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Generalized Hosoya polynomials of hexagonal chains

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Similar to the well-known Wiener index, Eu et al. [Int. J. Quantum Chem. 106 (2006) 423–435] introduced three families of topological indices including Schultz index and modified Schultz index, called generalized Wiener indices, and gave the similar formulae of generalized Wiener indices of hexagonal chains. They also mentioned three families of graph polynomials in x, called generalized Hosoya polynomials in contrast to the (standard) Hosoya polynomial, such that their first derivatives at $x = 1$ are equal to generalized Wiener indices. In this note we gave explicit analytical expressions for generalized Hosoya polynomials of hexagonal chains.

KEY WORDS: Hosoya polynomial, Wiener index, generalized Hosoya polynomial, Schultz index, modified Schultz index, hexagonal chain

1. Introduction

In 1988 Hosoya [8] introduced a distance-based polynomial associated with a connected graph G, denoted by $H(G, x)$. If we denote by $d_G(u, v)$ the distance between vertices u and v in G (subscript G is omitted when the graph is understood from the context), it is then defined as

$$H(G) \equiv H(G, x) := \sum_{\{u,v\} \subseteq V(G)} x^{d_G(u,v)}$$

nowadays called the "*Hosoya polynomial*." Directly from its definition, $H(G)$ has a main property that its first derivative at $x = 1$ is equal to a well-known *Wiener index* $W(G)$ of G ([9], the sum of distances of all vertex pairs of G). About the topic on the Hosoya polynomial we refer the reader to the papers [2, 11] for chemical applications, to the papers [4, 6, 14] for theoretical consideration and to the papers [1, 7, 13, 15, 16, 18] for computations.

Bearing in mind two topological indices for a graph G: *Schultz index* [12], denoted by $W_+(G)$ and *modified Schultz index* [10], denoted by $W_*(G)$, Gutman

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[5] constructed two graph polynomials having the property that their first derivatives at $x = 1$ are equal to the two indices, respectively. If we denote $\deg_G(v)$ for degree of vertex v in G (i.e., the number of its first neighbors), then these polynomials are

$$H_+(G) \equiv H_+(G, x) := \sum_{\{u,v\} \subseteq V(G)} (\deg_G(u) + \deg_G(v)) x^{d_G(u,v)}$$

and

$$H_*(G) \equiv H_*(G, x) := \sum_{\{u,v\} \subseteq V(G)} (\deg_G(u) \cdot \deg_G(v)) x^{d_G(u,v)}.$$

In particular in case of trees, Gutman [5] proved that $H_+(G)$ and $H_*(G)$ are related with $H(G)$.

As generalizations of Schultz and modified Schultz indices, recently Eu et al. [3] introduced families of *generalized Wiener indices* of a connected graph G for a real number a as follows:

$$W_{\ddagger}^{(a)}(G) := \sum_{\{u,v\} \subseteq V(G)} ((\deg_G(u))^a + (\deg_G(v))^a) d_G(u, v),$$

$$W_{+}^{(a)}(G) := \sum_{\{u,v\} \subseteq V(G)} (\deg_G(u) + \deg_G(v))^a d_G(u, v)$$

and

$$W_{*}^{(a)}(G) := \sum_{\{u,v\} \subseteq V(G)} (\deg_G(u))^a (\deg_G(v))^a d_G(u, v).$$

In case of hexagonal chains (unbranched catacondensed benzenoid systems), in that paper they gave not only linear relations between $W(G)$ and $W_+(G)$ and $W_*(G)$ respectively, but also the similar formulae for all generalized Wiener indices of G. Similar to the polynomials constructed by Gutman in [5], Eu et al. also mentioned some polynomials (termed *generalized Wiener polynomials* there, we call them *generalized Hosoya polynomials*, in contrast to the Hosoya polynomial) with the property that their first derivatives at $x = 1$ are exactly equal to corresponding generalized Wiener indices.

Our main aim of this paper is to give the explicit analytical expressions for all generalized Hosoya polynomials of hexagonal chains. The rest of the paper is organized as follows. In section 2 generalized Hosoya polynomials of a graph and the representations of hexagonal chains are introduced. In section 3 we deduce the analytical expressions of partial Hosoya polynomials of hexagonal chains. In section 4 we gave our main results (i.e., Theorem 4.3.) by means of the Divide-and-Conquer approach.

