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TREE-LIKE POLYPHENYL CHAINS WITH EXTREMAL DEGREE DISTANCE

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The degree distance of a connected graph *G=(V(G),E(G))*, denoted by $DD(G)$, is defined as $DD(G)=\sum_{\{u,v\}\subseteq V(G)}(d(u)+d(v))d(u,v)$, where *d(v)* is the degree of the vertex *v* and *d(u,v)* is the distance between vertices *u* and *v* in *G*. In this paper, we determine the polyphenyl chains with the maximum and minimum degree distances among all polyphenyl chains with *h* hexagons.

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1. Introduction

Let *G* be a graph with vertex set *V(G)* and edge set *E(G)*. For any two vertices *x* and *y* in *V(G)*, the distance between *x* and *y*, denoted by *d(x,y)*, is the length of the shortest path connecting *x* and *y*. The degree of a vertex *v* in *G* is the number of neighbors of *v* in *G*.

Numbers reflecting certain structural features of organic molecules that are obtained from the molecular graph are usually called graph invariants or more commonly topological indices. The oldest and most thoroughly examined use of a topological index in chemistry was by Wiener [1] in the study of paraffin boiling points, and the topological index was called Wiener index or Wiener number.The conventional generalization of W for an arbitrary molecular graph is due to Hosoya [2]. The Wiener index of the graph *G*, is equals to the sum of distances between all pairs of vertices of the respective molecular graph, i.e., $W(G)=\sum_{\{u,v\}\subseteq V(G)}d(u,v)$.

The degree distance of a connected graph *G=(V(G),E(G))*, denoted by $DD(G)$, is defined [3] as

$DD(G)=\sum_{\{u,v\}\subseteq V(G)}(d(u)+d(v))d(u,v)$. From the definition of degree distance, it is easy to see that $DD(G)$ is a degree analog of the Wiener index. For recent results on degree distance, the reader is referred to [4-11].

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A kind of macrocyclic aromatic hydrocarbons called polyphenyls and their derivatives has attracted the attention of chemists for many years [12, 13]. The molecular graphs of polyphenyls are called the polyphenyl system. A polyphenyl system is said to be tree-like if each vertex of *H* lies in a hexagon and the graph obtained by contracting each hexagon into a vertex in original molecular graphs is a tree. A hexagon *h* in a tree-like system has at least one and at most six neighboring hexagons. A hexagon *h* is said to be terminal if it has exactly one neighboring hexagon, and said to be branched if it has at least three neighboring hexagons. A polyphenyl system without branched hexagons is said to be a polyphenyl chain.

In this paper, we shall characterize the polyphenyl chains with the maximum and minimum degree distance among all polyphenyl chains with *h* hexagons.

2. Main results and discussion

Two vertices *u* and *v* of a hexagon *h* are said to be in *ortho*-position if there are adjacent in *h*. If two vertices *u* and *v* are at distance two, then they are said to be in *meta*-position, and if two vertices *u* and *v* are at distance three, then they are said to be in *para*-position. Examples of vertices in the above three types of positions are illustrated in Fig. 1.

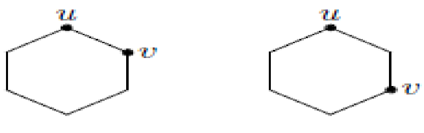

Fig. 1. ortho-, meta-, and para- positions of vertices in h.

An internal hexagon *h* in a polyphenyl chain is called a *ortho*-hexagon, *meta*- hexagon, or, *para*- hexagon if two vertices of *h* incident with two edges which connect other two hexagons are in *ortho*-position, *meta*-position, *para*-position, respectively. A polyphenyl chain of *h* hexagons is *ortho*- PPC_h and is denoted by O_h, if all its internal hexagons are *ortho*-hexagons. In a fully analogous manner, we can define *meta*- PPC_h (denoted by M_h) and *para*- PPC_h (denoted by L_h). See Fig. 2 for *ortho*- PPC_h, *meta*- PPC_h and *para*- PPC_h.

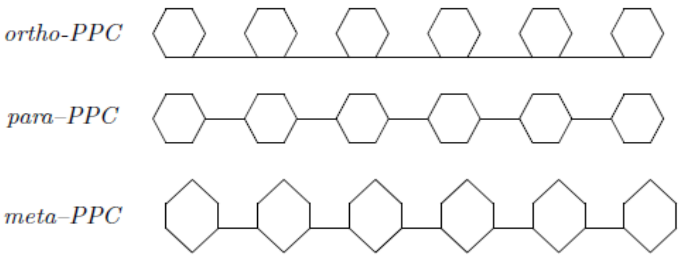

Fig. 2. ortho-, para-, and meta-Polyphenyl chains with six hexagons.

