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Research Article

Tingzeng Wu* and Huazhong Lü

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
\[
WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (d_G(u,v) + d_G^2(u,v)), \tag{1}
\]
where the summation goes over all pairs of vertices in \( G \). For two vertices \( u \) and \( v \) of \( G \), set \( a_G(u,v) = d_G(u,v)(d_G(u,v) + 1) \) and \( A_G(u) = \sum_v a_G(u,v) \), where this summation extends to all the vertices different from \( u \). Then (1) is expressed as follows.
\[
WW(G) = \frac{1}{2} \sum_{u,v \in V(G)} a_G(u,v). \tag{2}
\]

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.

*Corresponding Author: Tingzeng Wu: School of Mathematics and Statistics, Qinghai Nationalities University, Xining, Qinghai 810007, P.R. China, E-mail: mathtzwu@163.com
Huazhong Lü: School of Mathematical Sciences, University of Electronic Science and Technology of China, Chengdu, Sichuan 610054, P.R. China, E-mail: lvhz@uestc.edu.cn

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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.

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-spider if every leg of the polyphenyl spider is a polyphenyl ortho-chain. A polyphenyl spider is called a polyphenyl meta-spider if every leg of the polyphenyl spider is a polyphenyl meta-chain. A polyphenyl spider is called a polyphenyl para-spider if every leg of the polyphenyl spider is a polyphenyl para-chain. Clearly, a polyphenyl spider is a polyphenyl system.

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

$$WW(PC_n) = \frac{1}{2} \sum_{u,v \in V(PC_{n-1})} a_{PC_n}(u,v) + \frac{1}{2} \sum_{u,v \in V(C_6)} a_{PC_n}(u,v) + \frac{1}{2} \sum_{u \in V(PC_{n-1}), v \in V(C_6)} a_{PC_n}(u,v)$$

$$= WW(PC(n - 1)) + WW(C_6) + \frac{1}{2} a_{PC_n}(u_{n-1}, c_n) + \frac{1}{2} \sum_{u \in PC_{n-1}} a_{PC_n}(u, c_n)$$

$$+ \frac{1}{2} \sum_{v \in C_6} a_{PC_n}(u_{n-1}, v) + \frac{1}{2} \sum_{u \in V(PC_{n-1}), v \in V(C_6)} a_{PC_n}(u,v)$$

$$= WW(PC(n - 1)) + WW(C_6) + 1 + \frac{1}{2} \sum_{v \in V(C_6)} (d_{C_6}(c_n, v) + 1)(d_{C_6}(c_n, v) + 2)$$

$$+ \frac{1}{2} \sum_{u \in V(PC_{n-1})} (d_{PC_{n-1}}(u, u_{n-1}) + 1)(d_{PC_{n-1}}(u, u_{n-1}) + 2) + \frac{1}{2} M$$

$$= WW(PC(n - 1)) + WW(C_6) + 1 + \frac{1}{2} A_{PC_{n-1}}(u_{n-1}) + D_{PC_{n-1}}(u_{n-1}) + \frac{1}{2} A_{C_6}(c_n)$$

$$+ D_{C_6}(c_n) + 6n + \frac{1}{2} M,$$

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

Simplifying $M$, we have

$$M = \sum_{u \in V(PC_{n-1}), v \in V(C_6)} a_{PC_n}(u, v)$$

$$= \sum_{u \in V(PC_{n-1}), v \in V(C_6)} [d_{PC_{n-1}}(u, u_{n-1}) + 1 + d_{C_6}(c_n, v)][d_{PC_{n-1}}(u, u_{n-1})]$$

$$+ 2 + d_{C_6}(c_n, v)]$$

$$= \sum_{u \in V(PC_{n-1}), v \in V(C_6)} \sum_{u \in V(C_6)} [a_{PC_n}(u, u_{n-1}) + a_{C_6}(c_n, v)]$$

$$+ \sum_{u \in V(PC_{n-1}), v \in V(C_6)} \sum_{u \in V(C_6)} [d_{PC_{n-1}}(u, u_{n-1})(d_{C_6}(c_n, v) + 1)]$$

$$+ \sum_{u \in V(PC_{n-1}), v \in V(C_6)} \sum_{u \in V(C_6)} [d_{C_6}(c_n, v)(d_{PC_{n-1}}(u, u_{n-1}) + 1)]$$

$$+ \sum_{u \in V(PC_{n-1}), v \in V(C_6)} \sum_{u \in V(C_6)} [d_{PC_{n-1}}(u, u_{n-1}) + d_{C_6}(c_n, v) + 2]$$

$$= 5A_{PC_{n-1}}(u_{n-1}) + (6n - 5)A_{C_6}(c_n) + D_{PC_{n-1}}(u_{n-1})(D_{C_6}(c_n) + 5)$$

$$+ D_{C_6}(c_n)D_{PC_{n-1}}(u_{n-1}) + 6n - 7) + 5D_{PC_{n-1}}(u_{n-1}) + (6n - 7)D_{C_6}(c_n) + 10(6n - 7).$$

