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The Expected Value of Hosoya Index and Merrifield–Simmons Index in a Random Cyclooctylene Chain

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Abstract: The Hosoya index $m(G)$ and the Merrifield–Simmons index $i(G)$ of a graph G are the number of matchings and the number of independent sets in G. In this paper, we establish exact formulas for the expected value of the Hosoya index and Merrifield–Simmons index of the random cyclooctylene chains, which are graphs of a chemical chain consisting of n octagons, each of which is connected to the end of the previous octagon by an edge. In addition, we obtain the expected values and the average values of the two indexes through the relevant chemical diagrams and a series of accurate formulas with respect to the set of all cyclooctylene chains with n octagons.

Keywords: expected value; hosoya index; Merrifield–Simmons index; random cyclooctylene chain

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1. Introduction

Cyclooctylene and its derivatives have attracted the attention of chemists for many years, and have extensive industrial applications [1–4]. Cyclooctylene is an organic compound, fully known as "1, 3, 5, 7-cyclooctylene", which is a completely unsaturated derivative of cyclooctane. It is a colorless to golden liquid at room temperature. It belongs to cyclic polyolefin and its structure is similar to that of benzene. Unlike benzene, cyclooctylene is not aromatic. Its chemical properties are similar to those of unsaturated hydrocarbons [4]. It can undergo addition reaction and is easy to hydrogenate to form cyclooctane. It is also easy to oxidize and polymerize. There are many important compounds of cyclooctylene, which serve as precursors to many scientifically and commercially interesting materials.

The Hosoya index was redefined by a chemist in 1971, it is a structure descriptor defined on the basis of a molecular diagram, the chemist also showed that some of the physical and chemical properties of the Hosoya index in chemistry are strongly related to alkanes (saturated hydrocarbons). In a series of subsequent papers, Hosoya et al. [5–12] and others [13] also showed that the Hosoya index is related to a variety of physicochemical properties of alkanes. A series of other studies on this index have shown that the Hosoya index also has a wide applicability in the theory of conjugated π-electron systems [9,14–22]. In addition, the development of the Merrifield–Simmons index began with an unsuccessful theory in 1980—in this year, the chemists Merrifield and Simmons elaborated a theory aimed at describing molecular structure by means of finite-set topology, although not for the better at the time, but the topological formalism attracted the attention of colleagues and eventually became known as the Merrifield–Simmons index. This was the number of open sets of the finite topology, which is equal to the number of independent sets of vertices of the graph corresponding to that topology [23], and a series of articles [20,24–26] were published. The Hosoya index and the Merrifield–Simmons index are very popular in the development of combinatorial chemistry, and often used in mathematical chemistry as a typical example to demonstrate relevant conclusions. In recent years, a lot of research has been conducted on the extremal problem for these two indices. For a survey of results and techniques related to the Hosoya index and the Merrifield–Simmons index, see Wagner and Gutman [27]. For recent works along these lines see Andriatiana [28], Hosoya [29], Luthe et al. [30].

In this paper, we are going to give a series of explicit formulas for the expected values of the Hosoya index (i.e., the number of matchings) and the Merrifield-Simmons index (i.e., the number of independent sets) of a random cyclooctylene chain [31–34] and enrich the conclusions of Huang Kuang and Deng. In addition, we reach the average values of the two indexes with respect to the set of all cyclooctylene chains with n octagons [27,29,35].

All graphs mentioned in this paper are considered finite and simple graphs. We use $G = (V(G), E(G))$ to represent a graph, then the vertex set is represented by $V(G)$ and the edge set is represented by $E(G)$. According to the descriptions in these three men's (Guihua Huang, Meijun Kuang and Hanyuan Deng [29]) previous papers, we can know for a vertex $u \in V$, $G - u$ is the graph induced by $V - \{u\}$. For an edge $e \in E$, $G - e$ is the graph obtained from G by deleting the edge e. $N(v) = \{u|uv \in E\}$ denotes the neighbors of v in G, and $N_G[v] = \{v\} \cup N(v)$ is the closed neighborhood of v.

