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Hyper-Wiener indices of polyphenyl chains and polyphenyl spiders

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Abstract: Let G be a connected graph and u and v two vertices of G. The hyper-Wiener index of graph G is $WW(G) = \frac{1}{2}\sum_{u,v\in V(G)}(d_G(u,v)+d_G^2(u,v))$, where $d_G(u,v)$ is the distance between u and v. In this paper, we first give the recurrence formulae for computing the hyper-Wiener indices of polyphenyl chains and polyphenyl spiders. We then obtain the sharp upper and lower bounds for the hyper-Wiener index among polyphenyl chains and polyphenyl spiders, respectively. Moreover, the corresponding extremal graphs are determined.

Keywords: Hyper-Wiener index; Polyphenyl system, Polyphenyl chain; Polyphenyl spider

MSC: 05C12, 05C35, 92E20

1 Introduction

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The distance $d_G(u,v)$ between vertices u and v is the number of edges on a shortest path connecting these vertices in G. Let $u \in V(G)$. Denoted by $D_G(u)$ is the sum of the distances between u and all other vertices of G.

The *Wiener index* [1] of G is defined as the sum of distances between all pairs of vertices in G, i.e.,

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v).$$

The *hyper-Wiener index* of G, denoted by $WW(G)$, is defined as

$$WW(G) = \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}\left(d_G(u,v) + d_G^2(u,v)\right), \tag{1}$$

where the summation goes over all pairs of vertices in G. For two vertices u and v of G, set $\alpha_G(u,v) = d_G(u,v)(d_G(u,v)+1)$ and $A_G(u) = \sum_v \alpha_G(u,v)$, where this summation extends to all the vertices different from u. Then (1) is expressed as follows.

$$WW(G) = \frac{1}{2}\sum_{u,v\in V(G)} \alpha_G(u,v). \tag{2}$$

The hyper-Wiener index, which was first proposed by Milan Randić [2], is introduced as one of the distance-based molecular structure descriptors. Klein et al. [3] extended Randić's definition as a generalization of the Wiener index for all connected graphs. For more studies on hyper-Wiener index, see [5-25], among others.

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The polyphenyl system with n hexagons is obtained from two adjacent hexagons that are sticked by a path. Polyphenyl systems are of great importance for theoretical chemistry because they are natural molecular graph representations of benzenoid hydrocarbons [26].

A polyphenyl system is called a *polyphenyl chain* PC_n with n hexagons [4, 26], and it can be regarded as a polyphenyl chain PC_{n-1} with $n-1$ hexagons adjoining to a new terminal hexagon by a cut edge, the resulting graph see Figure 1.

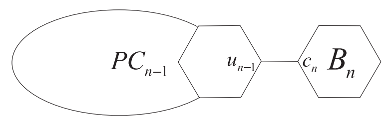

Figure 1: A polyphenyl chain PC_n with n hexagons.

Let $PC_n = B_1B_2 \cdots B_n$ be a polyphenyl chain with $n(n \geq 2)$ hexagons, where B_i is the i-th hexagon of PC_n attached to B_{i-1} by a cut edge $u_{i-1}c_i$, $i = 2, 3, \cdots, n$. A vertex v of H_i is said to be *ortho*-, *meta*- and *para*-vertex of H_i if the distance between v and c_i is 1, 2 and 3, denoted by o_i, m_i and p_i, respectively. In particular, A polyphenyl chain PC_n is a *polyphenyl ortho-chain* if $u_i = o_i$ for $2 \leq i \leq n-1$, denoted by PCO_n. A polyphenyl chain PC_n is a *polyphenyl meta-chain* if $u_i = m_i$ for $2 \leq i \leq n-1$, denoted by PCM_n. A polyphenyl chain PC_n is a *polyphenyl para-chain* if $u_i = p_i$ for $2 \leq i \leq n-1$, denoted by PCP_n.

A *polyphenyl spider*, denoted by $PS(r, s, t)$, is obtained by three nonadjacent vertices of a hexagon B joining a polyphenyl chain $PC_i(i = r, s, t)$, respectively, the resulting graph see Figure 2. In particular, the hexagon B is called the *center* of $PS(r, s, t)$, and three components of $PS(r, s, t)$ deleting the center B are called *legs* of $PS(r, s, t)$. A polyphenyl spider is called *a polyphenyl ortho-spiedr* if every leg of the polyphenyl spider is a polyphenyl ortho-chain. A polyphenyl spider is called *a polyphenyl meta-spiedr* if every leg of the polyphenyl spider is a polyphenyl meta-chain. A polyphenyl spider is called *a polyphenyl para-spiedr* if every leg of the polyphenyl spider is a polyphenyl para-chain. Clearly, a polyphenyl spider is a polyphenyl system.

