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The (n,n)-graphs with the first three extremal Wiener indices

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Let $G = (V, E)$ be a simple connected graph with vertex set V and edge set E. The Wiener index $W(G)$ of G is the sum of distances between all pairs of vertices in G, i.e., $W(G) = \sum_{\{u,v\}\subseteq G} d_G(u, v)$, where $d_G(u, v)$ is the distance between vertices u and v in G. In this paper, we first give a new formula for calculating the Wiener index of an (n,n)-graph according its structure, and then characterize the (n,n)-graphs with the first three smallest and largest Wiener indices by this formula.

KEY WORDS: (n,n)-graph, Wiener index, distance

1. Introduction

All graphs in this paper are simple, finite, and undirected. The vertex and edge sets of a graph G are $V(G)$ and $E(G)$, respectively. The number of vertices of G is denoted by $n(G)$ and it is called the order of G. The distance $d_G(u, v)$ between vertices u and v in G is the number of edges on a shortest path connecting these vertices in G. The distance of a vertex $v \in V(G)$, denoted by $d_G(v)$, is the sum of distances between v and all other vertices of G, i.e., $d_G(v) = \sum_{x\in V(G)} d_G(v, x)$. The Wiener index of G, denoted by $W(G)$, is defined as

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

The Wiener index is usual in chemical literature, since Wiener [1] in 1947 seems to be the first who considered it. Wiener himself used the name path number and conceived W 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].

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From the mid-1970s, the Wiener index gained much popularity and, since then, new results related to it are constantly being reported. For a review, historical details and further bibliography on the chemical applications of the Wiener index (see [3–5]). Results on the Wiener index of trees and hexagonal systems were summarized in [6–8].

In the present paper, we study the Wiener indices of (n,n)-graphs, i.e., simple and connected graphs with n vertices and n edges, and characterize the graphs with the first three largest and smallest Wiener indices among all the (n,n)-graphs.

2. A new formula for calculating the Wiener indices of (n,n)-graphs

Let $G = (V, E)$ be an (n,n)-graph with its unique circuit $C_m = v_1 v_2 \ldots v_m v_1$ of length m, $T_1, T_2, \ldots, T_k (0 \leqslant k \leqslant m)$ are all the nontrivial components (they are all nontrivial trees) of $G - E(C_m)$, u_i is the common vertex of T_i and C_m, $i = 1, 2, \ldots, k$. Such an (n,n)-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 $C_m(T_1)$ for $C_m^{u_1}(T_1)$; and $S_n + e$ for $C_3^{u_1}(S_{n-2})$. Let $n(T_i) = l_i + 1$, $i = 1, 2, \ldots, k$, then $l = l_1 + l_2 + \cdots + l_k = n - m$.

For calculating the Wiener indices of (n,n)-graphs, we need the following result of the Wiener indices of P_n and S_n.

Lemma 1. ([7]). $W(P_n) = \binom{n+1}{3}$ and $W(S_n) = (n-1)^2$, where P_n is the path of order n and S_n is the star of order n. If T is any tree of order n different from P_n and S_n, then

$$W(S_n) < W(T) < W(P_n).$$

The following lemma can be proved easily.

Lemma 2. Let C_n be the circuit of order n, u is a vertex on C_n. Then

$$d_{C_n}(u) = \begin{cases} \frac{1}{4}n^2, & \text{if } n \text{ is even,} \\ \frac{1}{4}(n^2-1), & \text{if } n \text{ is odd.} \end{cases}$$

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

Now, we give a new formula for calculating the Wiener index of (n,n)-graphs.

Theorem 3. Let $G = C_m^{u_1,u_2,\ldots,u_k}(T_1, T_2, \ldots, T_k)$ be an (n,n)-graph. Then

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

where $l_i = n(T_i) - 1$, $\omega_i = d_{T_i}(u_i)$, $i = 1, 2, \ldots, k$, $\omega = d_{C_m}(u)$, $u \in V(C_m)$.

Proof. We divide the distances between the vertices of G into the following four groups:

(i) the distances between the vertices of C_m; (ii) the distances between a vertex of C_m and a vertex of $T_i - \{u_i\}$; (iii) the distances between the vertices of $T_i - \{u_i\}$; (iv) the distances between a vertex of $T_i - \{u_i\}$ and a vertex of $T_j - \{u_j\}$, where $i \neq j$.

(i) The sum of distances between the vertices of C_m is the Wiener index $W_1 = W(C_m)$.

(ii) The sum of distances between a vertex of C_m and a vertex of $T_i - \{u_i\}$ is

$$\begin{aligned} W_2 &= \sum_{i=1}^{k}\sum_{x\in C_m}\sum_{y\in T_i-\{u_i\}} d_G(x, y) \\ &= \sum_{i=1}^{k}\sum_{x\in C_m}\sum_{y\in T_i-\{u_i\}} [d_G(x, u_i) + d_G(u_i, y)] \\ &= \sum_{i=1}^{k}\sum_{x\in C_m} [l_i d_{C_m}(x, u_i) + \omega_i] \\ &= \sum_{i=1}^{k} [l_i\omega + m\omega_i] \\ &= (n-m)\omega + m\sum_{i=1}^{k}\omega_i. \end{aligned}$$

(iii) The sum of distances between the vertices of $T_i - \{u_i\}$ is $W_3 = \sum_{i=1}^{k}[W(T_i) - \omega_i]$.