The set of edges in a graph G is called a matching M such that two edges from M have a vertex in common [36–38]. The size of a graph can be determined by the number of edges of M. Let us denote by $m_k(G)$ the number of matchings of size k in G. Obviously, $m_0(G) = 1$, $m_1(G) = |E|$. The total number of matchings in G is denoted by $m(G) = \sum_{k\geqslant 0} m_k(G)$. A set $S \subseteq V$ of vertices of G is an independent set in G if no two vertices of S are adjacent. $i_k(G)$ denotes the number of independent sets in G with k vertices. Clearly, $i_0(G) = 1$ and $i_1(G) = |V|$. The total number of independent sets in G is denoted by $i(G) = \sum_{k\geqslant 0} i_k(G)$. In chemical literature, the Hosoya index and the Merrifield–Simmons index are usually represented by $m(G)$ and $i(G)$ [39,40].

The following results belong to the mathematical folklore and will be used in the computations:

(i) Gutman and Polansky [41]: If uv is an edge of G, then
$$m(G) = m(G - uv) + m(G - \{u, v\}). \tag{1}$$
(ii) Gutman and Polansky [41]: If v is a vertex of G, then
$$i(G) = i(G - v) + i(G - N_G(v)). \tag{2}$$
(iii) Gutman and Polansky [41]: If G is a graph with components $G_1, G_2, \cdots, G_k$, then
$$m(G) = \prod_{i=1}^{k} m(G_i),\ i(G) = \prod_{i=1}^{k} i(G_i). \tag{3}$$
(iv) $m(P_2) = 2, m(P_3) = 3, m(P_4) = 5, m(P_5) = 8, m(P_6) = 13, m(P_7) = 21$ and $m(C_8) = 47$;
(v) $i(P_1) = 2, i(P_2) = 3, i(P_3) = 5, i(P_4) = 8, i(P_5) = 13, i(P_6) = 21, i(P_7) = 34$ and $i(C_8) = 47$

where P_n is the path on n vertices and C_n is the cycle on n vertices.

The graph discussed in this article is a connected graph in which no edge is contained in more than one cycle. A cyclooctylene in which no octagon has more than two cut-vertices is called a cyclooctylene chain. Obviously, each cyclooctylene chain contains exactly two octagons with only one cut-vertex. Those octagons are called terminal, all other octagons are internal. The number of octagons in a given cyclooctylene chain is called its length. Additionally, a cyclooctylene chain G_n with n octagons can be regarded as an octagonal chain G_{n-1} with $n - 1$ octagons to which a new terminal octagon has been adjoined by an edge, see Figure 1.

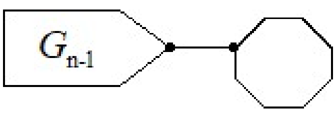

Figure 1. A cyclooctylene chain G_n with n octagons.

For $n \geqslant 3$, the final octagon can be joined in four manners, these connections can be represented by the following symbols: $G_n^1, G_n^2, G_n^3, G_n^4$, see Figure 2.

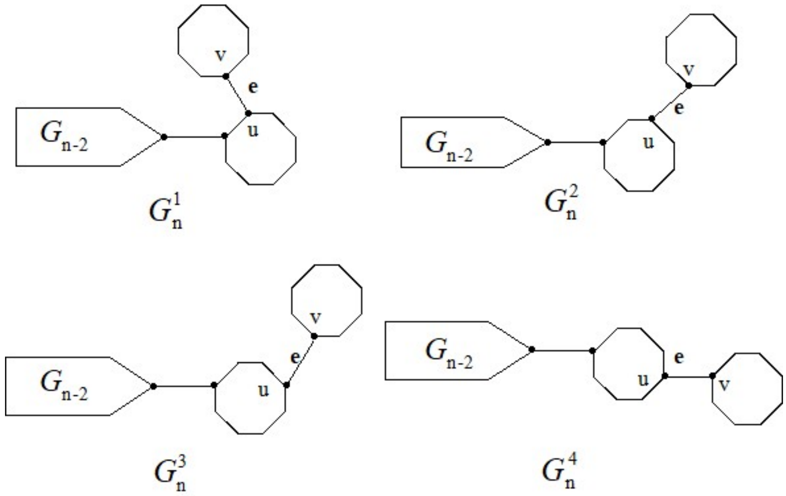

Figure 2. The four types of local arrangements in cyclooctylene chains.

