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Hosoya Polynomials of General Spiro Hexagonal Chains

Xianyong Li[a], Xiaofan Yang[a], Guoping Wang[b], Rongwei Hu[c]

[a] *College of Computer Science, Chongqing University, Chongqing 400044, P.R.China*
[b] *School of Mathematical Sciences, Xinjiang Normal University, Urumqi 830054, Xinjiang, P.R.China*
[c] *College of Mathematics and Systems Science, Xinjiang University, Urumqi 830046, Xinjiang, P.R.China*

Abstract. Spiro hexagonal chains are a subclass of spiro compounds which are an important subclass of Cycloalkynes in Organic Chemistry. This paper addresses general spiro hexagonal chains in which every hexagon represents a benzene ring, and establishes the formulae for computing the Hosoya polynomials of general spiro hexagonal chains.

1. Introduction

For a graph $G = (V, E)$, let $d_G(u, v)$ be the distance between vertices u and v in G. Then *Hosoya polynomial* (or Wiener polynomial) of G, which is introduced by Haruo Hosoya [6] in 1988, is defined as $H(G)= \sum_{\{u,v\}\subseteq V(G)} x^{d_G(u,v)}$. Its chemical applications and elementary properties are studied in [4, 9]. 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 [10], namely $W(G) = \frac{dH(G)}{dx}|_{x=1}$. Hosoya polynomial contains more information about distance in a graph than any of the hitherto proposed distance-based topological indices; cf. [5]. Abundant literatures appeared on this topic for the theoretical considerations and computations. The Hosoya polynomials of (catacondensed) benzenoid graphs, hexagonal chains, polyphenyl chains, polygonal chains and two-dimensional (2D) hexagonal patterns were determined in [5, 8, 12, 13, 15]. Also, the explicit analytical expressions for Hosoya polynomials of some kinds of nanotubes, such as zigzag polyhex, armchair open-ended and TUC_4C_8(S) nanotubes, were derived in [7, 11, 14].

In Organic Chemistry, spiro hexagonal chains are an significant subclass of spiro compounds. A *spiro hexagonal chain* is a kind of graph consisting of n hexagons $B_1, B_2, ..., B_n$ with the properties that (i) for any $1 \le i < j \le n$, B_i and B_j are linked by a spiro union (two hexagons have only one common vertex, this linkage is called *spiro union*, the common vertex is designated as *spiro vertex*) if and only if $j = i + 1$, and (ii) the spiro vertex should be the vertex with degree four in the spiro hexagonal chain (or six-membered ring spiro chain [1, 16], or chain hexagonal cactus [3]).

Recently, for spiro hexagonal chains, the Wiener index, numbers of the matching and independence sets, extremal Merrifield-Simmons and Hosoya indices and extremal energies were determined in [1–3, 16].

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Email addresses: xian-yong@163.com (Xianyong Li), xfyang1964@gmail.com (Xiaofan Yang)

Motivated by prior investigations, in this paper we compute the formulae for Hosoya polynomials of spiro ortho-, meta- and para-hexagonal chains (to be defined more precisely later) respectively, and then we establish the formulae for computing the Hosoya polynomials of general spiro hexagonal chains.

2. Main results

The number of hexagons in a spiro hexagonal chain is called its *length*. Denote by $\mathcal{G}(n)$ the set of all spiro hexagonal chain of length n. Let $G_n = B_1B_2\cdots B_n \in \mathcal{G}(n)$ where B_k is the k-th hexagon of G_n, and let c_k be the spiro vertex of B_k and B_{k+1}, $k = 1, 2, \cdots, n-1$. Then the sequence $(c_1, c_2, \cdots, c_{n-1})$ of length $n-1$ is called the *spiro vertex sequence* of G_n. G_n is called *spiro ortho-, meta-* and *para-hexagonal chain* if $d(c_i, c_{i+1}) = 1, 2$ and 3, respectively, for all $i = 1, 2, \cdots, n-1$. In what follows, we will denote by O_n, M_n and P_n the spiro ortho-, meta- and para-hexagonal chain of length n (see Fig. 1), respectively.