2. The generalized Hosoya polynomials and the representations of hexagonal chains

Definition 2.1. ([3]). For a connected graph G and a real number a, define families of generalized Hosoya polynomials of G as

$$H_{\ddagger}^{(a)}(G) \equiv H_{\ddagger}^{(a)}(G,x) := \sum_{\{u,v\}\subseteq V(G)} ((\deg_G(u))^a + (\deg_G(v))^a)x^{d_G(u,v)},$$

$$H_{+}^{(a)}(G) \equiv H_{+}^{(a)}(G,x) := \sum_{\{u,v\}\subseteq V(G)} (\deg_G(u) + \deg_G(v))^a x^{d_G(u,v)}$$

and

$$H_{*}^{(a)}(G) \equiv H_{*}^{(a)}(G,x) := \sum_{\{u,v\}\subseteq V(G)} (\deg_G(u))^a \cdot (\deg_G(v))^a x^{d_G(u,v)}.$$

Evidently, $W_{\ddagger}^{(a)}(G) = \frac{dH_{\ddagger}^{(a)}(G)}{dx}\Big|_{x=1}$, $W_{+}^{(a)}(G) = \frac{dH_{+}^{(a)}(G)}{dx}\Big|_{x=1}$, and $W_{*}^{(a)}(G) = \frac{dH_{*}^{(a)}(G)}{dx}\Big|_{x=1}$. For $a = 1$, the polynomials $H_{\ddagger}^{(a)}(G)$, $H_{+}^{(a)}(G)$ and $H_{*}^{(a)}(G)$ reduce to $H_{+}(G)$, $H_{+}(G)$ and $H_{*}(G)$, respectively.

A *hexagonal chain* is a connected plane graph without cut-vertices in which all inner faces are hexagons (and all hexagons are faces), such that two hexagons are either disjoint or have exactly one common edge (and are then said to be *adjacent*), no three hexagons share a common vertex and each hexagon is adjacent to two other hexagons, with the exception of exactly two terminal hexagons to which a single hexagon is adjacent. Among hexagonal chains with n hexagons, there is an extremal class, to be called the *linear hexagonal chain* and denoted by L_n, which is isomorphic to the linear polyacene (i.e., with no '*kink*'). A maximal linear hexagonal chain in a hexagonal chain is called a *segment*. A segment including a terminal hexagon is a *terminal segment*. The number of hexagons in a segment S is called its *length*, denoted by $l(S)$ (see figure 1).

Consider a nonterminal segment S and its two neighboring segments S_1 and S_2 embedded in the regular hexagonal lattice in the plane and draw a line through the centers of the hexagons of S (see figure 2). If S_1 and S_2 lie on the same side of the line, then S is called a *non-zigzag segment* (see figure 2(a)), otherwise, a *zigzag segment* (see figure 2(b)). We assume, for convenience, zigzag segments also include two terminal segments.

Let n be some positive integer. If a hexagonal chain H has n segments in turn denoted by $S_1, S_2, \ldots, S_n$, say $l(S_1) =: l_1$ and $l(S_i) =: l_i + 1$ for $2 \leqslant i \leqslant n$, then we say H consists of the set of segments $S_1, S_2, \ldots, S_n$ and use $Hl(l_1, l_2, \ldots, l_n)$ to denote such a chain (see figure 1). We also denote by $Hl(l_1, l_2, \ldots, l_i)$ the auxiliary hexagonal chain of $Hl(l_1, l_2, \ldots, l_n)$ consisting of the set of segments $S_1, S_2, \ldots, S_i$ for some i ($1 \leqslant i \leqslant n$). Obviously, $Hl(l_1, l_2, \ldots,$

