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The Hosoya Polynomial Decomposition for Polyphenyl Chains*

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Abstract: For a graph $G = (V, E)$ we denote by $d_G(u, v)$ the distance between vertices u and v in G, and the Hosoya polynomial of G is defined as $H(G)=\sum_{\{u,v\}\subseteq V(G)} x^{d_G(u,v)}$. In this paper, we compute formulae for Hosoya polynomials of general polyphenyl chains.

1 Introduction

Suppose that $G = (V, E)$ is a connected graph, and let $d_G(u, v)$ be the distance between u and v in G. Then $H(G) = \sum\limits_{\{u,v\}\subseteq V(G)} x^{d_G(u,v)}$ is called *Hosoya polynomial*, introduced by Hosoya in 1988 [1]. E. Estrada et al [2] studied the chemical applications of Hosoya polynomial. The main property of $H(G)$, which makes it interesting in chemistry, follows directly from its definition: its first derivative at $x = 1$ is equal to a well-known Wiener index $W(G)$ of G, the sum of distances of all vertex pairs of G, namely $W(G) = \frac{dH(G,x)}{dx}|_{x=1}$. Hosoya polynomial contains more information about distance in a graph than any of the hitherto proposed distance-based topological indices; cf. [3]. Abundant literature appeared on this topic for the theoretical consideration and computation. I. Gutman et al [3] had computed some exact formulae for the Hosoya polynomials of benzenoid graphs. Recently, S. Xu and H. Zhang gave explicit analytical expressions for Hosoya polynomials of catacondensed benzenoid graph [4], hexagonal chains [5], armchair open-ended nanotubes [6] and TUC_4C_8(S) nanotubes [7]. E. Mehdi and T. Bijan [8] gave a formula to compute Hosoya polynomial of zigzag polyhex nanotorus. A lot of results on

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Hosoya polynomial can also be found in [9].

The polyphenyls are widely used in industry and their detailed chemical application and physical properties can be found in [10-14].The molecular graph (or more precisely, the graph representing the carbon-atom) of polyphenyl is called *polyphenyl system.* A polyphenyl system is *tree-like* if each one of its vertices lies in a hexagon and the graph obtained by contracting every hexagon into a vertex in original molecular graphs is a tree. If a hexagon Y in a tree-like polyphenyl system has only one neighboring hexagon, then it is said to be *terminal.* If Y has three or more neighboring hexagons, then it is said to be *branched.* A tree-like polyphenyl system without branched hexagons is a *polyphenyl chain.*

In this paper, we first compute exact formulae for the Hosoya polynomials of three special polyphenyl chains, and then, by virtue of them, we further obtain the formula to compute Hosoya polynomials of general polyphenyl chains.

2 Main results

The number of hexagons in a polyphenyl chain is called its *length.* Denote by $\mathcal{G}(h)$ the set of all polyphenyl chains of length h. Let $G \in \mathcal{G}(h)$. If $h \geqslant 3$ then all but the two terminal hexagons of G are called the *internal hexagons.* The two vertices u and v of degree 3 on an internal hexagon Y are on *ortho-position* if they are adjacent, on *meta-position* if they are separated by a path of length 2 and on *para-position* if they are separated by a path of length 3; and correspondingly, Y is called *ortho-hexagon*, *meta-hexagon* and *para-hexagon*, respectively. G is an *ortho-polyphenyl chain* if all its internal hexagons are ortho-hexagons. The meta-polyphenyl chain and para-polyphenyl chain can also be analogously defined. In what follows, we will denote by O_h, M_h and L_h the ortho-polyphenyl chain, meta-polyphenyl chain and para-polyphenyl chain of length h, respectively.

If $G \in \mathcal{G}(h)$ then we also find the following two notations convenient. Firstly, let w be a vertex of G with $d_G(w) = m$, where $d_G(w)$ denotes the degree of w in G, and Y be a subgraph of G. Then we set $V_n(Y) = \{y \in V(Y) | d_Y(y) = n\}$, $H_{mn}(w, V_n(Y)) := \sum_{y \in V_n(Y)} x^{d_G(w,y)}$ and $H_{nn}(V_n(Y)) := \sum_{\{y,z\} \subseteq V_n(Y)} x^{d_G(y,z)}$. Secondly, if we set $H_{mn}(G) = \sum_{\substack{\{u,v\} \subseteq V(G), \\ d_G(u)=m, d_G(v)=n}} x^{d_G(u,v)}$, then clearly $H(G) = H_{22}(G) + H_{23}(G) + H_{33}(G)$.

