Research Article

Unicyclic Graphs with the Fourth Extremal Wiener Indices

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Received 30 August 2019; Accepted 21 November 2019; Published 15 April 2020

Guest Editor: Jia-Bao Liu

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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 \( C_{u_1,u_2}(S_3, S_n-4) \) attain the fourth minimum Wiener index, whereas \( C_{u_1,u_2}(P_3, P_n-4) \) 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

\[
W(G) = \frac{1}{2} \sum_{(u,v) \in E(G)} d_G(u, v) = \frac{1}{2} \sum_{u \in V(G)} d_G(u).
\]

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 pendant 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 \( k \) pendant 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 $C_m = v_1v_2\ldots v_mv_1$ of length $m$. Suppose that $T_1, T_2, \ldots, T_k$ ($0 \leq k \leq m$) 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 $C_m$, $i = 1, 2, \ldots, k$. Such a unicyclic graph is denoted by $C_m^{u_1, u_2, \ldots, u_k} (T_1, T_2, \ldots, T_k)$. Specially, $G = C_n$ for $k = 0$. And if $k = 1$, we write $C_m (T_k)$ for $C_m^{u_1} (T_1)$. Let $|V (T_i)| = l_i + 1$, $i = 1, 2, \ldots, k$. Then, $l = l_1 + l_2 + \ldots + l_k = n - m$. Denote by $T_n$ 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 $G = C_m^{u_1, u_2, \ldots, u_k} (T_1, T_2, \ldots, T_k)$ be a unicyclic graph. Then,

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

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

Lemma 2 (see [24]). Let $G_1 = C_m^{u_1, u_2, \ldots, u_k} (S_{i_1}, S_{i_2}, \ldots, S_{i_{l_1}})$ and $G_2 = C_m^{u_1, u_2, \ldots, u_k} (P_{l_1+1}, P_{l_2+1}, \ldots, P_{l_k+1})$, where $u_1, u_2, \ldots, u_k$ are the centers of $S_{i_1}, S_{i_2}, \ldots, S_{i_{l_1}}$, respectively, in $G_1$ and $u_1, u_2, \ldots, u_k$ are the pendant vertices of $P_{l_1+1}, P_{l_2+1}, \ldots, P_{l_k+1}$ respectively, in $G_2$. Then,

$$W (G_1) \leq W (G) \leq W (G_2),$$

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

Lemma 3 (see [24]). Let $G_1 = C_m^{u_1, u_2, \ldots, u_k} (S_{i_1+1}, S_{i_2+1}, \ldots, S_{i_{l_1}})$ and $l_i = n (T_i)$, $i = 1, 2, \ldots, k$. If $k \geq 1$, then

$$W (G_1) \geq W (C_m (S_{i_1+1})).$$

with the equality if and only if $G_1 \equiv C_m (S_{i_1+1})$, where $l = l_1 + l_2 + \ldots + l_k = n - m$.

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

$$W (G_2) \geq W (C_m (P_{l_1+1})).$$

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

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

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 $u'$. Then, $G_1$ be the graph obtained from $H, X,$ and $Y$ by identifying vertices $v, v', u$. Then,

$$W (G_1) < W (G) \text{ or } W (G_2) < W (G).$$

3. Results

3.1. Unicyclic Graphs with the Fourth Minimum Wiener Index. Let $C_3 (T_{n-5})$ 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 $G = C_m^{u_1, u_2, \ldots, u_k} (T_1, T_2, \ldots, T_k)$ is a unicyclic graph of order $n$, with $n \geq 7$. If $G \neq S_n + e$, $C_4 (S_{n-3}), C_3^{u_1, u_2} (S_2, S_{n-3})$, then

$$W (S_n + e) < W (C_4 (S_{n-3})) = W (C_3^{u_1, u_2} (S_2, S_{n-3}))$$

with equality if and only if

$$G \equiv \begin{cases} 
C_3 (T_{n-5}), & \text{if } n > 7, \\
C_3^{u_1, u_2} (S_3, S_3) \text{ or } C_3 (S_3), & \text{if } n = 7.
\end{cases}$$