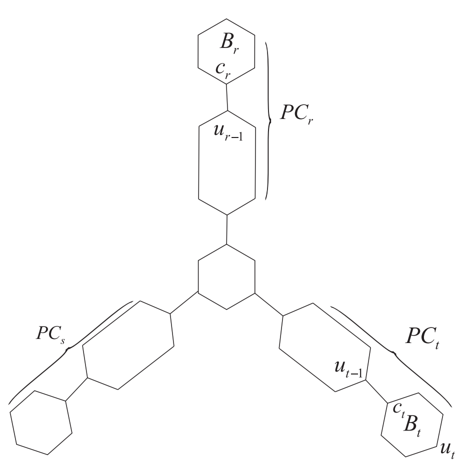

Figure 2: A polyphenyl spider $PS(r, s, t)$.

In this paper, we mainly investigate the properties of hyper-Wiener indices of polyphenyl chains and polyphenyl spiders. The rest of this paper is organized as follows. In Section 2, we present some properties of hyper-Wiener index of polyphenyl chains, and give the lower and upper bounds on the hyper-Wiener index among polyphenyl chains. In Section 3, we will give some properties of hyper-Wiener index of polyphenyl spiders, and the extremal polyphenyl spiders with respect to the hyper-Wiener index are obtained.

2 Hyper-Wiener index of polyphenyl chains

In this section, we will investigate some properties of hyper-Wiener index of polyphenyl chains.

Theorem 2.1. *Let PC_n be a polyphenyl chain with $n(n \geq 2)$ hexagons and $u_{n-1}c_n$ a cut edge of PC_n(see Figure 1). Then*

$$WW(PC_n) = WW(PC_{n-1}) + 3A_{PC_{n-1}}(u_{n-1}) + 15D_{PC_{n-1}}(u_{n-1}) + 174n - 130.$$

Proof. By Eq. (2), we obtain that

$$\begin{aligned}
WW(PC_n) &= \frac{1}{2}\sum_{u,v\in V(PC_{n-1})} \alpha_{PC_n}(u,v) + \frac{1}{2}\sum_{u,v\in V(C_6)} \alpha_{PC_n}(u,v) + \frac{1}{2}\sum_{u\in V(PC_{n-1}),v\in V(C_6)} \alpha_{PC_n}(u,v)\\
&= WW(PC(n-1)) + WW(C_6) + \frac{1}{2}\alpha_{PC_n}(u_{n-1},c_n) + \frac{1}{2}\sum_{u\in PC_{n-1}} \alpha_{PC_n}(u,c_n)\\
&+\frac{1}{2}\sum_{v\in C_6} \alpha_{PC_n}(u_{n-1},v) + \frac{1}{2}\sum_{u\in V(PC_{n-1}-u_{n-1}),v\in V(C_6-c_n)} \alpha_{PC_n}(u,v)\\
&= WW(PC(n-1)) + WW(C_6) + 1 + \frac{1}{2}\sum_{v\in V(C_6)} (d_{C_6}(c_n,v)+1)(d_{C_6}(c_n,v)+2) \qquad (3)\\
&+\frac{1}{2}\sum_{u\in V(PC_{n-1})} (d_{PC_{n-1}}(u,u_{n-1})+1)(d_{PC_{n-1}}(u,u_{n-1})+2) + \frac{1}{2}M\\
&= WW(PC(n-1)) + WW(C_6) + 1 + \frac{1}{2}A_{PC_{n-1}}(u_{n-1}) + D_{PC_{n-1}}(u_{n-1}) + \frac{1}{2}A_{C_6}(c_n)\\
&+D_{C_6}(c_n) + 6n + \frac{1}{2}M,
\end{aligned}$$

where $M = \sum_{u\in V(PC_{n-1}-u_{n-1}),v\in V(C_6-c_n)} \alpha_{PC_n}(u,v)$.