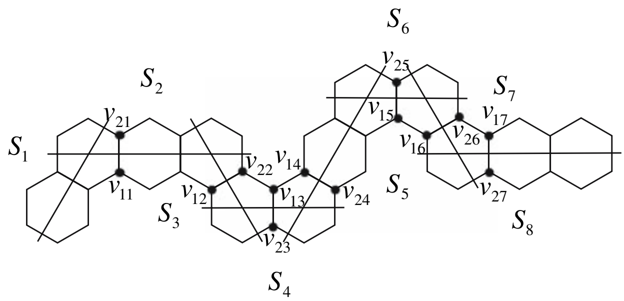

Figure 1. A hexagonal chain $Hl(2, 2, 1, 1, 2, 1, 1, 2)$ consisting of the set of segments $S_1, S_2, \cdots, S_8$ with length 2, 3, 2, 2, 3, 2, 2, 3, respectively and the edges $v_{1i}v_{2i}$ for $1 \leqslant i \leqslant 7$.

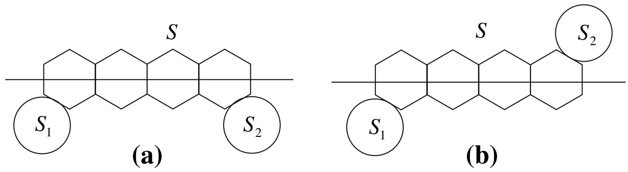

Figure 2. (a) A non-zigzag segment S and (b) a zigzag segment S.

$l_i, l_{i+1})$ can be obtained by identifying an edge, say $v_{1i}v_{2i}$ and v_{1i} adjacent to two degree-3 vertices belonging to the segment S_i, of $Hl(l_1, l_2, \ldots, l_i)$ and $L_{l_{i+1}}$ (see figure 1). Since two neighboring segments have always one hexagon in common, the number of hexagons of $Hl(l_1, l_2, \ldots, l_n)$ is exactly equal to $l_1 + l_2 + \cdots + l_n$.

Definition 2.2. For a vertex $u \in V(G)$ and subsets of vertices $U, V \subseteq V(G)$, we have the following partial Hosoya polynomials:

$$H(U, V; G) := \sum_{u \in U, v \in V} x^{d_G(u,v)}; \quad H(u, U; G) := \sum_{v \in U} x^{d_G(u,v)};$$
$$H(U; G) := \sum_{\{u,v\} \subseteq U} x^{d_G(u,v)}; \quad H(u; G) := \sum_{v \in V(G)} x^{d_G(u,v)}.$$

3. Partial Hosoya polynomials

First, we define two notations. For $1 \leqslant i \leqslant n$, let

$$\widehat{i} := \begin{cases} 0, & \text{if } S_i \text{ is a zigzag segment;} \\ 1, & \text{otherwise.} \end{cases} \tag{1}$$

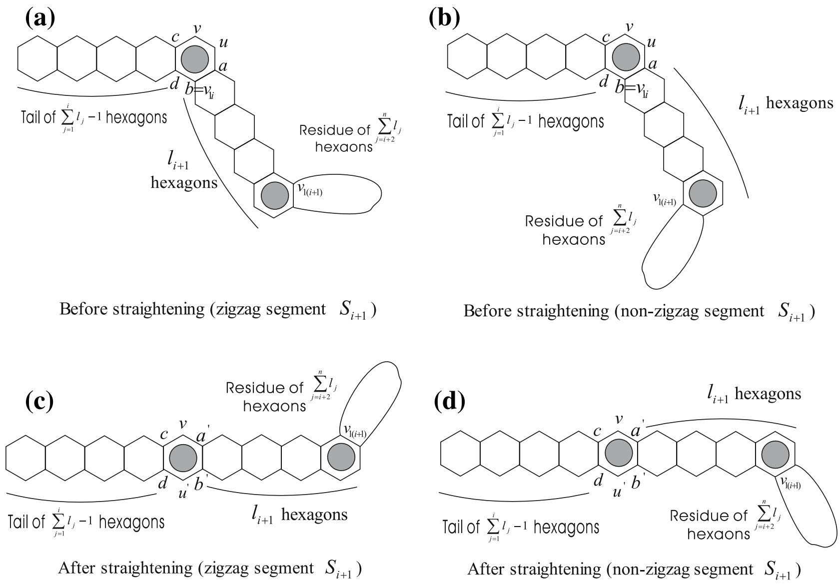

Figure 3. Changes in H_i^2 and H_i^3 as we straighten out a turn position.