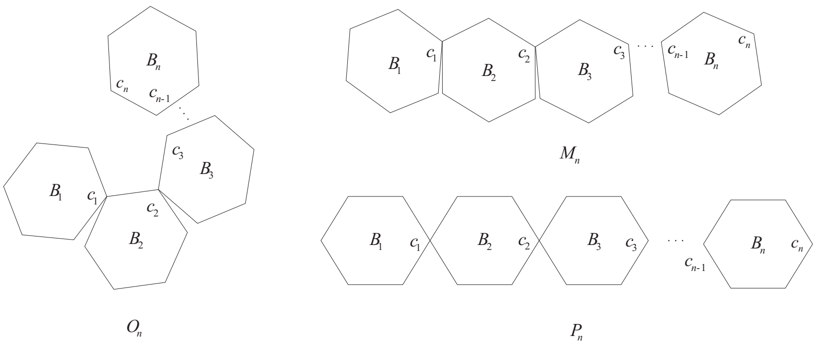

Fig. 1

Note that $H(O_1) = H(M_1) = H(P_1) = 6 + 6x + 6x^2 + 3x^3$. In the following we give the formulae for calculating the Hosoya polynomials of O_n, M_n and P_n ($n \geqslant 2$).

Theorem 2.1. *If $n \geqslant 2$ then*

$$H(O_n) = 6 + 6x + 6x^2 + 3x^3 + \frac{(n-1)(2x + 2x^2 + x^3)(3 - x + 2x^2 + x^3)}{1-x} - \frac{(2 + 2x + x^2)^2(1 - x^{n-1})x^3}{(1-x)^2},$$

$$H(M_n) = 6 + 6x + 6x^2 + 3x^3 + \frac{(n-1)(2x + 2x^2 + x^3)(3 + 2x - x^2 + x^3)}{1-x^2} - \frac{(2 + 2x + x^2)^2(1 - x^{2(n-1)})x^4}{(1-x^2)^2},$$

$$H(P_n) = 6 + 6x + 6x^2 + 3x^3 + \frac{(n-1)(2x + 2x^2 + x^3)(3 + 2x + 2x^2 - 2x^3)}{1-x^3} - \frac{(2 + 2x + x^2)^2(1 - x^{3(n-1)})x^5}{(1-x^3)^2}.$$

In order to prove the results of Theorem 2.1, we define a number of some useful terminologies and convenient notations. A vertex v of B_k in G_n is called ortho-, meta- *and* para-vertex *of B_k if the distance between v and c_{k-1} is 1, 2 and 3, denoted by o_{k-1}, m_{k-1} and p_{k-1}, respectively. Specially, we denote the ortho-vertex o_{n-1} of B_n in O_n by c_n (see Fig. 1). Analogously, we also denote the meta-vertex m_{n-1} and para-vertex p_{n-1} of B_n in M_n and P_n by c_n (see Fig. 1) respectively.*

If u be a vertex of G_n, then we set $H(G_n, u) := \sum_{v \in V(G_n)} x^{d_{G_n}(u,v)}$. Next we give the following important lemma.

Lemma 2.2. *If $n \geqslant 1$ then*

$$H(O_n, c_n) = \frac{(1 + x + 2x^2 + x^3) - (2 + 2x + x^2)x^{n+1}}{1-x},$$

$$H(M_n, c_n) = \frac{(1 + 2x + x^2 + x^3) - (2 + 2x + x^2)x^{2n+1}}{1-x^2},$$

$$H(P_n, c_n) = \frac{(1 + 2x + 2x^2) - (2 + 2x + x^2)x^{3n+1}}{1-x^3}.$$

Proof. If $n = 1$, the assertions are clearly.

If $n \geqslant 2$, by inspection of the graph O_n, we have

$$H(O_n, c_n) = H(O_n, o_{n-1}) = \sum_{v \in V(O_{n-1})} x^{d(v,o_{n-1})} + \sum_{v \in V(B_n \setminus o_{n-1})} x^{d(v,o_{n-1})}$$
$$= xH(O_{n-1}, c_{n-1}) + (1 + x + 2x^2 + x^3).$$

Analogously, we easily obtain

$$H(M_n, c_n) = x^2 H(M_{n-1}, c_{n-1}) + (1 + 2x + x^2 + x^3),$$
$$H(P_n, c_n) = x^3 H(P_{n-1}, c_{n-1}) + (1 + 2x + 2x^2).$$

