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Hyper–Wiener Index of Unicyclic Graphs

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Abstract

The hyper–Wiener index is one of the distance–based graph invariants, used as a structure–descriptor for predicting physicochemical properties of organic compounds. We determine the n-vertex unicyclic graphs of cycle length r with the smallest and the largest hyper–Wiener 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 $n \geq 5$.

1. INTRODUCTION

The Wiener index is the oldest and one of the most thoroughly studied molecular–graph–based structure–descriptors [1–6]. As a kind of extension of the Wiener index, the hyper–Wiener index, proposed by Randić [7] for trees and extended to all connected graphs by Klein, Lukovits and Gutman [8], is also used as a structure–descriptor for predicting physicochemical properties of organic compounds (often those significant for pharmacology, agriculture, environment–protection, etc.) [7, 8, 9].

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Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, $d_{uv} = d(u, v|G)$ denotes the distance between vertices u and v in G. The Wiener index of G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_{uv},$$

and the hyper–Wiener index of G is defined as

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

Lukovits [10] derived formulas for the hyper–Wiener index of chains and trees which contain one trivalent or tetravalent branching vertex. Diudea and Parv [11] proposed general formulas for the calculation of the hyper–Wiener index of regular dendrimers. Gutman et al. [12] determined trees with the smallest, the second smallest, the third smallest, the largest, the second largest and the third largest hyper–Wiener indices. Klavžar et al. [13] proposed an algorithm for the calculation of the hyper–Wiener index of benzenoid hydrocarbons. Aringhieri et al. [14] proposed an algorithm with a complexity linear in the number of vertices for calculating the Hyper–Wiener index of molecular trees. Cash et al. [15] proposed methods for calculating the hyper–Wiener index of molecular graphs, and found closed–form expressions for the hyper–Wiener indices of linear phenylenes, cyclic phenylenes, poly(azulenes), and several families of periodic hexagonal chains. Related and/or recent work may be found, e.g., in [16–20].

A unicyclic graph is a connected graph with a unique cycle. We determine the n-vertex unicyclic graphs of cycle length r with the smallest and the largest hyper–Wiener indices for $3 \le r \le n$, and the n-vertex unicyclic graphs with the smallest, the second smallest, the largest and the second largest hyper–Wiener indices for $n \ge 5$.

2. PRELIMINARIES

For a connected graph G with $u \in V(G)$, let $W_u(G) = \sum\limits_{v \in V(G)} d_{uv}$ and $WW_u(G) = \frac{1}{2} \sum\limits_{v \in V(G)} (d_{uv}^2 + d_{uv})$. Then $W(G) = \frac{1}{2} \sum\limits_{u \in V(G)} W_u(G)$ and $WW(G) = \frac{1}{2} \sum\limits_{u \in V(G)} WW_u(G)$.

Let S_n and P_n be respectively the n-vertex star and the n-vertex path.

Lemma 2.1. [12] *Let T be an n-vertex tree different from S_n and P_n. Then* $\frac{1}{2}(n-1)(3n-4) = WW(S_n) < WW(T) < WW(P_n) = \frac{1}{24}n(n-1)(n+1)(n+2)$.

The following two lemmas are easy to check.

Lemma 2.2. *Let T be an n-vertex tree with $u \in V(T)$, where $n \geq 3$. Let x and y be the center of the star S_n and a terminal vertex of the path P_n, respectively. Then $n-1 = W_x(S_n) \leq W_u(T) \leq W_y(P_n) = \binom{n}{2}$ with left equality if and only if $T = S_n$ and $u = x$, and with right equality if and only if $T = P_n$ and u is a terminal vertex.*

Lemma 2.3. *Let T be an n-vertex tree with $u \in V(T)$, where $n \geq 3$. Let x and y be the center of the star S_n and a terminal vertex of the path P_n, respectively. Then $n-1 = WW_x(S_n) \leq WW_u(T) \leq WW_y(P_n) = \binom{n+1}{3}$ with left equality if and only if $T = S_n$ and $u = x$, and with right equality if and only if $T = P_n$ and u is a terminal vertex.*

For $n \geq 5$, let S'_n be the tree formed by attaching a pendent vertex to a pendent vertex of the star S_{n-1}, and P'_n the tree formed by attaching a pendent vertex to the neighbor of one terminal vertex of P_{n-1}.