Note that $\widehat{1} = \widehat{n} = 0$. For $1 \leqslant p \leqslant q \leqslant n$, let

$$\alpha_{pq} := 2\sum_{k=p}^{q} l_k - \sum_{k=p}^{q} \widehat{k}. \tag{2}$$

For convenience, we set $\alpha_{pq} = 0$ for $q < p$.

For $k = 2, 3, i = 1, 2, \ldots, n-1$, if we define

$$H_i^k := H(v_{1i}, U_i^k; Hl(l_1, l_2, \ldots, l_n)),$$

where $U_i^k = \{u \in (V(Hl(l_1, l_2, \ldots, l_n)) - V(Hl(l_1, l_2, \ldots, l_i))) \cup \{v_{1i}, v_{2i}\} | \deg(u) = k\}$, then, by inspection of figure 3 , it follows for $1 \leqslant i \leqslant n-2$,

$$H_i^3 = \frac{x^{2l_{i+1}}-1}{x-1} + x^{2l_{i+1}-\widehat{i+1}} H_{i+1}^3, \tag{3}$$

$$H_i^2 = \frac{x(x^{2l_{i+1}}-1)}{x-1} + \widehat{i+1}(x^2-1)x^{2l_{i+1}-1} + x^{2l_{i+1}-\widehat{i+1}} H_{i+1}^2 \tag{4}$$

and

$$H_{n-1}^3 = \frac{x^{2l_n}-1}{x-1}, \qquad H_{n-1}^2 = \frac{x(x^{2l_n}-1)}{x-1} + (x+1)x^{2l_n}.$$

Lemma 3.1. For $1 \leqslant i \leqslant n-1$,

$$H_i^3 = \sum_{j=i}^{n-1} x^{\alpha(i+1)j} \frac{x^{2l_{j+1}}-1}{x-1}; \tag{5}$$

$$H_i^2 = \sum_{j=i}^{n-1} x^{\alpha(i+1)j+1} \frac{x^{2l_{j+1}}-1}{x-1} + (x+1)x^{\alpha(i+1)n} + (x^2-1) \sum_{\substack{j=i+1 \\ \widehat{j}=1}}^{n-1} x^{\alpha(i+1)j}. \tag{6}$$

Proof. We use induction on i. For the induction start, when $i = n-1$, the assertions hold. We assume that the assertions hold for more than i. In the following we prove the assertions for i. By equation (4) and induction hypothesis, we have

$$\begin{aligned}
H_i^2 &= \frac{x(x^{2l_{i+1}}-1)}{x-1} + \widehat{i+1}(x^2-1)x^{2l_{i+1}-1} + x^{2l_{i+1}-\widehat{i+1}} H_{i+1}^2 \quad \text{(by equation (4))} \\
&= \frac{x(x^{2l_{i+1}}-1)}{x-1} + \widehat{i+1}(x^2-1)x^{2l_{i+1}-1} + x^{2l_{i+1}-\widehat{i+1}} \\
&\quad \times \left(\sum_{j=i+1}^{n-1} x^{\alpha(i+2)j+1} \frac{x^{2l_{j+1}}-1}{x-1} + (x+1)x^{\alpha(i+2)n} + (x^2-1) \sum_{\substack{j=i+2 \\ \widehat{j}=1}}^{n-1} x^{\alpha(i+2)j} \right) \\
&\qquad \text{(by hypothesis induction)} \\
&= x^{\alpha(i+1)i+1} \frac{x^{2l_{i+1}}-1}{x-1} + \widehat{i+1}(x^2-1)x^{\alpha(i+1)(i+1)} \\
&\quad + \left(\sum_{j=i+1}^{n-1} x^{\alpha(i+1)j+1} \frac{x^{2l_{j+1}}-1}{x-1} + (x+1)x^{\alpha(i+1)n} + (x^2-1) \sum_{\substack{j=i+2 \\ \widehat{j}=1}}^{n-1} x^{\alpha(i+1)j} \right) \\
&= \sum_{j=i}^{n-1} x^{\alpha(i+1)j+1} \frac{x^{2l_{j+1}}-1}{x-1} + (x+1)x^{\alpha(i+1)n} + (x^2-1) \sum_{\substack{j=i+1 \\ \widehat{j}=1}}^{n-1} x^{\alpha(i+1)j}.
\end{aligned}$$

Similarly, we can also prove equation (5). □

In the following we compute explicit expressions of partial Hosoya polynomials of hexagonal chains. But our computation is based on the following lemma.