By (1) and definitions of $A_{C_6}(u)$ and $D_{C_6}(u)$, 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

$$WW(PC_n) = WW(PC_{n-1}) + WW(C_6) + 3(n - 1)A_{C_6}(c_n) + 3A_{PC_{n-1}}(u_{n-1})$$

$$+ 6(n - 1)D_{C_6}(c_n) + 6D_{PC_{n-1}}(u_{n-1}) + D_{PC_{n-1}}(u_{n-1})D_{C_6}(c_n) + 36(n - 1) + 2$$

$$= WW(PC_{n-1}) + WW(C_6) + 3A_{PC_{n-1}}(u_{n-1}) + 15D_{PC_{n-1}}(u_{n-1}) + 174n - 130.$$
By Theorem 2.1, (5) and (6), we have

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

The proof is completed. \qed

**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 \( D_C(u) \), we have

\[ D_{PCP_{n-1}}(u_{n-1}) = (4n - 5) + 2\left[ \frac{1 + 4n - 6 - (4n - 6)}{2} \right] - \frac{3 + 4n - 9 - (n - 2)}{2} - \frac{4 + 4n - 8 - (n - 2)}{2} \]

\[ = 12n^2 - 27n + 15. \] (5)

Similarly, by the definition of \( A_C(u) \), we obtain that

\[ A_{PCP_{n-1}}(u_{n-1}) = (4n - 5)^2 + (4n - 5) + 2\left[ (1^2 + 2^2 + \ldots + (4n - 6)^2) + (1 + 2 + \ldots + 4n - 6) \right] - \left[ 3^2 + 4^2 + 7^2 + 8^2 + \ldots + (4n - 9)^2 + 4n - 8 \right] - \frac{3 + 4n - 9(n - 2)}{2} \]

\[ - \frac{(4 + 4n - 8)(n - 2)}{2} \]

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

\[ - [9(n - 2) + 24(1 + 2 + \ldots + (n - 3)) + 16(1 + 2 + 3^2 + \ldots + (n - 3)^2)] \]

\[ - 4^2[1 + 2^2 + 3^2 + \ldots + (n - 2)^2] - 4n^2 + 13n - 10 \]

\[ = 32n^3 - 96n^2 + 92n - 28. \] (6)

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

\[ WW(PCP_n) = WW(PCP_{n-1}) + 96n^3 - 108n^2 + 45n + 11 \]

\[ = 479 + 96[1^3 + 2^3 + 3^3 + \ldots + (n - 1) + 3^3] - 108[1^2 + 2^2 + 3^2 + \ldots + (n - 1)^2 + n^2] \]

\[ + 45(1 + 2 + 3 + 4 + \ldots + n) + 11n - 864 + 540 - 135 - 22 \]

\[ = 479 + 24n^4 + 48n^3 + 24n^2 - 36n^3 - 54n^2 - 18n + \frac{45}{2}(n^2 + n) + 11n - 864 + 540 - 157 \]

\[ = 24n^4 + 12n^3 - \frac{15}{2}n^2 + \frac{31}{2}n - 2. \] \qed

**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 \( D_C(u) \), we have

\[ D_{PCO_{n-1}}(u_{n-1}) = \frac{(1 + 2n - 1)(2n - 1)}{2} + 2\left[ \frac{(1 + 2n - 2)(2n - 2)}{2} \right] - (2n - 3) \]

\[ = 6n^2 - 9n + 3. \] (7)

Similarly, by the definition of \( A_C(u) \), we have

\[ A_{PCO_{n-1}}(u_{n-1}) = \left[ (1^2 + 2^2 + \ldots + (2n - 1)^2) + (1 + 2 + \ldots + 2n - 1) \right] \]

\[ + 2\left[ (1^2 + 2^2 + \ldots + (2n - 2)^2) + (1 + 2 + \ldots + 2n - 2) \right] - (2n - 2)^2 - 2n \]

\[ = \frac{(2n - 1)(2n - 1 + 1)(2(2n - 1) + 1)}{6} + \frac{(1 + 2n - 1)(2n - 1)}{2} \]

\[ + 2\left[ \frac{(2n - 2)(2n - 2 + 1)(2(2n - 2) + 1)}{6} + \frac{(1 + 2n - 2)(2n - 2)}{2} \right] - (2n - 2)^2 - 2n \] (8)
Suppose \( \mathcal{G}_n \) be the set containing all polyphenyl chains with \( n \) hexagons. If \( PC_n \in \mathcal{G}_n \), then

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

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 \( n \geq 3 \).

By the definition of a polyphenyl chain, we know that any element \( PC_i = B_1B_2\ldots B_i \in \mathcal{G}_i \) 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 \( B_{i-1} \).

