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The Expected Values of Merrifield−Simmons Index in Random Phenylene Chains

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ABSTRACT

The Merrifield-Simmons index of a graph G is the number of independent sets in G. In this paper, we give exact formulae for the expected value of the Merrifield-Simmons index of random phenylene chains by means of auxiliary graphs.

1. INTRODUCTION

In 1980, the chemists Merrifield and Simmoms elaborated a theory aimed at describing molecular structure by means of finite-set topology, their theory was not particularly successful. However, the topological formalism attracted the attention of colleagues and eventually became known as the Merrifield-Simmons index. This was the number of independent sets of vertices of the graph corresponding to that topology [1], and a series of articles were published [2−5].

The Merrifield-Simmons index is a typical example of graph invariants used in mathematical chemistry for quantifying relevant details of molecular structure. In recent years, a lot of work has been done on the extremal problem for it. For a survey of results and techniques related to the Hosoya index and Merrifield-Simmons index, see [6]. For recent works, see [7−9]. Chen et al. give six-membered ring spiro chains with extremal

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Merrifield-Simmons index and Hosoya index, [10]. Li $et\ al.$ give the Hosoya polynomials of general spiro hexagonal chains [11], and Wiener index and Kirchhoff index of spiro chain were given by Peng [12, 13]. Bai $et\ al.$ give the exact formulae of extremal Merrifield-Simmons index and Hosoya index of polyphenylene chains, [14]. In 2015, Chen gives Merrifield-Simmons index in random phenylene chains and random hexagon chains [15]. In 2019, Liu $et\ al.$ give the expected values of Hosoya index and Merrifield-Simmons index in a random spiro chains [16].

In this paper, we will present explicit formulae for the expected values of the Merrifield-Simmons index of random phenylene chains. The results obtained by considering several auxiliary graphs.

2. PRELIMINARIES

All graphs considered here are finite and simple. For a given graph $G = (V; E)$, the set of its vertices is denoted by V and the set of its edges by E. For a vertex $u \in V$ by $G - u$ we denote the graph induced by $V - \{u\}$. The closed neighborhood of a vertex v is denoted by $N[v]$.

A set $S \in V$ of vertices of G is an independent set in G if no two vertices of S are adjacent. $i_k(G)$ denote the number of independent set in G with k vertices. Obviously, $i_0(G) = 1$ and $i_1(G) = |V|$. The total number of independent sets in G is denoted by $i(G) = \sum_{k\geq 0} i_k(G)$. In chemical literature, $i(G)$ is known as the Merrifield-Simmons index.

The following results belong to the mathematical folklore and will be used in the computations [16].

1. If v is a vertex of G, then

$$i(G) = i(G - v) + i(G - N[v]), \tag{1}$$

2. If G is a graph with components $G_1, G_2, \dots, G_k$, then

$$i(G) = \prod_{i=1}^{k} i(G_i), \tag{2}$$

3. $i(P_1) = 2, i(P_2) = 3, i(P_3) = 5, i(P_4) = 8, i(P_5) = 13$ and $i(C_6) = 18$, where P_n is the path on n vertices and C_n is the cycle on n vertices.

Let H be a cata-condensed hexagonal system. If a hexagon r has one neighbouring hexagon, then it is said to be terminal, and if it has three neighbouring hexagons, to be branched. If a hexagon adjacent to exactly two other hexagons is a kink if r possess two adjacent vertices of degree two, is linear otherwise. The dualist graph of H consists of vertices corresponding to hexagons of H, two vertices are adjacent if and only if the corresponding hexagons have a common edge. Obviously, the dualist graph of H is a tree. If H has n hexagons, then this tree has n vertices and none of its vertices have degree greater than three. A cata-condensed hexagonal system with no branched hexagons is said to be a hexagonal chain. A hexagonal chain with no kink is said to be a linear chain.

Let H be a cata-condensed hexagonal system with a least two hexagons. If we insert quadrilaterals (face where boundary is a $4-\text{cycle}$) between all pair of adjacent hexagons of H, the obtained graph G is called a phenylene. We say that H is the hexagonal squeeze of G. A phenylene containing n hexagons is called an $[n]-\text{phenylene}$. Clearly, there is one to one correspondence between a phenylene and its hexagonal squeeze, both possess the same number of hexagons. In addition, a phenylene with n hexagons has $n-1$ squares. The number of vertices of a phenylene and its hexagonal squeeze are $6n$ and $4n+2$, respectively. A phenylene chain with n hexagons can be regarded as a phenylene chain G_n, see Figure 1.

