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Tree-like polyphenyl systems with extremal Wiener indices *

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Abstract

The Wiener index of a connected graph is the sum of the distances between all pairs of vertices of the graph. In this paper, we determine the polyphenyl chains with minimum and maximum Wiener indices among all the polyphenyl chains with h hexagons, and the tree-like polyphenyl system with maximum Wiener index. Moreover, explicit formulas for the 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 for many years [1-3]. The derivatives of polyphenyls are very important organic chemicals, which can be used in organic 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 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 modul 36. In [2], the structures and relative contents of polyphenyl mixture by-products from the improved Ullmann reaction were determined, there are 23 polyphenyls found (see Fig.1).

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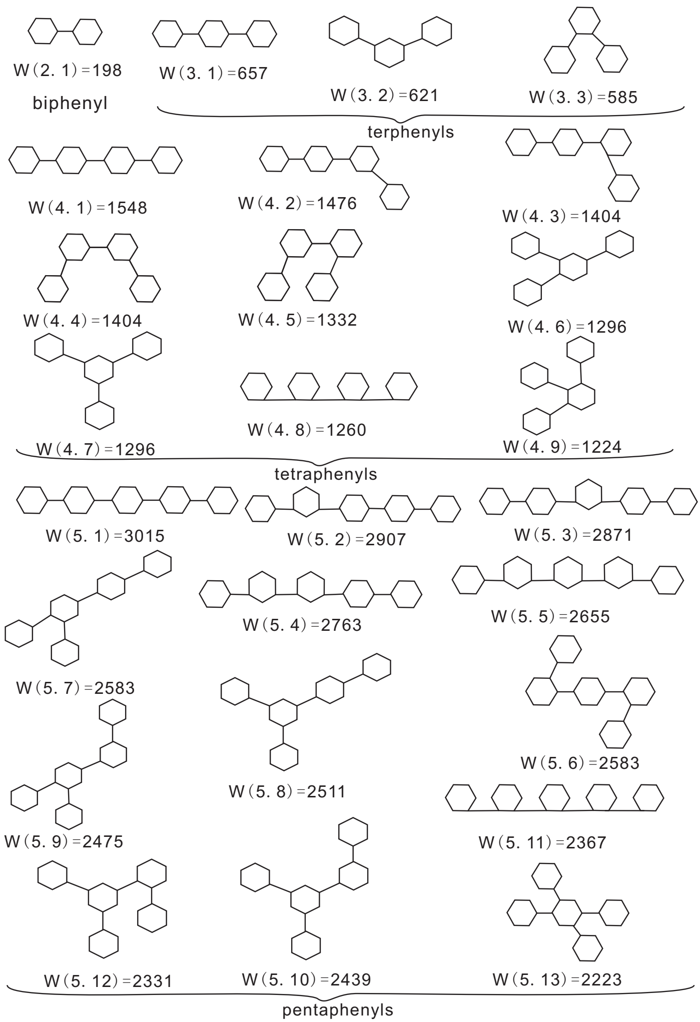

Fig. 1: All isomeric biphenyl, terphenyls, tetraphenyls and some isomeric pentaphenyls in [2]: $W(i.j)$ denotes by the polyphenyl with i hexagons and j-th large Wiener indices.

The Wiener index of a connected graph is the sum of the distances between all pairs of vertices of the graph. The Wiener index has been successfully used in $QSAR$ and $QSPR$ studies including pharmacological and biological activity [13-19]. The Wiener index has also been found to have interesting applications in organic and polymer chemistry, in studies of crystals and in drug design. A number of publications, reviews and books in the chemical and mathematical literature have been devoted to the Wiener index [16-19].

There have been two groups of closely related problems in the theory of Wiener index :
(1) How is the Wiener index related to the structure of a graph?
(2) How can we calculate the Wiener index of a graph efficiently (including the 'paper-and-pencil' method)?
The greatest progress in solving the above problems was made for trees and hexagonal systems [20-22]. For references on the Wiener indices of related molecular graphs with symmetry, see [23-28].

The ordering of Wiener indices can approximate the order of the boiling point of the tree-like polyphenyls and help their fractionation(see [2]). Therefore, it is reasonable to think that the order of the boiling point of the polyphenyls with less than 6 hexagons in [2] obeys the ordering of their Wiener indices (see Fig.1). In this paper, we characterize the polyphenyl chains with minimum and maximum Wiener indices among all polyphenyl chains with h hexagons, and tree-like polyphenyl systems with maximum Wiener index.

