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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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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 *pendent 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 *pendent path* (*internal path*, respectively) of length k, if one of the two vertices v_0, v_k is pendent 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 pendent 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

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

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 $\mathbb{ST}_{n,s}$ and $\mathbb{T}_{n,b}$ the classes of all n-vertex trees with s segments and b branching vertices, respectively, where $1 \le s \le n-1$ and $1 \le b \le (n/2) - 1$. In this note, we characterize all the trees attaining minimum W_p value from each of the two classes $\mathbb{ST}_{n,s}$ and $\mathbb{T}_{n,b}$ 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_v 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 $\mathbb{ST}_{n,1}$ consists of only the path graph P_n, and $\mathbb{ST}_{n,2}$ is empty. Thus, we proceed in this note with the assumption $3 \le s \le n-1$. Denote by $S_s^n \in \mathbb{ST}_{n,s}$ the starlike tree with $s-1$ pendent paths of length 1 (see Figure 1). Let $ST_{n,s}^* \subset \mathbb{ST}_{n,s}$ be the class of all n-vertex trees with exactly one internal path and $s-1$ pendent paths of length 1. For the tree(s) having the minimum Wiener Polarity index among all the members of the class $\mathbb{ST}_{n,s}$, we firstly prove some lemmas.

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

Proof. Suppose, contrarily, that $P = v_0, v_1, \ldots, v_s$ and $P' = v'_0, v'_1, \ldots, v'_l$ $(l, s \ge 2)$ are two pendent paths in T, where $d_{v_0} = d_{v'_0} = 1$ and $d_{v_s}, d_{v'_l} \ge 3$ (note that the vertices v'_l and v_s may coincide). If $T' = T - \{v_{s-1}v_{s-2}\} + \{v_{s-2}v'_0\}$, then $T' \in \mathbb{ST}_{n,s}$, and we have

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

a contradiction to the choice of T.

Lemma 1 ensures that the trees S_3^n and S_4^n have the minimum W_p value in the classes $\mathbb{ST}_{n,3}$ and $\mathbb{ST}_{n,4}$,

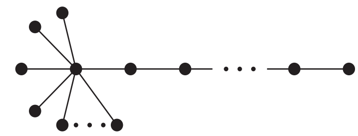

Figure 1: The graph S_s^n.

respectively. Also, it is obvious that the star graph S_n gives the minimum W_p value (that is, 0) in the class $\mathbb{ST}_{n,n-1}$. Therefore, we proceed with the assumption $5 \le s \le n-2$. Denote by $\mathbb{ST}_s \subset \mathbb{ST}_{n,s}$ the subclass consisting of all starlike trees. Moreover, by Lemma 1, S_s^n attains the minimum W_p value in the class $\mathbb{ST}_s$. Now, we consider the class $\mathbb{ST}_{n,s} \setminus \mathbb{ST}_s$ where $5 \le s \le n-2$. □

Lemma 2. *Let n and s be positive integers such that $5 \le s \le n-2$. If $T \in \mathbb{ST}_{n,s} \setminus \mathbb{ST}_s$ is a tree having minimum W_p value among all the members of $\mathbb{ST}_{n,s} \setminus \mathbb{ST}_s$, then each pendent path of T is of length 1.*

Proof. We contrarily assume that there is a pendent path $P{:} = v_0, v_1, \ldots, v_s$ of length $s \ge 2$ in T, where $d_{v_0} = 1$ and $d_{v_s} \ge 3$. 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 $d_u \ge 2$ and that u may coincide with v. Let $T' = T - \{v_s u, v_0 v_1\} + \{v_0 v_s, v_1 u\}$, it can be observed that $T' \in \mathbb{ST}_{n,s} \setminus \mathbb{ST}_s$, and we have $W_p(T) - W_p(T') = (d_u - 1)(d_{v_s} - 2) > 0$, a contradiction to the choice of T. □

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

$$W_p(T) \ge n - 3, \tag{3}$$

and the equality sign in (3) holds if and only if either $T \cong S_s^n$ (see Figure 1) or $T \in ST_{n,s}^*$.