Checking \( PC_{n-1} \), it can be known that \( d_{PC_{n-1}}(u, x) \leq d_{PC_{n-1}}(u, y) \leq d_{PC_{n-1}}(u, z) \), 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 \( PC_{n-1}^0 \) to denote \( PC_n \) obtained from \( PC_{n-1} \) by attaching a hexagon \( B_n \) to ortho-vertex of \( B_{n-1} \) in \( PC_{n-1} \), \( PC_{n-1}^m \) to denote \( PC_n \) obtained from \( PC_{n-1} \) by attaching a hexagon \( B_n \) to meta-vertex of \( B_{n-1} \) in \( PC_{n-1} \), and \( PC_{n-1}^p \) to denote \( PC_n \) obtained from \( PC_{n-1} \) by attaching a hexagon \( B_n \) to para-vertex of \( B_{n-1} \) in \( PC_{n-1} \). By Theorem 2.1, we obtain that \( WW(PC_{n-1}^0) < WW(PC_{n-1}^m) < WW(PC_{n-1}^p) \). 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 \( PS(r, s, t)(r \geq 2, s, t \geq 1) \) 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 \( M = \sum_{u \in V(PS(r-1,s,t)-u_{r-1}), v \in V(C_i-c_i)} a_{PS(r-1,s,t)}(u, v) \). By Eq. (2), we obtain that

\[
WW(PS(r, s, t)) = \frac{1}{2} \sum_{u,v \in V(PS(r-1,s,t))} a_{PS(r,s,t)}(u, v) + \frac{1}{2} \sum_{u,v \in V(C_i)} a_{PS(r,s,t)}(u, v) + \frac{1}{2} \sum_{u \in V(PS(r-1,s,t), v \in V(C_i)} a_{PS(r,s,t)}(u, v)
\]

\[
= WW(PS(r-1, s, t)) + WW(C_i) + \frac{1}{2} a_{PS(r,s,t)}(u_{r-1}, c_r) + \frac{1}{2} \sum_{u \in PS(r-1,s,t)} a_{PS(r,s,t)}(u, c_r)
\]
We shall use

\[ \{ \text{the proof is completed.} \] 

By (1) and definitions of \( A_C(u) \) and \( D_G(u) \), we have \( WW(C_6) = 42 \), \( A_C(c_r) = 28 \) and \( D_C(c_r) = 9 \).

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 \( \mathcal{T}(r, s, t) \) to denote the set of all polyphenyl spiders with three legs of lengths \( r, s, t \).

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

\[ WW(PSO(r, s, t)) \leq WW(PS(r, s, t)) \leq WW(PSP(r, s, t)), \]

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

**Proof.** Let \( \mathcal{T}(r, s, t) \) be the set of all polyphenyl spiders with three legs of lengths \( r, s, t \). Then \( \mathcal{T}(1, 1, 1) = \{ PSO(1, 1, 1) = PSM(1, 1, 1) = PSP(1, 1, 1) \} \). 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 \( PS(r, s, t) \in \mathcal{T}(r, s, t) \) is obtained from \( PS(r - 1, s, t)(PS(r - 1, s, t), or PS(r, s, t - 1)) \) 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 $A_{PS(r-1,s,t)}(u) < A_{PS(r-1,s,t)}(y) < A_{PS(r-1,s,t)}(z)$ 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 $B_t$ through three attaching. We use $PS^0(r, s, t)$ to denote $PS(r, s, t)$ obtained from $PS(r-1, s, t)$ by attaching a hexagon $B_t$ to ortho-vertex of $B_{r-1}$ 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 $B_t$ to meta-vertex of $B_{r-1}$ 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 $B_t$ to para-vertex of $B_{r-1}$ in $PC_{r-1}$. By Theorem 3.1, we obtain that $WW(PS^0(r, s, t)) < WW(PS^m(r, s, t)) < WW(PS^p(r, s, t)).$ 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 permanent 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 $PSO(r-1, s, t)$ is obtained from $PSO(r, s, t)$ by deleting the last hexagon $B_t$ of the leg $PC_t$ in $PSO(r, s, t)$ and attaching $B_t$ to ortho-vertex of $B_t$ in leg $PC_t$. We denote 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

$$WW(PSO(r, s, t)) = WW(PSO(r-1, s, t)) + 3A_{PSO(r-1,s,t)}(u_{r-1}) + 15d_{PSO(r-1,s,t)}(u_{r-1})$$

$$+ 174(r + s + t) + 44$$

(11)

and

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

(12)

For any vertex $x$ of leg $PC_t$ of $PSO(r-1, s, t)$, since $r - 1 < r \leq t$, $d_{PSO(r-1,s,t)}(u_{r-1}, x) < d_{PSO(r-1,s,t)}(u_{r-1})$. By the definitions of $A_G(u)$ and $D_G(u)$, we obtain that $A_{PSO(r-1,s,t)}(u_{r-1}) > A_{PSO(r-1,s,t)}(u_{r-1})$ and $d_{PSO(r-1,s,t)}(u_{r}) > d_{PSO(r-1,s,t)}(u_{r-1})$. 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 $B_t$ of the leg $PC_t$ in $PSP(r, s, t)$ and attaching $B_t$ 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

$$WW(PSP(r, s, t)) < WW(PSP(r-1, s, t+1)).$$
By Theorem 3.2 and Lemmas 3.5 and 3.8, the proof of Theorem 3.9 is straightforward.

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