2 Preliminaries

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

Under distance $d_G(u, v)$ between vertices $u, v \in V(G)$ we mean the standard distance of the simple graph G, i.e., the number of edges of a shortest path connecting these vertices in G [29]. The distance of a vertex $v \in V(G)$, $d_G(v)$ is the sum of distances between v and all other vertices of G.

The Wiener index (or Wiener number) W is a well-known distance-based topological index introduced originally for molecular graphs of alkanes [30]. For a cyclic graph G, the Wiener index is defined as the sum of distances between all unordered pairs of its vertices [31]:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v) = \frac{1}{2} \sum_{v \in V(G)} d_G(v)$$

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 is denoted by PPS and PPS_h, respectively.

Definition. 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.2)

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

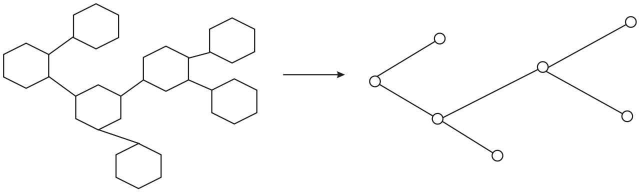

Fig. 2: A polyphenyl system and corresponding tree

if it has three or more neighboring hexagons to be *branched*.

Definition. 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.3)

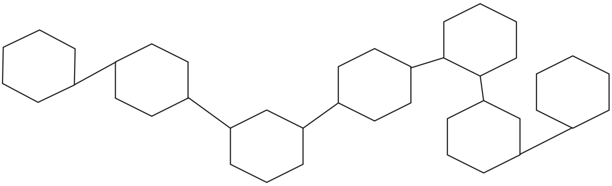

Fig. 3: A polyphenyl chain with 7 hexagons

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.4.

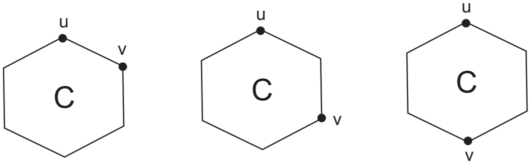

Fig. 4: *ortho*-, *meta*-, and *para*-Positions of vertices in C.

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.5)

The Wiener index of a graph can be expressed through the Wiener index of its subgraphs under some graph operations [20, 32, 33].

Lemma 2.1 *[20] 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 $W(G) = W(G_1)+W(G_2)+(n_1-1)d_{G_2}(v_2)+(n_2-1)d_{G_1}(v_1)$*

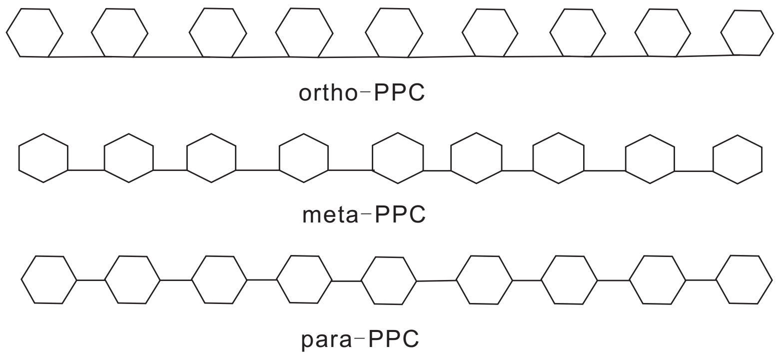

Fig. 5: *ortho*-, *meta*-, and *para*-Polyphenyl chains with 9 hexagons.

3 Tree-like polyphenyl system with respect to the Wiener index

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

Theorem 3.1 *Let G_h be a polyphenyl chain with h hexagons. Then $W(O_h) \leq W(G_h) \leq W(L_h)$. 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*-, a *meta*-, and a *para*-hexagon in the resulting chain. These three possibilities are shown in Fig.6.

