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The Polyphenyl Chains with Extremal Edge–Wiener Indices *

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Abstract

The edge-Wiener index of a connected graph is the sum of the distances between all pairs of edges of the graph. In this paper, we determine the polyphenyl chains with minimum and maximum edge-Wiener indices among all the polyphenyl chains with h hexagons. Moreover, explicit formulas for the edge-Wiener indices of extremal polyphenyl chains are obtained.

1 Introduction

A kind of macrocyclic aromatic hydrocarbons called polyphenyls and their derivatives attracted the attention of chemists form any years[1-3]. The derivatives of polyphenyls are very important organic chemicals, which can be used inorganic synthesis, drug synthesis, heat exchanger, etc. Biphenyl compounds also have extensive industrial applications. For example, 4,4-bis(chloromethyl) biphenyl can be used for the synthesis of brightening agents. Especially, polychlorinated biphenyls (PCBs) can be applied in print and dyeing extensively[4,5]. On the other side, PCBs are

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dangerous organic pollutants, which lead to global pollution. Many years ago, a series of linear and branched polyphenyls and their derivatives were synthesized and some physical properties were discussed[6-11]. Gutman [12] showed that the values which the Wiener indices of isomeric polyphenyls may assume are all congruent modulo 36. In [13], the present author and Fuji Zhang determine the polyphenyl chains with minimum and maximum Wiener indices among all the polyphenyl chains with h hexagons.

After Wiener, many topological indices were proposed by chemist and also by mathematicians, such as: Szeged index, PI index and detour index etc, and the corresponding edge versions of these topological indices are also considered. By now there do exist a lot of different types of such indices which capture different aspects of the molecular graphs associated to the molecules considered, for details one should consult the articles by Iranmanesh and Mahmiani [16, 17, 18, 19, 20, 21].

In this paper we are concerned with a quantity closely analogous to the Wiener index, namely the sum of all distances between all pairs of edges in a connected graph [22]. We determine the polyphenyl chains with minimum and maximum edge-Wiener indices among all the polyphenyl chains with h hexagons. Moreover, explicit formulas for the edge-Wiener indices of extremal polyphenyl chains are obtained.

2 Preliminaries

Throughout this paper all graphs are finite, undirected, simple connected. The vertex and edge sets of a graph G are $V(G)$ and $E(G)$.

Definition1: Let G be a connected graph. Then the edge-Wiener index of G is defined as the sum of the distance between all pairs of edges of G,

$$W_e(G) = \sum_{\{e,f\}\subseteq E(G)} d(e,f)$$

where the distance between two edges is the distance between the corresponding vertices in the line graph of G. In view of the above definition, the edge-Wiener index of a graph equals the ordinary Wiener index of its line graph.

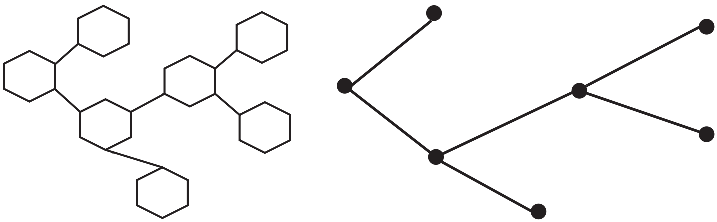

Fig.1: A polyphenyl system and corresponding tree

The molecular graphs (or more precisely, the graphs representing the carbon-atoms) of polyphenyls are called the polyphenyl system. The set of all polyphenyl systems and of all polyphenyl systems with h hexagons are denoted by PPS and PPS_h, respectively.

A polyphenyl system H is said to be tree-like, if each vertex of H lies in a hexagon and the graph obtained by contracting every hexagon into a vertex in original molecular graphs is a tree (see Fig.1). A hexagon r of a tree-like polyphenyl system has either one, two or three (at most six) neighboring hexagons. If r has one neighboring hexagon, then it is said to be terminal, and if it has three or more neighboring hexagons to be branched.