A random cyclooctylene chain $G_n(p_1, p_2, p_3)$ with n octagons, it is formed by continuing to join the octagons at the end of the last octagon in a cyclooctylene chain. At each step $k(=3, 4, \cdots, n)$, there are four different possible ways to connect, as shown below:

$$G_{k-1} \longrightarrow G_k^1 \quad \textit{with probability } p_1;$$

$$G_{k-1} \longrightarrow G_k^2 \quad \textit{with probability } p_2;$$

$$G_{k-1} \longrightarrow G_k^3 \quad \textit{with probability } p_3.$$

$$G_{k-1} \longrightarrow G_k^4 \quad \textit{with probability } p_4 = 1 - p_1 - p_2 - p_3$$

where the probabilities p_1, p_2, p_3 are constants, irrelative to the step parameter k.

Specially, G_n is the ortho-chain O_n, the meta-chain M_n' M_n'' and the para-chain L_n for $p_1 = 1, p_2 = 1, p_3 = 1$ and $p_4 = 1$, respectively.

2. The Expected Value of the Hosoya Index of a Random Cyclooctylene Chain

According to the description in the previous section, the octagonal chain $G_n(p_1, p_2, p_3)$ is obtained at random by attaching G_{n-1}, a new terminal octagon from one of the four possible constructions. This connection method is called a zeroth-order Markov Process. For $G_n(p_1, p_2, p_3)$, the Hosoya index is a random variable. In the second argument section, we are going to obtain a simple exact formula of its expected value $E(m(G_n(p_1, p_2, p_3)))$. There are four types of auxiliary random graphs A_k, B_k, C_k and D_k, where $A_k \in \{A_k^1, A_k^2, A_k^3, A_k^4\}$, $B_k \in \{B_k^1, B_k^2, B_k^3, B_k^4\}$, $C_k \in \{C_k^1, C_k^2, C_k^3, C_k^4\}$ and $D_k \in \{D_k^1, D_k^2, D_k^3, D_k^4\}$ shown in Figure 3.

(I) If $G_n = G_n^1$ in Figure 2, then by Equations (1) and (3),

(i) If $A_{n-2} = A_{n-2}^1$ in Figure 3, then by Equations (1) and (3),

$$m(A_{n-2}) = m(A_{n-2} - e) + m(A_{n-2} - \{u, v\}) = m(P_7)m(G_{n-2}) + m(P_6)m(A_{n-3}) = 21m(G_{n-2}) + 13m(A_{n-3}).$$

Similarly, we have:

(ii) If $A_{n-2} = A_{n-2}^2$, then

$$m(A_{n-2}) = m(P_7)m(G_{n-2}) + m(P_6)m(B_{n-3}) = 21m(G_{n-2}) + 13m(B_{n-3}).$$

(iii) If $A_{n-2} = A_{n-2}^3$, then

$$m(A_{n-2}) = m(P_7)m(G_{n-2}) + m(P_6)m(C_{n-3}) = 21m(G_{n-2}) + 13m(C_{n-3}).$$

(iv) If $A_{n-2} = A_{n-2}^4$, then

$$m(A_{n-2}) = m(P_7)m(G_{n-2}) + m(P_6)m(D_{n-3}) = 21m(G_{n-2}) + 13m(D_{n-3}).$$

(II) If $G_n = G_n^2$ in Figure 2, then by Equations (1) and (3),

$$m(G_n) = m(G_n - e) + m(G_n - \{u,v\}) = m(C_8)m(G_{n-1}) + m(P_7)m(B_{n-2}) = 47m(G_{n-1}) + 21m(B_{n-2}).$$