Using the above recurrence, we have

$$H(O_n, c_n) = x^{n-1} H(O_1, c_1) + (1 + x + \cdots + x^{n-2})(1 + x + 2x^2 + x^3),$$
$$H(M_n, c_n) = x^{2(n-1)} H(M_1, c_1) + (1 + x^2 + x^4 + x^6 + \cdots + x^{2(n-2)})(1 + 2x + x^2 + x^3),$$
$$H(P_n, c_n) = x^{3(n-1)} H(P_1, c_1) + (1 + x^3 + x^6 + \cdots + x^{3(n-2)})(1 + 2x + 2x^2).$$

Note that $H(O_1, c_1) = H(M_1, c_1) = H(P_1, c_1) = 1 + 2x + 2x^2 + x^3$. Thus, substituting these identities in above identities, we obtain the assertions. □

Proof of Theorem 2.1. By inspection of the graph O_n, we have

$$H(O_n) = H(O_{n-1}) + \sum_{u \in V(O_{n-1}), v \in V(B_n) \setminus c_{n-1}} x^{d(u,v)} + \sum_{\{u,v\} \subseteq V(B_n) \setminus c_{n-1}} x^{d(u,v)}$$
$$= H(O_{n-1}) + \sum_{u \in V(O_{n-1})} (2x^{d(u,c_{n-1})+1} + 2x^{d(u,c_{n-1})+2} + x^{d(u,c_{n-1})+3}) + \sum_{\{u,v\} \subseteq V(B_n) \setminus c_{n-1}} x^{d(u,v)}$$
$$= H(O_{n-1}) + H(O_{n-1}, c_{n-1})(2x + 2x^2 + x^3) + (4x + 4x^2 + 2x^3).$$

Using the recurrence, we have

$$H(O_n) = H(O_1) + \sum_{k=2}^{n} H(O_{k-1}, c_{k-1})(2x + 2x^2 + x^3) + (n-1)(4x + 4x^2 + 2x^3).$$

By Lemma 2.2, we obtain $H(O_{k-1}, c_{k-1}) = \frac{(1+x+2x^2+x^3)-(2+2x+x^2)x^k}{1-x}$. Substituting the identity in above identity and doing some manipulations, we obtain the assertion of $H(O_n)$. Analogously, we can obtain the assertions of $H(M_n)$ and $H(P_n)$. □

In order to describe general spiro hexagonal chains we give some additional terminologies and notations. An *spiro ortho-segment* of a spiro hexagonal chain is a subgraph that is a spiro ortho-hexagonal chain and is maximal with respect to this property. The spiro meta-segment and spiro para-segment can be analogously defined respectively. A segment is a *terminal segment* if it contains a terminal hexagon, and *internal segment* otherwise. Suppose that $S_1, S_2, \ldots, S_m$ are all segments of a spiro hexagonal chain $G_n = B_1 B_2 \cdots B_n$ and that S_i and S_{i+1} is connected by spiro vertex c'_i $(1 \leqslant i \leqslant m-1)$. Clearly, $c'_i \in \{c_1, c_2, \ldots, c_{n-1}\}$. Then we use $S_1 S_2 \cdots S_m$ instead of G_n to denote such a spiro hexagonal chain (see Fig. 2).

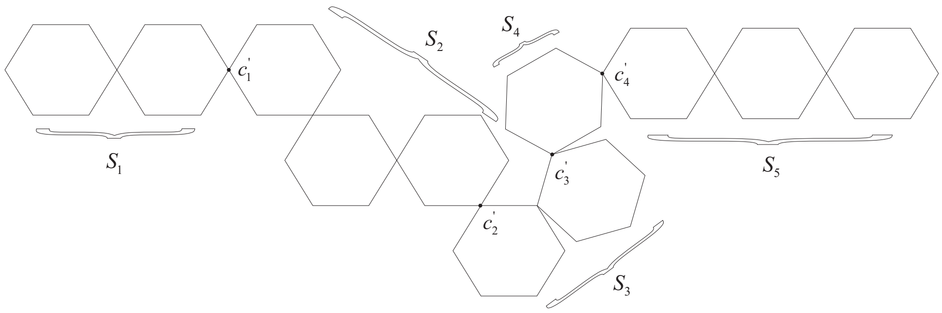

Fig. 2 A spiro hexagonal chain $G_{11} = S_1S_2S_3S_4S_5$ consisting of the set of segments S_1, S_2, S_3, S_4, S_5 with lengths 2, 3, 2, 1, 3 respectively and the spiro vertex c_i' $(1 \leqslant i \leqslant 4)$.