(iv) Let W_4 be the sum of distances between a vertex of $T_i - \{u_i\}$ and a vertex of $T_j - \{u_j\}$, where $i \neq j$. $\forall x \in T_i - \{u_i\}$, $\forall y \in T_j - \{u_j\}$, we have

$$d_G(x, y) = d_{T_i}(x, u_i) + d_{C_m}(u_i, u_j) + d_{T_j}(u_j, y).$$

and

$$\sum_{x\in T_i-\{u_i\}}\sum_{y\in T_j-\{u_j\}} d_G(x,y) = \sum_{x\in T_i-\{u_i\}}\sum_{y\in T_j-\{u_j\}} [d_{T_i}(x,u_i)+d_{C_m}(u_i,u_j) + d_{T_j}(u_j,y)] = l_i\omega_j + l_i l_j d_{C_m}(u_i,u_j) + l_j\omega_i.$$

So,

$$W_4 = \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} (l_i\omega_j + l_i l_j d_{C_m}(u_i,u_j) + l_j\omega_i).$$

And

$$W(G) = W_1 + W_2 + W_3 + W_4 = W(C_m) + (n-m)\omega + (m-1)\sum_{i=1}^{k}\omega_i + \sum_{i=1}^{k} W(T_i) + \sum_{i=1}^{k-1}\sum_{j=i+1}^{k}(l_i\omega_j + l_i l_j d_{C_m}(u_i,u_j) + l_j\omega_i).$$

Note that $n-1 \leqslant d_T(u) \leqslant \frac{1}{2}n(n-1)$ for any tree T of order n and a vertex u of T, with the left (or the right) equality if and only if $T \cong S_n$ and u is the center of S_n (or $T \cong P_n$ and u is a pendent vertex of P_n). Using lemma 1 and theorem 3, we have

Corollary 4. Let $G_1 = C_m^{u_1,u_2,\ldots,u_k}(S_{l_1+1}, S_{l_2+1}, \ldots, S_{l_k+1})$, $G_2 = C_m^{u_1,u_2,\ldots,u_k}(P_{l_1+1}, P_{l_2+1}, \ldots, P_{l_k+1})$, where $u_1, u_2, \ldots, u_k$ are the centers of $S_{l_1+1}, S_{l_2+1}, \ldots, S_{l_k+1}$, respectively, in G_1; and $u_1, u_2, \ldots, u_k$ are the pendent vertices of $P_{l_1+1}, P_{l_2+1}, \ldots, P_{l_k+1}$, respectively, in G_2. Then

$$W(G_1) \leqslant W(G) \leqslant W(G_2)$$

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

3. The (n,n)-graphs with the first three smallest Wiener indices

In this section, we characterize the (n,n)-graphs with the smallest, the second smallest and the third smallest Wiener indices among all the (n,n)-graphs.

Lemma 5. Let $G_1 = C_m^{u_1,u_2,\ldots,u_k}(S_{l_1+1}, S_{l_2+1}, \ldots, S_{l_k+1})$ and $l_i = n(T_i) - 1$, $i = 1, 2, \ldots, k$. If $k \geqslant 1$, then

$$W(G_1) \geqslant W(C_m^{u_1}(S_{l+1}))$$

with the equality if and only if $G_1 \cong C_m^{u_1}(S_{l+1})$, where $l = l_1 + l_2 + \cdots + l_k = n - m$.

Proof. By lemma 1 and theorem 3, we have

$$
\begin{aligned}
W(G_1) = {} & W(C_m) + (n-m)\omega + (m-1)\sum_{i=1}^{k} l_i + \sum_{i=1}^{k} l_i^2 \\
& + \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} (l_i l_j + l_i l_j d_{C_m}(u_i, u_j) + l_j l_i) \\
& = W(C_m) + (n-m)\omega + (m-1)l + l^2 + \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} l_i l_j d_{C_m}(u_i, u_j) \\
& \geqslant W(C_m) + (n-m)\omega + (m-1)l + l^2 \\
& = W(C_m^{u_1}(S_{l+1}))
\end{aligned}
$$

with the equality if and only if $k = 1$, i.e., $G_1 \cong C_m^{u_1}(S_{l+1})$.

Lemma 6. If $m > 3$, then $W(C_m^{u_1}(S_{n-m+1})) > W(C_{m-1}^{u_1}(S_{n-m+2}))$.

