A note on hyper-Wiener index

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Abstract

The hyper-Wiener index is a graph invariant that is used as a structure descriptor for predicting physicochemical properties of organic compounds. We determine the n-vertex unicyclic graphs with the third smallest and the third largest hyper-Wiener indices for $n \geq 5$.

1 Introduction

We consider simple graphs. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, d_{uv} denotes the distance between vertices u and v in G. The hyper-Wiener index of G is defined as [4, 5]

$$WW(G) = \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv}+1}{2} = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (d_{uv}^2 + d_{uv}).$$

Used as a structure descriptor (topological index) for predicting physicochemical properties of organic compounds [1], the hyper-Wiener index has been extensively studied, see, e.g., [2, 3, 6]. Among others, Xing et al. [6] determined the n-vertex unicyclic graphs (connected graphs with a unique cycle) of cycle length r with the smallest and the largest hyper-Wiener

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indices for $3 \leq r \leq n$, and the n-vertex unicyclic graphs with the smallest, the second smallest, the largest and the second largest hyper-Wiener indices for $n \geq 5$.

In this note, we determine the n-vertex unicyclic graphs with the third smallest and the third largest hyper-Wiener indices. By the results of [6], among the unicyclic graphs on $n \geq 6$ vertices, there are two graphs with the second smallest hyper-Wiener index, and two graphs with the second largest hyper-Wiener index. It is of interest to note that the results of this paper show that among the unicyclic graphs on n vertices, there is one graph for $n \geq 8$ with the third smallest hyper-Wiener index, and one graph for $n \geq 6$ with the third largest hyper-Wiener index.

2 Preliminaries

The number of vertices of G is denoted by $|G|$. Let C_n be the n-vertex cycle. Let $C_r(T_1, T_2, \ldots, T_r)$ be the graph constructed as follows. Let the vertices of the cycle C_r be labelled consecutively by $v_1, v_2, \ldots, v_r$. Let $T_1, T_2, \ldots, T_r$ be vertex-disjoint trees such that T_i and the cycle C_r have exactly one vertex v_i in common for $i = 1, 2, \ldots, r$. Then any n-vertex unicyclic graph G with a cycle on r vertices is of the form $C_r(T_1, T_2, \ldots, T_r)$, where $\sum_{i=1}^{r} |T_i| = n$. Let $t_i = |T_i|$ for $1 \leq i \leq r$.

Let G be a connected graph. Recall that the Wiener index of G is defined as $W(G) = \sum_{\{u,v\} \subseteq V(G)} d_{uv}$. For $u \in V(G)$, let $W_u(G) = \sum_{v \in V(G)} d_{uv}$ and $WW_u(G) = \sum_{v \in V(G)} \binom{d_{uv}+1}{2}$.

Lemma 2.1. [6] *For $r \geq 3$, let $G = C_3(T_1, T_2, T_3)$ with $t_3 = 1$. Then*

$$\begin{aligned} WW(G) &= \sum_{i=1}^{2} WW(T_i) + \sum_{i=1}^{2}(|G| - t_i) WW_{v_i}(T_i) + \sum_{i<j} t_i t_j \\ &\quad + \sum_{i=1}^{2} \sum_{j \neq i} t_j W_{v_i}(T_i) + W_{v_1}(T_1) W_{v_2}(T_2). \end{aligned}$$

For $t_1, t_2, \ldots, t_r \geq 1$, let $S_n(t_1, t_2, \ldots, t_r)$ be the n-vertex unicyclic graph formed by attaching $t_i - 1$ pendant vertices to vertex v_i of the cycle C_r, and $P_n(t_1, t_2, \ldots, t_r)$ the n-vertex unicyclic graph formed by attaching a path on $t_i - 1$ vertices (no path is attached if $t_i = 1$) to vertex v_i of the cycle C_r, where $t_1 + t_2 + \cdots + t_r = n$.