Figure 1: Examples of phenylene chain G_4

A phenylene chain G_n with n hexagons can be regard as a phenylene chain G_{n-1} with $n-1$ hexagons to which new terminal quadrilateral and hexagon have been adjoined, see Figure 2.

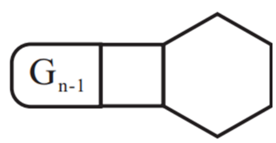

Figure 2: A phenylene chain G_n with n hexagons

For $n \geq 3$, the terminal quadrilateral and hexagon can be attached in three ways, which results in the local arrangement we describe as G_n^1, G_n^2, G_n^3, see Figure 3.

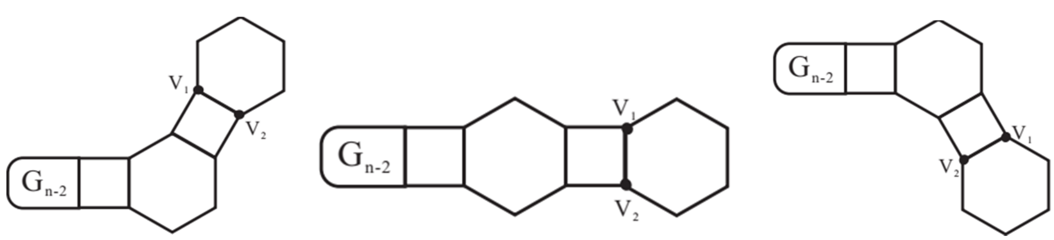

Figure 3: The three types of phenylene chains G_n^1, G_n^2, G_n^3, respectively.

A random phenylene chain $G_n(p, 1-2p, p)$ with n hexagons is a phenylene chain obtained by stepwise addition of terminal quadrilateral and hexagon. At each step k $(k \geq 3)$, a random selection is made from one of the three possible constructions:

1. $G_{n-1} \rightarrow G_n^1$ with probability p,
2. $G_{n-1} \rightarrow G_n^2$ with probability $1-2p$,
3. $G_{n-1} \rightarrow G_n^3$ with probability p;

where the probability p is a constant, satisfies the condition $0 \leq q \leq \frac{1}{2}$. Specially, the random phenylene chain $G_n(0,1,0)$ is the linear phenylene chain.

3. THE EXPECTED VALUES OF MERRIFIELD-SIMMONS INDEX OF A RANDOM PHENYLENE CHAIN

As described above, the phenylene chain $G_n(p, 1-2p, p)$ is obtained at random by attaching to G_{n-1} new quadrilateral and hexagon from one of the three possible constructions. The process is a zeroth-order Markov process. For $G_n(p, 1-2p, p)$, the Merrifield-Simmons index is a random variable. In this section, we will obtain a simple exact formula of its expected values $E(i(G_n))$. The results are obtained by considering auxiliary graphs. There are four types of auxiliary fandom graphs A_k, B_k and $\hat{A}_k, \hat{B}_k$, where $A_k \in \{A_k^1, A_k^2, A_k^3\}$, $B_k \in \{B_k^1, B_k^2, B_k^3\}$, and $\hat{A}_k \in \{\hat{A}_k^1, \hat{A}_k^2, \hat{A}_k^3\}$, $\hat{B}_k \in \{\hat{B}_k^1, \hat{B}_k^2, \hat{B}_k^3\}$, are shown in Figure 4, 5, 6, 7, respectively.

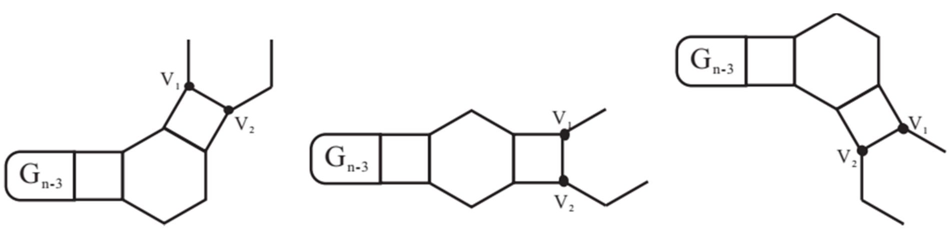

Figure 4: Graphs of $A_{n-2}^1, A_{n-2}^2, A_{n-2}^3$, respectively.

