ and $b$ where $a, b \in (3, \infty)$. Thus, we arrived at a contradiction to the choice of $T$. \square

Lemma 5. Let $b$ and $n$ be positive integers such that $2 \leq b \leq (n/2) - 1$. If $T \in \mathbb{T}_{n,b}$ is a tree with minimum $W_p$ among the trees from $\mathbb{T}_{n,b}$, such that $uv \in E(T)$ with $d_u = 1$ and $d_v \geq 4$, then a tree $T'$ in $\mathbb{T}_{n,b}$ can be obtained from $T$ as $T' = T - \{vw\} + \{uw\}$, where $w$ is a nonpendent neighbor of $v$, such that $W_p(T) \geq W_p(T')$.

Proof. It holds, as it is easy to see that $T' \in \mathbb{T}_{n,b}$. Also, using the facts $d_w \geq 2$ and $d_v \geq 4$, we have

$$W_p(T) - W_p(T') = (d_v - 1)(d_w - 1) + (d_v - 1)$$

$$= \sum_{x \in N(v), x \neq u, x \neq w} (d_x - 1) - (d_w - 1) - (d_v - 2) - (d_v - 2)$$

$$= d_w d_v - 2d_v - 2d_w + 4 + \sum_{x \in N(v), x \neq u, x \neq w} (d_x - 1) \geq 0,$$

which implies $W_p(T) \geq W_p(T')$. \square

Lemma 6. Let $b$ and $n$ be positive integers such that $2 \leq b \leq (n/2) - 1$. If $T \in \mathbb{T}_{n,b}$ is a tree having minimum $W_p$ value among all the members of $\mathbb{T}_{n,b}$, then every vertex of degree greater than 3 in $T$ has exactly one nonpendent neighbor.

Proof. We contrarily assume that the vertex $u \in V(T)$, with $N(u) = \{u_1, u_2, \ldots, u_{i-1}, u_{i+1}, \ldots, u_r\}$, has at least two nonpendent neighbors where $t \geq 4$. We consider the following cases:

Case 1. The vertex $u$ has at least one pendant neighbor. Without loss of generality, we assume that $d_{u_i} = 1$ for $1 \leq i \leq q$ and $d_{u_j} = 2$ for $q + 1 \leq j \leq t$. Then, $t - q \geq 2$ because $u$ has at least two nonpendent neighbors. Lemma 4 ensures that $d_{u_i} = 2$ for every $j$ satisfying $q + 1 \leq j \leq t$. If $T' = T - \{uu_i\} \cup \{u_iu_j\}$, then $T' \in \mathbb{T}_{n,b}$ and hence, because of the fact $t - q \geq 2$, we have

$$W_p(T) - W_p(T') = t - q - 1 > 0,$$

which is a contradiction.

Case 2. The vertex $u$ has nonpendent neighbor.

In this case, we have $d_{u_i} \geq 2$ for every $i$ satisfying $1 \leq i \leq t$. Here, Lemmas 3–5 ensure that there is a pendant vertex $v \in V(T)$ having the neighbor $w$ such that $d_w = 3$ for $d_v \geq 4$, where $1 \leq i \leq t$. Let $u_1$ be the neighbor of $u$ that lies on the unique $v$- $u$ path. If $T' = T - \{uu_i\} \cup \{v, u_i\}$, then $T' \in \mathbb{T}_{n,b}$, and we have

$$W_p(T) - W_p(T') = \sum_{x \in N(u), x \neq u_i} (d_x - 1) + (d_{u_i} - 2)(d_{u_i} - 1) - 2 > 0,$$

which is again a contradiction to the choice of $T$.

Theorem 2. Let $b$ and $n$ be positive integers such that $2 \leq b \leq (n/2) - 1$. If $T \in \mathbb{T}_{n,b}$, then
\[ W_p(T) \geq \begin{cases} 
\frac{n+b-5}{3}, & 2b < \frac{n-1}{3}, \\
4b - 4, & \frac{n-1}{3} \leq b \leq \frac{n}{2} - 1, \\
\end{cases} \]
and the equality holds if and only if \( T \in T^*_1 \), for \( 2b < (n - 1)/3 \), where \( T^*_1 = \{ T : T \) is a tree whose every vertex with degree \( \geq 4 \) has exactly one nonpendent neighbor and each internal path is of length at least 2\}, and \( T \in T^*_2 \), for \( (n - 1)/3 \leq b < (n/2) - 1 \), where \( T^*_2 \) is a class of trees with degree sequence \( (3,3,\ldots,3,2,2,\ldots,2,1,1,\ldots,1) \) such that each pendent vertex of \( T \in T^*_2 \) is adjacent to some branching vertex only.

\[ n \leq 3, \quad \text{or we have to add a starlike pendant vertex in such a way that every vertex with degree } \geq 4 \text{ has exactly one nonpendent neighbor that is } T \equiv T^*_1; \quad \text{Hence, } W_p(T) = n + b - 5, \quad \text{for } 2b < (n - 1)/3, \] which completes the proof.  

### Data Availability

The data used to support the findings of the study are available from the corresponding author upon request.

### Conflicts of Interest

The authors declare that they have no conflicts of interest.

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