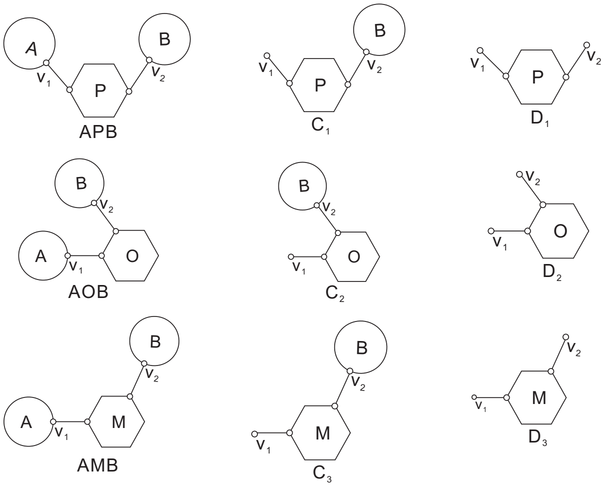

Fig. 6: Three ways of inserting a hexagon C or D between two polyphenyl chains, and their corresponding auxiliary graphs.

Let n_1 and n_2 be the order of A and B, respectively. According to Lemma 2.1, we have

$$\begin{aligned}
W(APB) &= W(A) + W(C_1) + (n_1-1)d_{C_1}(v_1) + (n_2+6)d_A(v_1)\\
&= W(A) + [W(D_1) + W(B) + 7d_B(v_2) + (n_2-1)d_{D_1}(v_2)]\\
&\quad +(n_1-1)d_{C_1}(v_1) + (n_2+6)d_A(v_1)\\
&= W(A) + W(D_1) + W(B) + 20(n_2-1) + 15(n_1-1)\\
&\quad +5n_2(n_1-1) + (n_1+6)d_B(v_2) + (n_2+6)d_A(v_1)\\
&= W(A) + 62 + W(B) + 20(n_2-1) + 15(n_1-1)\\
&\quad +5n_2(n_1-1) + (n_1+6)d_B(v_2) + (n_2+6)d_A(v_1)
\end{aligned}$$

Here we used the facts that $W(D_1) = 62$, $d_{D_1}(v_2) = 20$ and $d_{C_1}(v_1) = 15 + 5n_2 + d_B(v_2)$. In a similar way we obtain the expressions for $W(AOB)$ and $W(AMB)$:

$$\begin{aligned}
W(AOB) &= W(A) + W(C_2) + (n_1-1)d_{C_2}(v_1) + (n_2+6)d_A(v_1)\\
&= W(A) + [W(D_2) + W(B) + 7d_B(v_2) + (n_2-1)d_{D_2}(v_2)]\\
&\quad +(n_1-1)d_{C_2}(v_1) + (n_2+6)d_A(v_1)\\
&= W(A) + W(D_2) + W(B) + 18(n_2-1) + 15(n_1-1)\\
&\quad +3n_2(n_1-1) + (n_1+6)d_B(v_2) + (n_2+6)d_A(v_1)\\
&= W(A) + 60 + W(B) + 18(n_2-1) + 15(n_1-1)\\
&\quad +3n_2(n_1-1) + (n_1+6)d_B(v_2) + (n_2+6)d_A(v_1)
\end{aligned}$$

Finally,

$$\begin{aligned}
W(AMB) &= W(A) + W(C_3) + (n_1 - 1)d_{C_3}(v_1) + (n_2 + 6)d_A(v_1) \\
&= W(A) + [W(D_3) + W(B) + 7d_B(v_2) + (n_2 - 1)d_{D_3}(v_2)] \\
&\quad +(n_1 - 1)d_{C_3}(v_1) + (n_2 + 6)d_A(v_1) \\
&= W(A) + W(D_3) + W(B) + 19(n_2 - 1) + 15(n_1 - 1) \\
&\quad +3n_2(n_1 - 1) + (n_1 + 6)d_B(v_2) + (n_2 + 6)d_A(v_1) \\
&= W(A) + 61 + W(B) + 19(n_2 - 1) + 15(n_1 - 1) \\
&\quad +4n_2(n_1 - 1) + (n_1 + 6)d_B(v_2) + (n_2 + 6)d_A(v_1)
\end{aligned}$$

Now we can compute the differences:

$$\begin{aligned}
W(APB) - W(AMB) &= W(AMB) - W(AOB) \\
&= (n_2 - 1) + n_2(n_1 - 1) + 1 \\
&\geq 0
\end{aligned}$$

We have $W(AOB) \leq W(AMB) \leq W(APB)$. Hence, a polyphenyl chain with the maximum possible of Wiener index cannot contain an *ortho*- or a *meta*-hexagon. Similarly, a polyphenyl chain with the minimum possible of Wiener index cannot contain a *meta*- or a *para*-hexagon. □

According to Theorem 3.1, the maximum and minimum Wiener indices are obtained in polyphenyl chains. Note that the polyphenyl chain is a special tree-like polyphenyl system. In fact, we can further show that L_h has maximum Wiener index in all tree-like polyphenyl systems with h hexagons.