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

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

$$W (S_n + e) < W (C_4 (S_{n-3})) = W (C_3^{u_1, u_2} (S_2, S_{n-3}))$$

with equality if and only if

$$G \equiv \begin{cases} 
C_3 (T_{n-5}), & \text{if } n > 7, \\
C_3^{u_1, u_2} (S_3, S_3) \text{ or } C_3 (S_3), & \text{if } n = 7.
\end{cases}$$

Proof. By Lemma 1,

$$W (S_n + e) < W (C_4 (S_{n-3})) = W (C_3^{u_1, u_2} (S_2, S_{n-3})) < W (C_3 (T_{n-5})).$$

On the other hand, by Lemma 1, it is easily computed that
\[ W(C_5(S_{n-4})) = W(C_4^{u_1,u_2}(S_3, S_{n-4})) = n^2 - 10. \]  
\[ (11) \]

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

\[ \square \]

Case 1 \((m \geq 5)\). If \( k = 0 \), then \( G = C_m \). It is well known that
\[ W(C_m) = \begin{cases} 
\frac{1}{8}n^3, & \text{if } n \text{ is even,} \\
\frac{1}{8}n(n^2 - 1), & \text{otherwise.} 
\end{cases} \]
\[ (12) \]

Hence, if \( n \) is even, then
\[ W(G) - W(C_5(S_{n-4})) = \frac{1}{8}n^3 - (n^2 - 10) = \frac{1}{8}n^3 - n^2 + 10 > 0, \]
\[ (13) \]

and if \( n \) is odd, then
\[ W(G) - W(C_5(S_{n-4})) = \frac{1}{8}n(n^2 - 1) - (n^2 - 10) \\
= \frac{1}{8}n^3 - \frac{9}{8}n^2 + 10 > 0, \]
\[ (14) \]
as desired.

Now assume that \( k \geq 1 \). Then, by Lemmas 2, 3, and 5,
\[ W(G) \geq W(C_m^{u_1,u_2,...,u_k}(S_1, S_2, \ldots, S_n)) \geq W(C_m(S_{n+m-1})) = W(C_5(S_{n-4})), \]
\[ (15) \]
with equality if and only if \( G \equiv C_5(S_{n-4}) \).

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 \( G = C_4(T_1) \neq C_4(S_{n-3}) \), it has been shown in [25] that
\[ W(G) \geq W(C_4(T^1_{n-6})) = n^2 - 7. \]
\[ (16) \]

Hence, \( W(G) \geq W(C_4(T^1_{n-6})) = n^2 - 7 > n^2 - 10 = W(C_5(S_{n-4})) \), 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
\[ W(G) = W(C_4^{u_1,u_2}(T_1, T_2)) \geq W(C_4^{u_1,u_2}(S_1, S_2, \ldots, S_n)) = n^2 - n - 4 + \alpha l_2, \]
\[ (17) \]

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
\[ W(G) - W(C_5(S_{n-4})) \geq n^2 - n - 4 + \alpha l_1l_2 - (n^2 - 10) \\
= \alpha l_1l_2 - n + 6 \\
\geq 1 \times (n - 5) - n + 6 > 0. \]
\[ (18) \]

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

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 \( S_{n-3}, T^3_{n-5,1} \), and \( T^2_{n-6,1} \) has the minimum second minimum, and third minimum of Wiener index in \( T_{n-2} \). Since \( G \# S_n + e, C_3(T^1_{n-5,1}) \), we know \( T_1 \# S_{n-2}, T^1_{n-5,1} \). By Lemma 1,
\[ W(G) = W(C_3(T_1)) = W(C_3) + (n - 3)d_u(C_3) + 3d_{u_1}(T_1) + W(T_1). \]
\[ (20) \]