Proof. From theorem 3, it is known that

$$
\begin{aligned}
& W(C_m^{u_1}(S_{n-m+1})) - W(C_{m-1}^{u_1}(S_{n-m+2})) \\
& \quad = [W(C_m) + (n-m)d_{C_m}(u) + (m-1)(n-m) + W(S_{n-m+1})] \\
& \qquad -[W(C_{m-1}) + (n-m+1)d_{C_{m-1}}(u) + (m-2)(n-m+1) + W(S_{n-m+2})].
\end{aligned}
$$

If n is odd, then, by lemmas 1 and 2, we have

$$
\begin{aligned}
& W(C_m^{u_1}(S_{n-m+1})) - W(C_{m-1}^{u_1}(S_{n-m+2})) \\
& = \left[\frac{1}{8}m(m^2-1) + \frac{1}{4}(n-m)(m^2-1) + (m-1)(n-m) + (n-m)^2\right] \\
& \quad - \left[\frac{1}{8}(m-1)^3 + \frac{1}{4}(n-m+1)(m-1)^2 + (m-2)(n-m+1) + (n-m+1)^2\right] \\
& = \frac{1}{2}mn - \frac{3}{8}m^2 + \frac{1}{2}m - \frac{3}{2}n + \frac{7}{8} \\
& = \frac{1}{8}m^2 + \left(\frac{1}{2}t - 1\right)m + \left(\frac{7}{8} - \frac{3}{2}t\right) \quad \text{(where } t = n-m\text{)} \\
& > 0 \qquad \text{(since } m > 3 \text{ and } t \geqslant 0\text{)}.
\end{aligned}
$$

If n is even, then we have similarly that

$$W(C_m^{u_1}(S_{n-m+1})) - W(C_{m-1}^{u_1}(S_{n-m+2})) > 0.$$

The proof of lemma 6 is completed.

Theorem 7. Let $G = C_m^{u_1,u_2,\ldots,u_k}(T_1, T_2, \ldots, T_k)$ be an (n,n)-graph of order $n \geqslant 6$. If $G \ncong S_n + e, C_4(S_{n-3}), C_3^{u_1,u_2}(S_2, S_{n-3})$, or $C_3(T_{n-5,1}^1)$, then

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

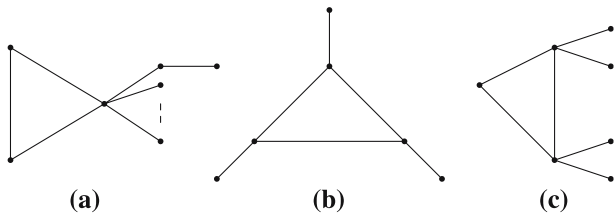

Figure 1. (a) $C_3(T^1_{n-5,1})$; (b) $C_3^{u_1,u_2,u_3}(S_2, S_2, S_2)$; (c) $C_3^{u_1,u_2}(S_3, S_3)$.

with the equality if and only if $G \cong C_3(T^1_{n-5,1})$, or $G \cong C_3^{u_1,u_2,u_3}(S_2, S_2, S_2)$, C_6 for $n = 6$, or $G \cong C_3^{u_1,u_2}(S_3, S_3)$ for $n = 7$, where $C_3(T^1_{n-5,1})$, $C_3^{u_1,u_2,u_3}(S_2, S_2, S_2)$ and $C_3^{u_1,u_2}(S_3, S_3)$ are showed in figure 1.

Proof. By calculating,

G	W(G)
$S_n + e$	$n^2 - 2n$
$C_4(S_{n-3})$	$n^2 - n - 4$
$C_3^{u_1,u_2}(S_2, S_{n-3})$	$n^2 - n - 4$
$C_3(T^1_{n-5,1})$	$n^2 - n - 3$

we have $W(S_n + e) < W(C_4(S_{n-3})) = W(C_3^{u_1,u_2}(S_2, S_{n-3})) < W(C_3(T^1_{n-5,1}))$.

In the following, we will prove that $W(G) > W(C_3(T^1_{n-5,1}))$ for $G \ncong S_n + e, C_4(S_{n-3}), C_3^{u_1,u_2}(S_2, S_{n-3})$, or $C_3(T^1_{n-5,1})$ and $n \geqslant 8$.

Case 1. $m > 4$.

(i) If $k = 0$, then $G = C_n$.
If n is even, then, by lemma 2, $W(G) - W(C_3(T^1_{n-5,1})) = \frac{1}{8}n^3 - (n^2 - n - 3)$ $= \frac{1}{8}(n^3 - 8n^2 + 8n + 24) = \frac{1}{8}(n-4)(n^2 - 4n - 8) - 1 \geqslant 0$ with the equality if and only if $n = 6$.
If n is odd, then, by lemma 2, $W(G) - W(C_3(T^1_{n-5,1})) = \frac{1}{8}n(n^2 - 1) - (n^2 - n - 3)$
$= \frac{1}{8}(n^3 - 8n^2 + 7n + 24) = \frac{1}{8}[(n-4)(n^2 - 4n - 9) - 12] > 0$ for $n \geqslant 7$.

(ii) If $k \geqslant 1$, then, by corollary 4, we have $W(G) \geqslant W(G_1)$ with the equality if and only if $G \cong G_1$, where

$$G_1 = C_m^{u_1,u_2,\ldots,u_k}(S_{l_1+1}, S_{l_2+1}, \ldots, S_{l_k+1})$$

$l = l_1 + l_2 + \cdots + l_k = n - m$.
By lemma 5,

$$W(G_1) \geqslant W(C_m^{u_1}(S_{l+1})) = W(C_m^{u_1}(S_{n-m+1}))$$

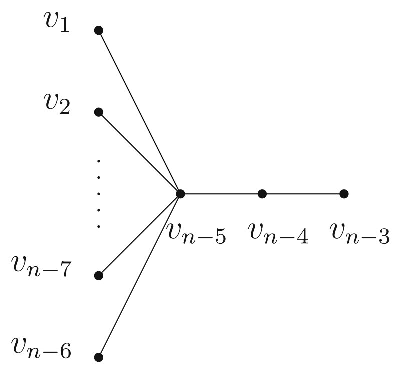

Figure 2. $T^1_{n-6,1}$ with order $n-3$ and $\geqslant 7$.

with the equality if and only if $G_1 \cong C_m^{u_1}(S_{l+1})$.