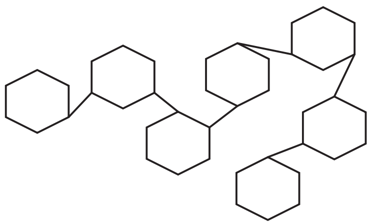

Fig.2: A polyphenyl chain with 7 hexagons

Definition2: A tree-like polyphenyl system without branched hexagons is called a polyphenyl chain. The sets of all polyphenyl chains and of all polyphenyl chains with h hexagons are denoted by PPC and PPC_h , respectively. It is known that all members of PPC_h have $6h$ vertices (see Fig.2).

Let us consider a hexagon C. Two vertices u and v of C are said to be in *ortho*-position if they are adjacent in C. If two vertices are at distance 2, they are in *meta*-

position. Finally, if u and v are at distance 3, we say that they are in *para*-position. Examples of pairs of vertices in *ortho*−, *meta*−, and *para*-position are shown in Fig.3.

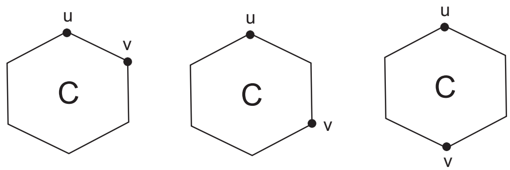

Fig.3: *ortho*−, *meta*−, and *para*-Positions of vertices in C

An internal hexagon C in a polyphenyl chain is called *ortho*-hexagon, *meta*-hexagon, or *para*-hexagon if the two vertices of C incident with two edges which connect other two hexagons are in *ortho*−, *meta*−, *para*-position, respectively. A polyphenyl chain with h hexagons is an $ortho-PPC_h$, if all its internal hexagons are *ortho*-hexagons. The $meta-PPC_h$ and $para-PPC_h$ are defined in a completely analogous manner. We denote the $ortho-PPC_h$, ($meta-PPC_h$ and $para-PPC_h$) by O_h (M_h, and L_h), respectively (see Fig.4).

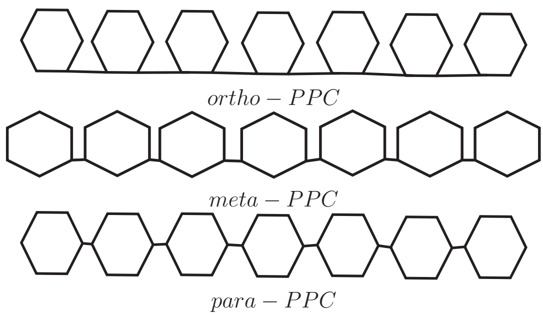

Fig.4: *ortho*−, *meta*−, and *para*-Polyphenyl chains with 7 hexagons

3 The polyphenyl chains with extremal edge-Wiener indices

Lemma 3.1. [23] *Let G be a graph obtained from arbitrary graphs G_1 and G_2 of order n_1 and n_2 by identifying vertices $v_1 \in V(G_1)$ and $v_2 \in V(G_2)$. Then:*

$$W(G) = W(G_1) + W(G_2) + (n_1 - 1)d_{G_2}(v_2) + (n_2 - 1)d_{G_1}(v_1)$$

Let h be the number of hexagons in the polyphenyl chain. Now we first give the explicit formula for the edge-Wiener index of the *para*−polyphenyl chain L_h.

Theorem 3.2. *Let L_h be a para-polyphenyl chain with h hexagons. Then*

$$W_e(L_h) = \frac{98}{3}h^3 - 14h^2 + \frac{25}{3}h$$

Proof. Let C and S be the subgraphs of $L(L_h)$ with common vertex x (see Fig.5), where $L(L_h)$ denotes the line graph of L_h. Using Lemma 3.1, we can write:

$$\begin{aligned} W_e(L_h) &= W(L(L_h)) = W(C) + W(S) + 6d_S(x) + (7h-8)d_C(x) \\ &= W(C) + W(L(L_{h-1})) + d_{L(L_{h-1})}(x) + 6d_S(x) + (7h-8)d_C(x) \\ &= W_e(L_{h-1}) + 98h^2 - 126h + 55 \end{aligned}$$