Simplifying M, we have

$$\begin{aligned}
M &= \sum_{u\in V(PC_{n-1}-u_{n-1}),v\in V(C_6-c_n)} \alpha_{PC_n}(u,v)\\
&= \sum_{u\in V(PC_{n-1}-u_{n-1}),v\in V(C_6-c_n)} [d_{PC_{n-1}}(u,u_{n-1}) + 1 + d_{C_6}(c_n,v)][d_{PC_{n-1}}(u,u_{n-1})\\
&+2 + d_{C_6}(c_n,v)]\\
&= \sum_{u\in V(PC_{n-1}-u_{n-1})}\sum_{v\in V(C_6-c_n)} [\alpha_{PC_{n-1}}(u,u_{n-1}) + \alpha_{C_6}(c_n,v)]\\
&+ \sum_{u\in V(PC_{n-1}-u_{n-1})}\sum_{v\in V(C_6-c_n)} [d_{PC_{n-1}}(u,u_{n-1})(d_{C_6}(c_n,v)+1)] \qquad (4)\\
&+ \sum_{u\in V(PC_{n-1}-u_{n-1})}\sum_{v\in V(C_6-c_n)} [d_{C_6}(c_n,v)(d_{PC_{n-1}}(u,u_{n-1})+1)]\\
&+ \sum_{u\in V(PC_{n-1}-u_{n-1})}\sum_{v\in V(C_6-c_n)} [d_{PC_{n-1}}(u,u_{n-1}) + d_{C_6}(c_n,v) + 2]\\
&= 5A_{PC_{n-1}}(u_{n-1}) + (6n-5)A_{C_6}(c_n) + D_{PC_{n-1}}(u_{n-1})(D_{C_6}(c_n)+5)\\
&+D_{C_6}(c_n)(D_{PC_{n-1}}(u_{n-1}) + 6n - 7) + 5D_{PC_{n-1}}(u_{n-1}) + (6n-7)D_{C_6}(c_n) + 10(6n-7).
\end{aligned}$$

By (1) and definitions of $A_G(u)$ and $D_G(u)$, we have $WW(C_6) = 42$, $A_{C_6}(c_n) = 28$ and $D_{C_6}(c_n) = 9$. By (9) and (10), we obtain that

$$\begin{aligned}
WW(PC_n) &= WW(PC_{n-1}) + WW(C_6) + 3(n-1)A_{C_6}(c_n) + 3A_{PC_{n-1}}(u_{n-1})\\
&+6(n-1)D_{C_6}(c_n) + 6D_{PC_{n-1}}(u_{n-1}) + D_{PC_{n-1}}(u_{n-1})D_{C_6}(c_n) + 36(n-1) + 2
\end{aligned}$$

$$= WW(PC_{n-1}) + 3A_{PC_{n-1}}(u_{n-1}) + 15D_{PC_{n-1}}(u_{n-1}) + 174n - 130.$$

The proof is completed. □

Lemma 2.2. *Let $PSP_n (n \geq 2)$ be a polyphenyl para-chain with n hexagons. Then*

$$WW(PCP_n) = 24n^4 + 12n^3 - \frac{15}{2}n^2 + \frac{31}{2}n - 2.$$

Proof. By the definition of $D_G(u)$, we have

$$\begin{aligned} D_{PCP_{n-1}}(u_{n-1}) &= (4n-5) + 2[\frac{(1+4n-6)(4n-6)}{2}] - \frac{(3+4n-9)(n-2)}{2} - \frac{(4+4n-8)(n-2)}{2} \\ &= 12n^2 - 27n + 15. \end{aligned} \tag{5}$$

Similarly, by the definition of $A_G(u)$, we obtain that

$$\begin{aligned} A_{PCP_{n-1}}(u_{n-1}) &= (4n-5)^2 + (4n-5) + 2[(1^2 + 2^2 + \ldots + (4n-6)^2) + (1 + 2 + \ldots + 4n-6)] \\ &\quad -[3^2 + 4^2 + 7^2 + 8^2 + \ldots + (4n-9)^2 + 4n-8)^2] - \frac{(3+4n-9)(n-2)}{2} \\ &\quad - \frac{(4+4n-8)(n-2)}{2} \\ &= (4n-5)^2 + (4n-5) + 2[\frac{(4n-6)(4n-6+1)(2(4n-6)+1)}{6} + \frac{(1+4n-6)(4n-6)}{2}] \\ &\quad -[9(n-2) + 24(1 + 2 + \ldots + (n-3)) + 16(1 + 2^2 + 3^2 + \ldots + (n-3)^2)] \\ &\quad -4^2[1 + 2^2 + 3^2 \ldots + (n-2)^2] - 4n^2 + 13n - 10 \\ &= 32n^3 - 96n^2 + 92n - 28. \end{aligned} \tag{6}$$

By Theorem 2.1, (5) and (6), we have

$$\begin{aligned} WW(PCP_n) &= WW(PCP_{n-1}) + 96n^3 - 108n^2 + 45n + 11 \\ &= 479 + 96[1^3 + 2^3 + 3^3 + \ldots + (n-1)^3 + n^3] - 108[1^2 + 2^2 + 3^2 + \ldots + (n-1)^2 + n^2] \\ &\quad +45(1 + 2 + 3 + 4 + \ldots + n) + 11n - 864 + 540 - 135 - 22 \\ &= 479 + 24n^4 + 48n^3 + 24n^2 - 36n^3 - 54n^2 - 18n + \frac{45}{2}(n^2 + n) + 11n - 864 + 540 - 157 \\ &= 24n^4 + 12n^3 - \frac{15}{2}n^2 + \frac{31}{2}n - 2. \end{aligned}$$