Lemma 2.4. [12] *Among the n-vertex trees with $n \geq 5$, S'_n is the unique tree with the second smallest hyper–Wiener index, which is equal to $\frac{1}{2}(3n^2 - n - 14)$, and P'_n is the unique tree with the second largest hyper–Wiener index, which is equal to* $\frac{1}{24}(n^4 + 2n^3 - 13n^2 + 10n + 72)$.

Let C_n be the n-vertex cycle with $n \geq 3$.

Lemma 2.5. [2, 8] *Let v be a vertex on the cycle C_n with $n \geq 3$. Then*

$$W_v(C_n) = \left\lfloor \frac{n^2}{4} \right\rfloor ,$$

$$WW(C_n) = \frac{n}{2}\, WW_v(C_n) = \begin{cases} \frac{n(n+1)(n-1)(n+3)}{48} & \text{if } n \text{ is odd,} \\ \frac{n^2(n+1)(n+2)}{48} & \text{if } n \text{ is even.} \end{cases}$$

The number of vertices of G is denoted by $|G|$. 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 $\sum_{i=1}^{r} |T_i| = n$.

When $C_r(T_1, T_2, \ldots, T_r)$ is considered, we write $d_{ij} = d(v_i, v_j|C_r)$, $WW_i(T_i) = WW_{v_i}(T_i)$, $W_i(T_i) = W_{v_i}(T_i)$, and $t_i = |T_i|$ for $1 \le i, j \le r$.

As in [21], we have

Proposition 2.1. *For $r \ge 3$, let $G = C_r(T_1, T_2, \ldots, T_r)$. Then*

$$\begin{aligned} WW(G) &= \sum_{i=1}^{r} WW(T_i) + \sum_{i=1}^{r}(|G| - t_i)WW_i(T_i) + \sum_{i<j} t_i t_j \binom{d_{ij}+1}{2} \\ &\quad + \sum_{i=1}^{r} \sum_{j \ne i} t_j d_{ij} W_i(T_i) + \sum_{i<j} W_i(T_i) W_j(T_j) . \end{aligned}$$

Proof. For $a \in V(T_i)$ and $b \in V(T_j)$ with $1 \le i < j \le r$, we have $d_{ab} = d_{av_i} + d_{ij} + d_{v_j b}$. It is easily seen that

$$\begin{aligned} & \sum_{1\le i<j\le r} \sum_{a\in V(T_i)} \sum_{b\in V(T_j)} (d_{ab}^2 + d_{ab}) \\ = & \sum_{1\le i<j\le r} \sum_{a\in V(T_i)} \sum_{b\in V(T_j)} \left[(d_{av_i} + d_{ij} + d_{v_j b})^2 + (d_{av_i} + d_{ij} + d_{v_j b})\right] \\ = & \sum_{1\le i<j\le r} \sum_{a\in V(T_i)} \sum_{b\in V(T_j)} \left[(d_{av_i}^2 + d_{av_i}) + (d_{v_j b}^2 + d_{v_j b})\right] \\ & + \sum_{1\le i<j\le r} \sum_{a\in V(T_i)} \sum_{b\in V(T_j)} (d_{ij}^2 + d_{ij}) \\ & + \sum_{1\le i<j\le r} \sum_{a\in V(T_i)} \sum_{b\in V(T_j)} (2d_{av_i} d_{ij} + 2d_{v_j b} d_{ij}) \\ & + \sum_{1\le i<j\le r} \sum_{a\in V(T_i)} \sum_{b\in V(T_j)} 2d_{av_i} d_{v_j b} \\ = & \ 2\sum_{i=1}^{r} (|G| - t_i)WW_i(T_i) + \sum_{i<j} t_i t_j (d_{ij}^2 + d_{ij}) \\ & +2\sum_{i=1}^{r} \sum_{j\ne i} t_j d_{ij} W_i(T_i) + 2\sum_{i<j} W_i(T_i) W_j(T_j) . \end{aligned}$$