Proof. If $T \in \mathbb{ST}_{n,s}$ contains more than one pendent path of length at least 2, then by the proof of Lemma 1, there exists a tree T^* having at most one pendent path of length at least 2 such that $W_p(T) > W_p(T^*)$. Thus, it is enough to prove the result when $T \in \mathbb{ST}_{n,s}$ contains at most one pendent path of length at least 2. In the remaining proof, we assume that $T \in \mathbb{ST}_{n,s}$ has at most one pendent path of length at least 2.

If either $T \cong S_s^n$ 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 $W_p(T) \ge n-3$ with equality if and only if $T \cong S_s^n$. Also, if $s = 5$, then by using Lemmas 1 and 2, we have $W_p(T) \ge n-3$ with equality if and only if either $T \cong S_5^n$ or $T \in ST_{n,5}^*$. Next, suppose that $6 \le s \le n-2$ and that the result holds for every s' satisfying $3 \le s' \le s-1$.

Let $P{:}\ w_1, w_2, \ldots, w_r$ be a longest path in T, where $r \ge 4$. Note that each of the two vertices w_2 and w_{r-1} has exactly one nonpendent neighbor in T. Since T contains at most one pendent path of length at least 2, at least one of the two vertices w_2 and w_{r-1} is branching. Without loss of generality, we assume that w_2 is branching. Let $N(w_2) = \{w_1, w_3, u_1, u_2, \ldots, u_t\}$ where $t \ge 1$ and $d_{u_i} = 1$ for every $i \in \{1, 2, \ldots, t\}$. Let

$T' = T - \{u_1\}$. Note that $T' \in \mathbb{ST}_{n-1,s-1}$ when $t \geq 2$, and $T' \in \mathbb{ST}_{n-1,s-2}$ when $t = 1$. Hence, by using the inductive hypothesis, we have

$$\begin{aligned} W_p(T) &= W_p(T') + (d_{w_3} - 1) \\ &\geq n - 4 + (d_{w_3} - 1) \\ &\geq n - 3. \end{aligned} \tag{4}$$

If $t \geq 2$, then the equality $W_p(T) = n - 3$ holds if and only if $d_{w_3} = 2$ and either $T' \in ST^*_{n-1,s-1}$ or $T' \cong S^{n-1}_{s-1}$. If $t = 1$, then the equality $W_p(T) = n - 3$ holds if and only if $d_{w_3} = 2$ and $T' \cong S^{n-1}_{s-2}$ (because in this case, the tree T' contains a pendent path of length at least 2). Thus, we conclude that $W_p(T) \geq n - 3$ with equality if and only if $T \cong S^n_s$ or $T \in ST^*_{n,s}$. This completes the induction and hence the proof. □

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_n 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 pendent path of T is of length 1.*

Let $x_{i,j}$ 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 pendent 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 $T' = T - \{vu, wz\} + \{wv, vz\}$, then it can be observed that $T' \in \mathbb{T}_{n,b}$, and we have

$$W_p(T) - W_p(T') = \sum_{x \in N(u), x \neq v} (d_x - 1) + d_w d_z - 2d_w - 2d_z + 3, \tag{5}$$

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. □

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

$$\begin{aligned} W_p(T) - W_p(T') &= (d_v - 1)(d_w - 1) + (d_v - 1) \\ &\sum_{z \in N(v), z \neq u, z \neq w} (d_z - 1) - (d_w - 1) - (d_v - 2) - (d_v - 2) \\ &\sum_{z \in N(v), z \neq u, z \neq w} (d_z - 1) \\ &= d_v d_w - 2d_v - 2d_w + 4 + \sum_{z \in N(v), z \neq u, z \neq w} (d_z - 1) \geq 0, \end{aligned} \tag{6}$$

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

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 $N(u) = \{u_1, u_2, \ldots, u_q, u_{q+1}, \ldots, u_t\}$, has at least two nonpendent neighbors where $t \geq 4$. We consider the following cases: □

Case 1. The vertex u has at least one pendent neighbor.