□

Lemma 2.3. *Let $PSO_n (n \geq 2)$ be a polyphenyl ortho-chain with n hexagons. Then*

$$WW(PCO_n) = 24n^4 + 12n^3 - \frac{15}{2}n^2 + \frac{31}{2}n - 2.$$

Proof. By the definition of $D_G(u)$, we have

$$\begin{aligned} D_{PCO_{n-1}}(u_{n-1}) &= \frac{(1+2n-1)(2n-1)}{2} + 2[\frac{(1+2n-2)(2n-2)}{2}] - (2n-3) \\ &= 6n^2 - 9n + 3. \end{aligned} \tag{7}$$

Similarly, by the definition of $A_G(u)$, we have

$$\begin{aligned} A_{PCO_{n-1}}(u_{n-1}) &= [(1^2 + 2^2 + \ldots + (2n-1)^2) + (1 + 2 + \ldots + 2n-1)] \\ &\quad +2[(1^2 + 2^2 + \ldots + (2n-2)^2) + (1 + 2 + \ldots + 2n-2)] - (2n-2)^2 - 2n \\ &= [\frac{(2n-1)(2n-1+1)(2(2n-1)+1)}{6} + \frac{(1+2n-1)(2n-1)}{2}] \\ &\quad +2[\frac{(2n-2)(2n-2+1)(2(2n-2)+1)}{6} + \frac{(1+2n-2)(2n-2)}{2}] - (2n-2)^2 - 2n \end{aligned} \tag{8}$$

$$= 8n^3 - 12n^2 + 8n - 4.$$

By Theorem 2.1, (7) and (8), we obtain that

$$\begin{aligned} WW(PCO_n) &= WW(PCO_{n-1}) + 3A_{PCO_{n-1}}(u_{n-1}) + 15D_{PCO_{n-1}}(u_{n-1}) + 174n - 130 \\ &= WW(PCO_{n-1}) + 24n^3 + 54n^2 + 63n - 97 \\ &= 479 + 24[1^3 + 2^3 + 3^3 + \ldots + (n-1)^3 + n^3] + 54[1^2 + 2^2 + 3^2 + \ldots + (n-1)^2 + n^2] \\ &\quad +63(1 + 2 + 3 + 4 + \ldots + n) - 97n - 481 \\ &= 6n^4 + 30n^3 + \frac{129}{2}n^2 - \frac{113}{2}n - 2. \end{aligned}$$

□

Theorem 2.4. *Let $\mathcal{G}_n$ be the set containing all polyphenyl chains with n hexagons. If $PC_n \in \mathcal{G}_n$, then*

$$6n^4 + 30n^3 + \frac{129}{2}n^2 - \frac{113}{2}n - 2 \le WW(PC_n) \le 24n^4 + 12n^3 - \frac{15}{2}n^2 + \frac{31}{2}n - 2,$$

where the first equality holds if and only if $PC_n \cong PCP_n$, and the second equality holds if and only if $PC_n \cong PCO_n$.

Proof. Since $\mathcal{G}_1 = \{PCP_1 = PCO_1 = PCM_1\}$, $\mathcal{G}_2 = \{PCP_2 = PCO_2 = PCM_2\}$, and $\mathcal{G}_3 = \{PCP_3, PCO_3, PCM_3\}$, it suffices to consider the case $n \ge 3$.

By the definition of a polyphenyl chain, we know that any element $PC_i = B_1B_2 \ldots B_{i-1}B_i \in \mathcal{G}_i$ can be obtained from a polyphenyl chain $PC_{i-1} = B_1B_2 \ldots B_{i-1}$ by attaching a hexagon B_i to ortho-, meta- or para-vertex of B_{i-1} in PC_{i-1}.

Checking PC_{n-1}, it can be known that $d_{PC_{n-1}}(u, x) \le d_{PC_{n-1}}(u, y) \le d_{PC_{n-1}}(u, z)$, where u is any vertex of PC_{n-1}, and x, y, z is an ortho-, meta- and para-vertex of B_{n-1} in PC_{n-1}. This implies, by the definitions of $A_G(u)$ and $D_G(u)$, that $A_{PC_{n-1}}(x) < A_{PC_{n-1}}(y) < A_{PC_{n-1}}(z)$ and $D_{PC_{n-1}}(x) < D_{PC_{n-1}}(y) < D_{PC_{n-1}}(z)$. By the definition of a polyphenyl chain, PC_n can be generated from PC_{n-1} by attaching a hexagon B_n through three attaching. We use PC_n^o to denote PC_n obtained from PC_{n-1} by attaching a hexagon B_n to ortho-vertex of B_{i-1} in PC_{n-1}, PC_n^m to denote PC_n obtained from PC_{n-1} by attaching a hexagon B_n to meta-vertex of B_{i-1} in PC_{n-1}, and PC_n^p to denote PC_n obtained from PC_{n-1} by attaching a hexagon B_n to para-vertex of B_{i-1} in PC_{n-1}. By Theorem 2.1, we obtain that $WW(PC_n^o) < WW(PC_n^m) < WW(PC_n^p)$. By Lemmas 2.2 and 2.3 and the definition of polyphenyl chain, the statement holds. □

3 Hyper-Wiener index of polyphenyl spiders

In this section, we will investigate the properties of hyper-Wiener index of polyphenyl chains.