Thus, we have

$$\begin{aligned} 2WW(G) &= \sum_{i=1}^{r} \sum_{j=1}^{r} \sum_{a\in V(T_i)} \sum_{b\in V(T_j)} (d_{ab}^2 + d_{ab}) \\ &= 2\sum_{i=1}^{r} WW(T_i) + \sum_{1\le i<j\le r} \sum_{a\in V(T_i)} \sum_{b\in V(T_j)} (d_{ab}^2 + d_{ab}) \end{aligned}$$

$$= 2\sum_{i=1}^{r} WW(T_i) + 2\sum_{i=1}^{r} (|G| - t_i) WW_i(T_i) + \sum_{i<j} t_i t_j (d_{ij}^2 + d_{ij})$$
$$+2\sum_{i=1}^{r} \sum_{j\neq i} t_j d_{ij} W_i(T_i) + 2\sum_{i<j} W_i(T_i) W_j(T_j) .$$

Now the result follows. ■

Let $S_{n,r}$ be the unicyclic graph obtained by attaching $n-r$ pendent vertices to a vertex of the cycle C_r, and $P_{n,r}$ the unicyclic graph obtained by attaching a path on $n-r$ vertices (at one terminal vertex) to the cycle C_r, where $3 \leq r \leq n$. In particular, $S_{n,n} = P_{n,n} = C_n$. Obviously, $S_{n,r}$ is the graph $C_r(T_1, T_2, \ldots, T_r)$ with $|T_1| = n - r + 1$, $|T_2| = \cdots = |T_r| = 1$ and T_1 is a star with center v_1, and $P_{n,r}$ is the graph $C_r(T_1, T_2, \ldots, T_r)$ with $|T_1| = n - r + 1$, $|T_2| = \cdots = |T_r| = 1$ and T_1 is a path with a terminal vertex v_1.

Let $\mathcal{U}_n$ be the set of n-vertex unicyclic graphs. Let Φ_n be the set of n-vertex unicyclic graphs with cycle length at least four. Let Γ_n be the set of n-vertex unicyclic graphs $C_3(T_1, T_2, T_3)$ with $|T_1| \geq |T_2| = |T_3| = 1$. Let Ψ_n be the set of n-vertex unicyclic graphs $C_3(T_1, T_2, T_3)$ with $|T_1| \geq |T_2| \geq \max\{|T_3|, 2\}$. Then, $\mathcal{U}_n = \Phi_n \cup \Gamma_n \cup \Psi_n$.

For an edge e of the graph G, $G - e$ denotes the graph obtained from G by deleting the edge e, and for an edge of the complement of G, $G + e$ denotes the graph obtained from G by adding the edge e.

3. UNICYCLIC GRAPHS WITH SMALL HYPER–WIENER INDICES

In this section, we determine the n-vertex unicyclic graph(s) of cycle length r with the smallest hyper–Wiener index for $3 \leq r \leq n$, and the n-vertex unicyclic graphs with the smallest and the second smallest hyper–Wiener indices for $n \geq 5$.

Proposition 3.1. *Let G be an n-vertex unicyclic graph with cycle length r. Then $WW(G) \geq WW(S_{n,r})$ with equality if and only if $G = S_{n,r}$, where*

$$WW(S_{n,r}) = \begin{cases} \frac{1}{48}(72n^2 - r^4 + 2nr^3 - 15r^3 + 18nr^2 + 25r^2 \\ \quad -98nr - 90n + 87r) & \text{if } r \text{ is odd,} \\ \frac{1}{48}(72n^2 - r^4 + 2nr^3 - 15r^3 + 18nr^2 + 22r^2 \\ \quad -92nr - 72n + 72r) & \text{if } r \text{ is even.} \end{cases}$$

Proof. To compute $WW(S_{n,r})$, consider the contributions of the pairs of vertices in the star $T_1 = S_{n-r+1}$, the pairs with one vertex in T_1 and the other vertex of the cycle both different from v_1, and the pairs of vertices of the cycle. It is easily seen that

$$\begin{aligned} WW(S_{n,r}) &= WW(S_{n-r+1}) + \left[\sum_{j\neq 1} \binom{1+d_{1j}+1}{2}\right] \cdot (n-r) + WW(C_r) \\ &= WW(S_{n-r+1}) + \frac{1}{2}(n-r)\sum_{j\neq 1}(d_{1j}^2 + 3d_{1j} + 2) + WW(C_r) \\ &= WW(S_{n-r+1}) + (n-r)(r-1) \\ &\quad +(n-r)[WW_{v_1}(C_r) + W_{v_1}(C_r)] + WW(C_r)\,. \end{aligned}$$

By Lemmas 2.1 and 2.5, we get the expressions for $WW(S_{n,r})$, as desired.