Lemma 3.2. (Shelling lemma [17]). If $V(G) = \biguplus_{i=1}^{k} U_i$ ($\biguplus$ stands for disjoint union), then

$$H(G) = \sum_{j=1}^{k} H(U_i; G) + \sum_{1 \leqslant i < j \leqslant k} H(U_i, U_j; G).$$

For a hexagonal chain G, we define

$$H^2(G) := H(V_2; G)$$

and

$$H^3(G) := H(V_3; G),$$

where V_2 and V_3 are the sets of degree-2 and degree-3 vertices of G, respectively.

Lemma 3.3. Let $G_1 := Hl(l_1, l_2, \ldots, l_n)$ be a hexagonal chain and let $l = \sum_{i=1}^{n} l_i$, then

$$\Delta H^3(G_1) := H^3(G_1) - H^3(L_l) = -x \sum_{i=1}^{n-1} \left(x^{2\sum_{j=1}^{i} l_j - 2} - 1 \right) \left(\frac{x^{2l_{i+1}} - 1}{x^2 - 1} + \widehat{i+1} \sum_{j=i+1}^{n-1} x^{\alpha(i+1)j} \frac{x^{2l_{j+1}} - 1}{x - 1} \right); \tag{7}$$

$$\begin{aligned}\Delta H^2(G_1) &:= H^2(G_1) - H^2(L_l) \\ &= -x(x^2 + x - 1) \sum_{i=1}^{n-1} \left(x^{2\sum_{j=1}^{i} l_j - 2} - 1 \right) \left(\frac{(x^2 + x - 1)(x^{2l_{i+1}} - 1)}{x^2 - 1} \right. \\ &\quad + \widehat{i+1} \left(-(x+1)x^{2l_{i+1}-1} + (x+1)x^{\alpha(i+1)n} \right. \\ &\quad \left. \left. + (x^2 - 1) \sum_{\substack{j=i+1 \\ \widehat{j+1}=1}}^{n-1} x^{\alpha(i+1)(j+1)} + \sum_{j=i+1}^{n-1} x^{\alpha(i+1)j} \frac{x(x^{2l_{j+1}} - 1)}{x - 1} \right) \right).\end{aligned} \tag{8}$$

Proof. First, from G_1 we can construct a sequence of hexagonal chains $Hl(l_1, l_2, \ldots, l_n) = G_1, G_2, \ldots, G_n$ such that for $1 \leqslant i \leqslant n - 1 G_{i+1}$ is obtained from G_i by straightening out the first turning hexagon (see figure 3 for illustration of turning G_i into G_{i+1}). Then G_i can be seen as comprising $\sum_{j=1}^{i} l_j - 1$ straight hexagons, then the turning hexagon, then a further l_{i+1} straight hexagons, then bending to the remaining $\sum_{j=i+2}^{n} l_j$ hexagons which are not necessarily straight, i.e., $G_i = Hl\left(\sum_{j=1}^{i} l_j, l_{i+1}, \ldots, l_n\right)$. Clearly, G_n is a linear hexagonal chain L_l. For example, if $G_1 = Hl(2, 3, 4)$, then $G_2 = Hl(5, 4), G_3 = L_9$. Clearly,

$$\Delta H^k(G_1) = \sum_{i=1}^{n-1}(H^k(G_i) - H^k(G_{i+1})), \quad k = 2, 3. \tag{9}$$

Second, we find $\Delta H^3(G_1)$ according to equation (9). By inspection of figure 3, we see that

- For any vertex behind a (including a) its distance to the tail does not change as we straighten the turn.
- For any degree-3 vertex behind b (including b), its distance to each of the $\left(2\sum_{j=1}^{i} l_j - 2\right)$ degree-3 vertices in the tail increases by one when we straighten the turn.