So, $W(G) \geqslant W(C_m^{u_1}(S_{l+1}))$, with the equality if and only if $G \cong C_m^{u_1}(S_{l+1})$.

From $m > 4$ and lemma 6, we have $W(C_m^{u_1}(S_{n-m+1})) \geqslant W(C_5(S_{n-4}))$. Then $W(G) \geqslant W(C_5(S_{n-4}))$. But $W(C_5(S_{n-4})) = n^2 + 2n - 15 > W(C_3(T^1_{n-5,1}))$. So, $W(G) > W(C_3(T^1_{n-5,1}))$.

Case 2. $m = 4$.

(i) If $k = 1$, we note that S_{n-3} and $T^1_{n-6,1}$ (see figure 2) are the trees with the smallest and the second smallest Wiener index, respectively, among all trees of order $n-3$ in [10]. By theorem 3, we have

$$W(C_4^{u_1}(T_1)) = W(C_4) + (n-4)d_u(C_4) + 3d_{u_1}(T_1) + W(T_1),$$
$$W(C_4^{u_1}(T^1_{n-6,1})) = W(C_4) + (n-4)d_u(C_4) + 3d_{u_1}(T^1_{n-6,1}) + W(T^1_{n-6,1}),$$

where u_1 is the vertex v_{n-5} with the maximum degree in $T^1_{n-6,1}$, T_1 is a tree of order $n-3$. Since, $G \ncong C_4(S_{n-3})$, $C_4^{u_1}(T_1) \ncong C_4(S_{n-3})$, and $d_{u_1}(T_1) \geqslant d_{u_1}(T^1_{n-6,1})$.
$W(C_4(S_{n-3})) < W(C_4^{u_1}(T^1_{n-6,1})) \leqslant W(C_4^{u_1}(T_1))$.
And, $W(C_4^{u_1}(T^1_{n-6,1})) - W(C_3(T^1_{n-5,1})) = n^2 - 9 - (n^2 - n - 3) = n - 6 > 0$.
So,

$$W(C_4(S_{n-3})) < W(C_3(T^1_{n-5,1})) < W(C_4^{u_1}(T^1_{n-6,1}) \leqslant W(C_4^{u_1}(T_1)).$$

(ii) If $k = 2$, then, by corollary 4, we have
$W(C_4^{u_1,u_2}(T_1, T_2)) \geqslant W(C_4^{u_1,u_2}(S_{l_1+1}, S_{l_2+1}))$
Using theorem 3, we have

$$W(C_4^{u_1,u_2}(S_{l_1+1}, S_{l_2+1}) = n^2 - n - 4 + \alpha l_1 l_2,$$

where $\alpha = 1$ if u_1 and u_2 are adjacent in C_4; otherwise $\alpha = 2$.

$$W(C_4^{u_1,u_2}(S_{l_1+1}, S_{l_2+1})) - W(C_3(T^1_{n-5,1})) = \alpha l_1 l_2 - 1 > 0.$$

So, $W(C_4^{u_1,u_2}(T_1, T_2) > W(C_3(T^1_{n-5,1}))$.

(iii) If $k = 3$, then, by corollary 4, we have
$W(C_4^{u_1,u_2,u_3}(T_1, T_2, T_3)) \geqslant W(C_4^{u_1,u_2,u_3}(S_{l_1+1}, S_{l_2+1}, S_{l_3+1}))$.
In the following, we prove that $W(C_4^{u_1,u_2,u_3}(S_{l_1+1}, S_{l_2+1}, S_{l_3+1})) > W(C_3(T^1_{n-5,1}))$.
Without loss of the generality, we assume that u_2 is adjacent to u_1 and u_3 in C_4.
By theorem 3,
$W(C_4^{u_1,u_2,u_3}(S_{l_1+1}, S_{l_2+1}, S_{l_3+1})) = n^2 - n - 4 + 2l_1l_3 + l_1l_2 + l_2l_3$
$W(C_4^{u_1,u_2,u_3}(S_{l_1+1}, S_{l_2+1}, S_{l_3+1})) - W(C_3(T^1_{n-5,1})) = 2l_1l_3 + l_1l_2 + l_2l_3 - 1 > 0$.
And $W(C_4^{u_1,u_2,u_3}(T_1, T_2, T_3)) > W(C_3(T^1_{n-5,1}))$.

(iv) If $k = 4$, then, by corollary 4, we have
$W(C_4^{u_1,u_2,u_3,u_4}(T_1, T_2, T_3, T_4)) \geqslant W(C_4^{u_1,u_2,u_3,u_4}(S_{l_1+1}, S_{l_2+1}, S_{l_3+1}, S_{l_4+1}))$.