Note $H(L_1) = H(M_1) = H(O_1) = 6 + 6x + 6x^2 + 3x^3$. Next we only give the formulae for calculating the Hosoya polynomials of O_h, L_h and M_h when $h \geqslant 2$.

Theorem 2.1. *If $h \geqslant 2$ then we have*

$$H(O_h) = 6h + (2+3h)x + 2(2+h)x^2 + (2+h)x^3 + x^{2h-1}$$
$$-\frac{x(2h-3+2(h-2)(x+1)^2+(h-1)x^2(x+1)^3-2(x^2+2x+2)(x^{2(h-1)}-1))}{x-1}$$
$$+\frac{x^2((x^{2h-3}-1)+x(x+1)(2(x^{2(h-2)}-1)+(x^3+x^2+2x-2)(x^{2(h-1)}-1)))}{(x-1)^2}\,.$$

Proof. We first prove by induction on h that following three results are true.

$$H_{33}(O_h) = 2(h-1) - \frac{(2h-3)x}{x-1} + \frac{x^2(x^{2h-3}-1)}{(x-1)^2}\,.$$

$$H_{22}(O_h) = 2+4h+(2+3h)x+2(2+h)x^2+(2+h)x^3+x^{2h-1} - \frac{(h-1)x^3(x+1)^3}{x-1}$$
$$+ \frac{x^3(x+1)(x^3+x^2+2x-2)(x^{2(h-1)}-1)}{(x-1)^2}\,.$$

$$H_{23}(O_h) = \frac{2x((2-h)(x+1)^2+(x^2+2x+2)(x^{2(h-1)}-1))}{x-1} + \frac{2x^3(x+1)(x^{2(h-2)}-1)}{(x-1)^2}\,.$$

The base step $h=2$ can be easily fulfilled. So suppose $h \geqslant 3$. Let $h=k+1$. Then O_{k+1} can be obtained from O_k by attaching to it a new hexagon Y_{k+1} through an edge uv as in Fig. 1(a). Thus we have

$$\begin{aligned}
H_{33}(O_{k+1}) &= H_{33}(O_k) + H_{33}(u, V_3(O_{k+1})) + H_{33}(v, V_3(O_{k+1}) \setminus \{u\}) \\
&= H_{33}(O_k) + (x + x^2 + \cdots + x^{2(k-1)}) + (1+x) + (1 + x^2 + \cdots + x^{2k-1}) \\
&= H_{33}(O_k) + \frac{x(x+1)(x^{2(k-1)}-1)}{x-1} + (2+x)\,, \\
H_{22}(O_{k+1}) &= H_{22}(O_k) - H_{32}(u, V_2(O_k)) + H_{22}(V_2(Y_{k+1})\setminus\{v\}) + H_{22}(p, V_2(O_k)\setminus\{u\}) \\
&+ H_{22}(q, V_2(O_k)\setminus\{u\}) + H_{22}(r, V_2(O_k)\setminus\{u\}) + H_{22}(s, V_2(O_k)\setminus\{u\}) \\
&+ H_{22}(t, V_2(O_k)\setminus\{u\}) = H_{22}(O_k) \\
&+ (-1+2x^2+2x^3+x^4)H_{22}(V_2(O_k) \setminus \{u\}) + H_{22}(V_2(Y_{k+1})\setminus\{v\}) - 1\,,
\end{aligned}$$

$$
\begin{aligned}
H_{23}(O_{k+1}) &= H_{23}(O_k) - H_{33}(u, V_3(O_{k+1}) \setminus \{u,v\}) + H_{32}(u, V_2(O_k) \setminus \{u\}) \\
&+ H_{32}(v, V_2(O_k) \setminus \{u\}) + H_{23}(p, V_3(O_{k+1})) + H_{23}(q, V_3(O_{k+1})) \\
&+ H_{23}(r, V_3(O_{k+1})) + H_{23}(s, V_3(O_{k+1})) + H_{23}(t, V_3(O_{k+1})) \\
&= H_{23}(O_k) - H_{33}(u, V_3(O_{k+1}) \setminus \{u,v\}) + (x+1)H_{32}(u, V_2(O_k) \setminus \{u\}) \\
&+ (2+2x+x^2)H_{23}(p, V_3(O_{k+1}))\ .
\end{aligned}
$$