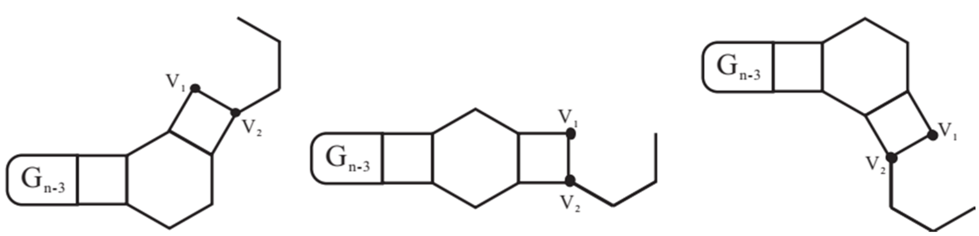

Figure 5: Graphs of $B_{n-2}^1, B_{n-2}^2, B_{n-2}^3$, respectively.

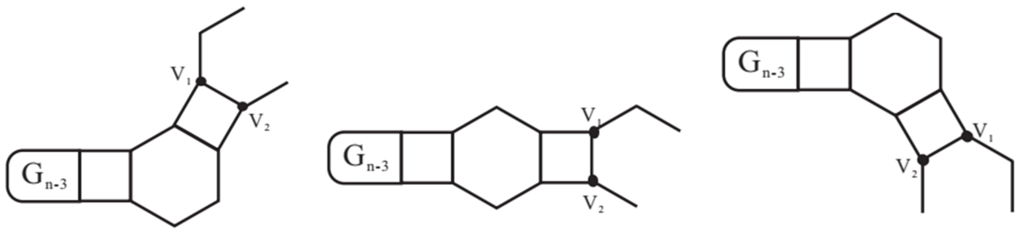

Figure 6: Graphs of $\hat{A}^1_{n-2}, \hat{A}^2_{n-2}, \hat{A}^3_{n-2}$, respectively.

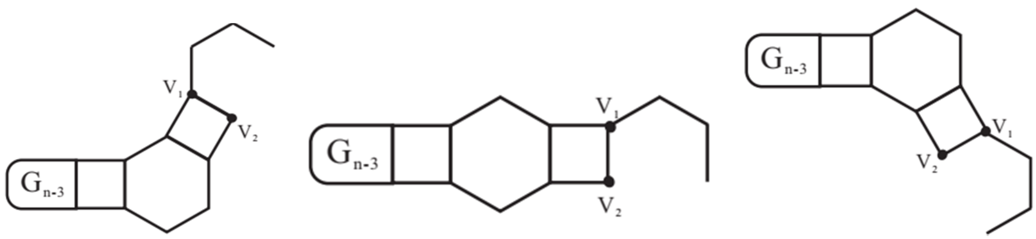

Figure 7: Graphs of $\hat{B}^1_{n-2}, \hat{B}^2_{n-2}, \hat{B}^3_{n-2}$, respectively.

If $G_n = G_n^1$ in Figure 2, then by (1) and (2), we have

$$\begin{aligned} i(G_n) &= i(G_n - v_1) + i(G_n - N[v_1]) \\ &= i(G_n - v_1 - v_2) + i(G_n - v_1 - N[v_2]) + i(G_n - N[v_1]) \\ &= i(P_4)i(G_{n-1}) + i(P_3)i(A_{n-2}) + i(P_3)i(B_{n-2}) \\ &= 8i(G_{n-1}) + 5i(A_{n-2}) + 5i(B_{n-2}), \end{aligned} \tag{3}$$

Similarly, if $G_n = G_n^2$,

$$\begin{aligned} i(G_n) &= i(G_n - v_1) + i(G_n - N[v_1]) \\ &= i(G_n - v_1 - v_2) + i(G_n - v_1 - N[v_2]) + i(G_n - N[v_1]) \\ &= i(P_4)i(G_{n-1}) + i(P_3)i(\hat{A}_{n-2}) + i(P_3)i(A_{n-2}) \\ &= 8i(G_{n-1}) + 5i(\hat{A}_{n-2}) + 5i(A_{n-2}), \end{aligned} \tag{4}$$