So $H^3(G_i) - H^3(G_{i+1}) = -x\left(x^{2\sum_{j=1}^{i} l_j - 2} - 1\right)\left(\frac{x^{2l_{i+1}} - 1}{x^2 - 1} + \widehat{i+1}x^{2l_{i+1}-1}H^3_{i+1}\right)$. Combining the above observation, equation (9) and lemma 3.1., we obtain equation (7).

Finally, we prove equation (8). We use the Shelling lemma and make the corresponding change in each category, then we have

$$\begin{aligned} H^2(G_i) = {} & H^2(\text{left side}; G_i) + H^2(\text{right side}; G_i) + H^2(\text{the turning hexagon}; G_i) \\ & + H^2(\text{turning hexagon, left side}; G_i) \\ & + H^2(\text{turning hexagon, right side}; G_i) \\ & + H^2(\text{left side, right side}; G_i). \end{aligned}$$

Straightening out the turn in G_i (then obtaining G_{i+1}) creates the following differences (see figure 3):

Within the left side and within the right side: no change.

The turning hexagon: $x - x^3$, as $d(u, v) = 1$ in figure 3 (a) and (b), $d(u', v) = 3$ in figure 3 (c) and (d).

From the turning hexagon to the left side: $(x^3 - x)\left(x + x^3 + \cdots + x^{2\sum_{j=1}^{i} l_j - 3} + x^{2\sum_{j=1}^{i} l_j - 2}\right) = (x^2 + x - 1)x^{2\sum_{j=1}^{i} l_j - 1} - x^2$, as only distances between degree-2 vertices behind d and u change and all decrease by two when we straighten the turn.

From the turning hexagon to the right side: No change for any vertex w behind a since $\mathrm{d}_{G_i}(w, v) = \mathrm{d}_{G_{i+1}}(w, u'), \mathrm{d}_{G_i}(w, u) = \mathrm{d}_{G_{i+1}}(w, v)$; $\big((x^2 + x^3) -$

$(x+x^2))\big(x+x^3+\cdots+x^{2l_{i+1}-1}+x^{2l_{i+1}}+\widehat{i+1}(x^{2l_{i+1}-1}H^2_{i+1}-x^{2l_{i+1}-1}-x^{2l_{i+1}})\big) = x(x^2-1)\big(\frac{(x^2+x-1)x^{2l_{i+1}}-x}{x^2-1}+\widehat{i+1}(x^{2l_{i+1}-1}H^2_{i+1}-(x+1)x^{2l_{i+1}-1})\big)$ as for any degree-2 vertex behind b, its distance to u and v decrease by one.

Between the left and the right sides: No change for vertices behind a; $(x-x^2)\Big(x+x^2+\cdots+x^{2\sum_{j=1}^{i}l_j-3}+2x^{2\sum_{j=1}^{i}l_j-2}+x^{2\sum_{j=1}^{i}l_j-1}\Big)\big(x+x^3+\cdots+x^{2l_{i+1}-1}+x^{2l_{i+1}}+\widehat{i+1}(x^{2l_{i+1}-1}H^2_{i+1}-x^{2l_{i+1}-1}-x^{2l_{i+1}})\big) = -\big((x^2+x-1)x^{2\sum_{j=1}^{i}l_j-1}-x^2\big)\big(\frac{(x^2+x-1)x^{2l_{i+1}}-x}{x^2-1}+\widehat{i+1}(x^{2l_{i+1}-1}H^2_{i+1}-(x+1)x^{2l_{i+1}-1})\big)$, as for vertices behind b, its distances to vertices in the tail increases by one when we straighten the turn.

After a simple computation we readily obtain equation (8). □

To compute partial Hosoya polynomials of hexagonal chains, we need the base values $H^2(L_n)$ and $H^3(L_n)$. The proof is trivial by mathematical induction.

Lemma 3.4. For a linear hexagonal chain L_n with n hexagons, we have

$$H^2(L_n) = 2x - \frac{2(3x^2-2)}{(x+1)(x-1)^2} + n\left(x^3-2x-\frac{2}{x-1}\right) + \frac{2(x^2+x-1)^2x^{2n}}{(x+1)(x-1)^2};$$

$$H^3(L_n) = x - \frac{2}{(x+1)(x-1)^2} - n\left(x+\frac{2}{x-1}\right) + \frac{2x^{2n}}{(x+1)(x-1)^2}.$$

By lemmas 3.3. and 3.4. we obtain partial Hosoya polynomials of hexagonal chains as follows.