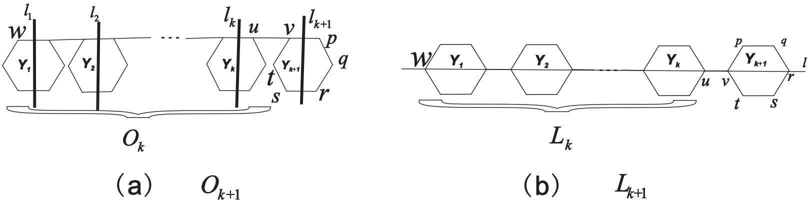

Fig. 1

To give more accurate expression of $H_{22}(O_{k+1})$ and $H_{23}(O_{k+1})$ draw an vertical line l_i through the center of the hexagon Y_i of O_{k+1} for each i, as in Fig. 1 (a). Let $V_m(Y_i, l_i(l))$ and $V_m(Y_i, l_i(r))$ denote sets of vertices of degree m lying on the left and the right sides of l_i in Y_i, respectively $(i = 1, 2, \ldots, k+1)$. Then we further have

$$
\begin{aligned}
H_{22}(O_{k+1}) &= H_{22}(O_k) + \left(-1+2x^2+2x^3+x^4\right)\left(H_{32}\left(u, \bigcup_{i=1}^{k} V_2(Y_i, l_i(l)) \backslash \{w\}\right)\right) \\
&+ H_{32}\left(u, \bigcup_{i=1}^{k} V_2(Y_i, l_i(r)) \backslash \{u\}\right) + x^{d(u,w)}\Bigg) + H_{22}(V_2(Y_{k+1}) \backslash \{v\}) - 1 \\
&= H_{22}(O_k) + \left(-1+2x^2+2x^3+x^4\right)\Bigg(\sum_{j=1}^{k}(x^{2j}+x^{2j+1}) \\
&+ \sum_{j=1}^{k}(x^{2j-1}+x^{2j}) + x^{2k-1}\Bigg) + \left(5+4x+4x^2+2x^3\right) - 1 \\
&= H_{22}(O_k) + \frac{x(x+1)^2(x^3+x^2+x-1)(x^{2k}-1)}{x-1} \\
&+ (x+1)(x^3+x^2+x-1)x^{2k-1} + (4+4x+4x^2+2x^3)\,,
\end{aligned}
$$

$$
\begin{aligned}
H_{23}(O_{k+1}) &= H_{23}(O_k) - H_{33}(u, V_3(O_{k+1}) \setminus \{u,v\}) \\
&+ (x+1)\left(H_{32}\left(u, \bigcup_{i=1}^{k} V_2(Y_i, l_i(r)) \setminus \{u\}\right)\right) + x^{d(u,w)} \\
&+ H_{32}\left(u, \bigcup_{i=1}^{k} V_2(Y_i, l_i(l)) \setminus \{u,w\}\right) + (2+2x+x^2)H_{23}(p, V_3(O_{k+1})) \\
&= H_{23}(O_k) - \sum_{j=1}^{2k-1} x^j + (x+1)\left(\sum_{j=1}^{2k} x^j + x^{2k-1} + \sum_{j=2}^{2k+1} x^j\right) \\
&+ (2+2x+x^2)\sum_{j=1}^{2k} x^j = H_{23}(O_k) \\
&- \frac{x((x^{2k-1}-1)-(2x^2+4x+3)(x^{2k}-1))}{x-1} + (x+1)x^{2k-1} .
\end{aligned}
$$

By the inductive hypothesis and direct calculation, $H_{33}(O_h)$, $H_{22}(O_h)$ and $H_{23}(O_h)$ are fulfilled for $h = k+1$. Hence they are fulfilled for all h. Finally, combining them, we obtain the last assertion of $H(O_h)$. □

Theorem 2.2. *If $h \geqslant 2$ then we have*

$$
\begin{aligned}
H(L_h) &= 6h + 3(1+h)x + 2(2+h)x^2 + 2hx^3 + x^{4h-1} \\
&- \frac{x((x+1)(5(h-1)x^2+4(h-2)) - 2(2x^4+x^2+2x+2)(x^{4(h-1)}-1))}{(x-1)(x^2+1)} \\
&+ \frac{x^3((4x^4+1)(x^{4(h-1)}-1)+4x^2(x^{4(h-2)}-1))}{(x-1)^2(x^2+1)^2} .
\end{aligned}
$$

Proof. We first prove by induction on h that following three results are true.

