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Research Article

Unicyclic Graphs with the Fourth Extremal Wiener Indices

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A graph is called unicyclic if the graph contains exactly one cycle. Unicyclic graphs with the fourth extremal Wiener indices are characterized. It is shown that, among all unicyclic graphs with $n \geq 8$ vertices, $C_5(S_{n-4})$ and $C_2^{u_1,u_2}(S_3, S_{n-4})$ attain the fourth minimum Wiener index, whereas $C_3^{u_1,u_2}(P_3, P_{n-4})$ attains the fourth maximum Wiener index.

1. Introduction

Let $G = (V(G), E(G))$ be a connected (molecular) graph with vertex set $V(G)$ and edge set $E(G)$. For any two vertices $u, v \in V(G)$, the distance $d_G(u, v)$ between them is defined as the number of edges in a shortest path connecting them. The distance of a vertex $u \in V(G)$, denoted by $d_G(u)$, is the sum of distances between u and all other vertices of G, i.e., $d_G(u) = \sum_{v \in V(G)} d_G(u, v)$. The famous Wiener index of G, denoted by $W(G)$, is defined as

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

The Wiener index of a graph is a well-known topological index, and it seems that Wiener [1] was the first who considered it. Wiener himself used the name path number and conceived $W(G)$ only for acyclic molecules. The definition of the Wiener index in terms of distances between vertices of a graph, such as in equation (1), was first given by Hosoya [2]. Since the middle of the 1970s, the Wiener index has been extensively studied. For research development on the Wiener index, the readers are referred to [3–7] and two special issues of MATCH [8] and Discrete Appl. Math. [9]. Analogous to the Wiener index, some other topological indices are introduced and studied (for example, see [10–13]).

As summarized in [14–16], studies on the Wiener index mainly focus on trees and hexagonal systems. Recently, Wiener indices of unicyclic graphs (i.e., connected graphs containing exactly one cycle) have attracted much attention. Studies along this line include relations between Wiener and Szeged indices of unicyclic graphs [17], minimum Wiener indices of unicyclic graphs of given order, cycle length and number of penden vertices [18], minimum Wiener indices of unicyclic graphs of given matching number [19], Wiener indices of unicyclic graphs with given girth [20], minimum Wiener indices of unicyclic graphs of order n with girth g and the matching number $\beta \geq 3g/2$ [21], minimum Wiener indices of unicyclic graphs of order n and girth g with k pendent vertices [22], minimum Wiener index of unicyclic graphs with given bipartition [23], and so on. In [24], Tang and Deng considered unicyclic graphs with the first three smallest and largest Wiener indices. However, their characterization turned out to be incomplete and two extremal graphs were missed. Later, Nasiri et al. [25] filled the gap and presented a complete characterization to these extremal graphs. On the basis of the previous work, in this paper, we characterize unicyclic graphs with the fourth smallest and largest Wiener indices.

2. Notations and Lemmas

Throughout the paper, the path, star, and cycle graphs on n vertices are denoted by P_n, S_n, and C_n, respectively. Let G be a unicyclic graph of order n with its unique cycle $C_m = v_1 v_2 \dots v_m v_1$ of length m. Suppose that $T_1, T_2, \dots, T_k$ $(0 \le k \le m)$ are all the nontrivial components (they are all nontrivial trees) of $G - E(C_m)$, and u_i is the common vertex of T_i and C_m, $i = 1, 2, \dots, k$. Such a unicyclic graph is denoted by $C_m^{u_1,u_2,\dots,u_k}(T_1, T_2, \dots, T_k)$. Specially, $G = C_n$ for $k = 0$. And if $k = 1$, we write $C_m(T_1)$ for $C_m^{u_1}(T_1)$. Let $|V(T_i)| = l_i + 1$, $i = 1, 2, \dots, k$. Then, $l = l_1 + l_2 + \dots + l_k = n - m$. Denote by $\mathcal{T}_n$ the set of all trees of order n.

In the following, we summarize some known results concerning Wiener indices of unicyclic graphs which will be used in the later.

Lemma 1 (see [24]). *Let $G = C_m^{u_1,u_2,\dots,u_k}(T_1, T_2, \dots, T_k)$ be a unicyclic graph. Then,*

$$W(G) = W(C_m) + (n-m)\omega + (m-1)\sum_{i=1}^{k}\omega_i + \sum_{i=1}^{k} W(T_i) + \sum_{i=1}^{k-1}\sum_{j=i+1}^{k}\left(l_i\omega_j + l_i l_j d_{C_m}(u_i, u_j) + l_j\omega_i\right), \quad (2)$$

where $\omega_i = d_{T_i}(u_i)$, $\omega = d_{C_m}(u)$, and $u \in C_m$.