Theorem 3.1. *Let $PS(r, s, t)(r \ge 2, s, t \ge 1)$ be a polyphenyl spider and $u_{r-1}c_r$ a cut edge of leg PC_r of $PS(r, s, t)$ (see Figure 2). Then*

$$WW(PS(r, s, t)) = WW(PS(r-1, s, t)) + 3A_{PS(r-1,s,t)}(u_{r-1}) + 15D_{PS(r-1,s,t)}(u_{r-1}) + 174(r + s + t) + 44.$$

Proof. Suppose $M = \sum_{u \in V(PS(r-1,s,t)-u_{r-1}), v \in V(C_6 - c_r)} \alpha_{PS(r,s,t)}(u, v)$. By Eq. (2), we obtain that

$$\begin{aligned} WW(PS(r, s, t)) &= \frac{1}{2}\sum_{u,v \in V(PS(r-1,s,t)} \alpha_{PS(r,s,t)}(u, v) + \frac{1}{2}\sum_{u,v \in V(C_6)} \alpha_{PS(r,s,t)}(u, v) \\ &\quad + \frac{1}{2}\sum_{u \in V(PS(r-1,s,t)), v \in V(C_6)} \alpha_{PS(r,s,t)}(u, v) \\ &= WW(PS(r-1, s, t)) + WW(C_6) + \frac{1}{2}\alpha_{PS(r,s,t)}(u_{r-1}, c_r) + \frac{1}{2}\sum_{u \in PS(r-1,s,t)} \alpha_{PS(r,s,t)}(u, c_r) \end{aligned}$$

$$+\frac{1}{2}\sum_{v\in C_6}\alpha_{PS(r,s,t)}(u_{r-1},v)+\frac{1}{2}\sum_{u\in V(PS(r-1,s,t)-u_{r-1}),v\in V(C_6-c_r)}\alpha_{PS(r,s,t)}(u,v)$$
$$= WW(PS(r-1,s,t))+WW(C_6)+1+\frac{1}{2}\sum_{v\in V(C_6)}(d_{C_6}(c_r,v)+1)(d_{C_6}(c_r,v)+2) \quad (9)$$
$$+\frac{1}{2}\sum_{u\in V(PS(r-1,s,t))}(d_{PS(r-1,s,t)}(u,u_{r-1})+1)(d_{PS(r-1,s,t)}(u,u_{r-1})+2)+\frac{1}{2}M$$
$$= WW(PS(r-1,s,t))+WW(C_6)+1+\frac{1}{2}A_{PS(r-1,s,t)}(u_{r-1})+D_{PS(r-1,s,t)}(u_{r-1})$$
$$+\frac{1}{2}A_{C_6}(c_r)+D_{C_6}(c_r)+6n+\frac{1}{2}M,$$

Simplifying M, we have

$$M = \sum_{u\in V(PS(r-1,s,t)-u_{r-1}),v\in V(C_6-c_n)}\alpha_{PS(r,s,t)}(u,v)$$
$$= \sum_{u\in V(PS(r-1,s,t)-u_{r-1}),v\in V(C_6-c_r)}[d_{PS(r-1,s,t)}(u,u_{n-1})+1+d_{C_6}(c_r,v)]$$
$$[d_{PS(r-1,s,t)}(u,u_{r-1})+2+d_{C_6}(c_r,v)]$$
$$= \sum_{u\in V(PS(r-1,s,t)-u_{n-1})}\sum_{v\in V(C_6-c_r)}[\alpha_{PS(r-1,s,t)}(u,u_{r-1})+\alpha_{C_6}(c_r,v)]$$
$$+\sum_{u\in V(PS(r-1,s,t)-u_{r-1})}\sum_{v\in V(C_6-c_r)}[d_{PS(r-1,s,t)}(u,u_{r-1})(d_{C_6}(c_r,v)+1)] \quad (10)$$
$$+\sum_{u\in V(PS(r-1,s,t)-u_{r-1})}\sum_{v\in V(C_6-c_r)}[d_{C_6}(c_r,v)(d_{PS(r-1,s,t)}(u,u_{r-1})+1)]$$
$$+\sum_{u\in V(PS(r-1,s,t)-u_{r-1})}\sum_{v\in V(C_6-c_r)}[d_{PS(r-1,s,t)}(u,u_{r-1})+d_{C_6}(c_r,v)+2]$$
$$= 5A_{PS(r-1,s,t)}(u_{r-1})+(6n-5)A_{C_6}(c_r)+D_{PS(r-1,s,t)}(u_{r-1})(D_{C_6}(c_r)+5)$$
$$+D_{C_6}(c_r)(D_{PS(r-1,s,t)}(u_{r-1})+6n-7)+5D_{PS(r-1,s,t)}(u_{r-1})+(6n-7)D_{C_6}(c_r)$$
$$+10(6n-7).$$