$$
\begin{aligned}
H_{33}(L_h) &= (h-1)(2+x) - \frac{(h-1)x^3(x+1)}{(x-1)(x^2+1)} + \frac{x^3(x^{4(h-1)}-1)}{(x-1)^2(x^2+1)^2} . \\
H_{22}(L_h) &= 2(1+2h+(h+2)x+(h+2)x^2+hx^3) + x^{4h-1} \\
&+ \frac{4x^3(x^2(x^{4(h-1)}-1)-(h-1)(x+1))}{(x-1)(x^2+1)} + \frac{4x^7(x^{4(h-1)}-1)}{(x-1)^2(x^2+1)^2} . \\
H_{23}(L_h) &= \frac{2x((x^2+2x+2)(x^{4(h-1)}-1)-2(h-2)(x+1))}{(x-1)(x^2+1)} + \frac{4x^5(x^{4(h-2)}-1)}{(x-1)^2(x^2+1)^2} .
\end{aligned}
$$

The base step $h = 2$ can be easily fulfilled. So suppose $h \geqslant 3$. Let $h = k + 1$. Then L_{k+1} can be obtained from L_k by attaching to it a new hexagon Y_{k+1} through an edge uv as in Fig. 1(b). Thus we have

$$\begin{aligned}
H_{33}(L_{k+1}) &= H_{33}(L_k) + H_{33}(u, V_3(L_k)) + H_{33}(v, V_3(L_k)) + (2 + x)\\
&= H_{33}(L_k) + (1 + x)H_{33}(u, V_3(L_k)) + (2 + x)\\
&= H_{33}(L_k) + (1 + x)\sum\nolimits_{j=0}^{k-2}(x^{3+4j} + x^{4+4j}) + (2 + x)\\
&= H_{33}(L_k) + \frac{x^3(x + 1)(x^{4(k-1)} - 1)}{(x - 1)(x^2 + 1)} + (2 + x)\,,\\
H_{22}(L_{k+1}) &= H_{22}(L_k) - H_{22}(u, V_2(L_k)) + H_{22}(V_2(Y_{k+1})\backslash\{v\}) + H_{22}(p, V_2(L_k) \setminus \{u\})\\
&+ H_{22}(q, V_2(L_k) \setminus \{u\}) + H_{22}(r, V_2(L_k) \setminus \{u\}) + H_{22}(s, V_2(L_k) \setminus \{u\})\\
&+ H_{22}(t, V_2(L_k) \setminus \{u\}) = H_{22}(L_k)\\
&+ (-1 + 2x^2 + 2x^3 + x^4)H_{22}(u, V_2(L_k) \setminus \{u\}) + H_{22}(V_2(Y_{k+1})\backslash\{v\}) - 1,\\
H_{23}(L_{k+1}) &= H_{23}(L_k) - H_{33}(u, V_3(L_k)) + H_{32}(u, V_2(L_k) \setminus \{u\}) + H_{32}(u, V_2(Y_{k+1}) \setminus \{v\})\\
&+ H_{32}(v, V_2(L_k) \setminus \{u\}) + H_{32}(v, V_2(Y_{k+1}) \setminus \{v\}) + H_{23}(p, V_3(L_k))\\
&+ H_{23}(q, V_3(L_k)) + H_{23}(r, V_3(L_k)) + H_{23}(s, V_3(L_k)) + H_{23}(t, V_3(L_k))\\
&= H_{23}(L_k) + (x + 1)H_{32}(u, V_2(L_k) \setminus \{u\}) + (x + 1)H_{32}(v, V_2(Y_{k+1}) \setminus \{v\})\\
&+ (-1 + 2x^2 + 2x^3 + x^4)H_{23}(u, V_3(L_k))\ .
\end{aligned}$$

To give more accurate expression of $H_{22}(L_{k+1})$ and $H_{23}(L_{k+1})$ draw a straight line l passing through all cut edges of L_{k+1}, as in Fig. 1(b). Denote by $V_m(L_{k+1}, l^+)$, $V_m(L_{k+1}, l)$ and $V_m(L_{k+1}, l^-)$ the sets of all vertices of degree m above l, on l and under l in L_{k+1}, respectively. Then we further have