Lemma 2 (see [24]). *Let $G_1 = C_m^{u_1,u_2,\dots,u_k}(S_{l_1+1}, S_{l_2+1}, \dots, S_{l_k+1})$ and $G_2 = C_m^{u_1,u_2,\dots,u_k}(P_{l_1+1}, P_{l_2+1}, \dots, P_{l_k+1})$, where $u_1, u_2, \dots, u_k$ are the centers of $S_{l_1+1}, S_{l_2+1}, \dots, S_{l_k+1}$, respectively, in G_1 and $u_1, u_2, \dots, u_k$ are the pendent vertices of $P_{l_1+1}, P_{l_2+1}, \dots, P_{l_k+1}$, respectively, in G_2. Then,*

$$W(G_1) \le W(G) \le W(G_2), \quad (3)$$

for any graph $G = C_m^{u_1,u_2,\dots,u_k}(T_1, T_2, \dots, T_k)$ and $|V(T_i)| = l_i + 1$, $i = 1, 2, \dots, k$, with the equality on the left (or on the right) if and only if $G \cong G_1$ (or $G \cong G_2$).

Lemma 3 (see [24]). *Let $G_1 = C_m^{u_1,u_2,\dots,u_k}(S_{l_1+1}, S_{l_2+1}, \dots, S_{l_k+1})$ and $l_i = n(T_i)$, $i = 1, 2, \dots, k$. If $k \ge 1$, then*

$$W(G_1) \ge W(C_m(S_{l+1})), \quad (4)$$

with the equality if and only if $G_1 \cong C_m(S_{l+1})$, where $l = l_1 + l_2 + \dots + l_k = n - m$.

Lemma 4 (see [24]). *Let $G_2 = C_m^{u_1,u_2,\dots,u_k}(P_{l_1+1}, P_{l_2+1}, \dots, P_{l_k+1})$ and $l_i = n(T_i)$, $i = 1, 2, \dots, k$. If $k \ge 1$, then*

$$W(G_2) \ge W(C_m(P_{l+1})), \quad (5)$$

with the equality if and only if $G_1 \cong C_m(P_{l+1})$, where $l = l_1 + l_2 + \dots + l_k = n - m$.

Lemma 5 (see [25]). *If $n \ge 8$ and $m \ge 3$, then $W(C_m(S_{n-m+1})) - W(C_{m-1}(S_{n-m+2})) > 0$.*

Besides, we also need the following result.

Lemma 6 (see [22]). *Let H, X, and Y be three connected pairwise vertex-set disjoint graphs. Suppose that u and v are the two vertices of H, v' is a vertex of X, and u' is a vertex of Y. Let G be the graph obtained from H, X, and Y by identifying v with v' and u with u', respectively. Let G_1^* be the graph obtained from H, X, and Y by identifying vertices v, v', and u', and let G_2^* be the graph obtained from H, X, and Y by identifying vertices u, v', u'. Then,*

$$W(G_1^*) < W(G) \text{ or } W(G_2^*) < W(G). \quad (6)$$

3. Results

3.1. Unicyclic Graphs with the Fourth Minimum Wiener Index. Let $C_3(T_{n-5,1}^1)$ be the unicyclic graph as shown in Figure 1(a). Then, unicyclic graphs with the first smallest Wiener indices are completely characterized in the following result.

Theorem 1 (see [25]). *Suppose $G = C_m^{u_1,u_2,\dots,u_k}(T_1, T_2, \dots, T_k)$ is a unicyclic graph of order n, with $n \ge 7$. If $G \ncong S_n + e$, $C_4(S_{n-3})$, $C_3^{u_1,u_2}(S_2, S_{n-3})$, then*

$$W(S_n + e) < W(C_4(S_{n-3})) = W(C_3^{u_1,u_2}(S_2, S_{n-3})) < W\left(C_3\left(T_{n-5,1}^1\right)\right) \le W(G), \quad (7)$$

with equality if and only if

$$G \cong \begin{cases} C_3\left(T_{n-5,1}^1\right), & \text{if } n > 7, \\ C_3^{u_1,u_2}(S_3, S_3) \text{ or } C_5(S_3), & \text{if } n = 7. \end{cases} \quad (8)$$

As illustrated in the following theorem, we show that $C_5(S_{n-4})$ and $C_3^{u_1,u_2}(S_3, S_{n-4})$ have the fourth smallest Wiener indices.

Theorem 2. *Suppose $G = C_m^{u_1,u_2,\dots,u_k}(T_1, T_2, \dots, T_k)$ is a unicyclic graph of order n, with $n \ge 8$. If $G \ncong S_n + e$, $C_4(S_{n-3})$, $C_3^{u_1,u_2}(S_2, S_{n-3})$, $C_3(T_{n-5,1}^1)$, then*

$$W(S_n + e) < W(C_4(S_{n-3})) = W(C_3^{u_1,u_2}(S_2, S_{n-3})) < W\left(C_3\left(T_{n-5,1}^1\right)\right) < W(C_5(S_{n-4})) = W(C_3^{u_1,u_2}(S_3, S_{n-4})) \le W(G), \quad (9)$$

with equality if and only if $G \cong C_5(S_{n-4})$ or $C_3^{u_1,u_2}(S_3, S_{n-4})$.