(i) If $B_{n-2} = B^1_{n-2}$ in Figure 3, then by Equations (1) and (3),

$$m(B_{n-2}) = m(B_{n-2} - e) + m(B_{n-2} - \{u,v\}) = m(P_7)m(G_{n-2}) + m(P_5)m(A_{n-3}) = 21m(G_{n-2}) + 8m(A_{n-3}).$$

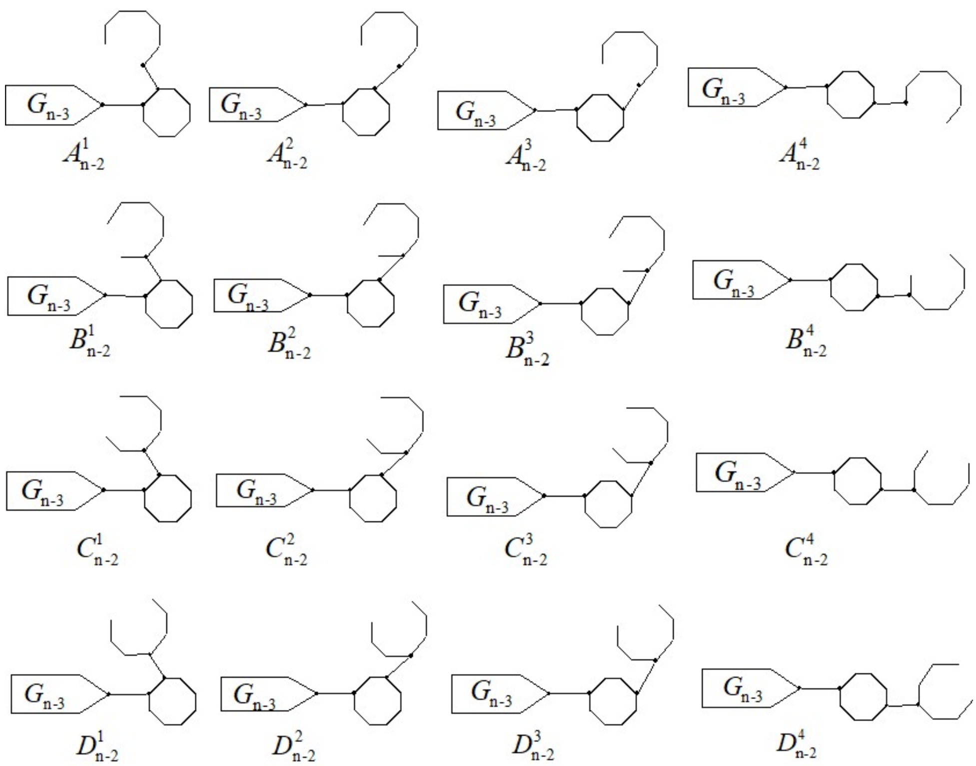

Figure 3. The four types of auxiliary graphs.

Similarly, we have:

(ii) If $B_{n-2} = B^2_{n-2}$, then
$$m(B_{n-2}) = m(P_7)m(G_{n-2}) + m(P_5)m(B_{n-3}) = 21m(G_{n-2}) + 8m(B_{n-3}).$$

(iii) If $B_{n-2} = B^3_{n-2}$, then
$$m(B_{n-2}) = m(P_7)m(G_{n-2}) + m(P_5)m(C_{n-3}) = 21m(G_{n-2}) + 8m(C_{n-3}).$$

(iv) If $B_{n-2} = B^4_{n-2}$, then
$$m(B_{n-2}) = m(P_7)m(G_{n-2}) + m(P_5)m(D_{n-3}) = 21m(G_{n-2}) + 8m(D_{n-3}).$$