Using theorem 3,
$W(C_4^{u_1,u_2,u_3,u_4}(S_{l_1+1}, S_{l_2+1}, S_{l_3+1}, S_{l_4+1})) = n^2 - n - 4 + 2l_1l_3 + l_1l_2 + l_2l_3 + 2l_2l_4$.
$W(C_4^{u_1,u_2,u_3,u_4}(S_{l_1+1}, S_{l_2+1}, S_{l_3+1}, S_{l_4+1})) - W(C_3(T^1_{n-5,1}))$
$= 2l_1l_3 + l_1l_2 + l_2l_3 + 2l_2l_4 - 1 > 0$.
So, $W(C_4^{u_1,u_2,u_3,u_4}(T_1, T_2, T_3, T_4)) > W(C_3(T^1_{n-5,1}))$.

Case 3. $m = 3$.

(i) If $k = 1$, we know from [10] that $T^1_{n-5,1}$ is the tree with the second smallest wiener index among all trees of order $n - 2$. For any tree T of order $n - 2$, if $T \ncong S_{n-2}, T^1_{n-5,1}$, then, by theorem 3, we can prove similarly as $W(C_4^{u_1}(T^1_{n-6,1})) \leqslant W(C_4^{u_1}(T_1))$ in case 2 (i) that
$W(C_3(T^1_{n-5,1})) < W(C_3^{u_1}(T))$.

(ii) If $k = 2$, then, by corollary 4, we have
$W(G) \geqslant W(C_3^{u_1,u_2}(S_{l_1+1}, S_{l_2+1}))$.
Now, we compare $W(C_3^{u_1,u_2}(S_{l_1+1}, S_{l_2+1}))$ with $W(C_3^{u_1}(T^1_{n-5,1}))$.
From theorem 3,

$$\begin{aligned} & W(C_3^{u_1,u_2}(S_{l_1+1}, S_{l_2+1})) \\ &= W(C_3) + 2(n-3) + 2(l_1 + l_2) + (l_1^2 + l_2^2) + 3l_1l_2 \\ &= 3 + 4(n-3) + (n-3)^2 + l_1l_2 \\ &= n^2 - 2n + l_1l_2 \\ &\geqslant n^2 - n - 4 (\text{since } l_1 + l_2 = n - 3 \text{ and } l_1 \geqslant 1, l_2 \geqslant 1) \end{aligned}$$

with the equality if and only if $l_1 = 1, l_2 = n-4$ or $l_1 = n-4, l_2 = 1$. If $l_1 \geqslant 2$ and $l_2 \geqslant 2$, then

$$W(C_3^{u_1,u_2}(S_{l_1+1}, S_{l_2+1})) \geqslant n^2 - 10 \geqslant n^2 - n - 3 = W(C_3(T_{n-5,1}^1))$$

with the equality if and only if $n = 7$ and $l_1 = l_2 = 2$. So, we have

$$W(C_3^{u_1,u_2}(S_{l_1+1}, S_{l_2+1})) > W(C_3(T_{n-5,1}^1)) > W(C_3^{u_1,u_2}(S_2, S_{n-3}))$$

for $n \geqslant 8$ and $W(C_3(T_{n-5,1}^1))) = W(C_3^{u_1,u_2}(S_3, S_3))$ for $n = 7$.

(iii) If $k = 3$, then, by corollary 4, we have

$$W(G) \geqslant W(C_3^{u_1,u_2,u_3}(S_{l_1+1}, S_{l_2+1}, S_{l_2+1}))$$

From theorem 3,

$$\begin{aligned} & W(C_3^{u_1,u_2,u_3}(S_{l_1+1}, S_{l_2+1}, S_{l_2+1})) \\ &= W(C_3) + (n-3)\omega + 2(l_1 + l_2 + l_3) + (l_1^2 + l_2^2 + l_3^2) + 3(l_1l_2 + l_1l_3 + l_2l_3) \\ &= W(C_3) + (n-3)\omega + 2(n-3) + (n-3)^2 + (l_1l_2 + l_1l_3 + l_2l_3) \\ &= n^2 - 2n + (l_1l_2 + l_1l_3 + l_2l_3). \end{aligned}$$

$$W(C_3^{u_1,u_2,u_3}(S_{l_1+1}, S_{l_2+1}, S_{l_3+1})) - W(C_3(T_{n-5,1}^1)) = l_1l_2 + l_1l_3 + l_2l_3 - n + 3 \geqslant 0$$

with the equality if and only if $l_1 = l_2 = l_3 = 1$ (and then $n = 6$).

Summarizing above, we have

$$W(G) \geqslant W(C_3^{u_1}(T_{n-5,1}^1)) > W(C_3^{u_1,u_2}(S_2, S_{n-3})) = W(C_4(S_{n-3})) > W(S_n + e)$$

with the equality if and only if $G \cong C_3(T_{n-5,1}^1)$, or $G \cong C_3^{u_1,u_2,u_3}(S_2, S_2, S_2), C_6$ for $n = 6$, or $G \cong C_3^{u_1,u_2}(S_3, S_3)$ for $n = 7$.

4. The (n,n)-graphs with the first three largest Wiener indices

In this section, we characterize the (n,n)-graphs with the largest, the second largest and the third largest Wiener indices among all the (n,n)-graphs.