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

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, \( T_1 \equiv S_2 \). By Lemma 1,
\[ W(G) = W(C_3^{u_1,u_2}(S_2, T_2)) = W(C_3) + (n - 3)\omega + (m - 1) \cdot (d_{u_1}(S_2) + d_{u_2}(T_2)) + W(S_2) + W(T_2) + l_1d_{u_1}(T_2) + l_2d_{u_2}(S_2). \]
\[ (22) \]
Since \( G \neq C_{m,n}^{(n)}(S_2, S_{n-3}) \), we have \( T_2 \neq S_{n-3} \). So \( W(T_2) \geq W(T_{n-6,1}^1) \) and \( d_{m_1}(T_2) \geq d_{m_1}(T_{n-6,1}^1) \). It thus follows that
\[
W(G) = W(C_{m,n}^{(n)}(S_2, T_2)) \leq W(C_{m,n}^{(n)}(S_2, T_{n-6,1}^1)).
\]

Again By Lemma 1, simple computation shows that \( W(C_{m,n}^{(n)}(S_2, T_{n-6,1}^1)) = n^2 - 7 \). Hence, we have \( W(G) \leq W(C_{m,n}^{(n)}(S_2, T_{n-6,1}^1)) = n^2 - 7 > n^2 - 10 = W(C_2(S_{n-4})) \).

(2) \( l_1 \geq 2 \). In this case, it is obvious that \( G \neq C_{m,n}^{(n)}(S_2, S_{n-3}) \). By Lemma 2, \( W(G) = W(C_{m,n}^{(n)}(T_1, T_2)) \geq W(C_{m,n}^{(n)}(S_1, S_{n-1})) \).

It has been computed in [24] that
\[
W(C_{m,n}^{(n)}(S_1, S_{n-1})) = n^2 - 2n + l_1 l_2.
\]

Bearing in mind that \( l_1 \geq 2 \) and \( l_1 + l_2 = n - 3 \), we readily have
\[
W(C_{m,n}^{(n)}(S_1, S_{n-1})) = n^2 - 2n + l_1 l_2 \geq n^2 - 2n + 2(n - 5) = n^2 - 10,
\]
with equality if and only if \( l_1 = 2 \) and \( l_2 = n - 5 \). Hence,
\[
W(G) = W(C_{m,n}^{(n)}(T_1, T_2)) \geq W(C_{m,n}^{(n)}(S_1, S_{n-1})) \geq W(C_{m,n}^{(n)}(S_3, S_{n-4})) = n^2 - 10,
\]
with equality if and only if \( G \equiv C_{m,n}^{(n)}(S_3, S_{n-4}) \).

Subcase 7 \((k = 3)\). In this case, \( G = C_{m,n}^{(n)}(T_1, T_2, T_3) \). It has been shown in [24] that
\[
W(G) \geq W(C_{m,n}^{(n)}(S_1, S_2, S_3)) = n^2 - 2n + l_1 l_2 + l_1 l_3 + l_2 l_3.
\]

Since \( l_1 + l_2 + l_3 = n - 3 \), we have
\[
l_1 l_2 + l_1 l_3 + l_2 l_3 = l_1 l_2 + (l_1 + l_2) l_3 = l_1 l_2 + (l_1 + l_2)
\cdot (n - 3 - (l_1 + l_2)),
\]
with equality if and only if \( G \equiv C_{m,n}^{(n)}(T_1, T_2, T_3) \).