(III) If $G_n = G^3_n$ in Figure 2, then by Equations (1) and (3),

$$m(G_n) = m(G_n - e) + m(G_n - \{u,v\}) = m(C_8)m(G_{n-1}) + m(P_7)m(C_{n-2}) = 47m(G_{n-1}) + 21m(C_{n-2}).$$

(i) If $C_{n-2} = C^1_{n-2}$ in Figure 3, then by Equations (1) and (3),

$$m(C_{n-2}) = m(C_{n-2} - e) + m(C_{n-2} - \{u,v\}) = m(P_7)m(G_{n-2}) + m(P_2)m(P_4)m(A_{n-3}) = 21m(G_{n-2}) + 10m(A_{n-3}).$$

Similarly, we have:

(ii) If $C_{n-2} = C^2_{n-2}$, then
$$m(C_{n-2}) = m(P_7)m(G_{n-2}) + m(P_2)m(P_4)m(B_{n-3}) = 21m(G_{n-2}) + 10m(B_{n-3}).$$

(iii) If $C_{n-2} = C^3_{n-2}$, then

$$m(C_{n-2}) = m(P_7)m(G_{n-2}) + m(P_2)m(P_4)m(C_{n-3}) = 21m(G_{n-2}) + 10m(C_{n-3}).$$

(iv) If $C_{n-2} = C_{n-2}^4$, then
$$m(C_{n-2}) = m(P_7)m(G_{n-2}) + m(P_2)m(P_4)m(D_{n-3}) = 21m(G_{n-2}) + 10m(D_{n-3}).$$

(IV) If $G_n = G_n^4$ in Figure 2, then by Equations (1) and (3),

$$m(G_n) = m(G_n - e) + m(G_n - \{u, v\}) = m(C_8)m(G_{n-1}) + m(P_7)m(D_{n-2}) = 47m(G_{n-1}) + 21m(D_{n-2}).$$

(i) If $D_{n-2} = D_{n-2}^1$ in Figure 3, then by Equations (1) and (3),

$$m(D_{n-2}) = m(D_{n-2} - e) + m(D_{n-2} - \{u, v\}) = m(P_7)m(G_{n-2}) + m(P_3)m(P_3)m(A_{n-3}) = 21m(G_{n-2}) + 9m(A_{n-3}).$$

Similarly, we have:

(ii) If $D_{n-2} = D_{n-2}^2$, then
$$m(D_{n-2}) = m(P_7)m(G_{n-2}) + m(P_3)m(P_3)m(B_{n-3}) = 21m(G_{n-2}) + 9m(B_{n-3}).$$

(iii) If $D_{n-2} = D_{n-2}^3$, then
$$m(D_{n-2}) = m(P_7)m(G_{n-2}) + m(P_3)m(P_3)m(C_{n-3}) = 21m(G_{n-2}) + 9m(C_{n-3}).$$

(iv) If $D_{n-2} = D_{n-2}^4$, then
$$m(D_{n-2}) = m(P_7)m(G_{n-2}) + m(P_3)m(P_3)m(D_{n-3}) = 21m(G_{n-2}) + 9m(D_{n-3}).$$

Note that $p_1 + p_2 + p_3 + p_4 = 1$, using the formulas in (I) to (IV), we can obtain the expected value $E(m(G_n))\ of\ m(G_n)$.

$E(m(G_n)) = p_1E(m(G_n^1)) + p_2E(m(G_n^2)) + p_3E(m(G_n^3)) + p_4E(m(G_n^4))$. Then,