Lemma 2.2. [6] *For $G = C_r(T_1, T_2, \ldots, T_r)$ with $|G| = n$,*

$$WW(S_n(t_1, t_2, \ldots, t_r)) \le WW(G) \le WW(P_n(t_1, t_2, \ldots, t_r))$$

with left equality if and only if $G = S_n(t_1, t_2, \ldots, t_r)$ and with right equality if and only if $G = P_n(t_1, t_2, \ldots, t_r)$.

Lemma 2.3. [6] *Let $G = S_n(t_1, t_2, \ldots, t_r)$. Suppose that there exist k and l with $1 \le k < l \le r$ such that $t_k, t_l \ge 2$. Let $a \in V(T_k), b \in V(T_l)$ with $a \ne v_k$ and $b \ne v_l$. If $WW_a(G) \le WW_b(G)$, then $WW(G) > WW(G - v_l b + v_k b)$.*

Lemma 2.4. [6] *Let $G = P_n(t_1, t_2, \ldots, t_r)$. Suppose that there exist k and l with $1 \le k < l \le r$ such that $t_k, t_l \ge 2$. Let $a \ne v_k$ and $b \ne v_l$ be end vertices of T_k and T_l and let c be the unique neighbor of b. If $WW_a(G) \ge WW_b(G)$, then $WW(G) < WW(G - cb + ab)$.*

Let $S_{n,r}$ be the unicyclic graph obtained by attaching $n - r$ pendant vertices to a vertex of the cycle C_r, $P_{n,r}$ the unicyclic graph obtained by attaching a path on $n - r$ vertices (at one terminal vertex) to the cycle C_r, where $3 \le r \le n$. In particular, $S_{n,n} = P_{n,n} = C_n$.

Lemma 2.5. [6] *Let G be an n-vertex unicyclic graph with cycle length r. Then $WW(G) \ge WW(S_{n,r})$ with equality if and only if $G = S_{n,r}$, where*

$$WW(S_{n,r}) = \begin{cases} \frac{72n^2+(2r^3+18r^2-98r-90)n-r^4-15r^3+25r^2+87r}{48} & \text{if } r \text{ is odd,} \\ \frac{72n^2+(2r^3+18r^2-92r-72)n-r^4-15r^3+22r^2+72r}{48} & \text{if } r \text{ is even.} \end{cases}$$

Lemma 2.6. [6] *Let G be an n-vertex unicyclic graph with cycle length r. Then $WW(G) \le WW(P_{n,r})$ with equality if and only if $G = P_{n,r}$, where*

$$WW(P_{n,r}) = \begin{cases} \frac{n^4+2n^3+(-3r^2+6r-4)n^2+(3r^3-12r^2+15r-8)n}{24} \\ +\frac{-r^4+11r^3-23r^2+13r}{48} & \text{if } r \text{ is odd,} \\ \frac{n^4+2n^3+(-3r^2+6r-1)n^2+(3r^3-12r^2+12r-2)n}{24} \\ +\frac{-r^4+11r^3-20r^2+4r}{48} & \text{if } r \text{ is even.} \end{cases}$$

Let $\mathbb{U}_n$ be the set of n-vertex unicyclic graphs. Let Γ_n be the set of n-vertex unicyclic graphs $C_3(T_1, T_2, T_3)$ with $|T_2| = |T_3| = 1$. Let Ψ_n be the set of n-vertex unicyclic graphs $C_3(T_1, T_2, T_3)$ with $|T_1| \ge |T_2| \ge \max\{|T_3|, 2\}$. Let Θ_n be the set of n-vertex unicyclic graphs $C_4(T_1, T_2, T_3, T_4)$ with $|T_2| = |T_3| = |T_4| = 1$. Let Ω_n be the set of n-vertex unicyclic graphs $C_4(T_1, T_2, T_3, T_4)$ with $|T_1| \ge |T_2| \ge 2$ or $|T_1| \ge |T_3| \ge 2$. Let Φ_n be the set of n-vertex unicyclic graphs with cycle length at least five.

Let S_n and P_n be respectively the n-vertex star and path. For $n \ge 5$, let S'_n be the tree formed by attaching a pendant vertex to a pendant vertex of the star S_{n-1}. Let P'_n be the tree formed by attaching a pendant vertex to the neighbor of one end vertex of P_{n-1}.