If $G_n = G_n^3$, we have

$$\begin{aligned} i(G_n) &= i(G_n - v_1) + i(G_n - N[v_1]) \\ &= i(G_n - v_1 - v_2) + i(G_n - v_1 - N[v_2]) + i(G_n - N[v_1]) \\ &= i(P_4)i(G_{n-1}) + i(P_3)i(\hat{B}_{n-2}) + i(P_3)i(\hat{A}_{n-2}) \\ &= 8i(G_{n-1}) + 5i(\hat{B}_{n-2}) + 5i(\hat{A}_{n-2}), \end{aligned} \tag{5}$$

Now, we search the case of auxiliary graphs A_{n-2}, B_{n-2} and $\hat{A}_{n-2}, \hat{B}_{n-2}$. If $A_{n-2} = A^1_{n-2}$, we have

$$\begin{aligned} i(A_{n-2}) &= i(A_{n-2}-v_1)+i(A_{n-2}-N[v_1]) \\ &= i(A_{n-2}-v_1-v_2)+i(A_{n-2}-v_1-N[v_2])+i(A_{n-2}-N[v_1]) \\ &= i(P_2)i(G_{n-2})+i(A_{n-3})+i(P_2)i(B_{n-3}) \\ &= 3i(G_{n-2})+i(A_{n-3})+3i(B_{n-3}), \end{aligned} \tag{6}$$

Similarly, if $A_{n-2} = A_{n-2}^2$, then

$$\begin{aligned} i(A_{n-2}) &= i(P_2)i(G_{n-2})+i(\hat{A}_{n-3})+i(P_2)i(A_{n-3}) \\ &= 3i(G_{n-2})+i(\hat{A}_{n-3})+3i(A_{n-3}), \end{aligned} \tag{7}$$

if $A_{n-2} = A_{n-2}^3$, we have

$$\begin{aligned} i(A_{n-2}) &= i(P_2)i(G_{n-2})+i(\hat{B}_{n-3})+i(P_2)i(\hat{A}_{n-3}) \\ &= 3i(G_{n-2})+i(\hat{B}_{n-3})+3i(\hat{A}_{n-3}). \end{aligned} \tag{8}$$

If $B_{n-2} = B_{n-2}^1$, then

$$\begin{aligned} i(B_{n-2}) &= i(P_3)i(G_{n-2})+i(P_2)i(A_{n-3})+i(P_3)i(B_{n-3}) \\ &= 5i(G_{n-2})+3i(A_{n-3})+5i(B_{n-3}), \end{aligned} \tag{9}$$

If $B_{n-2} = B_{n-2}^2$, then

$$\begin{aligned} i(B_{n-2}) &= i(P_3)i(G_{n-2})+i(P_2)i(\hat{A}_{n-3})+i(P_3)i(A_{n-3}) \\ &= 5i(G_{n-2})+3i(\hat{A}_{n-3})+5i(A_{n-3}), \end{aligned} \tag{10}$$

If $B_{n-2} = B_{n-2}^3$, then

$$\begin{aligned} i(B_{n-2}) &= i(P_3)i(G_{n-2})+i(P_2)i(\hat{B}_{n-3})+i(P_3)i(\hat{A}_{n-3}) \\ &= 5i(G_{n-2})+3i(\hat{B}_{n-3})+5i(\hat{A}_{n-3}), \end{aligned} \tag{11}$$

If $\hat{A}_{n-2} = \hat{A}_{n-2}^1$, then

$$\begin{aligned} i(\hat{A}_{n-2}) &= i(P_2)i(G_{n-2})+i(P_2)i(A_{n-3})+i(B_{n-3}) \\ &= 3i(G_{n-2})+3i(A_{n-3})+i(B_{n-3}), \end{aligned} \tag{12}$$