Lemma 8. Let $G_2 = C_m^{u_1,u_2,\ldots,u_k}(P_{l_1+1}, P_{l_2+1}, \ldots, P_{l_k+1})$. If $k \geqslant 1$, then $W(G_2) \leqslant W(C_m^{u_1}(P_{l+1}))$ with the equality if and only if $G_2 \cong C_m^{u_1}(P_{l+1})$, where $l = l_1 + l_2 + \cdots + l_k = n - m$.

Proof. By lemma 1 and theorem 3, we have

$$
\begin{aligned}
&W\left(C_m^{u_1}(P_{l+1})\right) - W(G_2)\\
&= \left(W(C_m) + (n-m)\omega + (m-1)(1+2+\cdots+l) + \binom{l+2}{3}\right)\\
&\quad -\Bigg(W(C_m) + (n-m)\omega + (m-1)\sum_{i=1}^{k}(1+2+\cdots+l_i) + \sum_{i=1}^{k}\binom{l_i+2}{3}\\
&\quad + \sum_{i=1}^{k-1}\sum_{j=i+1}^{k}[l_i(1+2+\cdots+l_j) + l_i l_j d_{C_m}(u_i,u_j) + l_j(1+2+\cdots+l_i)]\Bigg)\\
&= (m-1)\left[\tfrac{1}{2}l(l+1) - \tfrac{1}{2}\sum_{i=1}^{k} l_i(l_i+1)\right] + \tfrac{1}{6}\left[(l^3+3l^2+2l) - \sum_{i=1}^{k}(l_i^3+3l_i^2+2l_i)\right]\\
&\quad - \sum_{i=1}^{k-1}\sum_{j=i+1}^{k}[\tfrac{1}{2}l_i l_j(l_j+1) + l_i l_j d_{C_m}(u_i,u_j) + \tfrac{1}{2}l_j l_i(l_i+1)]\\
&= (m-1)\left(\sum_{i=1}^{k-1}\sum_{j=i+1}^{k} l_i l_j\right) + \sum_{i,j,t} l_i l_j l_t - \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} l_i l_j d_{C_m}(u_i,u_j)
\end{aligned}
$$

(where the summation $\sum_{i,j,t}$ goes over all i, j, t of $1, 2, \ldots, k$ and i, j, t are not equal each other.)

$$
\begin{aligned}
&= \sum_{i,j,t} l_i l_j l_t + \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} l_i l_j[(m-1) - d_{C_m}(u_i,u_j)]\\
&\geqslant 0.
\end{aligned}
$$

with the equality if and only if $k = 1$, (i.e., $G_2 \cong C_m^{u_1}(P_{l+1})$) or $k = 2$ and $d_{C_m}(u_1,u_2) = m-1$, but $d_{C_m}(u_1,u_2) = m-1$ is not possible.

Theorem 9. Let $G = C_m^{u_1,u_2,\ldots,u_k}(T_1, T_2, \ldots, T_k)$ be an (n,n)-graph of order $n \geqslant 6$. If $G \ncong C_3(P_{n-2}), C_4(P_{n-3})$, then

$$W(G) \leqslant W(C_3^{u_1}(T(n-5,1,1))) < W(C_4(P_{n-3})) < W(C_3(P_{n-2}))$$

with the equality if and only if $G \cong C_3^{u_1}(T(n-5,1,1))$, where $C_3^{u_1}(T(n-5,1,1))$ is showed in figure 3.

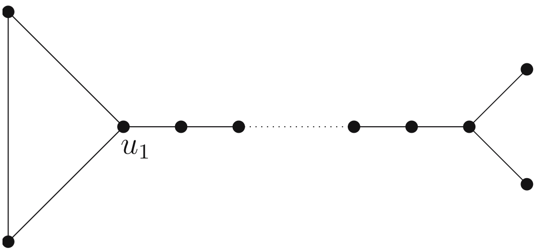

Figure 3. $C_3^{u_1}(T(n-5,1,1))$.

Proof. By calculating,

G	W(G)
$C_3^{u_1}(T(n-5,1,1))$	$\frac{1}{6}(n^3-13n+30)$
$C_4(P_{n-3})$	$\frac{1}{6}(n^3-13n+36)$
$C_3(P_{n-2})$	$\frac{1}{6}(n^3-7n+12)$

we have $W(C_3^{u_1}(T(n-5,1,1))) < W(C_4(P_{n-3})) < W(C_3(P_{n-2}))$.

Case 1. $m \geqslant 5$.

(i) If $k=0$, then $G=C_n$.
If n is even, then, from lemma 2,
$W(G) - W(C_3^{u_1}(T(n-5,1,1))) = \frac{1}{8}n^3 - \frac{1}{6}(n^3-13n+30) = -\frac{1}{24}(n^3-52n+120) = -\frac{1}{24}[n(n-8)(n+8)+12n+120] < 0$ for $n \geqslant 6$.
If n is odd,
$W(G) - W(C_3^{u_1}(T(n-5,1,1))) = \frac{1}{8}n(n^2-1) - \frac{1}{6}(n^3-13n+36) = -\frac{1}{24}(n^3 - 49n+120) = -\frac{1}{24}[n(n-7)(n+7)+120] < 0$ for $n \geqslant 7$.