Lemma 2.7. [3] *Among the n-vertex trees with $n \geq 5$, different from S_n, S'_n is the unique tree with the smallest hyper-Wiener index, which is equal to $\frac{1}{2}(3n^2 - n - 14)$, and among the n-vertex trees with $n \geq 5$, different from P_n, P'_n is the unique tree with the largest hyper-Wiener index, which is equal to $\frac{1}{24}(n^4 + 2n^3 - 13n^2 + 10n + 72)$.*

3 The third smallest hyper-Wiener index

Among the graphs in $\mathbb{U}_n$ with $n \geq 5$, we showed in [6] that $S_{5,3}$ and C_5 for $n = 5$, and $S_{n,3}$ for $n \geq 6$ are the unique graphs with the smallest hyper-Wiener index, which is equal to $\frac{1}{2}(3n^2 - 7n)$, and that $S_6(3,2,1)$, $S_{6,4}$ and $S_{6,5}$ for $n = 6$, and $S_n(n-3,2,1)$ and $S_{n,4}$ for $n = 5$ and $n \geq 7$ are the unique graphs with the second smallest hyper-Wiener index, which is equal to $\frac{1}{2}(3n^2 - n - 24)$. In this section, we determine the graphs with the third smallest hyper-Wiener index in $\mathbb{U}_n$ with $n \geq 5$, which are just the graphs with the smallest hyper-Wiener index in $\mathbb{U}_5 \setminus \{S_{5,3}, C_5, S_5(2,2,1), S_{5,4}\}$ for $n = 5$, $\mathbb{U}_6 \setminus \{S_{6,3}, S_6(3,2,1), S_{6,4}, S_{6,5}\}$ for $n = 6$, and $\mathbb{U}_n \setminus \{S_{n,3}, S_n(n-3,2,1), S_{n,4}\} = (\Gamma_n \setminus \{S_{n,3}\}) \cup (\Psi_n \setminus \{S_n(n-3,2,1)\}) \cup (\Theta_n \setminus \{S_{n,4}\}) \cup \Omega_n \cup \Phi_n$ for $n \geq 7$.

For $n \geq 5$ and $3 \leq r \leq n-2$, let $S'_{n,r}$ be the n-vertex unicyclic graph formed by attaching a path on two vertices and $n - r - 2$ pendant vertices to a (common) vertex of the cycle C_r. Evidently, $S'_{n,3} \in \Gamma_n$ and $S'_{n,4} \in \Theta_n$. Note that $\mathbb{U}_5 \setminus \{S_{5,3}, C_5, S_5(2,2,1), S_{5,4}\} = \{S'_{5,3}\}$.

Lemma 3.1. [6] *Among the graphs in $\Gamma_n \setminus \{S_{n,3}\}$ with $n \geq 5$, $S'_{n,3}$ is the unique graph with the smallest hyper-Wiener index, which is equal to $\frac{1}{2}(3n^2 - n - 18)$.*

Lemma 3.2. *Among the graphs in $\Psi_n \setminus \{S_n(n-3,2,1)\}$ with $n \geq 6$, $S_6(2,2,2)$ for $n = 6$ and $S_n(n-4,3,1)$ for $n \geq 7$ are the unique graphs with the smallest hyper-Wiener index, which is equal to 42 for $n = 6$ and $\frac{1}{2}(3n^2 + 5n - 60)$ for $n \geq 7$.*

Proof. The case $n = 6$ may be checked directly. Suppose that $n \geq 7$. Let $H_n = C_3(S'_{n-3}, S_2, S_1)$ where v_1 has degree $n - 3$. It may be checked that

$$WW(H_n) = \frac{1}{2}(3n^2 + 5n - 40) > \frac{1}{2}(3n^2 + 5n - 60) = WW(S_n(n-4,3,1)).$$

Let $G = C_3(T_1, T_2, T_3) \in \Psi_n \setminus \{S_n(n-3,2,1)\}$ with $t_1 \geq t_2 \geq \max\{t_3, 2\}$.