Theorem 3.2 *Let G_h be a any tree-like polyphenyl system with h hexagons. Then $W(G_h) \leq W(L_h)$, the upper bound is realized if and only if $G_h = L_h$.*

Before giving the proof of Theorem 3.2, we need to define the following removed transformation:

Let r be a branched hexagon of any tree-like polyphenyl system H, and A, B, C, D, E, F be connected components adjacent to r. We assume that B is a *para*-polyphenyl chain, and for any one of the other nonempty connected components adjacent to r, let us delete the component from H and link it to a vertex on the terminal hexagon of B with *para*-position, then a polyphenyl system H' is obtained. We say that H' is obtained from H by a removed transformation.

Lemma 3.3 *Let r be a branched hexagon of any tree-like polyphenyl system H, and A, B, C, D, E, F be connected components adjacent to r in which B is a para-polyphenyl chain. Then $W(H') > W(H)$, where H' is obtained from H by a removed transformation.*

Proof. Let n_i, $i = 1, 2, \cdots, 6$ be the orders of A, B, C, D, E and F, respectively. By assumption, r is a branched hexagon, then there are at least three connected components which are nonempty. Suppose that H' is obtained by a removed transformation from H by deleting the component F from H, and linking it to a vertex on the terminal hexagon of B with *para*-position. According to Lemma 2.1, we can calculate the Wiener indices of H and

H' (see Fig.7).

$$\begin{aligned}
W(H) &= W(F)+W(S_1)+(n_6-1)d_{S_1}(x_6)+(n_1+n_2+n_3+n_4+n_5+6)d_F(x_6)\\
&= W(F)+[1+W(S_0)+d_{S_0}(y)+(n_1+n_2+n_3+n_4+n_5+5)]\\
&\quad +(n_6-1)d_{S_1}(x_6)+(n_1+n_2+n_3+n_4+n_5+6)d_F(x_6)\\
&= W(F)+W(S_0)+1+(n_1+n_2+n_3+n_4+n_5+5)+(n_1+n_2+n_3+n_4\\
&\quad +n_5+6)d_F(x_6)+d_{S_0}(y)+(n_6-1)d_{S_1}(x_6)
\end{aligned}$$

$$\begin{aligned}
W(H') &= W(F)+W(S_2)+(n_6-1)d_{S_2}(x_6)+(n_1+n_2+n_3+n_4+n_5+6)d_F(x_6)\\
&= W(F)+[1+W(S_0)+d_{S_0}(x_0)+(n_1+n_2+n_3+n_4+n_5+5)]\\
&\quad +(n_6-1)d_{S_2}(x_6)+(n_1+n_2+n_3+n_4+n_5+6)d_F(x_6)\\
&= W(F)+W(S_0)+1+(n_1+n_2+n_3+n_4+n_5+5)+(n_1+n_2+n_3+n_4\\
&\quad +n_5+6)d_F(x_6)+d_{S_0}(x_0)+(n_6-1)d_{S_2}(x_6)
\end{aligned}$$