Proof. By Lemma 1,

$$W(S_n + e) < W(C_4(S_{n-3})) = W(C_3^{u_1,u_2}(S_2, S_{n-3})) < W\left(C_3\left(T_{n-5,1}^1\right)\right) = n^2 - n - 3. \quad (10)$$

On the other hand, by Lemma 1, it is easily computed that

$$W(C_5(S_{n-4})) = W(C_3^{u_1,u_2}(S_3, S_{n-4})) = n^2 - 10. \quad (11)$$

Hence, for $n \geq 8$, $W(S_n + e) < W(C_4(S_{n-3})) = W(C_3^{u_1,u_2}(S_2, S_{n-3})) < W(C_3(T^1_{n-5,1})) < W(C_5(S_{n-4})) = W(C_3^{u_1,u_2}(S_3, S_{n-4}))$. So, it suffices to show that if G is a n-vertex unicyclic graph ($n \geq 8$), such that $G \ncong S_n + e, C_4(S_{n-3}), C_3^{u_1,u_2}(S_2, S_{n-3}), C_3(T^1_{n-5,1})$, then $W(C_5(S_{n-4})) \leq W(G)$, with equality if and only if $G \cong C_5(S_{n-4})$ or $C_3^{u_1,u_2}(S_3, S_{n-4})$. To this end, for convenience, we distinguish three cases that $m = 3, 4$ or $m \geq 5$. □

Case 1 ($m \geq 5$). If $k = 0$, then $G = C_n$. It is well known that

$$W(C_n) = \begin{cases} \frac{1}{8}n^3, & \text{if } n \text{ is even}, \\ \frac{1}{8}n(n^2-1), & \text{otherwise}. \end{cases} \quad (12)$$

Hence, if n is even, then

$$W(G) - W(C_5(S_{n-4})) = \frac{1}{8}n^3 - (n^2 - 10) = \frac{1}{8}n^3 - n^2 + 10 > 0, \quad (13)$$

and if n is odd, then

$$\begin{aligned} W(G) - W(C_5(S_{n-4})) &= \frac{1}{8}n(n^2-1) - (n^2 - 10) \\ &= \frac{1}{8}n^3 - \frac{9}{8}n^2 + 10 > 0, \end{aligned} \quad (14)$$

as desired.

Now assume that $k \geq 1$. Then, by Lemmas 2, 3, and 5,

$$\begin{aligned} W(G) &\geq W\left(C_m^{u_1,u_2,\ldots,u_k}\left(S_{l_1+1}, S_{l_2+1}, \ldots, S_{l_k+1}\right)\right) \\ &\geq W(C_m(S_{n-m+1})) \geq W(C_5(S_{n-4})), \end{aligned} \quad (15)$$

with equality if and only if $G \cong C_5(S_{n-4})$.

Case 2 ($m = 4$). In this case, we consider four subcases that k = 1, 2, 3, or 4.

Subcase 1 ($k = 1$). In this case, $G = C_4(T_1)$. Since $G = C_4(T_1) \ncong C_4(S_{n-3})$, it has been shown in [25] that

$$W(G) \geq W\left(C_4\left(T^1_{n-6,1}\right)\right) = n^2 - 7. \quad (16)$$

Hence, $W(G) \geq W(C_4(T^1_{n-6,1})) = n^2 - 7 > n^2 - 10 = W(C_5(S_{n-4}))$, as desired.

Subcase 2 ($k = 2$). In this case, $G = C_4^{u_1,u_2}(T_1, T_2)$. It has been shown in [24] that

$$\begin{aligned} W(G) = W(C_4^{u_1,u_2}(T_1, T_2)) &\geq W\left(C_4^{u_1,u_2}\left(S_{l_1+1}, S_{l_2+1}\right)\right) \\ &= n^2 - n - 4 + \alpha l_1 l_2, \end{aligned} \quad (17)$$

where $\alpha = 1$ if u_1 and u_2 are adjacent in C_4; otherwise, $\alpha = 2$. Noticing that $l_1 + l_2 = n - 4$, we have

$$\begin{aligned} W(G) - W(C_5(S_{n-4})) &\geq n^2 - n - 4 + \alpha l_1 l_2 - (n^2 - 10) \\ &= \alpha l_1 l_2 - n + 6 \\ &\geq 1 \times (n-5) - n + 6 > 0. \end{aligned} \quad (18)$$

Subcase 3 ($k = 3$). In this case, $G = C_4^{u_1,u_2,u_3}(T_1, T_2, T_3)$. Let G_1^* be the graph obtained from G by first removing T_1 from G and then identifying the root of T_1 with u_2, and let G_2^* be the graph obtained from G by first removing T_2 from G and then identifying the root of T_2 with u_1. Then, by Lemma 6, $W(G_1^*) < W(G)$ or $W(G_2^*) < W(G)$. Suppose that $W(G_1^*) < W(G)$. Then, according to the proof of Subcase 2, we know that $W(G_1^*) > W(C_5(S_{n-4}))$. Hence, we have $W(G) > W(C_5(S_{n-4}))$, as desired.