$$\begin{aligned}
H_{22}(L_{k+1}) &= H_{22}(L_k) + (x + 1)(x^3 + x^2 + x - 1)(2H_{22}(u, V_2(L_k, l^+) \setminus \{u\})\\
&+ H_{22}(u, V_2(L_k, l) \setminus \{u\})) + H_{22}(V_2(Y_{k+1})\backslash\{v\}) - 1\\
&= H_{22}(L_k) + (x + 1)(x^3 + x^2 + x - 1)\left(2\sum_{j=1}^{k}(x^{4j-3} + x^{4j-2}) + x^{4k-1}\right)
\end{aligned}$$

$$
\begin{aligned}
&+ \quad (4+4x+4x^2+2x^3) \\
&= \quad H_{22}(L_k)+(x+1)(x^3+x^2+x-1)\left(\frac{2x(x^{4k}-1)}{(x-1)(x^2+1)}+x^{4k-1}\right) \\
&+ \quad (4+4x+4x^2+2x^3),
\end{aligned}
$$

$$
\begin{aligned}
H_{23}(L_{k+1}) &= H_{23}(L_k)+(x+1)(2H_{32}(u,V_2(L_k,l^+)\setminus\{u\})+H_{32}(u,V_2(L_k,l)\setminus\{u\})) \\
&+ (x+1)(2H_{32}(v,V_2(Y_{k+1},l^+)\setminus\{v\})+H_{32}(v,V_2(Y_{k+1},l)\setminus\{v\})) \\
&+ (-1+2x^2+2x^3+x^4)H_{33}(u,V_3(L_k)) \\
&= H_{23}(L_k)+(x+1)\left(2\sum_{j=0}^{k-1}(x^{1+4j}+x^{2+4j})+x^{3+4(k-1)}\right) \\
&+ (x+1)(2x+2x^2+x^3)+(-1+2x^2+2x^3+x^4)\sum_{j=2}^{k}\left(x^{3+4(j-2)}+x^{4(j-1)}\right) \\
&= H_{23}(L_k)+(x+1)\left(\frac{2x(x^{4k}-1)}{(x-1)(x^2+1)}+x^{3+4(k-1)}\right)+x(x+1)(x^2+2x+2) \\
&+ (-1+2x^2+2x^3+x^4)\,\frac{x^3(x^{4(k-1)}-1)}{(x-1)(x^2+1)}\ .
\end{aligned}
$$

By the inductive hypothesis and direct calculation, $H_{33}(L_h)$, $H_{22}(L_h)$ and $H_{23}(L_h)$ are fulfilled for $h=k+1$. Hence they are fulfilled for all h. Finally, combining them, we obtain the last assertion of $H(L_h)$. $\square$

Let w be the unique vertex of degree 3 on a terminal hexagon Y of a polyphenyl chain. Then a vertex x of degree 2 on Y is *ortho*, *meta* and *para* if $d_Y(x,w)=1,2$ and 3, respectively. If u is a vertex of a graph G and X is a subgraph of G, then we define $H(u|G):=\sum_{v\in V(G)}x^{d_G(u,v)}$ and $H(u,V(X)):=\sum_{y\in V(X)}x^{d_G(u,y)}$. Next we give two auxiliary lemmas to obtain the formula of $H(M_h)$.

Lemma 2.1. *Suppose that u and v are para and meta on the same terminal hexagon of L_h, respectively. Then we have*

$$
\begin{aligned}
H(u|L_h) &= (1+2x+2x^2+x^3)+\frac{x^4(x^2+x+1)(x^{4(h-1)}-1)}{(x-1)(x^2+1)}, \\
H(v|L_h) &= (1+2x+2x^2+x^3)+\frac{x^3(x^2+x+1)(x^{4(h-1)}-1)}{(x-1)(x^2+1)}\ .
\end{aligned}
$$

Proof. Drawing a straight auxiliary line l in L_h as in the proof of Theorem 2.2, we have

$$\begin{aligned} H(u|L_h) &= H(u|Y_1) + H(u, V(L_h, l^+)\backslash V(Y_1)) + H(u, V(L_h, l)\backslash V(Y_1)) \\ &+ H(u, V(L_h, l^-)\backslash V(Y_1)) \\ &= H(u|Y_1) + x(2H(v, V(L_h, l^+)\backslash V(Y_1)) + H(v, V(L_h, l)\backslash V(Y_1))) \\ &= (1 + 2x + 2x^2 + x^3) + x\left(2\sum_{i=1}^{h-1}(x^{4i} + x^{4i+1}) + \sum_{i=1}^{h-1}(x^{4i-1} + x^{4i+2})\right) \\ &= (1 + 2x + 2x^2 + x^3) + \frac{x^4(x^2 + x + 1)(x^{4(h-1)} - 1)}{(x-1)(x^2+1)} . \end{aligned}$$