The result is obvious for $r = n-1, n$. Suppose that $r \leq n-2$. Let $G = C_r(T_1, \ldots, T_r)$ be a graph with the smallest hyper–Wiener index in the set of n-vertex unicyclic graphs with cycle length r. By Proposition 2.1 and Lemmas 2.1–2.3, T_i is a star with center v_i for $i = 1, 2, \ldots, r$. Suppose that there exist k and l with $1 \leq k < l \leq r$ such that $t_k, t_l \geq 2$. Let $a \in V(T_k)$, $b \in V(T_l)$ with $a \neq v_k$ and $b \neq v_l$. Suppose without loss of generality that $WW_a(G) \leq WW_b(G)$. For $G' = G - v_l b + v_k b$, we have $WW(G') - WW_b(G') = \frac{1}{2} \sum_{\{u,v\}\subseteq V(G)\setminus\{b\}} (d_{uv}^2 + d_{uv}) = WW(G) - WW_b(G)$, and then

$$\begin{aligned} WW(G') - WW(G) &= WW_b(G') - WW_b(G) = WW_a(G') - WW_b(G) \\ &= WW_a(G) + 3 - \frac{1}{2}\left(d_{ab}^2 + d_{ab}\right) - WW_b(G) \\ &= WW_a(G) - WW_b(G) - \frac{1}{2}\left(d_{kl}^2 + 5d_{kl}\right) < 0, \end{aligned}$$

which is a contradiction to the choice of G. Thus $r-1$ of $t_1, t_2, \ldots, t_r$ are equal to 1 and the remaining one is equal to $n-(r-1)$, i.e., $G = S_{n,r}$. ■

Proposition 3.2. *Among the graphs in $\mathcal{U}_n$ with $n \geq 3$, $S_{n,3}$ and C_n for $n = 4, 5$, and $S_{n,3}$ for $n \neq 4, 5$ are the unique graphs with the smallest hyper–Wiener index, which is equal to $\frac{1}{2}(3n^2 - 7n)$.*

Proof. Note that the number of edges of G is n. It is easily seen that

$$WW(G) \geq \frac{1}{2} \cdot (1^2+1) \cdot n + \frac{1}{2} \cdot (2^2+2) \cdot \left[\binom{n}{2} - n\right] = \frac{3n^2 - 7n}{2}$$

with equality if and only if the diameter of G is at most 2. The result follows. ■

By previous proposition, the graphs in $\mathcal{U}_n = \Phi_n \cup \Gamma_n \cup \Psi_n$ for $n \geq 5$ with the second smallest hyper–Wiener index are just the graphs in $\mathcal{U}_5 \setminus \{S_{5,3}, C_5\} = (\Phi_5 \setminus \{C_5\}) \cup (\Gamma_5 \setminus \{S_{5,3}\}) \cup \Psi_5$ for $n = 5$ and in $\mathcal{U}_n \setminus \{S_{n,3}\} = \Phi_n \cup (\Gamma_n \setminus \{S_{n,3}\}) \cup \Psi_n$ for $n \geq 6$ with the smallest hyper–Wiener index.

Lemma 3.1. *Among the graphs in $\Phi_5 \backslash \{C_5\}$, $S_{5,4}$ is the unique graph with the smallest hyper–Wiener index, which is equal to 23. Among the graphs in Φ_n with $n \geq 6$, $S_{6,4}$ and $S_{6,5}$ for $n = 6$, and $S_{n,4}$ for $n \geq 7$ are the unique graphs with the smallest hyper–Wiener index, which is equal to $\frac{1}{2}(3n^2 - n - 24)$.*

Proof. The case $n = 5$ is trivial. Suppose that $n \geq 6$.