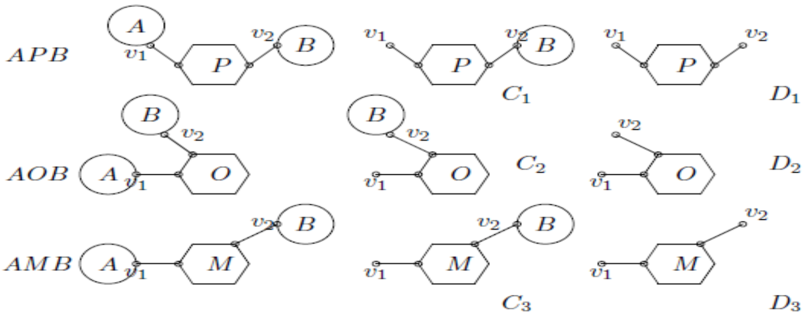

Fig. 3 Three ways of inserting a hexagon between two polyphenyl chains A and B.

Concerning the Wiener index of polyphenyl chains, Bian and Zhang obtained the following result.

Theorem 1([14]). *Let* G_h *be a polyphenyl chain with h hexagons. Then*

$$W(O_h) \le W(G_h) \le W(L_h),$$

where the left-hand side equality holds in the above inequality if and only if $G_h \cong O_h$ *and right-hand one holds in the above inequality if and only if* $G_h \cong L_h$.

According to the definition of Wiener index (*W(G)*) and degree distance (*DD(G)*), one can deduce an explicit relation between *W(G)*) and *DD(G)* when *G* is a polyphenyl chain.

Proposition 1. *Let* G_h *be a polyphenyl chain with h hexagons. Then*

$$DD(G_h) = 4W(G_h) + W_{23}(G_h) + 2W_{33}(G_h),$$

where $W_{23}(G_h) = \sum_{\substack{\{u,v\}\subseteq V(G_h) \\ d(u)=2,d(v)=3, \\ or, d(u)=3,d(v)=2}} d(u,v)$ *and* $W_{23}(G_h) = \sum_{\substack{\{u,v\}\subseteq V(G_h) \\ d(u)=d(v)=3}} d(u,v)$.

Proof. According to the definition of degree distance, we have

$$DD(G) = \sum_{\{u,v\}\subseteq V(G)} (d(u)+d(v))d(u,v)$$

$$= 4\sum_{\substack{\{u,v\}\subseteq V(G_h) \\ d(u)=d(v)=2}} d(u,v) + 5\sum_{\substack{\{u,v\}\subseteq V(G_h) \\ d(u)=2,d(v)=3, \\ or, d(u)=3,d(v)=2}} d(u,v) + 6\sum_{\substack{\{u,v\}\subseteq V(G_h) \\ d(u)=d(v)=3}} d(u,v)$$

$$= 4W(G_h) + W_{23}(G_h) + 2W_{33}(G_h).$$

This completes the proof. ■

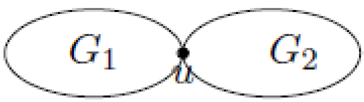

Fig. 4 The graph used in Lemma 1.

For j=2, 3, we let $n_j(H)$ be the number of vertices of degree j in a graph H and let $d_H^j(x)$ be the sum of distance between a vertex *x* and all vertices of degree *j* in *H*. By means of these notation, we thus have:

Lemma 1. *Let* G *be a connected graph as shown in Fig. 4 with* $G_1-\{u\}$ *and* $G_2-\{u\}$ *being two connected components of* $G-\{u\}$. *Then we have*

(i). $W_{23}(G)=\left\{\begin{matrix}W_{23}(G_1)+W_{23}(G_2)+n_3(G_2-\{u\})d^2_{G_1}(u)+n_2(G_1-\{u\})d^3_{G_2}(u)+\\ n_2(G_2-\{u\})d^3_{G_1}(u)+n_3(G_1-\{u\})d^2_{G_2}(u)\end{matrix}\right\}$;

(ii). $W_{33}(G)=\left\{\begin{matrix}W_{33}(G_1)+W_{33}(G_2)+\\ n_3(G_2-\{u\})d^3_{G_1}(u)+n_3(G_1-\{u\})d^3_{G_2}(u)\end{matrix}\right\}$.