By (1) and definitions of $A_G(u)$ and $D_G(u)$, we have $WW(C_6)=42$, $A_{C_6}(c_r)=28$ and $D_{C_6}(c_r)=9$.
By (9) and (10), we obtain that

$$WW(PS(r,s,t)) = WW(PS(r-1,s,t))+3A_{PS(r-1,s,t)}(u_{r-1})+15D_{PS(r-1,s,t)}(u_{r-1})+174(r+s+t)+44.$$

The proof is completed. □

We shall use $\mathscr{T}(r,s,t)$ to denote the set of all polyphenyl spiders with three legs of lengths r,s,t.

Theorem 3.2. *Let $PS(r,s,t)\in\mathscr{T}(r,s,t)$ be a polyphenyl spider. Then*

$$WW(PSO(r,s,t))\le WW(PS(r,s,t))\le WW(PSP(r,s,t)),$$

where the first equality holds if and only if $PS(r,s,t)\cong PSO(r,s,t)$, and the second equality holds if and only if $PS(r,s,t)\cong PSP(r,s,t)$.

Proof. Let $\mathscr{T}(r,s,t)$ be the set of all polyphenyl spiders with three legs of lengths r,s,t. Then $\mathscr{T}(1,1,1)=\{PSO(1,1,1)=PSM(1,1,1)=PSP(1,1,1)\}$. Thus we assume that two of r,s,t are more than one.

By the definitions of polyphenyl chain and polyphenyl spider, it can be known that any element $PS(r,s,t)\in\mathscr{T}(r,s,t)$ is obtained from $PS(r-1,s,t)(PS(r,s-1,t)$, or $PS(r,s,t-1))$ by attaching a hexagon B_i to ortho-, meta- or para-vertex of B_{i-1} in PC_{i-1}, where $i=r,s$ or t. Without loss of generality, we only consider the case that $PS(r,s,t)$ is generated by $PS(r-1,s,t)$.

Checking $PS(r-1,s,t)$, we know that $d_{PS(r-1,s,t)}(u,x) \leq d_{PS(r-1,s,t)}(u,y) \leq d_{PS(r-1,s,t)}(u,z)$, where u is any vertex of $PS(r-1,s,t)$, and x,y,z is a ortho-, meta- and para-vertex of B_{r-1} in leg $PC(r-1)$. This implies, by the definitions $A_G(u)$ and $D_G(u)$, that $A_{PS(r-1,s,t)}(x) < A_{PS(r-1,s,t)}(y) < A_{PS(r-1,s,t)}(z)$ and $D_{PS(r-1,s,t)}(x) < D_{PS(r-1,s,t)}(y) < D_{PS(r-1,s,t)}(z)$. By the definition of a polyphenyl spider, $PS(r,s,t)$ can be obtained from $PS(r-1,s,t)$ by attaching a hexagon B_r through three attaching. We use $PS^o(r,s,t)$ to denote $PS(r,s,t)$ obtained from $PS(r-1,s,t)$ by attaching a hexagon B_r to ortho-vertex of B_{i-1} in PC_{r-1}. And $PS^m(r,s,t)$ denotes $PS(r,s,t)$ obtained from $PS(r-1,s,t)$ by attaching a hexagon B_r to meta-vertex of B_{i-1} in PC_{r-1}. And $PS^p(r,s,t)$ denotes $PS(r,s,t)$ obtained from $PS(r-1,s,t)$ by attaching a hexagon B_r to para-vertex of B_{i-1} in PC_{r-1}. By Theorem 3.1, we obtain that $WW(PS^o(r,s,t)) < WW(PS^m(r,s,t)) < WW(PS^p(r,s,t))$. By the definition of $PS(r,s,t)$, the theorem holds. □

Next we shall introduce a graph operation that can be considered as graph transformations, and we shall show that generally, the transformed graph will have larger permanental sum than that of the original graph.

Definition 3.3. *Let $PSO(r,s,t)$ be a polyphenyl ortho-spider and $r \leq s \leq t$. The polyphenyl ortho-spider $PSO(r-1,s,t+1)$ is obtained from $PSO(r,s,t)$ by deleting the last hexagon B_r of the leg PC_r in $PSO(r,s,t)$ and attaching B_r to ortho-vertex of B_t in leg PC_t. We define the transformation from $PSO(r,s,t)$ to $PSO(r-1,s,t+1)$ as type* **I**.