Suppose first that r is odd with $r \geq 7$. By Proposition 3.1,

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

Let $f_1(n)$ be the expression in the right side of the above equation. Since $n \geq r \geq 7$, we have $f_1'(n) = 2r^3 + 18r^2 - 98r - 210 > 0$, and then $f_1(n)$ is increasing for $n \geq r$. It follows that

$$48[WW(S_{n,r}) - WW(S_{n,5})] = f_1(n) \geq f_1(r) = r^4 + 3r^3 - 73r^2 - 123r + 1440 > 0,$$

and then $WW(S_{n,r}) > WW(S_{n,5})$. Now suppose that r is even with $r \geq 6$. By Proposition 3.1,

$$\begin{aligned} & 48[WW(S_{n,r}) - WW(S_{n,4})] \\ = \ & (2r^3 + 18r^2 - 92r - 48)n - r^4 - 15r^3 + 22r^2 + 72r + 576 \,. \end{aligned}$$

Similarly, $WW(S_{n,r}) > WW(S_{n,4})$.

It is easily seen that $WW(S_{n,4}) - WW(S_{n,5}) = -3(n-6)$. Now the result follows easily. ■

For $n \geq 5$, let $S'_{n,3}$ be the n-vertex unicyclic graph formed by attaching $n - 5$ pendent vertices and a path P_2 to one vertex of a triangle. Evidently, $S'_{n,3} \in \Gamma_n$. By Proposition 3.2, $S_{n,3}$ is the unique graph in Γ_n with the smallest hyper–Wiener index.

Lemma 3.2. *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* $\frac{1}{2}(3n^2 - n - 18)$.

Proof. The cases for $n = 5, 6$ may be checked easily. Suppose that $n \geq 7$. Let $G = C_3(T_1, T_2, T_3) \in \Gamma_n \setminus \{S_{n,3}\}$. Note that $|T_1| = n - 2 \geq 5$. It is easily seen that

$$WW(G) \;=\; 3 + WW(T_1) + 2 \sum_{u \in V(T_1)\setminus\{v_1\}} \binom{d_{uv_2} + 1}{2}$$

which, together with Lemma 2.4, implies that $S'_{n,3}$ is the unique graph in $\Gamma_n \setminus \{S_{n,3}\}$ with the smallest index, and we have

$$\begin{aligned} WW(S'_{n,3}) &= 3 + WW(S'_{n-2}) + 2 \cdot \frac{1}{2} \cdot [(4+2)(n-4) + 9 + 3] \\ &= \frac{1}{2}(3n^2 - n - 18). \end{aligned}$$

This proves the lemma. ■

Let $S_n(a, b, c)$ be the n-vertex unicyclic graph formed by attaching $a - 1$, $b - 1$ and $c - 1$ pendent vertices to the three vertices of a triangle, respectively, where $a \geq b \geq c \geq 1$ and $a + b + c = n$.

Lemma 3.3. *Among the graphs in* Ψ_n *with* $n \geq 5$, $S_n(n-3, 2, 1)$ *is the unique graph with the smallest hyper–Wiener index, which is equal to* $\frac{1}{2}(3n^2 - n - 24)$.

Proof. For $n \geq 5$, let $G = C_3(T_1, T_2, T_3) \in \Psi_n$ with $a \geq b \geq \max\{c, 2\}$ and $a + b + c = n$, where $a = |T_1|$, $b = |T_2|$ and $c = |T_3|$.