If $\hat{A}_{n-2} = \hat{A}_{n-2}^2$, then

$$\begin{aligned} i(\hat{A}_{n-2}) &= i(P_2)i(G_{n-2})+i(P_2)i(\hat{A}_{n-3})+i(A_{n-3}) \\ &= 3i(G_{n-2})+3i(\hat{A}_{n-3})+i(A_{n-3}), \end{aligned} \tag{13}$$

If $\hat{A}_{n-2} = \hat{A}_{n-2}^3$, then

$$\begin{aligned} i(\hat{A}_{n-2}) &= i(P_2)i(G_{n-2})+i(P_2)i(\hat{B}_{n-3})+i(\hat{A}_{n-3}) \\ &= 3i(G_{n-2})+3i(\hat{B}_{n-3})+i(\hat{A}_{n-3}), \end{aligned} \tag{14}$$

If $\hat{B}_{n-2} = \hat{B}_{n-2}^1$, then

$$\begin{aligned} i(\hat{B}_{n-2}) &= i(P_3)i(G_{n-2})+i(P_3)i(A_{n-3})+i(P_2)i(B_{n-3}) \\ &= 5i(G_{n-2})+5i(A_{n-3})+3i(B_{n-3}), \end{aligned} \tag{15}$$

If $\widehat{B}_{n-2} = \widehat{B}^2_{n-2}$, then

$$\begin{aligned} i(\widehat{B}_{n-2}) &= i(P_3)i(G_{n-2}) + i(P_3)i(\hat{A}_{n-3}) + i(P_2)i(A_{n-3}) \\ &= 5i(G_{n-2}) + 5i(\hat{A}_{n-3}) + 3i(A_{n-3}), \end{aligned} \tag{16}$$

If $\widehat{B}_{n-2} = \widehat{B}^3_{n-2}$, then

$$\begin{aligned} i(\widehat{B}_{n-2}) &= i(P_3)i(G_{n-2}) + i(P_3)i(\widehat{B}_{n-3}) + i(P_2)i(\hat{A}_{n-3}) \\ &= 5i(G_{n-2}) + 5i(\widehat{B}_{n-3}) + 3i(\hat{A}_{n-3}), \end{aligned} \tag{17}$$

From above, we can get the expected values $E(i(G_n))$, $E(i(A_{n-2}))$, $E(i(B_{n-2}))$, $E(i(\hat{A}_{n-2}))$, $E(i(\widehat{B}_{n-2}))$ of $i(G_n)$, $i(A_{n-2})$, $i(B_{n-2})$, $i(\hat{A}_{n-2})$, $i(\widehat{B}_{n-2})$, respectively.

From (3), (4), (5), we have

$$\begin{aligned} E(i(G_n)) = & \; pE(i(G_n^1)) + (1-2p)E(i(G_n^2)) + pE(i(G_n^3)) \\ = & \; 8pE(i(G_{n-1})) + 5pE(i(A_{n-2})) + 5pE(i(B_{n-2})) + 8(1-2p)E(i(G_{n-1})) \\ & +5(1-2p)E(i(\hat{A}_{n-2})) + 5(1-2p)E(i(A_{n-2})) + 8pE(i(G_{n-1})) \\ & +5pE(i(\widehat{B}_{n-2})) + 5pE(i(\hat{A}_{n-2})) \\ = & \; 8E(i(G_{n-1})) + (5-5p)E(i(A_{n-2})) + 5pE(i(B_{n-2})) \\ & +(5-5p)E(i(\hat{A}_{n-2})) + 5pE(i(\widehat{B}_{n-2})) \end{aligned} \tag{18}$$

From (6), (7), (8), we have

$$\begin{aligned} E(i(A_{n-2})) = & \; pE(i(A^1_{n-2})) + (1-2p)E(i(A^2_{n-2})) + pE(i(A^3_{n-2})) \\ = & \; 3E(i(G_{n-2})) + (3-5p)E(i(A_{n-3})) + 3pE(i(B_{n-3})) \\ & +(1+p)E(i(\hat{A}_{n-3})) + pE(i(\widehat{B}_{n-3})). \end{aligned} \tag{19}$$