Lemma 3.5.

$$\begin{aligned} &H^2(Hl(l_1,l_2,\ldots,l_n)) \\ &= 2x - \frac{2(3x^2-2)}{(x+1)(x-1)^2} + \left(\sum_{i=1}^{n} l_i\right)\left(x^3-2x-\frac{2}{x-1}\right) + \frac{(x^2+x-1)^2}{x^2-1}x^{2l_1-1} \\ &\quad + \frac{(x^2+x-1)^2}{(x-1)^2}x^{2\sum_{i=1}^{n}l_i-1} + \frac{x(x^2+x-1)^2}{x^2-1}\sum_{i=1}^{n-1}(x^{2l_{i+1}}-1) - x(x+1)(x^2+x-1) \\ &\quad \times \sum_{\substack{i=1\\ \widehat{i+1}}}^{n-1}\left(x^{2\sum_{j=1}^{i}l_j-2}-1\right)\left(-x^{2l_{i+1}-1}+x^{\alpha(i+1)n}+(x-1)\sum_{\substack{j=i+1\\ \widehat{j+1}=1}}^{n-1}x^{\alpha(i+1)(j+1)}\right) \end{aligned}$$

$$-\frac{(x^2+x-1)x^2}{x-1}\sum_{\substack{i=1\\ \widehat{i+1=1}}}^{n-1}\sum_{j=i+1}^{n-1}(x^{2l_{j+1}}-1)\left(x^{2\sum_{j=1}^{i}l_j-2}-1\right)x^{\alpha(i+1)j};$$

$H^{3}(Hl(l_1,l_2,\cdots,l_n))$

$$=x-\frac{2}{(x+1)(x-1)^2}-\left(\sum_{i=1}^{n}l_i\right)(x+\frac{2}{x-1})+\frac{1}{x^2-1}x^{2l_1-1}+\frac{1}{(x-1)^2}x^{2\sum_{i=1}^{n}l_i-1}$$

$$+\frac{x}{x^2-1}\sum_{i=1}^{n-1}(x^{2l_{i+1}}-1)-\frac{x}{x-1}\sum_{\substack{i=1\\ \widehat{i+1=1}}}^{n-1}\sum_{j=i+1}^{n-1}(x^{2l_{j+1}}-1)\left(x^{2\sum_{j=1}^{i}l_j-2}-1\right)x^{\alpha(i+1)j}.$$

4. Main results

Recall that the Shelling lemma can be considered as the version about Hosoya polynomials. Similarly, we also apply the Shelling lemma to generalized Hosoya polynomials.

Lemma 4.1. Let G be any hexagonal chain, V_2 and V_3 are the sets of degree-2 and -3 vertices of G, respectively, then

$$H_{\ddagger}^{(a)}(G)=(2^a+3^a)H(G)+(2^a-3^a)(H^2(G)-H^3(G));$$
$$H_{+}^{(a)}(G)=5^aH(G)+(4^a-5^a)H^2(G)+(6^a-5^a)H^3(G);$$
$$H_{*}^{(a)}(G)=6^aH(G)+(4^a-6^a)H^2(G)+(9^a-6^a)H^3(G).$$

Proof. We merely have to observe that the hexagonal chain G only have vertices of degree 2 and 3, $H(G)=H(V_2,V_3;G)+H(V_2;G)+H(V_3;G)$ and this lemma follows immediately from the Shelling lemma. □

The above observation is crucial to computing generalized Hosoya polynomials of hexagonal chains.

In Ref. [14] we have given Hosoya polynomials for hexagonal chains as follows (note that there is a bit difference in the form of analytical expressions because there is a bit change of the notation α_{ij}).

Lemma 4.2. ([14]).