Proof. We only prove (i) here. The proof of (ii) can be conducted by the same way.

$$W_{23}(G)=W_{23}(G_1)+W_{23}(G_2)+\sum_{\substack{x\in V(G_1)-\{u\}\\ d(x)=2}}\sum_{\substack{y\in V(G_2)-\{u\}\\ d(y)=3}}d(x,y)+\sum_{\substack{x\in V(G_1)-\{u\}\\ d(x)=3}}\sum_{\substack{y\in V(G_2)-\{u\}\\ d(y)=2}}d(x,y)$$

$$=W_{23}(G_1)+W_{23}(G_2)+\sum_{\substack{x\in V(G_1)-\{u\}\\ d(x)=2}}\sum_{\substack{y\in V(G_2)-\{u\}\\ d(y)=3}}(d(x,u)+d(u,y))+\sum_{\substack{x\in V(G_1)-\{u\}\\ d(x)=3}}\sum_{\substack{y\in V(G_2)-\{u\}\\ d(y)=2}}(d(x,u)+d(u,y))$$

$$=W_{23}(G_1)+W_{23}(G_2)+\sum_{\substack{x\in V(G_1)-\{u\}\\ d(x)=2}}[n_3(G_2-\{u\})d(x,u)+d^3_{G_2-\{u\}}(u)]+$$

$$\sum_{\substack{x\in V(G_1)-\{u\}\\ d(x)=3}}[n_2(G_2-\{u\})d(x,u)+d^2_{G_2-\{u\}}(u)]$$

$$=W_{23}(G_1)+W_{23}(G_2)+n_3(G_2-\{u\})d^2_{G_1-\{u\}}(u)+n_2(G_1-\{u\})d^3_{G_2-\{u\}}(u)+$$

$$n_2(G_2-\{u\})d^3_{G_1-\{u\}}(u)+n_3(G_1-\{u\})d^2_{G_2-\{u\}}(u)$$

$$=W_{23}(G_1)+W_{23}(G_2)+n_3(G_2-\{u\})d^2_{G_1}(u)+n_2(G_1-\{u\})d^3_{G_2}(u)+$$

$$n_2(G_2-\{u\})d^3_{G_1}(u)+n_3(G_1-\{u\})d^2_{G_2}(u),$$

as desired. ■

In the following two theorems, we shall deduce two results similar to Theorem 1 w. r. t. the extremal values of W_{23} and W_{33} for a polyphenyl chain.

Theorem 2. *Let* G_h *be a polyphenyl chain with h hexagons. Then*

$W_{23}(O_h)\le W_{23}(G_h)\le W_{23}(L_h)$,

where the left-hand side equality holds in the above inequality if and only if $G_h\cong O_h$ *and right-hand one holds in the above inequality if and only if* $G_h\cong L_h$.

Proof. Let *A* and *B* be two polyphenyl chains such that the number of hexagons in these two chains add up to $n-1$. Obviously, there are three ways of inserting a hexagon between them and

eventually forming a polyphenyl chain with h hexagons. Denoted by *AOB*, *AMB* and *APB*, respectively, the resulting polyphenyl chains upon the case when the inserted hexagon is an *ortho*-, a *meta*- , or a *para*-hexagon.
According to Lemma 1, we have

$$W_{23}(APB) = W_{23}(A) + W_{23}(C_1) + n_3(C_1 - \{v_1\})d_A^2(v_1) + n_2(A - \{v_1\})d_{C_1}^3(v_1) +$$
$$n_2(C_1 - \{v_1\})d_A^3(v_1) + n_3(A - \{v_1\})d_{C_1}^2(v_1).$$

From Fig. 3, one can deduce that

$$\begin{cases} n_3(C_1 - \{v_1\}) = n_3(B) + 2 \\ n_2(A - \{v_1\}) = n_2(A) \\ n_2(C_1 - \{v_1\}) = n_2(B) + 4 \\ n_3(A - \{v_1\}) = n_3(A) - 1 \end{cases}, \quad \begin{cases} d_{C_1}^3(v_1) = 5 + \sum\limits_{\substack{y \in B \\ d(y)=3}} [d(v_2, y) + 5] = 5 + 5n_3(B) + d_B^3(v_2) \\ d_{C_1}^2(v_1) = 10 + 5n_2(B) + d_B^2(v_2) \end{cases}.$$

Also, we have

$$W_{23}(C_1) = W_{23}(B) + W_{23}(D_1) + n_3(B - \{v_2\})d_{D_1}^2(v_2) + n_2(D_1 - \{v_2\})d_B^3(v_2) +$$
$$n_2(B - \{v_2\})d_{D_1}^3(v_2) + n_3(D_1 - \{v_2\})d_B^2(v_2),$$

$$\begin{cases} n_3(B - \{v_2\}) = n_3(B) - 1 \\ n_2(D_1 - \{v_2\}) = n_2(D_1) = 4 \\ n_2(B - \{v_2\}) = n_2(B) \\ n_3(D_1 - \{v_2\}) = n_3(D_1) - 1 = 3 \end{cases}, \quad \begin{cases} d_{D_1}^2(v_2) = 10 \\ d_{D_1}^3(v_2) = 10 \end{cases}, \quad \text{and } W_{23}(D_1) = 32.$$