Subcase 4 ($k = 4$). The same argument as Subcase 3 shows that

$$W(G) = W(C_4^{u_1,u_2,u_3,u_4})(T_1, T_2, T_3, T_4) > W(C_5(S_{n-4})). \quad (19)$$

Case 3 ($m = 3$). For convenience, we distinguish the following three cases.

Subcase 5 ($k = 1$). In this case, $G = C_3(T_1)$. Let $C_3(T^2_{n-6,1})$ be the graph shown in Figure 1(b) . Then, it is well known that S_{n-3}, $T^1_{n-5,1}$, and $T^2_{n-6,1}$ has the minimum, second minimum, and third minimum of Wiener index in $\mathcal{T}_{n-2}$. Since $G \ncong S_n + e, C_3(T^1_{n-5,1})$, we know $T_1 \ncong S_{n-2}, T^1_{n-5,1}$. By Lemma 1,

$$\begin{aligned} W(G) = W(C_3(T_1)) &= W(C_3) + (n-3)d_u(C_3) \\ &+ 3d_{u_1}(T_1) + W(T_1). \end{aligned} \quad (20)$$

Noticing that $W(T_1) \geq W(T^2_{n-6,1})$ and $d_{u_1}(T_1) \geq d_{u_1}(T^2_{n-6,1})$, we readily have

$$W(G) \geq W\left(C_3\left(T^2_{n-6,1}\right)\right) = n^2 - 8 > W(C_5(S_{n-4})). \quad (21)$$

Subcase 6 ($k = 2$). In this case, $G = C_3^{u_1,u_2}(T_1, T_2)$. Without loss of generality, we assume that $l_1 \leq l_2$. Now, we consider the following two cases:

(1) $l_1 = 1$. In this case, $T_1 \cong S_2$. By Lemma 1,

$$\begin{aligned} W(G) = W(C_3^{u_1,u_2}(S_2, T_2)) &= W(C_3) + (n-3)\omega + (m-1) \\ &\cdot \left(d_{u_1}(S_2) + d_{u_2}(T_2)\right) + W(S_2) + W(T_2) \\ &+ l_1 d_{u_2}(T_2) + l_1 l_2 d_{C_3}(u_1, u_2) + l_2 d_{u_1}(S_2). \end{aligned} \quad (22)$$

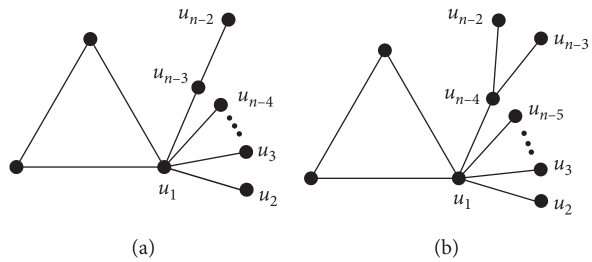

Figure 1: Unicyclic graphs $C_3(T^1_{n-5,1})$ (a) and $C_3(T^1_{n-6,2})$ (b).

Since $G \not\cong C_3^{u_1,u_2}(S_2, S_{n-3})$, we have $T_2 \not\cong S_{n-3}$. So $W(T_2) \geq W(T^1_{n-6,1})$ and $d_{u_2}(T_2) \geq d_{u_2}(T^1_{n-6,1})$. It thus follows that

$$W(G) = W\left(C_3^{u_1,u_2}(S_2, T_2)\right) \geq W\left(C_3^{u_1,u_2}\left(S_2, T^1_{n-6,1}\right)\right). \tag{23}$$

Again By Lemma 1, simple computation shows that $W(C_3^{u_1,u_2}(S_2, T^1_{n-6,1})) = n^2 - 7$. Hence, we have $W(G) \geq W(C_3^{u_1,u_2}(S_2, T^1_{n-6,1})) = n^2 - 7 > n^2 - 10 = W(C_5(S_{n-4}))$.

(2) $l_1 \geq 2$. In this case, it is obvious that $G \not\cong C_3^{u_1,u_2}(S_2, S_{n-3})$. By Lemma 2,

$$W(G) = W\left(C_3^{u_1,u_2}(T_1, T_2)\right) \geq W\left(C_3^{u_1,u_2}\left(S_{l_1+1}, S_{l_2+1}\right)\right). \tag{24}$$

It has been computed in [24] that

$$W\left(C_3^{u_1,u_2}\left(S_{l_1+1}, S_{l_2+1}\right)\right) = n^2 - 2n + l_1 l_2. \tag{25}$$

Bearing in mind that $l_1 \geq 2$ and $l_1 + l_2 = n - 3$, we readily have

$$W\left(C_3^{u_1,u_2}\left(S_{l_1+1}, S_{l_2+1}\right)\right) = n^2 - 2n + l_1 l_2 \geq n^2 - 2n + 2(n-5) = n^2 - 10, \tag{26}$$

with equality if and only if $l_1 = 2$ and $l_2 = n - 5$. Hence,

$$W(G) = W\left(C_3^{u_1,u_2}(T_1, T_2)\right) \geq W\left(C_3^{u_1,u_2}\left(S_{l_1+1}, S_{l_2+1}\right)\right) \geq W\left(C_3^{u_1,u_2}(S_3, S_{n-4})\right) = n^2 - 10, \tag{27}$$

with equality if and only if $G \cong C_3^{u_1,u_2}(S_3, S_{n-4})$.