If $t_2 = 2$ and $t_3 = 1$, then by Lemmas 2.1 and 2.7, we have $WW(G) \geq WW(H_n) > WW(S_n(n-4,3,1))$. Suppose that $(t_2, t_3) \neq (2,1)$. By Lemma 2.2, we have $WW(G) \geq WW(S_n(t_1,t_2,t_3))$. If $t_i \geq 2$ in $S_n(t_1,t_2,t_3)$, then u_i denotes a pendant vertex of T_i and $u_i \neq v_i$ for $i = 1, 2, 3$. It is easy to check that if $t_i \geq t_j \geq 2$, then $WW_{u_i}(S_n(t_1, t_2, t_3)) \leq WW_{u_j}(S_n(t_1, t_2, t_3))$ for $i, j = 1, 2, 3$ with $i \neq j$. Now by Lemma 2.3, we have $WW(G) > WW(S_n(n-4, 3, 1))$ for $t_2 = 2$ and $t_3 = 2$, and $WW(G) \geq WW(S_n(t_1 + t_3 - 1, t_2, 1)) \geq WW(S_n(n-4, 3, 1))$ with equalities if and only if $t_2 = 3$ and $t_3 = 1$ for $t_2 \geq 3$. □

Lemma 3.3. *Among the graphs in $\Theta_n \setminus \{S_{n,4}\}$ with $n \geq 6$, $S'_{n,4}$ is the unique graph with the smallest hyper-Wiener index, which is equal to $\frac{1}{2}(3n^2 + 5n - 40)$.*

Proof. Let $G = C_4(T_1, T_2, T_3, T_4) \in \Theta_n \setminus \{S_{n,4}\}$. Note that $WW(C_4) = 10$. Then

$$WW(G) = 10 + WW(T_1) + \sum_{u \in V(T_1) \setminus \{v_1\}} \left[2\binom{d_{uv_2} + 1}{2} + \binom{d_{uv_3} + 1}{2} \right],$$

which, together with Lemma 2.7, implies that $S'_{n,4}$ is the unique graph in $\Theta_n \setminus \{S_{n,4}\}$ with the smallest hyper-Wiener index, which is equal to $\frac{1}{2}(3n^2 + 5n - 40)$. □

For $G = C_4(T_1, T_2, T_3, T_4) = S_n(t_1, t_2, t_3, t_4)$, let u_i be a pendant vertex of T_i with $u_i \neq v_i$ if $t_i \geq 2$ for $1 \leq i \leq 4$. The following two properties are easily seen: For $\{i, j\} = \{1, 3\}$ or $\{2, 4\}$, we have $WW_{u_i}(G) \leq WW_{u_j}(G)$ if $t_i \geq t_j \geq 2$; For the cycle $v_i v_j v_l v_k$, we have $WW_{u_i}(G) \leq WW_{u_j}(G)$ if $t_i \geq t_j \geq 2$ and $t_k = t_l = 1$.

Lemma 3.4. *Among the graphs in Ω_n with $n \geq 6$, $S_n(n-4, 2, 1, 1)$ is the unique graph with the smallest hyper-Wiener index, which is equal to $\frac{1}{2}(3n^2 + 5n - 54)$.*

Proof. It is easily seen that $WW(S_n(n-4, 2, 1, 1)) = \frac{1}{2}(3n^2 + 5n - 54)$. Let $G = C_4(T_1, T_2, T_3, T_4) \in \Omega_n$. Suppose without loss of generality that $t_1 \geq \max\{t_2, t_3, t_4\}$ and $t_2 \geq t_4$. By Lemma 2.2, we have $WW(G) \geq WW(S_n(t_1, t_2, t_3, t_4))$ with equality if and only if $G = S_n(t_1, t_2, t_3, t_4)$. Suppose that $G = S_n(t_1, t_2, t_3, t_4)$. By Lemma 2.3, if $t_2 = 1$, then $WW(G) \geq WW(S_n(n-4, 1, 2, 1)) = \frac{1}{2}(3n^2 + 13n - 94) > WW(S_n(n-4, 2, 1, 1))$, and if $t_2 \geq 2$, then

$$\begin{aligned} WW(G) &\geq WW(S_n(t_1 + t_3 - 1, t_2 + t_4 - 1, 1, 1)) \\ &\geq WW(S_n(n-4, 2, 1, 1)) \end{aligned}$$

with equalities if and only if $t_3 = t_4 = 1$ and $t_2 = 2$, i.e., $G = S_n(n-4, 2, 1, 1)$. The result follows. □