Similarly, we can obtain $H(v|L_h) = (1 + 2x + 2x^2 + x^3) + \frac{x^3(x^2+x+1)(x^{4(h-1)}-1)}{(x-1)(x^2+1)}$. □

Lemma 2.2. *Suppose that u is meta on a terminal hexagon of M_h. Then we have $H(u|M_h) = \frac{(x+1)(x^{3h}-1)}{x-1}$.*

Proof. Draw a straight line l through the centers of all hexagons in M_h so that all vertices of degree 3 are above l. Then we have $H(u|M_h) = H(u, V(M_h, l^+)) + H(u, V(M_h, l^-)) = \sum_{i=0}^{3h-1} x^i + \sum_{i=1}^{3h} x^i = \frac{(x+1)(x^{3h}-1)}{x-1}$. □

Theorem 2.3. *If $h \geqslant 2$ then we have*

$$\begin{aligned} H(M_h) &= 6h + 3(h+1)x + 2(h+2)x^2 + 2hx^3 + x^{4h-1} \\ &- \frac{x(x+1)[(h-2)(x^5 + x^4 + x^3 + 4) + 5(h-1)x^2]}{(x-1)(x^2+1)} \\ &+ 2x\frac{(2x^4 + x^2 + 2x + 2)(x^{4(h-1)} - 1)}{(x-1)(x^2+1)} \\ &+ \frac{x^2(x+1)(x^5(x^{3(h-2)} - 1) - x^{3h}(x^2 + x + 1)(x^{h-2} - 1))}{(x-1)^2(x^2+1)} \\ &+ \frac{x^3((4x^4+1)(x^{4(h-1)} - 1) + x^2(x^5 + x^4 + x^3 + 4)(x^{4(h-2)} - 1))}{(x-1)^2(x^2+1)^2} . \end{aligned}$$

Proof. Let Y_i be the i-th hexagon of L_h, and suppose that Y_i and Y_{i+1} are connected by w_iu_i and that v_i is a vertex of Y_{i+1} that is adjacent to u_i $(1 \leqslant i \leqslant h-1)$, as in Fig. 2.

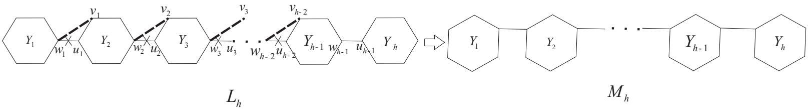

Fig. 2

Let G_k be the chain obtained from L_h by deleting the cut edges $w_1u_1, \ldots, w_ku_k$ and then adding cut edges $w_1v_1, \ldots, w_kv_k$ $(k = 1, \ldots, h-2)$. Then $G_{h-2} = M_h$. Set $G_0 = L_h$. Then by Lemmas 2.1 and 2.2, we have

$$\begin{aligned} H(G_{k+1}) - H(G_k) &= H(w_{k+1}|M_{k+1})(H(v_{k+1}|L_{h-k-1}) - H(u_{k+1}|L_{h-k-1})) \\ &= -\frac{(x+1)(x^{3(k+1)}-1)}{x-1} \cdot \frac{x^4(x^2+x+1)(x^{4(h-k-2)}-1)}{x^2+1} \\ &= -\frac{x^4(x+1)(x^2+x+1)(x^{4h-k-5} - x^{4(h-k-2)} - x^{3(k+1)} + 1)}{(x-1)(x^2+1)} . \end{aligned}$$

Since $H(M_h) - H(L_h) = \sum\limits_{k=0}^{h-3}(H(G_{k+1}) - H(G_k))$, substituting $H(L_h)$ into it, we can obtain the assertion. □

Lemma 2.3. *Suppose that u is ortho on a terminal hexagon of O_h. Then we have* $H(u|O_h) = \frac{(x^{2h-1}-1)+x(x+1)(x^{2h}-1)}{x-1}$.