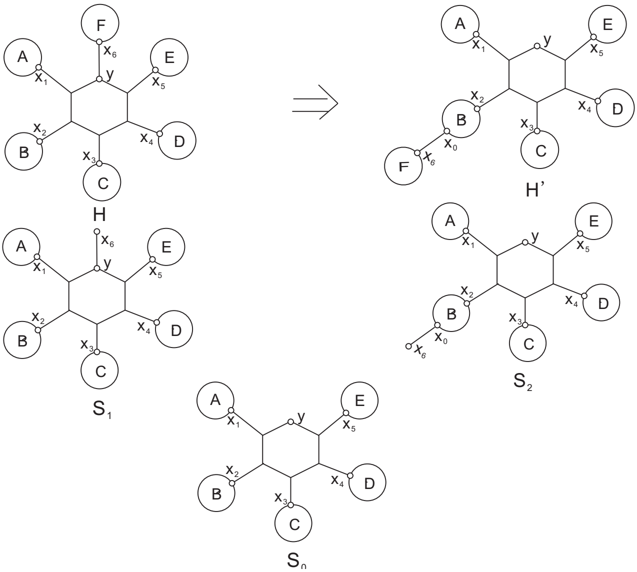

Fig. 7: H' is obtained by a removed transformation from H in which B is a *para*-polyphenyl chain (A, C, D, E may be empty) and three auxiliary graphs.

where

$$\begin{aligned}
d_{S_0}(y) &= 9+2n_1+3n_2+4n_3+3n_4+2n_5+d_A(x_1)+d_B(x_2)+d_C(x_3)+d_D(x_4)+d_E(x_5)\\
d_{S_1}(x_6) &= 15+3n_1+4n_2+5n_3+4n_4+3n_5+d_A(x_1)+d_B(x_2)+d_C(x_3)+d_D(x_4)+d_E(x_5)
\end{aligned}$$

$$\begin{aligned}
d_{S_0}(x_0) &= d_B(x_0) + [d(x_0,x_2)+1] + [d(x_0,x_2)+2]\cdot 2 + [d(x_0,x_2)+3]\cdot 2 + [d(x_0,x_2)+4] \\
&\quad +[d(x_0,x_2)+3]n_1 + d_A(x_1) + [d(x_0,x_2)+4]n_3 + d_C(x_3) \\
&\quad +[d(x_0,x_2)+4]n_4 + d_D(x_4) + [d(x_0,x_2)+5]n_5 + d_E(x_5) \\
&= 15 + 3n_1 + 3n_3 + 4n_4 + 5n_5 + (n_1+n_3+n_4+n_5+6)d(x_0,x_2) \\
&\quad +d_B(x_0) + d_A(x_1) + d_C(x_3) + d_D(x_4) + d_E(x_5)
\end{aligned}$$

$$\begin{aligned}
d_{S_2}(x_6) &= n_2 + d_B(x_0) + [d(x_0,x_2)+2] + [d(x_0,x_2)+3]\cdot 2 + [d(x_0,x_2)+4]\cdot 2 + [d(x_0,x_2)+5] \\
&\quad +[d(x_0,x_2)+4]n_1 + d_A(x_1) + [d(x_0,x_2)+4]n_3 + d_C(x_3) \\
&\quad +[d(x_0,x_2)+5]n_4 + d_D(x_4) + [d(x_0,x_2)+6]n_5 + d_E(x_5) \\
&= 21 + 4n_1 + 4n_3 + 5n_4 + 6n_5 + n_2 + (n_1+n_3+n_4+n_5+6)d(x_0,x_2) \\
&\quad +d_B(x_0) + d_A(x_1) + d_C(x_3) + d_D(x_4) + d_E(x_5)
\end{aligned}$$

Since B is a *para*-polyphenyl chain, we have $d_B(x_0) = d_B(x_2)$, and $2d(x_0,x_2) \geq n_2$ ($d(x_0,x_2) \geq 3$). By comparing with various items of $W(H)$ and $W(H')$, we have the desired result.

If H' is obtained by a removed transformation from H by deleting A (or C, or D, or E) from H, and link it to a vertex on the terminal hexagon of B with *para*-position, the computing and results are analogous. □

Proof of Theorem 3.2. Let G be a extremal tree-like polyphenyl system with maximum Wiener index. We first claim that all internal hexagons (which are not branched hexagons) are all *para*-hexagons. Suppose, on the contrary, that there exists one internal hexagon r (which is not a branched hexagon) such that r is not *para*-hexagon. Similarly to the proof of theorem 3.1, we can transform it into a *para*-hexagon. Then we obtain a polyphenyl system G' with greater Wiener index than G, this contradicts the maximum of G. Furthermore, we can show that there exists no branched hexagons in G. Otherwise, G has a branched hexagon which has three or more neighbors. Starting from any terminal hexagon go through the adjacent hexagon until first meet a branched hexagon r', then this is a *para*-polyphenyl chain adjacent to r' which contains the terminal hexagon. Then we can obtain a polyphenyl system G' by a removed transformation as in Lemma 3.3, then $W(G') > W(G)$, a contradiction. This completes the proof. □