It is not difficult to see that:

$$\begin{aligned} W(C) &= 39 \\ d_{L(L_{h-1})}(x) &= 14h^2 - 30h + 16; \\ d_S(x) &= 0 + d_{L(L_{h-1})}(x) = 14h^2 - 30h + 16; \\ d_C(x) &= 12 \end{aligned}$$

where $d_G(v)$ is the sum of distances between v and all other vertices of G. Thus, using the G above recurrence relation and simple calculations, an explicit expression for $W_e(L_h)$ can be obtained.

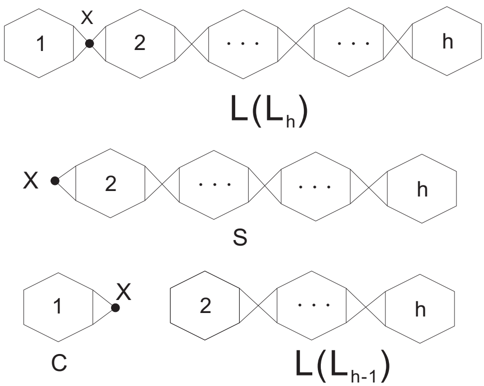

Fig.5

By the same reasoning as for O_h and M_h, we get the following two theorems.

Theorem 3.3. *Let O_h be an ortho-polyphenyl chain with h hexagons. Then*

$$W_e(O_h) = \frac{49}{3}h^3 + 35h^2 - \frac{73}{3}h$$

Theorem 3.4. *Let M_h be a meta-polyphenyl chain with h hexagons. Then*

$$W_e(M_h) = \frac{49}{2}h^3 - \frac{35}{2}h^2 - 36h$$

By comparing the edge-Wiener indices of O_h, M_h, L_h, we can show that $W_e(O_h) \leq W_e(M_h) \leq W_e(L_h)$. This double inequality remains valid even if M_h is replaced by any polyphenyl chain $G_h \in PPC_h$.

Theorem 3.5. *Let G_h be a polyphenyl chain with h hexagons. Then $W_e(O_h) \leq W_e(G_h) \leq W_e(L_h)$. The lower bound is realized if and only if $G_h = O_h$, and the upper bound is realized if and only if $G_h = L_h$.*

Proof. Let A and B be two polyphenyl chains such that the number of hexagons add to $h-1$. There are three ways of inserting a hexagon between them and forming a polyphenyl chain with h hexagons. We denote by AOB, AMB, and APB the cased when the inserted hexagon is an *ortho*$-$, *meta*$-$, and *para*$-$hexagon in the resulting chain. These three possibilities are shown in Fig.6.

Let n_1 and n_2 be the order of A' and B', respectively. According to Lemma 3.1, we have:

$$\begin{aligned}
W_e(APB) = W(A'P'B') &= W(A') + W(C_1) \\
&\quad + (n_1 - 1)d_{C_1}(u) + (n_2 + 6)d_{A'}(u) \\
&= W(A') + [W(D_1) + W(B') + 7d_{B'}(v) + (n_2 - 1)d_{D_1}(v)] \\
&\quad + (n_1 - 1)d_{C_1}(u) + (n_2 + 6)d_{A'}(u) \\
&= W(A') + W(D_1) + W(B') + 7d_{B'}(v) + 16(n_2 - 1) \\
&\quad + 12(n_1 - 1) + 4n_2(n_1 - 1) + (n_1 - 1)d'_B(u) + (n_2 + 6)d_{A'}(u) \\
&= W(A') + 55 + W(B') + 16(n_2 - 1) + 12(n_1 - 1) \\
&\quad + 4n_2(n_1 - 1) + (n_1 + 6)d_{B'}(v) + (n_2 + 6)d_{A'}(u)
\end{aligned}$$

Here we used the facts that $W(D_1) = 55, d_{D_1}(v) = 16$ and $d_{C_1}(u) = 12 + 4n_2 + d_{B'}(v)$.