$H(Hl(l_1,l_2,\ldots,l_n))$

$$=-4-x+\frac{2(3-5x)}{(x-1)^2}+\frac{2(x+1)x^{2l_1+2}}{(x-1)^2}+\left(\sum_{i=1}^{n}l_i\right)\left(x^3-3x-4-\frac{8}{x-1}\right)$$

$$+\frac{x+1}{(x-1)^2}\sum_{i=1}^{n-1}(x^{2l_{i+1}}-1)\big((x-1)x^3+(x+1)x^{2l_i}+(x^2-1)x^{\alpha_{1i}}\big)$$
$$+\frac{(x+1)^2}{(x-1)^2}\sum_{i=1}^{n-1}\sum_{j=i+1}^{n-1}(x^{2l_i}-1)(x^{2l_{j+1}}-1)x^{\alpha_{(i+1)j}}$$
$$+(x^2+x+1)(x+1)^2\sum_{\substack{i=1\\ \widehat{i+1}=1}}^{n-1}\sum_{j=i+1}^{n-1}(x^{2l_{j+1}}-1)x^{\alpha_{(i+1)j}}.$$

From Lemmas 3.5, 4.1 and 4.2, we get our main results as follows.

Theorem 4.3. Let the notations $\widehat{i}$ and α_{ij} are defined as (1) and (2), respectively, then

$$\widetilde{H}(Hl(l_1,l_2,\ldots,l_n))$$
$$=-4a_1+(-a_1+2a_2+a_3)x+\frac{2a_1(3-5x)}{(x-1)^2}-\frac{6a_2x^2-4a_2+2a_3}{(x+1)(x-1)^2}$$
$$+\frac{2a_1x^3(x+1)^2+a_2(x-1)(x^2+x-1)^2+a_3(x-1)}{(x+1)(x-1)^2}x^{2l_1-1}$$
$$+\left(\sum_{i=1}^{n}l_i\right)\left((a_1+a_2)x^3-(3a_1+2a_2+a_3)x-4a_1-\frac{2(4a_1+a_2+a_3)}{x-1})\right)$$
$$+\frac{a_2(x^2+x-1)^2+a_3}{(x-1)^2}x^{2\sum_{i=1}^{n}l_i-1}+\frac{1}{(x+1)(x-1)^2}\sum_{i=1}^{n-1}(x^{2l_{i+1}}-1)$$
$$\times\Big(x(x-1)\big(a_2(x^2+x-1)^2+a_3\big)+a_1(x+1)^2\big((x-1)x^3$$
$$+(x+1)x^{2l_i}+(x^2-1)x^{\alpha_{1i}}\big)\Big)-a_2x(x+1)(x^2+x-1)$$
$$\times\sum_{\substack{i=1\\ \widehat{i+1}=1}}^{n-1}(x^{2\sum_{k=1}^{i}l_k-2}-1)\Bigg(-x^{2l_{i+1}-1}+x^{\alpha_{(i+1)n}}+(x-1)\sum_{\substack{j=i+1\\ \widehat{j+1}=1}}^{n-1}x^{\alpha_{(i+1)(j+1)}}\Bigg)$$
$$+\frac{a_1(x+1)^2}{(x-1)^2}\sum_{i=1}^{n-1}\sum_{j=i+1}^{n-1}(x^{2l_i}-1)(x^{2l_{j+1}}-1)x^{\alpha_{(i+1)j}}$$

$$+\sum_{\substack{i=1\\ \widehat{i+1}=1}}^{n-1}\sum_{j=i+1}^{n-1}\Bigg(a_1(x^2+x+1)(x+1)^2$$

$$-\frac{x\big(a_2x(x^2+x-1)+a_3\big)(x^{2\sum_{k=1}^{i}l_k-2}-1)}{x-1}\Bigg)(x^{2l_{j+1}}-1)x^{\alpha_{(i+1)j}},$$

where the vector (a_1, a_2, a_3) is equal to $(2^a+3^a, 2^a-3^a, 3^a-2^a)$ for $H_{\ddagger}^{(a)}$, $(5^a, 4^a-5^a, 6^a-5^a)$ for $H_{+}^{(a)}$, $(6^a, 4^a-6^a, 9^a-6^a)$ for $H_{*}^{(a)}$. In particular, $(5, -1, 1)$ for H_+ and $(6, -2, 3)$ for H_*.

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