If \( l_1 + l_2 = n - 4 \), then \( l_1 l_2 \geq n - 5 \) and thus \( l_1 l_3 + l_1 l_2 + l_2 l_3 \geq n - 5 + (n - 4)(n - 3 - (n - 4)) = 2n - 9 \); otherwise, \( 2 \leq l_1 + l_2 \leq n - 5 \), then \( l_1 l_2 \geq 1 \) and thus \( l_1 l_2 + l_1 l_3 + l_1 l_2 \geq 1 + (n - 5)(n - 3 - (n - 3)) = 2n - 9 \). Hence, in both cases, we have \( l_1 l_2 + l_1 l_3 + l_2 l_3 \geq 2n - 9 \) and consequently,
\[
W(G) \geq W(C_{m,n}^{(n)}(S_1, S_2, S_3)) \geq n^2 - 2n + (2n - 9) = n^2 - 9 > n^2 - 10.
\]

\[
\tag{30}
\]

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 \( G = C_{m,n}^{(n)}(T_1, T_2, \ldots, T_k) \) is a unicyclic graph of order \( n \), with \( n \geq 6 \). If \( G \neq C_3(P_{n-2}), C_4(P_{n-3}), \) and \( C_{m,n}^{(n)}(P_2, P_{n-3}) \), then
\[
W(G) \leq W(C_3(T(n - 5, 1, 1))) < W(C_4(P_{n-3})) = W(C_{m,n}^{(n)}(P_2, P_{n-3})) < W(C_3(P_{n-2})),
\]
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 \( G = C_{m,n}^{(n)}(T_1, T_2, \ldots, T_k) \) is a unicyclic graph of order \( n \), with \( n \geq 8 \). If \( G \neq C_3(P_{n-2}), C_4(P_{n-3}), C_{m,n}^{(n)}(P_2, P_{n-3}) \), and \( C_3(T(n - 5, 1, 1)) \), then
\[
W(G) \leq W(C_{m,n}^{(n)}(P_2, P_{n-3})) < W(C_3(T(n - 5, 1, 1))) < W(C_4(P_{n-3})) = W(C_{m,n}^{(n)}(P_2, P_{n-3})) < W(C_3(P_{n-2})),
\]
with equality if and only if \( G = C_{m,n}^{(n)}(P_3, P_{n-4}) \).

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

Figure 1: Unicyclic graphs \( C_3(T_{n-5,1}) \) (a) and \( C_3(T_{n-6,1}) \) (b).
\[
\frac{1}{6}(n^3 - 19n + 72) = W(C_3^{u_1, u_2} (P_3, P_{n-4}))
\]

(33)

\[
< \frac{1}{6}(n^3 - 13n + 30) = W(C_3(T(n - 5, 1, 1))).
\]

Hence, according to Theorem 4, we only need to show that for \( n \geq 8 \), if \( G \not\cong C_3(P_{n-2}), C_4(P_{n-3}), C_5^{u_1, u_2} (P_2, P_{n-3}), \) and \( C_4(T(n - 5, 1, 1)) \), 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 \( m \).

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

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

\[
W(C_n) - W(C_3^{u_1, u_2} (P_3, P_{n-4})) = \frac{1}{8}n^3 - \frac{1}{6}(n^3 - 19n + 72)
\]

(34)

\[
= -\frac{1}{24}n^3 + \frac{19}{6}n - 12 < 0.
\]

If \( n \) is odd, then

\[
W(C_n) - W(C_3^{u_1, u_2} (P_3, P_{n-4})) = \frac{1}{8}n^3 - 1
\]

(35)

\[
= -\frac{1}{24}n^3 + \frac{73}{24}n - 12 < 0.
\]

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

\underline{Subcase 9 \((k \geq 1)\):} By Lemmas 2 and 4,

\[
W(G) \leq W(C_m^{u_1, u_2} (P_{i_1}, P_{i_2}, \ldots, P_{i_{m-1}})) \leq W(C_m(P_{i_1})).
\]

(36)

We now prove that \( W(C_m(P_{i_1}))) < W(C_3^{u_1, u_2} (P_3, P_{n-4})) \). We first assume that \( m \) is even. Then, \( m \geq 6 \) and by Lemma 1,

\[
W(C_m(P_{i_1})) = \frac{1}{6}[n^3 + \left(\frac{3}{2}m^2 + 3m - 1\right)n + \left(\frac{5}{4}m^3 - 3m^2 + m\right)].
\]