Lemma 3.5. *Among the graphs in $\Phi_n \setminus \{S_{6,5}\}$ with $n \geq 6$, C_6 for $n = 6$ and $S_{n,5}$ for $n \geq 7$ are the unique graphs with the smallest hyper-Wiener index, which is equal to 42 for $n = 6$ and $\frac{1}{2}(3n^2 + 5n - 60)$ for $n \geq 7$.*

Proof. The result holds trivially for $n = 6$. Suppose that $n \geq 7$. By the expression for $WW(S_{n,r})$ given in Lemma 2.5, if r is odd and $7 \leq r \leq n$, then we have

$$\begin{aligned} & 48[WW(S_{n,r}) - WW(S_{n,5})] \\ = \; & (2r^3 + 18r^2 - 98r - 210)n - r^4 - 15r^3 + 25r^2 + 87r + 1440 \\ \geq \; & (2r^3 + 18r^2 - 98r - 210)r - r^4 - 15r^3 + 25r^2 + 87r + 1440 \\ = \; & r^4 + 3r^3 - 73r^2 - 123r + 1440 > 0, \end{aligned}$$

and thus $WW(S_{n,r}) > WW(S_{n,5})$, and if r is even and $6 \leq r \leq n$, then we have

$$\begin{aligned} & 48[WW(S_{n,r}) - WW(S_{n,5})] \\ = \; & (2r^3 + 18r^2 - 92r - 192)n - r^4 - 15r^3 + 22r^2 + 72r + 1440 \\ \geq \; & (2r^3 + 18r^2 - 92r - 192)r - r^4 - 15r^3 + 22r^2 + 72r + 1440 \\ = \; & r^4 + 3r^3 - 70r^2 - 120r + 1440 > 0, \end{aligned}$$

and thus $WW(S_{n,r}) > WW(S_{n,5})$. The result follows from Lemma 2.5. □

Proposition 3.1. *Among the graphs in $\mathbb{U}_n$ with $n \geq 5$, $S'_{n,3}$ for $n = 5$ and $n \geq 8$, $S'_{6,3}$, $S_6(2,2,2)$, $S_6(2,2,1,1)$ and C_6 for $n = 6$, and $S'_{7,3}$, $S_7(3,3,1)$ and $S_{7,5}$ for $n = 7$ are the unique graphs with the third smallest hyper-Wiener index, which is equal to $\frac{1}{2}(3n^2 - n - 18)$.*

Proof. The case $n = 5$ is trivial. By the discussion at the beginning of this section, the third smallest hyper-Wiener index of graphs in $\mathbb{U}_n$ is equal to the minimum of the values of the hyper-Wiener indices appearing in Lemmas 3.1–3.5. These values and the corresponding graphs are listed in Table 1, from which the result follows easily. □

4 The third largest hyper-Wiener index

Among the graphs in $\mathbb{U}_n$, with $n \geq 5$, we showed in [6] that $P_{n,3}$ is the unique graph with the largest hyper-Wiener index, which is equal to $\frac{1}{24}(n^4 + 2n^3 - 13n^2 + 10n + 24)$, and that $P_n(n-3, 2, 1)$ and $P_{n,4}$ are the unique graphs with the second largest hyper-Wiener index, which is equal to $\frac{1}{24}(n^4 +$

Table 1: Graphs and their hyper-Wiener indices in Lemmas 3.1–3.5.