If $G = S_n(a, b, c)$ and $G \neq S_n(n-3, 2, 1)$, then it is easily seen that $WW_x(G) \leq WW_y(G)$ for pendent vertices $x \in V(T_1)$ and $y \in V(T_2) \cup V(T_3)$, and by the proof of Proposition 3.1, we have

$$WW(S_n(a, b, c)) \geq WW(S_n(a + c - 1, b, 1)) \geq WW(S_n(n-3, 2, 1)),$$

and at least one inequality is strict, where

$$\begin{aligned} WW(S_n(n-3, 2, 1)) &= WW(S_{n-1,3}) + \frac{1}{2} \cdot [2 + 6 + 6 + 12(n-4)] \\ &= \frac{3n^2 - n - 24}{2}. \end{aligned}$$

If $G \neq S_n(a, b, c)$, then as in the proof of Proposition 3.1, we have $WW(G) > WW(S_n(a, b, c)) \geq WW(S_n(n-3, 2, 1))$. ■

By Lemmas 3.1–3.3, we have:

Proposition 3.3. *Among the graphs in $\mathcal{U}_n$ with $n \geq 5$, $S_6(3,2,1)$, $S_{6,4}$ 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 $\frac{1}{2}(3n^2 - n - 24)$.*

4. UNICYCLIC GRAPHS WITH LARGE HYPER–WIENER INDICES

In this section, we determine the n-vertex unicyclic graph(s) of cycle length r with the largest hyper–Wiener index for $3 \leq r \leq n$, and the n-vertex unicyclic graphs with the largest and the second largest hyper–Wiener indices for $n \geq 5$.

Proposition 4.1. *Let G be an n-vertex unicyclic graph with cycle length r. Then $WW(G) \leq WW(P_{n,r})$ with equality if and only if $G = P_{n,r}$, where*

$$WW(P_{n,r}) = \begin{cases} \frac{1}{48}(2n^4 + 4n^3 + 6nr^3 - 6n^2r^2 + 12n^2r - 24nr^2 - 8n^2 \\ \quad +30nr - 16n - r^4 + 11r^3 - 23r^2 + 13r) & \text{if } r \text{ is odd,} \\ \frac{1}{48}(2n^4 + 4n^3 + 6nr^3 - 6n^2r^2 + 12n^2r - 24nr^2 - 2n^2 \\ \quad +24nr - 4n - r^4 + 11r^3 - 20r^2 + 4r) & \text{if } r \text{ is even.} \end{cases}$$

Proof. It is easily seen that

$$\begin{aligned} WW(P_{n,r}) &= WW(P_{n-r+1}) + \sum_{k=1}^{n-r} \sum_{j \neq 1} \binom{k + d_{1j} + 1}{2} + WW(C_r) \\ &= WW(P_{n-r+1}) + \frac{1}{2} \sum_{j \neq 1} \sum_{k=1}^{n-r} (k^2 + k + 2d_{1j}k) \\ &\quad + \sum_{j \neq 1} \sum_{k=1}^{n-r} \binom{d_{1j}}{2} + WW(C_r) \\ &= WW(P_{n-r+1}) + \frac{(r-1)(n-r)(n-r+1)(n-r+2)}{6} \\ &\quad + \frac{1}{2}(n-r)(n-r+1)W_{v_1}(C_r) + (n-r)WW_{v_1}(C_r) + WW(C_r)\,. \end{aligned}$$

By Lemmas 2.1 and 2.5, we get the expressions for $WW(P_{n,r})$, as desired.

The result is obvious for $r = n-1, n$. Suppose that $r \leq n-2$. Let $G = C_r(T_1, \ldots, T_r)$ be a graph with the largest hyper–Wiener index in the set of n-vertex unicyclic graphs with cycle length r. By Proposition 2.1 and Lemmas 2.1–2.3, T_i is a path with v_i as one of its end vertices for $i = 1, 2, \ldots, r$. Suppose that there exist k and l with $1 \leq k < l \leq r$ such that $t_k, t_l \geq 2$. Let $a \neq v_k$ and $b \neq v_l$ be end vertices of T_k and T_l, respectively. Let $L_G(a,b) = \binom{d_{ab}+1}{2}$. Suppose without loss of generality that $WW_a(G) \geq WW_b(G)$. Let c be the neighbor of b in G. For $G' = G - cb + ab$, we have

$$\begin{aligned}
& WW(G') - WW(G) \\
= \;& WW_b(G') - WW_b(G) \\
= \;& \sum_{u \in V(G)\setminus\{b\}} \binom{1 + d_{ua} + 1}{2} - WW_b(G) \\
= \;& \sum_{u \in V(G)\setminus\{b\}} \binom{d_{ua} + 1}{2} + \sum_{u \in V(G)\setminus\{b\}} (d_{ua} + 1) - WW_b(G) \\
= \;& WW_a(G) - WW_b(G) + n - 1 + \sum_{u \in V(G)\setminus\{a,b\}} d_{ua} - L_G(a,b)\,.
\end{aligned}$$