Subcase 7 ($k = 3$). In this case, $G = C_3^{u_1,u_2,u_3}(T_1, T_2, T_3)$. It has been shown in [24] that

$$W(G) \geq W\left(C_3^{u_1,u_2,u_3}\left(S_{l_1+1}, S_{l_2+1}, S_{l_3+1}\right)\right) = n^2 - 2n + l_1 l_2 + l_1 l_3 + l_2 l_3. \tag{28}$$

Since $l_1 + l_2 + l_3 = n - 3$, we have

$$l_1 l_2 + l_1 l_3 + l_2 l_3 = l_1 l_2 + (l_1 + l_2) l_3 = l_1 l_2 + (l_1 + l_2) \cdot (n - 3 - (l_1 + l_2)). \tag{29}$$

If $l_1 + l_2 = n - 4$, then $l_1 l_2 \geq n - 5$ and thus $l_1 l_2 + l_1 l_3 + l_2 l_3 \geq n - 5 + (n-4)(n - 3 - (n-4)) = 2n - 9$; otherwise, $2 \leq l_1 + l_2 \leq n - 5$, then $l_1 l_2 \geq 1$ and thus $l_1 l_2 + l_1 l_3 + l_2 l_3 \geq 1 + (n-5)(n - 3 - (n-5)) = 2n - 9$. Hence, in both cases, we have $l_1 l_2 + l_1 l_3 + l_2 l_3 \geq 2n - 9$ and consequently,

$$W(G) \geq W\left(C_3^{u_1,u_2,u_3}\left(S_{l_1+1}, S_{l_2+1}, S_{l_3+1}\right)\right) \geq n^2 - 2n + (2n - 9) = n^2 - 9 > n^2 - 10. \tag{30}$$

□

3.2. Unicyclic Graphs with the Fourth Maximum Wiener Index. Unicyclic graphs with the first three largest Wiener indices were first characterized by Tang and Deng [24], but one extremal graph was missed. Then, Nasiri et al. [25] gave a complete characterization.

Theorem 3 (see [25]). *Suppose $G = C_m^{u_1,u_2,\ldots,u_k}(T_1, T_2, \ldots, T_k)$ is a unicyclic graph of order n, with $n \geq 6$. If $G \not\cong C_3(P_{n-2}), C_4(P_{n-3})$, and $C_3^{u_1,u_2}(P_2, P_{n-3})$, then*

$$W(G) \leq W\left(C_3(T(n-5,1,1))\right) < W\left(C_4(P_{n-3})\right) = W\left(C_3^{u_1,u_2}(P_2, P_{n-3})\right) < W\left(C_3(P_{n-2})\right), \tag{31}$$

with equality if and only if $G = C_3(T(n-5,1,1))$. Here, $T(n-5,1,1)$ is a unicyclic graph depicted in Figure 2(a).

Now, we characterize unicyclic graphs with the fourth largest Wiener indices.

Theorem 4. *Suppose that $G = C_m^{u_1,u_2,\ldots,u_k}(T_1, T_2, \ldots, T_k)$ is a unicyclic graph of order n, with $n \geq 8$. If $G \not\cong C_3(P_{n-2}), C_4(P_{n-3}), C_3^{u_1,u_2}(P_2, P_{n-3})$, and $C_3(T(n-5,1,1))$, then*

$$W(G) \leq W\left(C_3^{u_1,u_2}(P_3, P_{n-4})\right) < W\left(C_3(T(n-5,1,1))\right) < W\left(C_4(P_{n-3})\right) = W\left(C_3^{u_1,u_2}(P_2, P_{n-3})\right) < W\left(C_3(P_{n-2})\right), \tag{32}$$

with equality if and only if $G = C_3^{u_1,u_2}(P_3, P_{n-4})$.