Hence, we have

$$W_{23}(APB) = W_{23}(A) + W_{23}(B) + 22 + 10(n_2(B) + n_3(B)) + 4d_B^3(v_2) + 3d_B^2(v_2) +$$
$$(n_3(B) + 2)d_A^2(v_1) + n_2(A)d_B^3(v_2) + (n_2(B) + 4)d_A^3(v_1) + (n_3(A) - 1)d_B^2(v_2) +$$
$$5n_2(A)(n_3(B) + 1) + 5(n_2(B) + 2)(n_3(A) - 1).$$

By the same reasoning, we have

$$W_{23}(AMB) = W_{23}(A) + W_{23}(B) + 36 + 11(n_3(B) - 1) + 8n_2(B) + 4d_B^3(v_2) + 3d_B^2(v_2) +$$
$$(n_3(B) + 2)d_A^2(v_1) + n_2(A)d_B^3(v_2) + (n_2(B) + 4)d_A^3(v_1) + (n_3(A) - 1)d_B^2(v_2) +$$
$$4n_2(A)(n_3(B) + 1) + (4n_2(B) + 11)(n_3(A) - 1)$$

and

$$W_{23}(AOB) = W_{23}(A) + W_{23}(B) + 36 + 12(n_3(B) - 1) + 6n_2(B) + 4d_B^3(v_2) + 3d_B^2(v_2) +$$
$$(n_3(B) + 2)d_A^2(v_1) + n_2(A)d_B^3(v_2) + (n_2(B) + 4)d_A^3(v_1) + (n_3(A) - 1)d_B^2(v_2) +$$
$$3n_2(A)(n_3(B) + 1) + 3(n_2(B) + 4)(n_3(A) - 1).$$

An elementary calculation gives $W_{23}(AOB) < W_{23}(AMB) < W_{23}(APB)$. Now, we conclude that a polyphenyl chain with the maximum possible value of W_{23} can not have an *ortho*-, or a *meta*-hexagon. Similarly, a polyphenyl chain with the minimum possible value of W_{23} can not have an *meta*-, or a *para*-hexagon. This completes the proof. ■

Theorem 3. *Let* G_h *be a polyphenyl chain with h hexagons. Then* $W_{33}(O_h) \le W_{33}(G_h) \le W_{33}(L_h)$,

where the left-hand side equality holds in the above inequality if and only if $G_h \cong O_h$ *and right-hand one holds in the above inequality if and only if* $G_h \cong L_h$.

Proof. Let *AOB*, *AMB* and *APB* be the polyphenyl chains introduced as in Theorem 2. Analogous to Theorem 2, we have

$$W_{33}(APB) = W_{33}(A) + W_{33}(B) + 18 + 10(n_3(B) - 1) + 3d_B^3(v_2) + (n_3(B) + 2)d_A^3(v_1) + (n_3(A) - 1)d_B^3(v_2) + 5(n_3(B) + 1)(n_3(A) - 1),$$

$$W_{33}(AMB) = W_{33}(A) + W_{33}(B) + 14 + 8(n_3(B) - 1) + 3d_B^3(v_2) + (n_3(B) + 2)d_A^3(v_1) + (n_3(A) - 1)d_B^3(v_2) + 4(n_3(B) + 1)(n_3(A) - 1),$$

and

$$W_{33}(AOB) = W_{33}(A) + W_{33}(B) + 10 + 6(n_3(B) - 1) + 3d_B^3(v_2) + (n_3(B) + 2)d_A^3(v_1) + (n_3(A) - 1)d_B^3(v_2) + 3(n_3(B) + 1)(n_3(A) - 1).$$

By an elementary calculation, we have $W_{23}(AOB) < W_{23}(AMB) < W_{23}(APB)$. Now, we conclude that a polyphenyl chain with the maximum possible value of W_{33} can not have an *ortho*- or a *meta*-hexagon. Similarly, a polyphenyl chain with the minimum possible value of W_{33} can not have an *meta*- or a *para*-hexagon. This completes the proof. ■

Now, we are in a position to state and prove our main result of this paper.

Theorem 4. *Let* G_h *be a polyphenyl chain with h hexagons. Then* $DD(O_h) \le DD(G_h) \le DD(L_h)$,

where the left-hand side equality holds in the above inequality if and only if $G_h \cong O_h$ *and right-hand one holds in the above inequality if and only if* $G_h \cong L_h$.

Proof. In view of Theorems 1, 2 and 3, we have

$$W_{23}(O_h) \le W_{23}(G_h) \le W_{23}(L_h),$$

$$W_{33}(O_h) \le W_{33}(G_h) \le W_{33}(L_h).$$

$$W(O_h) \le W(G_h) \le W(L_h).$$

Combining Proposition 1 and the above three inequalities, we have actually obtained our desired result. ■

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