4 Wiener indices for three type of polyphenyl chains: L_h, O_h and M_h

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

Theorem 4.1 *Let L_h be a para-polyphenyl chain with h hexagons. Then $W(L_h) = 24h^3 + 3h$.*

Proof. Let C and S be the subgraphs of L_h with common vertex x (see Fig.8). Using Lemma 2.1, we can write:

$$\begin{aligned}
W(L_h) &= W(C) + W(S) + 5d_S(x) + 6(h-1)d_C(x) \\
&= W(C) + [1 + W(L_{h-1}) + d_{L_{h-1}}(y) + 6(h-1) - 1] + 5d_S(x) + 6(h-1)d_C(x) \\
&= W(L_{h-1}) + 72h^2 - 72h + 27
\end{aligned}$$

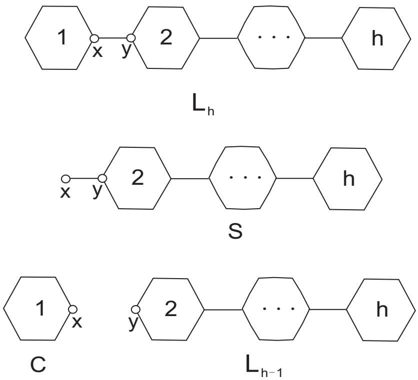

Fig. 8: a *para*-chain L_h and three auxiliary graphs for L_h.

It is not difficult to see that:

$$\begin{aligned} d_{L_{h-1}}(y) &= 12(h-1)^2 - 3(h-1); \\ d_S(x) &= 12h^2 - 21h + 9; \\ d_C(x) &= 9 \end{aligned}$$

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

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

Theorem 4.2 *Let O_h be an ortho-polyphenyl chain with h hexagons. Then* $W(O_h) = 12h^3 + 36h^2 - 21h$.

□

Theorem 4.3 *Let M_h be a meta-polyphenyl chain with h hexagons. Then* $W(M_h) = 18h^3 + 18h^2 - 9h$.

□

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References

[1] D. R. Flower, *On the properties of bit string-based measures of chemical similarity*, J. Chem. Inf. Comput. Sci. 38 (1998) 379-386.

[2] Q. R. Li, Q. Yang, H. Yin, S. Yang, *Analysis of by-products from improved Ullmann reaction using TOFMS and GCTOFMS*, J. Univ. Sci. Technol. China, 34 (2004) 335-341.

[3] S. Tepavcevic, A. T. Wroble, M. Bissen, D. J. Wallace, Y. Choi, L. Hanley, *Photoemission studies of polythiophene and polyphenyl films produced via surface polymerization by ion-assisted deposition*, J. Phys. Chem. B 109 (2005) 7134-7140.

[4] G. Luthe, J. A. Jacobus, L. W. Robertson, *Receptor interactions by polybrominated diphenyl ethers versus polychlorinated biphenyls: A theoretical structure-activity assessment*, Environ. Tox. Pharm. 25 (2008) 202-210.

[5] M. Bureš, V. Pekárek, T. Ocelka, *Thermochemical properties and relative stability of polychlorinated biphenyls*, Environ. Tox. Pharm. 25 (2008) 148-155.

[6] S. Ozasa, N. Hatada, Y. Fujioka, E. Ibuki, *Studies of polyphenyls and polyphenylenes. II. The synthesis and physical properties of polphenyls containing para linkage*, Bull. Chem. Soc. Jpn. 53 (1980) 2610-2617.

[7] E. Ibuki, S. Ozasa, Y. Fujioka, H. Kitamura, *Syntheses and physical properties of several symmetrical sexiphenyls*, Chem. Pharm. Bull., 28 (1980) 1468-1476.

[8] S. Ozasa, Y. Fujioka, M. Fujiwara, E. Ibuki, *Syntheses and physical properties of several octiphenyls and a septiphenyl*, Chem. Pharm. Bull., 28 (1980) 3210-3222.

[9] S. Ozasa, Y. Fujioka, M. Tsukada, E. Ibuki, *Syntheses and physical properties of several octiphenyls containing mixed linkages*, Chem. Pharm. Bull., 29 (1980) 344-355.