Proof. Drawing auxiliary vertical lines $l_1, l_2, \ldots, l_h$ as in the proof of Theorem 2.1, we have

$$\begin{aligned} H(u|O_h) &= H(u, \cup_{i=1}^{h} V_2(Y_i, l_i(l)) \backslash \{u, w\}) + H(u, \cup_{i=1}^{h} V_2(Y_i, l_i(r)) \backslash \{u, w\}) \\ &+ H(u, V_3(O_h)) + x^{d(u,w)} = \sum_{i=1}^{h}(x^{2i-1} + x^{2i}) + \sum_{i=1}^{h}(x^{2i} + x^{2i+1}) \\ &+ \sum_{i=0}^{2h-2} x^i + x^{d(u,w)} = \frac{(x^{2h-1}-1) + x(x+1)(x^{2h}-1)}{x-1} . \end{aligned}$$

□

An *ortho-segment* of a polyphenyl chain is a subgraph that is an ortho-polyphenyl chain and is maximal with respect to this property. The meta-segment and para-segment can be analogously defined. A segment is a *terminal segment* if it contains a terminal hexagon, and *internal segment* otherwise. Suppose that $S_1, S_2, \ldots, S_n$ are all segments of a polyphenyl chain G and that S_i and S_{i+1} are connected by the edge u_iv_i $(1 \leqslant i \leqslant n-1)$ (See Fig. 3).

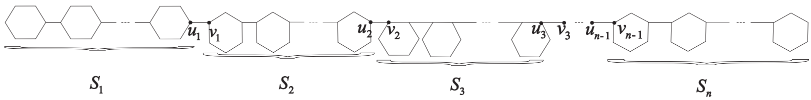

Fig. 3 A polyphenyls chain $G(S_1, S_2, \cdots, S_n)$ and the edges u_iv_i for $i = 1, 2, \cdots, n-1$.

Then we use $G(S_1, S_2, \ldots, S_n)$ instead of G to denote such a polyphenyl chain. If $G(S_i, \ldots, S_n)$ is a partial chain of G, then we let $\widehat{i} = 0$, and for $i+1 \leqslant j \leqslant n$, set

$$\widehat{j} := \begin{cases} 1, & \text{if } S_j \text{ is an ortho-segment;} \\ 2, & \text{if } S_j \text{ is a meta-segment;} \\ 3, & \text{if } S_j \text{ is a para-segment.} \end{cases}$$

Theorem 2.4. *Let $G = G(S_1, S_2, \cdots, S_n)$ be a polyphenyls chain of length h. Then we have*

$$H(G) = \sum_{i=1}^{n} H(S_i) + x\sum_{i=1}^{n-1} f(l_i)f(l_{i+1}) + \sum_{m=1}^{n-2} f(l_m) \sum_{k=m+1}^{n-1} x^{\sum_{j=m+1}^{k}(\widehat{j}+1)l_j+1} f(l_{k+1}),$$

where l_i is the length of the segment S_i $(1 \leqslant i \leqslant n)$, and

$$f(l_i) := \begin{cases} \frac{(x^{2l_i-1}-1)+x(x+1)(x^{2l_i}-1)}{x-1}, & \textit{if } S_i \textit{ is an ortho-segment;} \\ \frac{(x+1)(x^{3l_i}-1)}{x-1}, & \textit{if } S_i \textit{ is a meta-segment;} \\ (1+2x+2x^2+x^3) + \frac{x^4(x^2+x+1)(x^{4(l_i-1)}-1)}{(x-1)(x^2+1)}, & \textit{if } S_i \textit{ is a para-segment.} \end{cases}$$

Proof. Draw a straight line passing through all cut edges of G. Then we can observe that all shortest paths between a vertex in the segment S_i and a vertex in S_j $(j > i)$ pass through the vertices lying on the straight line and above the straight line. Thus we have

$$\begin{aligned} H(G) &= \sum_{i=1}^{n} H(S_i) + \sum_{i=1}^{n-1} xH(u_i|S_i)H(v_i|G(S_{i+1}, \cdots, S_n)) \\ &= \sum_{i=1}^{n} H(S_i) + xH(u_1|S_1)\sum_{i=2}^{n} H(v_1|S_i) + xH(u_2|S_2)\sum_{i=3}^{n} H(v_2|S_i) \\ &+ \cdots + xH(u_{n-2}|S_{n-2}) \sum_{i=n-1}^{n} H(v_{n-2}|S_i) + xH(u_{n-1}|S_{n-1})H(v_{n-1}|S_n) \ . \end{aligned}$$