graphs	hyper-Wiener indices		
	n	6	7
$S'_{n,3}$ $(n \geq 6)$	$\frac{1}{2}(3n^2 - n - 18)$	42	61
$S_6(2,2,2)$ $(n = 6)$		42	
$S_n(n-4,3,1)$ $(n \geq 7)$	$\frac{1}{2}(3n^2 + 5n - 60)$		61
$S'_{n,4}$ $(n \geq 6)$	$\frac{1}{2}(3n^2 + 5n - 40)$	49	71
$S_n(n-4,2,1,1)$ $(n \geq 6)$	$\frac{1}{2}(3n^2 + 5n - 54)$	42	64
C_6 $(n = 6)$		42	
$S_{n,5}$ $(n \geq 7)$	$\frac{1}{2}(3n^2 + 5n - 60)$		61

$2n^3 - 25n^2 + 46n + 72)$. In this section, we determine the third largest hyper-Wiener index in $\mathbb{U}_n$ with $n \geq 5$, which are just the graphs with the largest hyper-Wiener index in $\mathbb{U}_n \setminus \{P_{n,3}, P_n(n-3,2,1), P_{n,4}\} = (\Gamma_n \setminus \{P_{n,3}\}) \cup (\Psi_n \setminus \{P_n(n-3,2,1)\}) \cup (\Theta_n \setminus \{P_{n,4}\}) \cup \Omega_n \cup \Phi_n$. If $n = 5$, then $\mathbb{U}_n \setminus \{P_{n,3}, P_n(n-3,2,1), P_{n,4}\}$ contains exactly $S_{5,3}$ and C_5 with equal hyper-Wiener index 20. So we assume that $n \geq 6$.

For $n \geq 6$ and $3 \leq r \leq n-2$, let $P'_{n,r}$ be the n-vertex unicyclic graph formed by attaching a pendant vertex to the neighbor of the pendant vertex of $P_{n-1,r}$.

Lemma 4.1. [6] *Among the graphs in* $\Gamma_n \setminus \{P_{n,3}\}$ *with* $n \geq 6$, $P'_{n,3}$ *is the unique graph with the largest hyper-Wiener index, which is equal to* $\frac{1}{24}(n^4 + 2n^3 - 25n^2 + 22n + 120)$.

Lemma 4.2. *Among the graphs in* $\Psi_n \setminus \{P_n(n-3,2,1)\}$ *with* $n \geq 6$, $P_6(2,2,2)$ *for* $n = 6$ *and* $P_n(n-4,3,1)$ *for* $n \geq 7$ *are the unique graphs with the largest hyper-Wiener index, which is equal to* 42 *for* $n = 6$ *and* $\frac{1}{24}(n^4 + 2n^3 - 37n^2 + 106n + 144)$ *for* $n \geq 7$.

Proof. The case $n = 6$ may be checked directly. Suppose that $n \geq 7$. Let $L_n = C_3(P'_{n-3}, P_2, P_1)$ where v_1 has degree 3. Note that $WW(P_n(n-4,3,1)) = \frac{1}{24}(n^4 + 2n^3 - 37n^2 + 106n + 144) > WW(L_n) = \frac{1}{24}(n^4 + 2n^3 - 37n^2 + 58n + 192)$. Let $G = C_3(T_1, T_2, T_3) \in \Psi_n \setminus \{P_n(n-3,2,1)\}$ with $t_1 \geq t_2 \geq \max\{t_3, 2\}$.

If $t_2 = 2$, $t_3 = 1$, by Lemmas 2.1 and 2.7, we have $WW(G) \leq WW(L_n) < WW(P_n(n-4,3,1))$. Suppose that $(t_2, t_3) \neq (2,1)$. By Lemma 2.2, we have $WW(G) \leq WW(P_n(t_1, t_2, t_3))$.

If $t_i \geq 2$ in $P_n(t_1, t_2, t_3)$, then u_i denotes a pendant vertex of T_i and $u_i \neq v_i$ for $i = 1, 2, 3$. It is easy to check that if $t_i \geq t_j \geq 2$, then

$WW_{u_i}(P_n(t_1,t_2,t_3)) \geq WW_{u_j}(P_n(t_1,t_2,t_3))$ for $i,j = 1,2,3$ with $i \neq j$. Now by Lemma 2.4, we have $WW(G) < WW(P_n(n-4,3,1))$ for $t_2 = 2$ and $t_3 = 2$, and $WW(G) \leq WW(P_n(t_1+t_3-1,t_2,1)) \leq WW(P_n(n-4,3,1))$ with equalities if and only if $t_2 = 3$ and $t_3 = 1$ for $t_2 \geq 3$. □