(ii) If $k \geqslant 1$, then, by corollary 4 and lemma 8, we have

$$W(G) \leqslant W(C_m^{u_1}(P_{n-m+1}))$$

with the equality if and only if $G \cong C_m^{u_1}(P_{n-m+1})$.

Now, we prove that $W(C_m^{u_1}(P_{n-m+1})) < W(C_3^{u_1}(T(n-5,1,1)))$ for $m \geqslant 5$.

If m is even, then $m \geqslant 6$. By theorem 3, we have

$$W\left(C_m^{u_1}(P_{n-m+1})\right) = \frac{1}{6}\left[n^3 + \left(-\frac{3}{2}m^2+3m-1\right)n + \left(\frac{5}{4}m^3-3m^2+m\right)\right].$$

$$\begin{aligned}
&W\left(C_3^{u_1}(T(n-5,1,1))\right) - W(C_m^{u_1}(P_{n-m+1}))\\
&= \frac{1}{6}(n^3 - 13n + 30) - \frac{1}{6}\left[n^3 + \left(-\frac{3}{2}m^2 + 3m - 1\right)n + \left(\frac{5}{4}m^3 - 3m^2 + m\right)\right]\\
&= \frac{1}{6}\left[\left(\frac{3}{2}m^2 - 3m - 12\right)n - \left(\frac{5}{4}m^3 - 3m^2 + m - 30\right)\right]\\
&= \frac{1}{4}(m-4)(m+2)n - \frac{1}{24}[(m-4)(5m^2 + 8m + 30) + 6m]\\
&\geqslant \frac{1}{4}(m-4)(m+2)m - \frac{1}{24}[(m-4)(5m^2 + 8m + 30) + 6m]\\
&= \frac{1}{24}(m-4)[(m+2)^2 - 40] - 1 > 0
\end{aligned}$$

So, $W(C_3^{u_1}(T(n-5,1,1))) > W(C_m^{u_1}(P_{n-m+1})$.

If m is odd, then

$$\begin{aligned}
W(C_m^{u_1}(P_{n-m+1})) = &\frac{1}{6}\left[n^3 + \left(-\frac{3}{2}m^2 + 3m - 1\right)n + \left(\frac{5}{4}m^3 - 3m^2 + m\right)\right]\\
&-\frac{1}{4}n + \frac{1}{8}m.
\end{aligned}$$

$$\begin{aligned}
&W(C_3^{u_1}(T(n-5,1,1))) - W(C_m^{u_1}(P_{n-m+1}))\\
&= \frac{1}{6}\left(n^3 - 13n + 30\right) - \frac{1}{6}\left[n^3 + \left(-\frac{3}{2}m^2 + 3m - 1\right)n + \left(\frac{5}{4}m^3 - 3m^2 + m\right)\right]\\
&\quad + \frac{1}{4}n - \frac{1}{8}m > \frac{1}{6}\left[\left(\frac{3}{2}m^2 - 3m - 12\right)n - \left(\frac{5}{4}m^3 - 3m^2 + m - 30\right)\right] > 0.
\end{aligned}$$

So, $W(C_3^{u_1}(T(n-5,1,1))) > W(C_m^{u_1}(P_{n-m+1})$.

Case 2. $m = 4$.

Calculating by theorem 3, we have
$W(C_4^{u_1}(T(n-6,1,1))) = \frac{1}{6}(n^3 - 19n + 54)$.
So, $W(C_3^{u_1}(T(n-5,1,1))) > W(C_4^{u_1}(T(n-6,1,1)))$.

Note that $T(n-6,1,1)$ is the tree with the second largest Wiener index among all trees of order $n-3$ from [9].

If $k = 1$, and $T_1 \ncong P_{n-3}$, then $d_{T_1}(u) < d_{T(n-6,1,1)}(u_1)$, where T_1 is a tree of order $n-3$, u is any vertex of T_1, u_1 is the pendant vertex with the largest distance from the maximum degree vertex in $T(n-6,1,1)$. By theorem 3, we have
$W(C_4^{u_1}(T(n-6,1,1))) > W(C_4^{u}(T_1))$.

If $k = 2$, then, by corollary 4, we have,

$W(G) \leqslant W(C_4^{u_1,u_2}(P_{l_1+1}, P_{l_2+1}))$.

$$\begin{aligned}
&W(C_4^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})) - W(C_4^{u_1}(T(n-6,1,1))) \\
&\quad = \frac{3}{2}[l_1(l_1+1) + l_2(l_2+1)] + \frac{1}{6}[(l_1+2)(l_1+1)l_1 + (l_2+2)(l_2+1)l_2] \\
&\qquad + \frac{1}{2}[l_1 l_2(l_2+1) + \alpha l_1 l_2 + l_2 l_1(l_1+1)] - \left[\frac{3}{2}(n-5)(n-2) + \frac{1}{6}(n^3 - 19n + 54)\right] \\
&\quad = \frac{1}{6}[(l_1+l_2)^3 + 12(l_1+l_2)^2 + 11(l_1+l_2) - (18-6\alpha)l_1 l_2] - \frac{1}{6}(n^3 + 9n^2 - 82n + 144) \\
&\quad = \frac{1}{6}[(n-4)^3 + 12(n-4)^2 + 11(n-4) - (18-6\alpha)l_1 l_2] - \frac{1}{6}(n^3 + 9n^2 - 82n + 144) \\
&\quad = -\frac{1}{6}(9n^2 - 45n + 60 + (18-6\alpha)l_1 l_2) < 0.
\end{aligned}$$