Proof. By Lemma 1, it is easily computed that for $n \geq 8$,

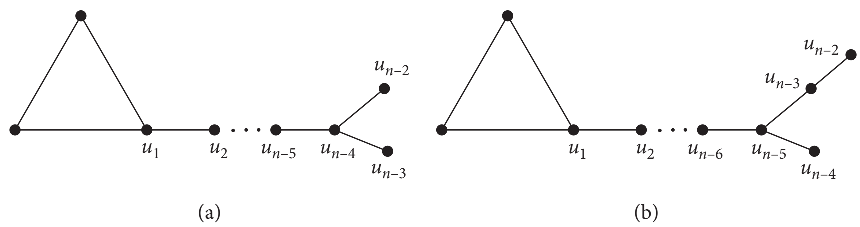

FIGURE 2: Unicyclic graphs $C_3(T(n-5,1,1))$ (a) and $C_3(T(n-6,1,2))$ (b).

$$\frac{1}{6}\left(n^3 - 19n + 72\right) = W\left(C_3^{u_1,u_2}(P_3, P_{n-4})\right) < \frac{1}{6}\left(n^3 - 13n + 30\right) = W\left(C_3(T(n-5,1,1))\right). \quad (33)$$

Hence, according to Theorem 4, we only need to show that for $n \geq 8$, if $G \ncong C_3(P_{n-2}), C_4(P_{n-3}), C_3^{u_1,u_2}(P_2, P_{n-3})$, and $C_3(T(n-5,1,1))$, then $W(G) \leq W(C_3^{u_1,u_2}(P_3, P_{n-4}))$, with equality if and only if $G \cong C_3^{u_1,u_2}(P_3, P_{n-4})$. To prove our result, we distinguish the following three cases according to m. □

Case 4 ($m \geq 5$). In this case, we consider two subcases that $k = 0$ and $k \geq 1$.

Subcase 8 ($k = 0$). In this case $G \cong C_n$. If n is even, then

$$W(C_n) - W\left(C_3^{u_1,u_2}(P_3, P_{n-4})\right) = \frac{1}{8}n^3 - \frac{1}{6}\left(n^3 - 19n + 72\right) = -\frac{1}{24}n^3 + \frac{19}{6}n - 12 < 0. \quad (34)$$

If n is odd, then

$$W(C_n) - W\left(C_3^{u_1,u_2}(P_3, P_{n-4})\right) = \frac{1}{8}n\left(n^2 - 1\right) - \frac{1}{6}\left(n^3 - 19n + 72\right) = -\frac{1}{24}n^3 + \frac{73}{24}n - 12 < 0. \quad (35)$$

Hence, $W(G) < W(C_3^{u_1,u_2}(P_3, P_{n-4}))$ as desired.

Subcase 9 ($k \geq 1$). By Lemmas 2 and 4,

$$W(G) \leq W\left(C_m^{u_1,u_2,\ldots,u_k}\left(P_{l_1+1}, P_{l_2+1}, \ldots, P_{l_k+1}\right)\right) \leq W\left(C_m(P_{l+1})\right). \quad (36)$$

We now prove that $W(C_m(P_{l+1})) < W(C_3^{u_1,u_2}(P_3, P_{n-4}))$. We first assume that m is even. Then, $m \geq 6$ and by Lemma 1,

$$W\left(C_m(P_{l+1})\right) = \frac{1}{6}\left[n^3 + \left(-\frac{3}{2}m^2 + 3m - 1\right)n + \left(\frac{5}{4}m^3 - 3m^2 + m\right)\right]. \quad (37)$$

Thus,

$$\begin{aligned} &W\left(C_3^{u_1,u_2}(P_3, P_{n-4})\right) - W\left(C_m(P_{l+1})\right) \\ &= \frac{1}{6}\left(n^3 - 19n + 72\right) - \frac{1}{6}\left[n^3 + \left(-\frac{3}{2}m^2 + 3m - 1\right)n + \left(\frac{5}{4}m^3 - 3m^2 + m\right)\right] \\ &= \frac{1}{4}\left(m^2 - 2m - 12\right)n - \frac{1}{24}\left(5m^3 - 12m^2 + 4m - 288\right) \\ &\geq \frac{1}{4}\left(m^2 - 2m - 12\right)m - \frac{1}{24}\left(5m^3 - 12m^2 + 4m - 288\right) \\ &= \frac{1}{24}m^3 - \frac{19}{6}m + 12 > 0. \end{aligned} \quad (38)$$

Now assume that m is odd. Then, $m \geq 5$ and by Lemma 1

$$W\left(C_m(P_{l+1})\right) = \frac{1}{6}\left[n^3 + \left(-\frac{3}{2}m^2 + 3m - 1\right)n + \left(\frac{5}{4}m^3 - 3m^2 + m\right) - \frac{1}{4}n + \frac{1}{8}m\right]. \quad (39)$$

Thus,

$$\begin{aligned} &W\left(C_3^{u_1,u_2}(P_3, P_{n-4})\right) - W\left(C_m(P_{l+1})\right) \\ &= \frac{1}{6}\left(n^3 - 19n + 72\right) - \frac{1}{6}\left[n^3 + \left(-\frac{3}{2}m^2 + 3m - 1\right)n + \left(\frac{5}{4}m^3 - 3m^2 + m\right)\right] + \frac{1}{4}n - \frac{1}{8}m \\ &= \frac{1}{4}\left(m^2 - 2m - 11\right)n - \frac{1}{24}\left(5m^3 - 12m^2 + 7m - 288\right) \\ &\geq \frac{1}{4}\left(m^2 - 2m - 11\right)m - \frac{1}{24}\left(5m^3 - 12m^2 + 7m - 288\right) \\ &= \frac{1}{24}m^3 - \frac{73}{24}m + 12 > 0. \end{aligned} \quad (40)$$

Therefore, we could conclude that $W(C_m(P_{l+1})) < W(C_3^{u_1,u_2}(P_3, P_{n-4}))$. □

Case 5 ($m = 4$). We consider subcases that $k = 1, 2, 3$, or 4.