From (9), (10), (11), we have

$$\begin{aligned} E(i(B_{n-2})) = & \; pE(i(B^1_{n-2})) + (1-2p)E(i(B^2_{n-2})) + pE(i(B^3_{n-2})) \\ = & \; 5E(i(G_{n-2})) + (5-7p)E(i(A_{n-3})) + 5pE(i(B_{n-3})) \\ & +(3-p)E(i(\hat{A}_{n-3})) + 3pE(i(\widehat{B}_{n-3})). \end{aligned} \tag{20}$$

From (12), (13), (14), we have

$$\begin{aligned} E(i(\hat{A}_{n-2})) = & \; pE(i(\hat{A}^1_{n-2})) + (1-2p)E(i(\hat{A}^2_{n-2})) + pE(i(\hat{A}^3_{n-2})) \\ = & \; 3E(i(G_{n-2})) + (1+p)E(i(A_{n-3})) + pE(i(B_{n-3})) \\ & +(3-5p)E(i(\hat{A}_{n-3})) + 3pE(i(\widehat{B}_{n-3})). \end{aligned} \tag{21}$$

From (15), (16), (17), we have

$$\begin{aligned} E(i(\hat{B}_{n-2})) &= pE(i(\hat{B}^1_{n-2})) + (1-2p)E(i(\hat{B}^2_{n-2})) + pE(i(\hat{B}^3_{n-2})) \\ &= 5E(i(G_{n-2})) + (3-p)E(i(A_{n-3})) + 3pE(i(B_{n-3})) \\ &\quad +(5-7p)E(i(\hat{A}_{n-3})) + 5pE(i(\hat{B}_{n-3})). \end{aligned} \tag{22}$$

From (18), (19), (20), (21), (22), we have

$$\begin{aligned} E(i(G_n)) = {} & 8E(i(G_{n-1})) + (30+20p)E(i(G_{n-2})) + (20-20p^2)E(i(A_{n-3})) \\ & + (20p+20p^2)E\big(i(B_{n-3})\big) + (20-20p^2)E\left(i\big(\hat{A}_{n-3}\big)\right) \\ & +(20p+20p^2)E(i(\hat{B}_{n-3})), \end{aligned}$$

andwith the same method, we have

$$\begin{aligned} E(i(G_n)) = {} & 8E(i(G_{n-1})) + (30+20p)E(i(G_{n-2})) + (120+200p+80p^2)E(i(G_{n-3})) \\ & +(80+80p-80p^2-80p^3)E(i(A_{n-4})) + (80p+160p^2+80p^3)E(i(B_{n-4})) \\ & +(80+80p-80p^2-80p^3)E(i(\hat{A}_{n-4})) + (80p+160p^2+80p^3)E(i(\hat{B}_{n-4})). \end{aligned} \tag{23}$$

From above (19), (20), (21), (22), we have

$$\begin{aligned} & (80+80p-80p^2-80p^3)E(i(A_{n-4})) + (80p+160p^2+80p^3)E(i(B_{n-4})) \\ + {} & (80+80p-80p^2-80p^3)E(i(\hat{A}_{n-4})) + (80p+160p^2+80p^3)E(i(\hat{B}_{n-4})) \\ = {} & (480+1280p+1120p^2+320p^3)E(i(G_{n-4})) \\ & +(4+4p)(80+80p-80p^2-80p^3)E(i(A_{n-5})) \\ & +(4+4p)(80p+160p^2+80p^3)E(i(B_{n-5})) \\ & +(4+4p)(80+80p-80p^2-80p^3)E(i(\hat{A}_{n-5})) \\ & +(4+4p)(80p+160p^2+80p^3)E(i(\hat{B}_{n-5})). \end{aligned} \tag{24}$$

Let

$$\begin{aligned} H = {} & (4+4p)(80+80p-80p^2-80p^3)E(i(A_{n-5})) + (4+4p)(80p+160p^2+80p^3)E(i(B_{n-5})) \\ + {} & (4+4p)(80+80p-80p^2-80p^3)E\left(i\big(\hat{A}_{n-5}\big)\right) + (4+4p)(80p+160p^2+80p^3)E\left(i\big(\hat{B}_{n-5}\big)\right). \end{aligned} \tag{25}$$

From (23), (24), (25), we have

$$\begin{aligned} H = {} & (4+4p)[E(i(G_{n-1})) - 8E(i(G_{n-2})) \\ & - (30+20p)E(i(G_{n-3})) - (120+200p+80p^2)E(i(G_{n-4}))]. \end{aligned}$$