If $S_1 \cdots S_i$ is a partial chain of G_n, then we let $\widehat{1} = \widehat{i+1} = 0$, and for $2 \leqslant j \leqslant i$ set

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

Theorem 2.3. *Let $G_n = S_1S_2 \cdots S_m$ be a spiro hexagonal chain of length n. Then we have*

$$H(G_n) = \sum_{r=3}^{m} \sum_{k=2}^{r-1} x^{\sum_{i=k}^{r-1} \widehat{i} l_i} g(l_{k-1}) g(l_r) + g(l_1)g(l_2) + \sum_{r=1}^{m} H(S_r) - \sum_{r=2}^{m} g(l_r),$$

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

$$g(l_i) := \begin{cases} \dfrac{(1 + x + 2x^2 + x^3) - (2 + 2x + x^2)x^{l_i+1}}{1 - x}, & \text{if } S_i \text{ is a spiro ortho-segment;} \\ \dfrac{(1 + 2x + x^2 + x^3) - (2 + 2x + x^2)x^{2l_i+1}}{1 - x^2}, & \text{if } S_i \text{ is a spiro meta-segment;} \\ \dfrac{(1 + 2x + 2x^2) - (2 + 2x + x^2)x^{3l_i+1}}{1 - x^3}, & \text{if } S_i \text{ is a spiro para-segment.} \end{cases}$$

Proof. By inspection of the graph $G_n = S_1S_2 \cdots S_m$, we have

$$H(G_n) = H(S_1S_2 \cdots S_{m-1}) + H(S_1S_2 \cdots S_{m-1}, c'_{m-1})H(S_m, c'_{m-1}) + (H(S_m) - H(S_m, c'_{m-1})).$$

Using the definition of $\widehat{1} = \widehat{i+1} = 0$ and $\widehat{j}$ $(2 \leqslant j \leqslant i)$ in the partial chain $S_1 \cdots S_i$ of $G_n = S_1S_2 \cdots S_n$, we further have

$$\begin{aligned} H(G_n) &= H(S_1S_2 \cdots S_{m-1}) + (x^{\widehat{2}l_2 + \widehat{3}l_3 + \cdots + \widehat{m-1}l_{m-1}} H(S_1, c_1') + x^{\widehat{3}l_3 + \widehat{4}l_4 + \cdots + \widehat{m-1}l_{m-1}} H(S_2, c_2') \\ &\quad + \cdots + x^{\widehat{m-1}l_{m-1}} H(S_{m-2}, c'_{m-2}))H(S_m, c'_{m-1}) + (H(S_m) - H(S_m, c'_{m-1})) \\ &= H(S_1S_2 \cdots S_{m-1}) + \sum_{k=2}^{m-1} x^{\sum_{i=k}^{m-1} \widehat{i} l_i} H(S_{k-1}, c'_{k-1})H(S_m, c'_{m-1}) + (H(S_m) - H(S_m, c'_{m-1})). \end{aligned}$$

Note that c'_{k-1} is an ortho-, meta- and para-vertex on the terminal hexagon of S_{k-1} if S_{k-1} is a spiro ortho-, meta- and para-segment respectively $(2 \leqslant k \leqslant m-1)$, and that c'_{m-1} has similar properties on the terminal hexagon of S_m. Therefore, combining the results of Lemma 2.2 with the definition of $g(l_i)$, we obtain

$$H(G_n) = H(S_1S_2 \cdots S_{m-1}) + \sum_{k=2}^{m-1} x^{\sum_{i=k}^{m-1} \widehat{i} l_i} g(l_{k-1})g(l_m) + (H(S_m) - g(l_m)).$$

Using the recurrence, we have

$$H(G_n) = H(S_1S_2) + \sum_{r=3}^{m}\sum_{k=2}^{r-1} x^{\sum_{i=k}^{r-1} \widehat{il_i}} g(l_{k-1})g(l_r) + \sum_{r=3}^{m}(H(S_r) - g(l_r)).$$

Then we derive the assertion from $H(S_1S_2) = H(S_1) + g(l_1)g(l_2) + (H(S_2) - g(l_2))$. □

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