(where $\alpha = 1$ if u_1 and u_2 are adjacent; otherwise $\alpha = 2$)

So, $W(C_4^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})) < W(C_4^{u_1}(T(n-6,1,1)))$.
If $k = 3$ or $k = 4$, then we can similarly see that
$W(C_4^{u_1,u_2,u_3}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1})) < W(C_4^{u_1}(T(n-6,1,1)))$, or
$W(C_4^{u_1,u_2,u_3,u_4}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1}, P_{l_4+1})) < W(C_4^{u_1}(T(n-6,1,1)))$

Case 3. $m = 3$. Then $1 \leqslant k \leqslant 3$.

If $k = 1$, then $T_1 \ncong P_{n-2}$, $T(n-5,1,1)$ since $G = C_3^{u_1}(T_1) \ncong C_3^{u_1}(P_{n-2})$, $C_3^{u_1}(T(n-5,1,1))$. By theorem 3,
$W(C_3^{u_1}(T_1)) = W(C_3) + (n-3)\omega + 2d_{T_1}(u_1) + W(T_1)$.

Note that $T(n-5,1,1)$ is the tree with the second largest Wiener index among all trees of order $n-2$ from [9], and $T_1 \ncong T(n-5,1,1)$. Then $W(T(n-5,1,1)) > W(T_1)$, and $d_{T(n-5,1,1)}(u_1) > d_{T_1}(u_1)$. So, $W(C_3^{u_1}(T(n-5,1,1))) \geqslant W(C_3^{u_1}(T_1))$.

If $k = 2$, then, by lemma 8, $W(G) \leqslant W(C_3^{u_1,u_2}(P_{l_1+1}, P_{l_2+1}))$ with the equality if and only if $G \cong C_3^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})$.

$$\begin{aligned}
&W(C_3^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})) - W(C_3^{u_1}(T(n-5,1,1))) \\
&\quad = W(C_3) + (n-3)\omega + 2d_{P_{l_1+1}}(u_1) + 2d_{P_{l_2+1}}(u_2) + W(P_{l_1+1}) + W(P_{l_2+1}) \\
&\qquad - [W(C_3) + (n-3)\omega + 2d_{T(n-5,1,1)}(u_1) + W(T(n-5,1,1))] \\
&\quad = 2d_{P_{l_1+1}}(u_1) + 2d_{P_{l_2+1}}(u_2) + W(P_{l_1+1}) + W(P_{l_2+1}) \\
&\qquad - 2d_{T(n-5,1,1)}(u_1 - W(T(n-5,1,1))). \\
&\quad = l_1(l_1+1) + l_2(l_2+1) + \frac{1}{6}(l_1^3 - l_1) + \frac{1}{6}(l_1^3 - l_1) \\
&\qquad - (n-2)(n-4) + \frac{1}{6}(n^3 - 6n^2 + 6n + 22) \\
&\quad = \frac{1}{6}(n - 6l_1 l_2 - 3)
\end{aligned}$$

$W(C_3^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})) < W(C_3^{u_1}(T(n-5,1,1)))$ since $l_1 + l_2 = n - 3$, and $min\{l_1 l_2 | l_1 + l_2 = n-3, l_1 \geqslant 1, l_2 \geqslant 1\} = n - 4$.

If $k = 3$, then, by lemma 8, $W(G) \leqslant W(C_3^{u_1,u_2,u_3}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1}))$ with the equality if and only if $G \cong C_3^{u_1,u_2,u_3}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1})$.

From theorem 3, we have

$$W(C_3^{u_1,u_2,u_3}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1})) = \frac{1}{6}(n^3 - 12n + 27 - l_1 l_2 l_3) - l_1 l_2 - l_2 l_3 - l_1 l_3.$$

$$\begin{aligned} &W\left(C_3^{u_1}(T(n-5,1,1))\right) - W(C_3^{u_1,u_2,u_3}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1})) \\ &= \frac{1}{6}(n^3 - 13n + 30) - \left[\frac{1}{6}(n^3 - 12n + 27 - l_1 l_2 l_3) - l_1 l_2 - l_2 l_3 - l_1 l_3\right] \\ &= \frac{1}{6}(l_1 l_2 l_3 - n + 3) + l_1 l_2 + l_2 l_3 + l_1 l_3 \end{aligned}$$

$W(C_3^{u_1}(T(n-5,1,1)))) > W(C_3^{u_1,u_2,u_3}(P_{l_1+1}, P_{l_2+1}, P_{l_3+1}))$ since $n - 3 = l_1 + l_2 + l_3$ and l_1, l_2, l_3 are positive integers.

Summarizing above, we have

$$W(G) \leqslant W(C_3^{u_1}(T(n-5,1,1))) < W(C_4(P_{n-3})) < W(C_3(P_{n-2}))$$

with the equality if and only if $G \cong C_3^{u_1}(T(n-5,1,1))$.

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