Lemma 3.4. *Let $PSO(r,s,t)$ and $PSO(r-1,s,t+1)$ be two polyphenyl ortho-spiders and $r \leq s \leq t$. Then*

$$WW(PSO(r,s,t)) < WW(PSO(r-1,s,t+1)).$$

Proof. By Theorem 3.1, we have

$$\begin{aligned} WW(PSO(r,s,t)) = {} & WW(PSO(r-1,s,t)) + 3A_{PSO(r-1,s,t)}(u_{r-1}) + 15D_{PSO(r-1,s,t)}(u_{r-1}) \\ & +174(r+s+t)+44 \end{aligned} \tag{11}$$

and

$$\begin{aligned} & WW(PSO(r-1,s,t+1)) \\ = {} & WW(PSO(r-1,s,t)) + 3A_{PSO(r-1,s,t)}(u_t) + 15D_{PSO(r-1,s,t)}(u_t) + 174(r+s+t)+44. \end{aligned} \tag{12}$$

For any vertex x of leg PCO_s in $PSO(r-1,s,t)$, since $r-1 < r \leq t$, $d_{PSO(r-1,s,t)}(u_{r-1},x) < d_{PSO(r-1,s,t)}(u_t,x)$. By the definitions of $A_G(u)$ and $D_G(u)$, we obtain that $A_{PSO(r-1,s,t)}(u_t) > A_{PSO(r-1,s,t)}(u_{r-1})$ and $D_{PSO(r-1,s,t)}(u_t) > D_{PSO(r-1,s,t)}(u_{r-1})$. By (11) and (12), we have

$$WW(PSO(r-1,s,t+1)) - WW(PSO(r-1,s,t)) > 0.$$

The proof is completed. □

By repeated applications of Transformation **I**, we can obtain the following result.

Lemma 3.5. *Let $PSO(r,s,t)$ be a polyphenyl ortho-spider and $r \leq s \leq t$. Then*

$$WW(PSO(r,s,t)) \leq WW(PSO(1,1,r+s+t-2)),$$

where the equality holds if and only if $PSO(r,s,t) \cong PSO(1,1,r+s+t-2)$).

Definition 3.6. *Let $PSP(r,s,t)$ be a polyphenyl para-spider and $r \leq s \leq t$. The polyphenyl para-spider $PSP(r-1,s,t+1)$ is obtained from $PSP(r,s,t)$ by deleting the last hexagon B_r of the leg PC_r in $PSP(r,s,t)$ and attaching B_r to para-vertex of B_t in leg PC_t. We define the transformation from $PSP(r,s,t)$ to $PSP(r-1,s,t+1)$ as type* **II**.

Lemma 3.7. *Let $PSP(r,s,t)$ and $PSP(r-1,s,t+1)$ be two polyphenyl para-spiders and $r \leq s \leq t$. Then*

$$WW(PSP(r,s,t)) < WW(PSP(r-1,s,t+1)).$$

Proof. Similarly, by Theorem 3.1, we have

$$\begin{aligned} & WW(PSP(r,s,t)) - WW(PSP(r-1,s,t+1)) \\ = {} & 3[A_{PSP(r-1,s,t)}(u_{r-1}) - A_{PSP(r-1,s,t)}(u_t)] + 15[D_{PSP(r-1,s,t)}(u_{r-1}) - D_{PSP(r-1,s,t)}(u_t)]. \end{aligned} \tag{13}$$

For any vertex x of leg PCP_s in $PSP(r-1,s,t)$, since $r-1 < r \le t$, $d_{PSP(r-1,s,t)}(u_{r-1},x) < d_{PSP(r-1,s,t)}(u_t,x)$. By the definitions of $A_G(u)$ and $D_G(u)$, we obtain that $A_{PSP(r-1,s,t)}(u_t) > A_{PSP(r-1,s,t)}(u_{r-1})$ and $D_{PSP(r-1,s,t)}(u_t) > D_{PSP(r-1,s,t)}(u_{r-1})$. Thus $WW(PSP(r,s,t)) - WW(PSP(r-1,s,t+1)) > 0$. □

By repeated applications of Transformation **II**, we can obtain a result as follows.

Lemma 3.8. *Let $PSP(r,s,t)$ be a polyphenyl para-spider and $r \le s \le t$. Then*

$$WW(PSP(r,s,t)) \le WW(PSP(1,1,r+s+t-2)).$$

where the equality holds if and only if $PSP(r,s,t) \cong PSP(1,1,r+s+t-2)$).