Without loss of generality, we assume that $d_{u_i} = 1$ for $1 \leq i \leq q$ and $d_{u_j} = d_j \geq 2$ for $q + 1 \leq j \leq t$. Then, $t - q \geq 2$ because u has at least two nonpendent neighbors. Lemma 4 ensures that $d_j = 2$ for every j satisfying $q + 1 \leq j \leq t$. If $T' = T - \{uu_t\} + \{u_t u_1\}$, then $T' \in \mathbb{T}_{n,b}$ and hence, because of the fact $t - q \geq 2$, we have

$$W_p(T) - W_p(T') = t - q - 1 > 0, \tag{7}$$

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 pendent vertex $v \in V(T)$ having the neighbor w such that $d_w = 3$ for $d_{u_i} \geq 2$, where $1 \leq i \leq t$. Let u_1 be the neighbor of u that lies on the unique v - u path. If $T' = T - \{uu_t\} + \{vu_t\}$, then $T' \in \mathbb{T}_{n,b}$, and we have

$$W_p(T) - W_p(T') = \sum_{x \in N(u), x \neq u_t} (d_x - 1) + (d_u - 2)(d_{u_t} - 1) - 2 > 0, \tag{8}$$

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*

$$W_P(T) \geq \begin{cases} n+b-5, & 2 \leq b < \dfrac{n-1}{3}, \\ \\ 4b-4, & \dfrac{n-1}{3} \leq b \leq \dfrac{n}{2} - 1, \end{cases} \quad (9)$$

and the equality holds if and only if $T \in \mathbb{T}_1^*$, *for* $2 \leq b < (n - 1/3)$, *where* $\mathbb{T}_1^* = \{T\text{: } T$ *is a tree whose every vertex with degree* ≥ 4 *has exactly one nonpendent neighbor and each internal path is of length at least 2*$\}$, *and* $T \in \mathbb{T}_2^*$, *for* $(n - 1/3) \leq b \leq (n/2) - 1$, *where* $\mathbb{T}_2^*$ *is a class of trees with degree sequence* $(\underbrace{3,3,\ldots,3}_{b}, \underbrace{2,2,\ldots,2}_{n-2b-2}, \underbrace{1,1,\ldots,1}_{b+2})$ *such that each pendent vertex of* $T \in \mathbb{T}_2^*$ *is adjacent to some branching vertex only.*

Proof. Denote by N_i the number of vertices of degree i in a graph G. Let T be a tree that minimizes W_p among the class $\mathbb{T}_{n,b}$. Lemma 3 and Lemma 4 conclude that whenever $(n - 1/3) \leq b \leq (n/2) - 1$, every branching vertex in T has degree 3 such that the vertices of degree 2 are placed between the adjacent vertices of degree 3 in such a way that no two vertices of degree 2 are adjacent if there are adjacent vertices of degree 3. Note that, for $(n - 1/3) \leq b \leq (n/2) - 1$, we have $N_3 = b$, $N_1 = b + 2$ and $N_2 = n - 2b - 2$. Hence, $W_p(T) = 4b - 4$.

Now, Lemmas 3–6 conclude that every internal path has a length of at least 2. Also, Lemma 5 ensures that, to obtain minimal graph T, either we have to insert the vertices of degree 2 between any vertex of degree 2 and vertex of degree 3, or we have to add a starlike pendent vertex in such a way that every vertex with degree ≥ 4 has exactly one nonpendent neighbor that is $T \cong \mathbb{T}_1^*$. Hence, $W_p(T) = n + b - 5$, for $2 \leq b < (n - 1/3)$, 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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