Subcase 10 ($k = 1$). In this case, $G = C_4(T_1)$ with T_1 being a tree of order $n-3$. By assumption, $G \ncong C_4(P_{n-3})$ and so $T_1 \ncong P_{n-3}$. By Lemma 1,

$$W(G) = W(C_4(T_1)) = W(C_4) + (n-3)\omega + 3d_{u_1}(T_1) + W(T_1). \quad (41)$$

Noticing that $T(n-6,1,1)$ has the second maximum Wiener index in $\mathcal{T}_{n-3}$ and $d_{T_1}(u_1) \le d_{T(n-6,1,1)}(u_1)$, we have

$$W(G) = W(C_4(T_1)) \le W(C_4(T(n-6,1,1))) = \frac{1}{6}\left(n^3 - 19n + 54\right). \quad (42)$$

Thus, we have

$$W(G) \le \frac{1}{6}\left(n^3 - 19n + 54\right) < \frac{1}{6}\left(n^3 - 19n + 72\right) = W(C_3^{u_1,u_2}(P_3, P_{n-4})), \quad (43)$$

as desired.

Subcase 11 ($k = 2$). By Lemma 2, we have

$$W(G) = W(C_4^{u_1,u_2}(T_1, T_2)) \le W\left(C_4^{u_1,u_2}\left(P_{l_1+1}, P_{l_2+1}\right)\right). \quad (44)$$

In addition, it has been shown in [24] that

$$W(C_3^{u_1,u_2}(P_3, P_{n-4})) - W\left(C_4^{u_1,u_2}\left(P_{l_1+1}, P_{l_2+1}\right)\right) = (3-\alpha)l_1 l_2 - n + 6, \quad (45)$$

where $\alpha = 1$ if u_1 and u_2 are adjacent and 2, otherwise. Bearing in mind that $l_1 + l_2 = n - 4$, $l_1 l_2 \ge n - 5$ and

$$W(C_3^{u_1,u_2}(P_3, P_{n-4})) - W\left(C_4^{u_1,u_2}\left(P_{l_1+1}, P_{l_2+1}\right)\right) > (3-2)(n-5) - n + 6 = 1 > 0. \quad (46)$$

So we have $W(C_3^{u_1,u_2}(P_3, P_{n-4})) - W(G) > 0$ as desired.

Subcase 12 ($k = 3$ or $k = 4$). In this case, it has been shown in [24] that

$$\begin{aligned} W(C_4^{u_1,u_2,u_3})(T_1, T_2, T_3) &\le W(C_4^{u_1,u_2,u_3})\left(P_{l_1+1}, P_{l_2+1}, P_{l_3+1}\right) < W(C_4(T(n-6,1,1))), \\ W(C_4^{u_1,u_2,u_3,u_4})(T_1, T_2, T_3, T_4) &\le W(C_4^{u_1,u_2,u_3,u_4})\left(P_{l_1+1}, P_{l_2+1}, P_{l_3+1}, P_{l_4+1}\right) < W(C_4(T(n-6,1,1))). \end{aligned} \quad (47)$$

As shown in Subcase 10, $W(C_4(T(n-6,1,1))) < W(C_3^{u_1,u_2}(P_3, P_{n-4}))$. Thus, it is done.

Case 6 ($m = 3$). We distinguish three cases according to $k = 1, 2$, or 3.

Subcase 13 ($k = 1$). In this case, $G = C_3(T_1)$. By assumption, $C_3(T_1) \ncong C_3(P_{n-2}), C_3(T(n-5,1,1))$ and so $T_1 \ncong P_{n-2}, T(n-5,1,1)$. By Lemma 1,

$$W(C_3(T_1)) = W(C_3) + W(T_1) + 2(n-3) + 2d_{T_1}(u_1). \quad (48)$$

Since $T(n-6,1,2)$ has the third maximum Wiener index in $\mathcal{T}_{n-2}$ and $T_1 \ncong P_{n-2}, T(n-5,1,1)$, we readily have $W(C_3(T_1)) \le W(C_3(T(n-6,1,2)))$. It is easily verified that

$$W(C_3(T(n-6,1,2))) = \frac{1}{6}\left(n^3 - 19n + 48\right) < W(C_3^{u_1,u_2}(P_3, P_{n-4})), \quad (49)$$

as desired.