(37)

Thus,

\[
W(C_3^{u_1, u_2} (P_3, P_{n-4})) - W(C_m(P_{i_1}))
\]

\[
= \frac{1}{6}(n^3 - 19n + 72) - \frac{1}{6}n^3 + \left(\frac{3}{2}m^2 + 3m - 1\right)n + \left(\frac{5}{4}m^3 - 3m^2 + m\right)
\]

\[
+ \left(\frac{5}{4}m^3 - 3m^2 + m\right)
\]

\[
= \frac{1}{6}(m^2 - 2m - 12)n - \frac{1}{24}(5m^3 - 12m^2 + 4m - 288)
\]

\[
\geq \frac{1}{4}(m^2 - 2m - 12)m - \frac{1}{24}(5m^3 - 12m^2 + 4m - 288)
\]

\[
= \frac{1}{24}m^3 - \frac{19}{6}m + 12 > 0.
\]

Therefore, we could conclude that \( W(C_m(P_{i_1}))) < W(C_3^{u_1, u_2} (P_3, P_{n-4})) \).

\underline{Case 5 \((m = 4)\):} We consider subcases that \( k = 1, 2, 3, \) or 4.
Subcase 10 ($k = 1$). In this case, $G = C_n(T_i)$ with $T_i$ being a tree of order $n - 3$. By assumption, $G \not= C_n(P_{n-3})$ and so $T_i \not= P_{n-3}$. By Lemma 1,

$$W(G) = W(C_n(T_i)) = W(C_n) + (n - 3)\omega + 3d_{T_i}(T_i) + W(T_i).$$

(41)

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

$$W(G) = W(C_n(T_i)) \leq W(C_n(T(n - 6, 1, 1)))$$

$$= \frac{1}{6}(n^3 - 19n + 54).$$

(42)

Thus, we have

$$W(G) \leq \frac{1}{6}(n^3 - 19n + 54) < \frac{1}{6}(n^3 - 19n + 72)$$

$$= W(c_{3}^{u_1,u_2}(P_3, P_{n-4})),$$

(43)

as desired.

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

$$W(G) = W(C_4^{u_1,u_2}(T_1, T_2)) \leq W(c_4^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})).$$

(44)

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

$$W(c_4^{u_1,u_2}(P_3, P_{n-4})) - W(c_4^{u_1,u_2}(P_{l_1+1}, P_{l_2+1}))$$

$$= (3 - \alpha)l_1l_2 - n + 6,$$

(45)

where $\alpha = 1$ if $u_1$ and $u_2$ are adjacent and 2, otherwise. Bearing in mind that $l_1 + l_2 = n - 4$, $l_1l_2 \geq n - 5$ and

$$W(c_4^{u_1,u_2}(P_3, P_{n-4})) - W(c_4^{u_1,u_2}(P_{l_1+1}, P_{l_2+1}))$$

$$> (3 - 2)(n - 5) - n + 6 = 1 > 0.$$ 

(46)

So we have $W(c_4^{u_1,u_2}(P_3, P_{n-4})) - W(G) > 0$ as desired.

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

$$W(C_4^{u_1,u_2,u_3}(T_1, T_2, T_3)) \leq W(C_4^{u_1,u_2,u_3}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1}))$$

$$< W(C_4(T(n - 6, 1, 1))).$$

(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 $k = 1, 2, \text{ or } 3$.