Theorem 3.9. *Let $\mathscr{S}$ be the set containing all polyphenyl spiders with $r+s+t+1$ hexagons. Then the polyphenyl ortho-spider $PSO(1,1,r+s+t-2)$ and para-spider $PSP(1,1,r+s+t-2)$ have the minimum and maximum hyper-Wiener index in $\mathscr{S}$, respectively.*

Proof. By Theorem 3.2 and Lemmas 3.5 and 3.8, the proof of Theorem 3.9 is straightforward. □

Competing interests
The authors declare that they have no competing interests.

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References

[1] Wiener H., Structural determination of paraffin boiling points, J. Am. Chem. Soc., 1947, 69, 17–20
[2] Randić M., Novel molecular descriptor for structure-property studies, Chem. Phys. Lett., 1993, 211, 478–483
[3] Klein D.J., Lukovits I., Gutman I., On the definition of the hyper-Wiener index for cycle-containing structures, J. Chem. Inf. Comput. Sci., 1995, 35, 50–52
[4] Deng H., Wiener indices of spiro and polyphenyl hexagonal chains, Math. Comput. Mod., 2012, 55, 634–644
[5] Behtoei A., Jannesari M., Taeri B., Maximum Zagreb index, minimum hyper-Wiener index and graph connectivity, Appl. Math. Lett., 2009, 22, 1571–1576
[6] Diudea M., Wiener and hyper-Wiener numbers in a single matrix, J. Chem. Inf. Comput. Sci., 1996, 3, 833–836
[7] Dobrynin A., Gutman I., Piottukh-Peletskii V., Hyper-Wiener index for acyclic structures, J. Structrual Chem., 1999, 40, 293–298
[8] Eliasi M., Iranmanesh A., The hyper-Wiener index of the generalized hierarchical product of graphs, Discrete Appl. Math., 2011, 159, 866–871
[9] Feng L., Liu W., Yu G., Li S., The hyper-Wiener index of graphs with given bipartition, Utilitas Math., 2014, 96, 99–108
[10] Feng L., Ilić A., Zagreb, Harary and hyper-Wiener indices of graphs with a given matching number, Appl. Math. Lett., 2010, 23, 943–948
[11] Feng L., Ilić A., Yu G., The hyper-Wiener index of unicyclic graphs, Utilitas Math., 2010, 82, 215–225
[12] Feng L., The hyper-Wiener index of unicyclic graphs with given matching number, Ars Comb., 2011, 100, 9–17
[13] Feng L., Liu W., Xu K., The hyper-Wiener index of bicyclic graphs, Utilitas Math., 2011, 84, 97–104
[14] Gutman I., Relation between hyper-Wiener and Wiener index, Chem. Phys. Lett., 2002, 364, 352–356

[15] Gutman I., Linert W., Lukovits I., Dobrynin A., Trees with extremal hyper-Wiener index: mathematical basis and chemical applications, J. Chem. Inf. Comput. Sci., 1997, 37, 349–354
[16] Khalifeh M., Yousefi-Azari H., Ashrafi A., The hyper-Wiener index of graph operations, Comput. Math. Appl., 2008, 56, 1402–1407
[17] Lang R., Li T., Mo D., Shi Y., A novel method for analyzing inverse problem of topological indices of graphs using competitive agglomeration, Appl. Math. Comp., 2016, 291, 115–121
[18] Lei H., Li T., Shi Y., Wang H., Wiener polarity index and its generalization in trees, MATCH Commun. Math. Comput. Chem., 2017, 78, 199–212
[19] Liu M., Liu B., Trees with the seven smallest and fifteen greatest hyper-Wiener indices, MATCH Commun. Math. Comput. Chem., 2010, 63, 151–170
[20] Ma J., Shi Y., Wang Z., Yue J., On Wiener polarity index of bicyclic networks, Sci. Rep., 2016, 6, 19066
[21] Mansour T., Schork M., Wiener, hyper-Wiener, detour and hyper-detour indices of bridge and chain graphs, J. Math. Chem., 2010, 47, 72–79
[22] Xu K., TrinajstićN., Hyper-Wiener and Harary indices of graphs with cut edges, Utilitas Math, 2011, 84, 153–163
[23] Xu K., Liu M., Das K., Gutman I., Furtula B., A survey on graphs extremal with respect to distance-based topological indices, MATCH Commun. Math. Comput. Chem., 2014, 71, 461–508
[24] Yu G., Feng L., Ilić A., The hyper-Wiener index of trees with given parameters. Ars Comb., 2010, 96, 395–404
[25] Zhou B., Gutman I., Relations between Wiener, hyper-Wiener and Zagreb indices, Chem. Phys. Lett., 2004, 394, 93–95
[26] Gutman I., Polansky O., Mathematical Concepts in Organic Chemistry, 1986, Springer, Berlin