Lemma 4.3. *Among the graphs in $\Theta_n \setminus \{P_{n,4}\}$ with $n \geq 6$, $P'_{n,4}$ is the unique graph with the largest hyper-Wiener index, which is equal to $\frac{1}{24}(n^4+2n^3-37n^2+58n+192)$.*

Proof. Let $G = C_4(T_1,T_2,T_3,T_4) \in \Theta_n \setminus \{P_{n,4}\}$. By similar arguments as in the proof of Lemma 3.3, we have

$$WW(G) = 10 + WW(T_1) + \sum_{u \in V(T_1)\setminus\{v_1\}} \left[2\binom{d_{uv_2}+1}{2} + \binom{d_{uv_3}+1}{2}\right],$$

which, together with Lemma 2.7, implies that $P'_{n,4}$ is the unique graph in $\Theta_n \setminus \{P_{n,4}\}$ with the largest hyper-Wiener index, which is equal to $\frac{1}{24}(n^4+2n^3-37n^2+58n+192)$. □

For $G = C_4(T_1,T_2,T_3,T_4) = P_n(t_1,t_2,t_3,t_4)$, let u_i be a pendant vertex of T_i with $u_i \neq v_i$ if $t_i \geq 2$ for $1 \leq i \leq 4$. The following two properties are easily seen: For $\{i,j\} = \{1,3\}$ or $\{2,4\}$, we have $WW_{u_i}(G) \geq WW_{u_j}(G)$ if $t_i \geq t_j \geq 2$; For the cycle $v_iv_jv_lv_k$, we have $WW_{u_i}(G) \geq WW_{u_j}(G)$ if $t_i \geq t_j \geq 2$ and $t_k = t_l = 1$.

Lemma 4.4. *Among the graphs in Ω_n with $n \geq 6$, $P_n(n-4,1,2,1)$ is the unique graph with the largest hyper-Wiener index, which is equal to $\frac{1}{24}(n^4+2n^3-37n^2+106n+72)$.*

Proof. It is easily checked that $WW(P_n(n-4,1,2,1) = \frac{1}{24}(n^4+2n^3-37n^2+106n+72)$. Let $G = C_4(T_1,T_2,T_3,T_4) \in \Omega_n$. Suppose without loss of generality that $t_1 \geq \max\{t_2,t_3,t_4\}$ and $t_2 \geq t_4$. By Lemma 2.2, we have $WW(G) \leq WW(P_n(t_1,t_2,t_3,t_4))$ with equality if and only if $G = P_n(t_1,t_2,t_3,t_4)$. Suppose that $G = P_n(t_1,t_2,t_3,t_4)$. By Lemma 2.4, if $t_2 = 1$, then $WW(G) \leq WW(P_n(n-4,1,2,1))$ with equality if and only if $t_3 = 2$, i.e., $G = P_n(n-4,1,2,1)$, and if $t_2 \geq 2$, then

$$\begin{aligned} WW(G) &\leq WW(P_n(t_1+t_3-1,t_2+t_4-1,1,1)) \\ &\leq WW(P_n(n-4,2,1,1)) \\ &= \frac{1}{24}(n^4+2n^3-49n^2+142n+192) \\ &< WW(P_n(n-4,1,2,1)). \end{aligned}$$

The result follows. □

Lemma 4.5. *Among the graphs in Φ_n with $n \geq 6$, C_6 for $n = 6$, and $P_{n,5}$ for $n \geq 7$ are the unique graphs with the largest hyper-Wiener index, which is equal to 42 for $n = 6$ and $\frac{1}{24}(n^4 + 2n^3 - 49n^2 + 142n + 120)$ for $n \geq 7$.*