Since $\sum\limits_{u \in V(G)\setminus\{a,b\}} d_{ua} > \sum\limits_{i=1}^{d_{ab}-1} i = \binom{d_{ab}}{2}$, we have $n - 1 + \sum\limits_{u \in V(G)\setminus\{a,b\}} d_{ua} - L_G(a,b) > 0$. Thus, $WW(G') > WW(G)$, which is a contradiction to the choice of G. It follows that $G = P_{n,r}$. ■

Proposition 4.2. *Among the graphs in $\mathcal{U}_n$ with $n \geq 3$, $P_{4,3}$ and C_4 for $n = 4$, and $P_{n,3}$ for $n \neq 4$ are the unique graphs with the largest hyper–Wiener index, which is equal to* $\frac{1}{24}(n^4 + 2n^3 - 13n^2 + 10n + 24)$.

Proof. Suppose first that r is odd with $r \geq 5$. By Proposition 4.1,

$$\begin{aligned}
& 48[WW(P_{n,r}) - WW(P_{n,3})] \\
= \;& (-6r^2 + 12r + 18)n^2 + (6r^3 - 24r^2 + 30r - 36)n - r^4 + 11r^3 - 23r^2 + 13r - 48\,.
\end{aligned}$$

Let $g_1(n)$ be the expression in the right side of equation above. Since $n \geq r$, we have

$$\begin{aligned}
g_1'(n) &= -12(r+1)(r-3)n + 6r^3 - 24r^2 + 30r - 36 \\
&\leq -12(r+1)(r-3)r + 6r^3 - 24r^2 + 30r - 36 \\
&= -6r(r^2 - 11) - 36 < 0,
\end{aligned}$$

and then $g_1(n)$ is decreasing for $n \geq r$. It follows that

$$48[WW(P_{n,r}) - WW(P_{n,3})] = g_1(n) \leq g_1(r) = -r^4 - r^3 + 25r^2 - 23r - 48 < 0,$$

and thus, for odd $r \geq 5$, we have $WW(P_{n,r}) < WW(P_{n,3})$. Now suppose that r is even and $r \geq 4$. By Proposition 4.1,

$$48[WW(P_{n,r}) - WW(P_{n,3})]$$

$$= \quad (-6r^2+12r+24)n^2+(6r^3-24r^2+24r-24)n-r^4+11r^3-20r^2+4r-48\,.$$

Let $g_2(n)$ be the expression in the right side of the above equation. Since $n \geq r$, we have

$$\begin{aligned} g_2'(n) &= -12(r^2-2r-4)n+6r^3-24r^2+24r-24 \\ &\leq -12(r^2-2r-4)r+6r^3-24r^2+24r-24 \\ &= -6r(r^2-12)-24<0, \end{aligned}$$

and then $g_2(n)$ is decreasing for $n \geq r$. It follows that

$$48[WW(P_{n,r})-WW(P_{n,3})]=g_2(n)\leq g_2(r)=-r^4-r^3+28r^2-20r-48\leq 0,$$

and thus, for even $r \geq 4$, we have $WW(P_{n,r}) \leq WW(P_{n,3})$ with equality if and only if $n=r=4$. Then the result follows. ■

By previous proposition, the graphs in $\mathcal{U}_n=\Phi_n\cup\Gamma_n\cup\Psi_n$ for $n\geq 5$ with the second largest hyper–Wiener index are just the graphs in $\Phi_n\cup(\Gamma_n\setminus\{P_{n,3}\})\cup\Psi_n$ with the largest hyper–Wiener index.

For $n \geq 5$, let $P'_{n,3}$ be the n-vertex unicyclic graph formed by attaching a pendent vertex to the neighbor of the pendent vertex of $P_{n-1,3}$.

Lemma 4.1. *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* $\frac{1}{24}(n^4+2n^3-25n^2+22n+120)$.