Subcase 13 ($k = 1$). In this case, $G = C_3(T_i)$. By assumption, $C_3(T_i) \not= C_3(P_{n-2}, C_3(T(n - 5, 1, 1))$ and so $T_i \not= P_{n-2}, T(n - 5, 1, 1)$. By Lemma 1,

$$W(C_3(T_i)) = W(C_3) + W(T_i) + 2(n - 3) + 2d_{T_i}(u_i).$$

(48)

Since $T(n - 6, 1, 2)$ has the third maximum Wiener index in $\mathcal{T}_{n-3}$ and $T_i \not= P_{n-2}, T(n - 5, 1, 1)$, we readily have $W(C_3(T_i)) \leq W(C_3(T(n - 6, 1, 2)))$. It is easily verified that

$$W(C_3(T(n - 6, 1, 2))) = \frac{1}{6}(n^3 - 19n + 48)$$

$$< W(c_3^{u_1,u_2}(P_3, P_{n-4})),$$

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 $l_1 \leq l_2$. For convenience, we distinguish the following two cases:

(1) $l_1 = 1$; that is, $T_1 \equiv P_2$. Since $G \not= C_3(P_2, P_{n-3})$, $T_2 \not= P_{n-3}$. It is easy to compute that

$$W(C_3(P_2, T_2)) = W(C_3(P_3)) + W(T_2) + 3d_{T_2}(u_2) + 2(n - 4).$$

(50)

Since $T(n - 6, 1, 1)$ has the second maximum Wiener index in $\mathcal{T}_{n-3}$ and $T_2 \not= P_{n-3}$, we have

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

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

$$W(G) = W(C_3^{u_1,u_2}(T_1, T_2)) \leq W(c_3^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})).$$

(52)

By Lemma 1, simple calculation shows that

$$W(c_3^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})) = \frac{1}{6}n^3 - \frac{7}{6}n - l_1l_2 + 2.$$ 

(53)

On the other hand,

$$W(c_3^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})) - W(c_3^{u_1,u_2}(P_3, P_{n-4}))$$

$$= \frac{1}{6}n^3 - \frac{7}{6}n - l_1l_2 + 2 - \frac{1}{6}(n^3 - 19n + 72)$$

$$= 2n - 10 - l_1l_2 \leq 2n - 10 - 2(n - 5) = 0,$$ 

(54)
with equality if and only if $l_1 = 2$ (and thus, $l_2 = n - 5$), that is, if and only if $C_3^{l_1,l_2}(P_{l_1+1}, P_{l_2+1}) \equiv C_3^{l_1,l_2}(P_3, P_{n-4})$. Hence, $W(G) = W(C_3^{l_1,l_2}(T_1, T_2)) \leq W(C_3^{l_1,l_2}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1}))$, with equality if and only if $G \equiv C_3^{l_1,l_2}(P_3, P_{n-4})$.

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

$$W(G) = W(C_3^{l_1,l_2,l_3}(T_1, T_2, T_3)) \leq W(C_3^{l_1,l_2,l_3}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1})).$$

(55)

It has been shown in [25] that

$$W(C_3^{l_1,l_2,l_3}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1})) = \frac{1}{6} n^3 - \frac{7}{6} n + 2 - (l_1 l_2 l_3 + l_1 l_2 + l_1 l_3 + l_2 l_3).$$

(56)

Hence,

$$W(C_3^{l_1,l_2,l_3}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1})) - W(C_3^{l_1,l_2,l_3}(P_3, P_{n-4})) = \frac{1}{6} n^3 - \frac{7}{6} n + 2 - (l_1 l_2 l_3 + l_1 l_2 + l_1 l_3 + l_2 l_3)$$

$$- \frac{1}{6} (n^3 - 19n + 72)$$

$$= 2n - 10 - (l_1 l_2 l_3 + l_1 l_2 + l_1 l_3 + l_2 l_3).$$

(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

$$W(C_3^{l_1,l_2,l_3}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1})) - W(C_3^{l_1,l_2,l_3}(P_3, P_{n-4})) < 0,$$

(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.

**Acknowledgments**

This research was funded by the National Natural Science Foundation of China (through grant nos. 116711347 and 11861032) and the project ZR2019YQ02 by the Shandong Provincial Natural Science Foundation.

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