[10] S. Ozasa, Y. Fujioka, M. Okada, H. Izumi, E. Ibuki, *Syntheses and physical properties of several deuterium-labelled polyphenyls*, Chem. Pharm. Bull., 29 (1980) 370-378.

[11] E. Ibuki, S. Ozasa, Y. Fujioka, M. Okada, Y. Yanagihara, *Polyphenyl synthesis by means of the Kharash-type Grignard Cross-coupling Reaction*, Chem. Pharm. Bull., 30 (1982) 2369-2379.

[12] I. Gutman, G. Dömötör, *Wiener number of polyphenyls and phenylenes*, Z. Naturforsch. 49a (1994) 1040-1044.

[13] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1983; 2nd ed. 1992.

[14] D. H. Rouvray, *Should we have designs on topological indices?* in: R. B. King (Ed.), *Chemical Application of Topology and Graph Theory*, Elsevier, Amsterdam, 1983, pp. 159-177.

[15] A. T. Balaban, I. Motoc, D. Bonchev, O. Mekenyan, *Topological indices for structure-activity correlations*, Top. Curr. Chem. 114 (1983) 21-55.

[16] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin , 1986.

[17] I. Gutman, Y. N. Yeh, S. L. Lee, Y. L. Luo, *Some results in the theory of the Wiener number*, Indian J. Chem., Sect. A 32 (1993) 651-661.

[18] S. Nikolić, N. Trinajstić, Z. Mihalić, *The Wiener index: developments and applications*, Croat. Chem. Acta. 68 (1995) 105-129.

[19] I. Gutman, J. H. Potgieter, *Wiener index and intermolecular forces*, J. Serb. Chem. Soc. 62 (1997) 185-192.

[20] A. A. Dobrynin, R. Entringer, I. Gutman, *Wiener index of trees: theory and applications*, Acta Appl. Math. 66 (2001) 211-249.

[21] A. A. Dobrynin, I. Gutman, *The Wiener index for trees and graphs of hexagonal systems*, Diskretn. Anal. Issled. Oper. Ser. 2 5(2) (1998) 34-60 (in Russian).

[22] R. C. Entringer, *Distance in graphs: trees*, J. Combin. Math. Combin. Comput. 24 (1997) 65-84.

[23] I. Gutman, S. Klavžar, *Relations between Wiener numbers of benzenoid hydrocarbons and phenylenes*, ACH Models Chem. 135 (1998) 45-55.

[24] I. Gutman, S. Marković, L. Popović, Z. Spalević, L. Pavlović, *The relation between the Wiener indices of phenylenes and their hexagonal squeezes*, J. Serb. Chem. Soc. 62 (1997) 207-210.

[25] L. Pavlovic, I. Gutman, *Wiener numbers of phenylenes: an exact result*, J. Chem. Inf. Comput. Sci. 37 (1997) 355-358.

[26] F. J. Zhang, H. E. Li, *Calculating Wiener numbers of molecular graphs with symmetry*, Fifty years of the Wiener index. MATCH Commun. Math. Comput. Chem. 35 (1997) 213-226.

[27] H. E. Li, F. J. Zhang, *Note on calculating Wiener numbers of molecular graphs with symmetry*, Appl. Math. J. Chinese Uni. Ser. B. 14 (1999) 191-196.

[28] P. W. Fowler, G. Caporossi, P. Hansen, *Distance matrices, Wiener indices, and related invariants of fullerenes*, J. Phys. Chem. A. 105 (2001), 6232-6242.

[29] F. Buckley, F. Harary, *Distance in Graphs*, Addison-Wesley, Redwood, 1990.

[30] H. Wiener, *Structural determination of paraffin boiling points*, J. Amer. Chem. Soc. 69 (1947) 17-20.

[31] H. Hosoya, *Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons*, Bull. Chem. Soc. Jpn. 4 (1971) 2332-2339.

[32] O. E. Polansky, D Bonchev, *Theory of the Wiener numbers of graphs. II. transfer graphs and some of their metric properties*, MATCH Commun. Math. Comput. Chem. 21 (1986) 133-186.

[33] O. E. Polansky, D Bonchev, *The Wiener number of graphs. I. general theory and changes due to some graph operations*, MATCH Commun. Math. Comput. Chem. 25 (1990) 3-39.