Proof. The cases for $n=6,7$ may be checked easily. Suppose that $n\geq 8$. Let $G=C_3(T_1,T_2,T_3)\in\Gamma_n\setminus\{P_{n,3}\}$. Obviously,

$$WW(G) \quad = \quad 3+WW(T_1)+2\sum_{u\in V(T_1)\setminus\{v_1\}}\binom{d_{uv_2}+1}{2}$$

which, together with Lemma 2.4, implies that $P'_{n,3}$ is the unique graph in $\Gamma_n\setminus\{P_{n,3}\}$ with the largest hyper–Wiener index, and

$$\begin{aligned} WW(P'_{n,3}) &= 3+WW(P'_{n-2})+\sum_{i=2}^{n-3}(i^2+i)+(n-3)^2+(n-3) \\ &= \frac{n^4+2n^3-25n^2+22n+120}{24}, \end{aligned}$$

as desired. ■

Let $P_n(a,b,c)$ be the n-vertex unicyclic graph formed by attaching P_{a-1}, P_{b-1} and P_{c-1} to the three vertices of a triangle, respectively, where $a \geq b \geq c \geq 1$ and $a+b+c=n$.

Lemma 4.2. *Among the graphs in Ψ_n with $n \geq 5$, $P_n(n-3,2,1)$ is the unique graph with the largest hyper–Wiener index, which is equal to $\frac{1}{24}(n^4+2n^3-25n^2+46n+72)$.*

Proof. For $n \geq 5$, let $G = C_3(T_1,T_2,T_3) \in \Psi_n$ with $a \geq b \geq \max\{c,2\}$ and $a+b+c=n$, where $a=|T_1|$, $b=|T_2|$ and $c=|T_3|$.

If $G = P_n(a,b,c)$ and $G \neq P_n(n-3,2,1)$, then it is easily seen that $WW_x(G) \geq WW_y(G)$ for pendent vertices $x \in V(T_1)$ and $y \in V(T_2) \cup V(T_3)$, and by the proof of Proposition 4.1, we have

$$WW(P_n(a,b,c)) \leq WW(P_n(a+c-1,b,1)) \leq WW(P_n(n-3,2,1)),$$

and at least one inequality is strict, where

$$\begin{aligned} WW(P_n(n-3,2,1)) &= WW(P_{n-1,3}) + \frac{1}{2}\left[2+6+\sum_{i=2}^{n-2}(i^2+i)\right] \\ &= \frac{n^4+2n^3-25n^2+46n+72}{24}. \end{aligned}$$

If $G \neq P_n(a,b,c)$, then as in the proof of Proposition 4.1, we have $WW(G) < WW(P_n(a,b,c)) \leq WW(P_n(n-3,2,1))$. ■

Proposition 4.3. *Among the graphs in $\mathcal{U}_n$ with $n \geq 5$, $P_n(n-3,2,1)$ and $P_{n,4}$ are the unique graphs with the second largest hyper–Wiener index, which is equal to $\frac{1}{24}(n^4+2n^3-25n^2+46n+72)$.*

Proof. If $G \in \Phi_n$, then by similar arguments as in the proof of Proposition 4.2 and noting that $WW(P_{n,4}) - WW(P_{n,5}) = n^2-4n-2 > 0$, we have $WW(G) \leq \frac{1}{24}(n^4+2n^3-25n^2+46n+72)$ with equality if and only if $G = P_{n,4}$. Now the result follows from Lemmas 4.1 and 4.2. ■

5. COMMENTS

We have determined in Propositions 3.2 and 3.3 the graphs in $\mathcal{U}_n$, $n \geq 5$, with the smallest and the second smallest hyper–Wiener indices, and in Propositions 4.2 and

4.3 the graphs in $\mathcal{U}_n$, $n \geq 5$, with the largest and the second largest hyper–Wiener indices. By Propositions 3.3 and 4.3, among graphs in $\mathcal{U}_n$ with $n \geq 5$, there are three graphs for $n = 6$ and two graphs for $n \neq 6$ with the second smallest hyper–Wiener index, and there are two graphs with the second largest hyper–Wiener index.

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