From (23), (24), (25), then

$$E(i(G_n)) = (12+4P)E(i(G_{n-1})) - (2+12p)E(i(G_{n-2})). \tag{26}$$

We know that

$$E(i(G_1)) = E(i(C_6)) = 18, E(i(G_2)) = 274.$$

Theorem 3.1. *The expected value of the Merrifield-Simmons index of a random phenylene chain* $G_n(p, 1-2p, p)$ *is*

$$\begin{aligned} E(i(G_n)) &= \frac{192-50p-72p^2+(-29+36p)\sqrt{4p^2+12p+34}}{(2+12p)\sqrt{4p^2+12p+34}}\left(6+2p+\sqrt{4p^2+12p+34}\right)^n \\ &- \frac{192-50p-72p^2-(-29+36p)\sqrt{4p^2+12p+34}}{(2+12p)\sqrt{4p^2+12p+34}}\left(6+2p-\sqrt{4p^2+12p+34}\right)^n. \end{aligned} \tag{27}$$

Proof. From (26), we know that

$$E\big(i(G_n)\big) = (12+4P)E\big(i(G_{n-1})\big) - (2+12p)E\big(i(G_{n-2})\big),$$

and

$$E(i(G_1)) = E(i(C_6)) = 18, E(i(G_2)) = 274.$$

Next, we use the second order method for solving the recurrence relation with constant coefficient. It is well known that $x^2 - (12+4p)x + (2+12p) = 0$ is the characteristic equation of the recursive relationship $E(i(G_n)) = (12+4p)E(i(G_{n-1})) - (2+12p)E(i(G_{n-2}))$, the characteristic root of this characteristic equation is

$$p_1 = \frac{12+4p+2\sqrt{4p^2+12p+34}}{2}, p_2 = \frac{12+4p-2\sqrt{4p^2+12p+34}}{2}$$

Let

$$E(i(G_n)) = Ap_1^n - Bp_2^n.$$

We know that

$$E(i(G_1)) = Ap_1 - Bp_2 = 18, E(i(G_2)) = Ap_1^2 - Bp_2^2 = 274.$$

Then

$$redA = \frac{274-18p_1}{p_2^2-p_1p_2}, B = \frac{274-18p_2}{p_1^2-p_1p_2}.$$

Finally, the result can be obtained. ■

Corollary 3.2. *The Merrifield-Simmons index of linear phenylene chain* L_n *is*

$$i(L_n) = \frac{192-29\sqrt{34}}{2\sqrt{34}}(6+\sqrt{34})^n - \frac{192+29\sqrt{34}}{2\sqrt{34}}(6-\sqrt{34})^n,$$

and the Merrifield-Simmons index of all-kinky phenylene chain P_n is

$$i(P_n) = \frac{149-11\sqrt{41}}{8\sqrt{41}}(7+\sqrt{41})^n - \frac{149+11\sqrt{41}}{8\sqrt{41}}(7-\sqrt{41})^n.$$

Proof. From (27), when $p = 0$ and $p = \frac{1}{2}$, respectively, we can get results. ■

4. THE AVERAGE VALUES OF THE MERRIFIELD-SIMMONS INDEX OF A RANDOM PHENYLENE CHAIN

Let $\mathcal{G}_n$ be the set of all phenylene chain with n hexagons. The average value of the Merrifield-Simmons index with respect to $\mathcal{G}_n$ is

$$i_{avr}(\mathcal{G}_n) = \frac{1}{|\mathcal{G}_n|}\sum_{G\in\mathcal{G}_n} i(G).$$

In order to obtain the average value $i_{avr}(\mathcal{G}_n)$, we only need to take $p = \frac{1}{3}$ in the expected value $E(i(G_n))$. From Theorem 3.1, we have

Theorem 4.1. *The average value of the Merrifield-Simmons index with respect to $\mathcal{G}_n$ is*

$$i_{avr}(\mathcal{G}_n) = \frac{502-17\sqrt{346}}{6\sqrt{346}}\left(\frac{20+\sqrt{346}}{3}\right)^n - \frac{502+17\sqrt{346}}{6\sqrt{346}}\left(\frac{20-\sqrt{346}}{3}\right)^n.$$

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