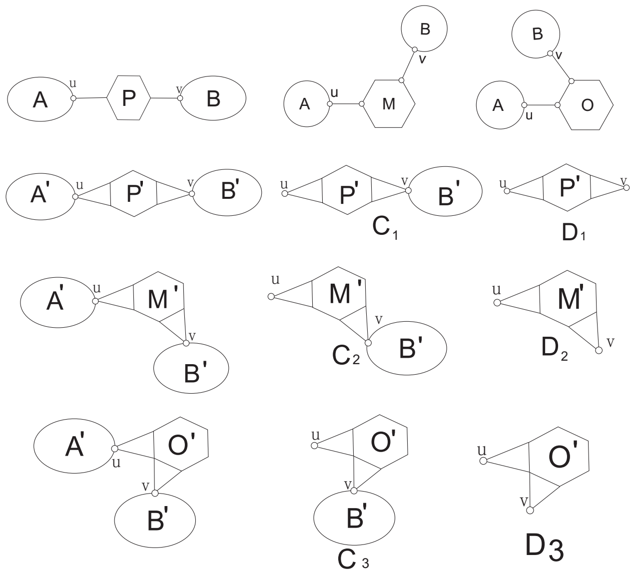

Fig.6: Three ways of inserting a hexagon C or D between two polyphenyl chains, and their corresponding auxiliary graphs.

In a similar way we obtain the expressions for $W_e(AOB)$ and $W_e(AMB)$:

$$\begin{aligned}
W_e(AMB) &= W(A'M'B') = W(A') + W(C_2) \\
&\quad + (n_1-1)d_{C_2}(u) + (n_2+6)d_{A'}(u) \\
&= W(A') + [W(D_2) + W(B') + 7d_{B'}(v) + (n_2-1)d_{D_2}(v)] \\
&\quad + (n_1-1)d_{C_2}(u) + (n_2+6)d_{A'}(u) \\
&= W(A') + W(D_2) + W(B') + 7d_{B'}(v) + 15(n_2-1) \\
&\quad + 12(n_1-1) + 3n_2(n_1-1) + (n_1-1)d_{B'}(u) + (n_2+6)d_{A'}(u) \\
&= W(A') + 54 + W(B') + 15(n_2-1) + 12(n_1-1) \\
&\quad + 3n_2(n_1-1) + (n_1+6)d_{B'}(v) + (n_2+6)d_{A'}(u)
\end{aligned}$$

$$\begin{aligned}
W_e(AOB) = W(A'O'B') &= W(A') + W(C_3) \\
&\quad + (n_1 - 1)d_{C_3}(u) + (n_2 + 6)d_{A'}(u) \\
&= W(A') + [W(D_3) + W(B') + 7d_{B'}(v) + (n_2 - 1)d_{D_3}(v)] \\
&\quad + (n_1 - 1)d_{C_3}(u) + (n_2 + 6)d_{A'}(u) \\
&= W(A') + W(D_3) + W(B') + 7d_{B'}(v) + 14(n_2 - 1) \\
&\quad + 12(n_1 - 1) + 2n_2(n_1 - 1) + (n_1 - 1)d_{B'}(u) + (n_2 + 6)d_{A'}(u) \\
&= W(A') + 53 + W(B') + 14(n_2 - 1) + 12(n_1 - 1) \\
&\quad + 2n_2(n_1 - 1) + (n_1 + 6)d_{B'}(v) + (n_2 + 6)d_{A'}(u)
\end{aligned}$$

Now we can compute the differences

$$W_e(APB) - W_e(AMB) = W_e(AMB) - W_e(AOB) = n_1 n_2 > 0$$

We have $W_e(AOB) \leq W_e(AMB) \leq W_e(APB)$.

Hence, a polyphenyl chain with the maximum possible of edge-Wiener index cannot contain an *ortho*−or a *meta*−hexagon. Similarly, a polyphenyl chain with the minimum possible of edge-Wiener index cannot contain a *meta*− or a *para*−hexagon.

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