Subcase 14 ($k = 2$). In this case, $G = C_3^{u_1,u_2}(T_1, T_2)$. Without loss of generality, we suppose that $l_1 \le l_2$. For convenience, we distinguish the following two cases:

(1) $l_1 = 1$; that is, $T_1 \cong P_2$. Since $G \ncong C_3(P_2, P_{n-3})$, $T_2 \ncong P_{n-3}$. It is easy to compute that

$$W(C_3(P_2, T_2)) = W(C_3(P_2)) + W(T_2) + 3d_{T_2}(u_2) + 2(n-4). \quad (50)$$

Since $T(n-6,1,1)$ has the second maximum Wiener index in $\mathcal{T}_{n-3}$ and $T_2 \ncong P_{n-3}$, we have

$$W(C_3(P_2, T_2)) \le W(C_3(P_2, T(n-6,1,1))) = \frac{1}{6}\left(n^3 - 19n + 54\right). \quad (51)$$

Noticing that $W(C_3(P_2, T(n-6,1,1))) < W(C_3^{u_1,u_2}(P_3, P_{n-4}))$, we complete the proof.

(2) $l_1 \ge 2$. In this case, we have

$$W(G) = W(C_3^{u_1,u_2}(T_1, T_2)) \le W\left(C_3^{u_1,u_2}\left(P_{l_1+1}, P_{l_2+1}\right)\right). \quad (52)$$

By Lemma 1, simple calculation shows that

$$W\left(C_3^{u_1,u_2}\left(P_{l_1+1}, P_{l_2+1}\right)\right) = \frac{1}{6}n^3 - \frac{7}{6}n - l_1 l_2 + 2. \quad (53)$$

On the other hand,

$$\begin{aligned} &W\left(C_3^{u_1,u_2}\left(P_{l_1+1}, P_{l_2+1}\right)\right) - W(C_3^{u_1,u_2}(P_3, P_{n-4})) \\ &= \frac{1}{6}n^3 - \frac{7}{6}n - l_1 l_2 + 2 - \frac{1}{6}\left(n^3 - 19n + 72\right) \\ &= 2n - 10 - l_1 l_2 \le 2n - 10 - 2(n-5) = 0, \end{aligned} \quad (54)$$

with equality if and only if $l_1 = 2$ (and thus, $l_2 = n - 5$), that is, if and only if $C_3^{u_1,u_2}(P_{l_1+1}, P_{l_2+1}) \cong C_3^{u_1,u_2}(P_3, P_{n-4})$. Hence, $W(G) = W(C_3^{u_1,u_2}(T_1, T_2)) \leq W(C_3^{u_1,u_2}(P_3, P_{n-4}))$, with equality if and only if $G \cong C_3^{u_1,u_2}(P_3, P_{n-4})$.

Subcase 15 ($k = 3$). By Lemma 2, we have

$$\begin{aligned} W(G) &= W\left(C_3^{u_1,u_2,u_3}(T_1, T_2, T_3)\right) \\ &\leq W\left(C_3^{u_1,u_2,u_3}\left(P_{l_1+1}, P_{l_2+1}, P_{l_3+1}\right)\right). \end{aligned} \tag{55}$$

It has been shown in [25] that

$$\begin{aligned} W\left(C_3^{u_1,u_2,u_3}\left(P_{l_1+1}, P_{l_2+1}, P_{l_3+1}\right)\right) &= \frac{1}{6}n^3 - \frac{7}{6}n + 2 \\ &\quad - \left(l_1 l_2 l_3 + l_1 l_2 + l_1 l_3 + l_2 l_3\right). \end{aligned} \tag{56}$$

Hence,

$$\begin{aligned} &W\left(C_3^{u_1,u_2,u_3}\left(P_{l_1+1}, P_{l_2+1}, P_{l_3+1}\right)\right) - W\left(C_3^{u_1,u_2}(P_3, P_{n-4})\right) \\ &= \frac{1}{6}n^3 - \frac{7}{6}n + 2 - \left(l_1 l_2 l_3 + l_1 l_2 + l_1 l_3 + l_2 l_3\right) \\ &\quad - \frac{1}{6}\left(n^3 - 19n + 72\right) \\ &= 2n - 10 - \left(l_1 l_2 l_3 + l_1 l_2 + l_1 l_3 + l_2 l_3\right). \end{aligned} \tag{57}$$

Since it has been shown in the proof of Theorem 2 that $l_1 l_2 + l_1 l_3 + l_2 l_3 \geq 2n - 9$, it immediately follows that

$$W\left(C_3^{u_1,u_2,u_3}\left(P_{l_1+1}, P_{l_2+1}, P_{l_3+1}\right)\right) - W\left(C_3^{u_1,u_2}(P_3, P_{n-4})\right) < 0, \tag{58}$$

and the proof is complete. □

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare no conflicts of interest.

Authors' Contributions

All authors contributed equally to this paper.

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