Proof. By the expression for $WW(P_{n,r})$ given in Lemma 2.6, if r is odd and $7 \leq r \leq n$, then

$$\begin{aligned}
& 48[WW(P_{n,r}) - WW(P_{n,5})] \\
= \;& (-6r^2 + 12r + 90)n^2 + (6r^3 - 24r^2 + 30r - 300)n \\
& -r^4 + 11r^3 - 23r^2 + 13r - 240 \\
\leq \;& (-6r^2 + 12r + 90)rn + (6r^3 - 24r^2 + 30r - 300)n \\
& -r^4 + 11r^3 - 23r^2 + 13r - 240 \\
= \;& (-12r^2 + 120r - 300)n - r^4 + 11r^3 - 23r^2 + 13r - 240 \\
\leq \;& (-12r^2 + 120r - 300)r - r^4 + 11r^3 - 23r^2 + 13r - 240 \\
= \;& -r^4 - r^3 + 97r^2 - 287r - 240 < 0,
\end{aligned}$$

and thus $WW(P_{n,r}) < WW(P_{n,5})$, and if r is even and $8 \leq r \leq n$, then

$$\begin{aligned}
& 48[WW(P_{n,r}) - WW(P_{n,5})] \\
= \;& (-6r^2 + 12r + 96)n^2 + (6r^3 - 24r^2 + 24r - 288)n \\
& -r^4 + 11r^3 - 20r^2 + 4r - 240 \\
\leq \;& (-6r^2 + 12r + 96)rn + (6r^3 - 24r^2 + 24r - 288)n \\
& -r^4 + 11r^3 - 20r^2 + 4r - 240 \\
= \;& (-12r^2 + 120r - 288)n - r^4 + 11r^3 - 20r^2 + 4r - 240 \\
\leq \;& (-12r^2 + 120r - 288)r - r^4 + 11r^3 - 20r^2 + 4r - 240 \\
= \;& -r^4 - r^3 + 100r^2 - 284r - 240 < 0,
\end{aligned}$$

and thus $WW(P_{n,r}) < WW(P_{n,5})$. For $r = 6$ and $n \geq 7$, we have $24[WW(P_{n,6}) - WW(P_{n,5})] = -24(n-3)^2 + 288 < 0$. For $n = r = 6$, we have $42 = WW(C_6) > WW(P_{6,5}) = 39$. The result follows from Lemma 2.6. $\square$

Proposition 4.1. *Among the graphs in $\mathbb{U}_n$ with $n \geq 5$, $S_{5,3}$ and C_5 for $n = 5$, $P_6(2,1,2,1)$ for $n = 6$, $P_7(3,3,1)$ for $n = 7$ and $P'_{n,3}$ for $n \geq 8$ are the unique graphs with the third largest hyper-Wiener index, which is equal to 20 for $n = 5$, 46 for $n = 6$, 90 for $n = 7$ and $\frac{1}{24}(n^4+2n^3-25n^2+22n+120)$ for $n \geq 8$.*

Proof. The case $n = 5$ is trivial. Suppose that $n \geq 6$. By the discussion at the beginning of this section, the third largest hyper-Wiener index of graphs in $\mathbb{U}_n$ is equal to the maximum of the values of the hyper-Wiener indices appearing in Lemmas 4.1–4.5. These values and the corresponding graphs are listed in Table 2, from which the result follows easily. □

Table 2: Graphs and their hyper-Wiener indices in Lemmas 4.1–4.5.

graphs	hyper-Wiener indices		
	n	6	7
$P'_{n,3}$ $(n \geq 6)$	$\frac{1}{24}(n^4+2n^3-25n^2+22n+120)$	45	89
$P_6(2,2,2)$ $(n=6)$		42	
$P_n(n-4,3,1)$ $(n \geq 7)$	$\frac{1}{24}(n^4+2n^3-37n^2+106n+144)$		90
$P'_{n,4}$ $(n \geq 6)$	$\frac{1}{24}(n^4+2n^3-37n^2+58n+192)$	39	78
$P_n(n-4,1,2,1)$ $(n \geq 6)$	$\frac{1}{24}(n^4+2n^3-37n^2+106n+72)$	46	87
C_6 $(n=6)$		42	
$P_{n,5}$ $(n \geq 7)$	$\frac{1}{24}(n^4+2n^3-49n^2+142n+120)$		75

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