By the definitions of $\widehat{i}$ and $\widehat{j}$ $(i+1 \leqslant j \leqslant n)$ in the partial chain $G(S_i, \ldots, S_n)$ of $G(S_1, S_2, \ldots, S_n)$, we further have

$$\begin{aligned} H(G) &= \sum_{i=1}^{n} H(S_i) + xH(u_1|S_1)(H(v_1|S_2) + \sum_{k=2}^{n-1} x^{\sum_{j=2}^{k}(\widehat{j}+1)l_j} H(v_k|S_{k+1})) \\ &+ xH(u_2|S_2)(H(v_2|S_3) + \sum_{k=3}^{n-1} x^{\sum_{j=3}^{k}(\widehat{j}+1)l_j} H(v_k|S_{k+1})) \\ &+ \cdots + xH(u_{n-2}|S_{n-2})\left(H(v_{n-2}|S_{n-1}) + x^{(\widehat{n-1}+1)l_{n-1}} H(v_{n-1}|S_n)\right) \\ &+ xH(u_{n-1}|S_{n-1})H(v_{n-1}|S_n) \ . \end{aligned}$$

Note that both v_i and u_{i+1} are ortho, meta and para on the terminal hexagons of S_{i+1} if S_{i+1} is an ortho-segment, meta-segment and para-segment, respectively $(1 \leqslant i \leqslant n-2)$, and that u_1 and v_{n-1} have similar properties on two terminal segments S_1 and S_n, respectively. Therefore, combining lemmas 2.1, 2.2 and 2.3 with the definition of $f(l_i)$, we obtain

$$\begin{aligned} H(G) &= \sum_{i=1}^{n} H(S_i) + xf(l_1)(f(l_2) + \sum_{k=2}^{n-1} x^{\sum_{j=2}^{k}(\widehat{j}+1)l_j} f(l_{k+1})) \\ &+ xf(l_2)(f(l_3) + \sum_{k=3}^{n-1} x^{\sum_{j=3}^{k}(\widehat{j}+1)l_j} f(l_{k+1})) \\ &+ \cdots + xf(l_{n-2})\left(f(l_{n-1}) + x^{(\widehat{n-1}+1)l_{n-1}} f(l_n)\right) + xf(l_{n-1})f(l_n) \\ &= \sum_{i=1}^{n} H(S_i) + x\sum_{i=1}^{n-1} f(l_i)f(l_{i+1}) + \sum_{m=1}^{n-2} f(l_m) \sum_{k=m+1}^{n-1} x^{\sum_{j=m+1}^{k}(\widehat{j}+1)l_j+1} f(l_{k+1}) \ . \quad \Box \end{aligned}$$

References

[1] H. Hosoya, On some counting polynomials in chemistry, *Discr. Appl. Math.* **19** (1988) 239–257.

[2] E. Estrada, O. Ivanciuc, I. Gutman, A. Gutierrez, L. Rodriguez, Extended Wiener indices. A new set of descriptors forquantitative structureproperty studies, *New J. Chem.* **22** (1998) 819–822.

[3] I. Gutman, S. Klavžar, M. Petkovšek, P. Žigert, On Hosoya polynomials of benzenoid graphs, *MATCH Commun. Math. Comput. Chem.* **43** (2001) 49–66.

[4] S. Xu, H. Zhang, The Hosoya polynomials decomposition for catacondensed benzenoid graph, *Discr. Appl. Math.* **156** (2008) 2930–2938.

[5] S. Xu, H. Zhang, The Hosoya polynomials decomposition for hexagonal chains, *Math. Comput. Model.* **48** (2008) 601–609.

[6] S. Xu, H. Zhang, Hosoya polynomials of armchair open-ended nanotubes, *J. Quant. Chem.* **107** (2007) 586–596.

[7] S. Xu, H. Zhang, Hosoya polynomials of TUC_4C_8(S) nanotubes, *J. Math. Chem.* **45** (2009) 488–502.

[8] E. Mehdi ,T. Bijan, Hosoya polynomial of zigzag polyhex nanotorus, *J. Serb. Chem. Soc.* **73** (2008) 311–319.

[9] A. A. Dobrynin, I. Gutman, The average Wiener index of trees and chemical trees, *J. Chem. Inf. Comput. Sci.* **39** (1999) 679–683.

[10] C. A. Draxl, J. A. Majewski, P. Vogl, G. Leising, First-principles studies of the structural and optical properties of crystalline poly (para-polyphenylene), *Phys. Rev. B.* **51** (1995) 9668–9676.

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

[12] L. Marynowski, F. Czechowski, B. R. T. Simoneit, Phenylnaphthalenes and polyphenyls in Palaeozoic source rocks of the Holy Cross Mountains, Poland, *Org. Geochem.* **32** (2001) 69–85.

[13] 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.

[14] 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.