$$\begin{aligned}
E(m(G_n^1)) &= 47E(m(G_{n-1})) + 21E(m(A_{n-2})) \\
&= 47E(m(G_{n-1})) + 21[21p_1E(m(G_{n-2})) + 13p_1E(m(A_{n-3})) \\
&\quad +21p_2E(m(G_{n-2})) + 13p_2E(m(B_{n-3})) + 21p_3E(m(G_{n-2})) \\
&\quad +13p_3E(m(C_{n-3})) + 21p_4E(m(G_{n-2})) + 13p_4E(m(D_{n-3}))] \\
&= 47E(m(G_{n-1})) + 441E(m(G_{n-2})) + 273p_1E(m(A_{n-3})) \\
&\quad +273p_2E(m(B_{n-3})) + 273p_3E(m(C_{n-3})) + 273p_4E(m(D_{n-3})). \\
E(m(G_n^2)) &= 47E(m(G_{n-1})) + 21E(m(B_{n-2})) \\
&= 47E(m(G_{n-1})) + 21[21p_1E(m(G_{n-2})) + 8p_1E(m(A_{n-3})) \\
&\quad +21p_2E(m(G_{n-2})) + 8p_2E(m(B_{n-3})) + 21p_3E(m(G_{n-2})) \\
&\quad +8p_3E(m(C_{n-3})) + 21p_4E(m(G_{n-2})) + 8p_4E(m(D_{n-3}))] \\
&= 47E(m(G_{n-1})) + 441E(m(G_{n-2})) + 168p_1E(m(A_{n-3})) \\
&\quad +168p_2E(m(B_{n-3})) + 168p_3E(m(C_{n-3})) + 168p_4E(m(D_{n-3})).
\end{aligned}$$

$$\begin{aligned}
E(m(G_n^3)) &= 47E(m(G_{n-1})) + 21E(m(C_{n-2})) \\
&\quad a + 21p_2E(m(G_{n-2})) + 10p_2E(m(B_{n-3})) + 21p_3E(m(G_{n-2})) \\
&\quad +10p_3E(m(C_{n-3})) + 21p_4E(m(G_{n-2})) + 10p_4E(m(D_{n-3}))] \\
&= 47E(m(G_{n-1})) + 441E(m(G_{n-2})) + 210p_1E(m(A_{n-3})) \\
&\quad +210p_2E(m(B_{n-3})) + 210p_3E(m(C_{n-3})) + 210p_4E(m(D_{n-3})). \\
E(m(G_n^4)) &= 47E(m(G_{n-1})) + 21E(m(D_{n-2})) \\
&= 47E(m(G_{n-1})) + 21[21p_1E(m(G_{n-2})) + 9p_1E(m(A_{n-3})) \\
&\quad +21p_2E(m(G_{n-2})) + 9p_2E(m(B_{n-3})) + 21p_3E(m(G_{n-2})) \\
&\quad +9p_3E(m(C_{n-3})) + 21p_4E(m(G_{n-2})) + 9p_4E(m(D_{n-3}))] \\
&= 47E(m(G_{n-1})) + 441E(m(G_{n-2})) + 189p_1E(m(A_{n-3})) \\
&\quad +189p_2E(m(B_{n-3})) + 189p_3E(m(C_{n-3})) + 189p_4E(m(D_{n-3})).
\end{aligned}$$

$$\begin{aligned}
E(m(G_n)) &= 47E(m(G_{n-1})) + 441E(m(G_{n-2})) \\
&\quad +(273p_1^2 + 168p_1p_2 + 210p_1p_3 + 189p_1p_4)E(m(A_{n-3})) \\
&\quad +(273p_1p_2 + 168p_2^2 + 210p_2p_3 + 189p_2p_4)E(m(B_{n-3})) \\
&\quad +(273p_1p_3 + 168p_2p_3 + 210p_3^2 + 189p_3p_4)E(m(C_{n-3})) \\
&\quad +(273p_1p_4 + 168p_2p_4 + 210p_3p_4 + 189p_4^2)E(m(D_{n-3})).
\end{aligned} \tag{4}$$

Similarly, we can obtain the expected values $E(m(A_{n-3}))$ of $m(A_{n-3})$, $E(m(B_{n-3}))$ of $m(B_{n-3})$, $E(m(C_{n-3}))$ of $m(C_{n-3})$ and $E(m(D_{n-3}))$ of $m(D_{n-3})$,

$$\begin{aligned} E(m(A_{n-3})) &= p_1E(m(A^1_{n-3})) + p_2E(m(A^2_{n-3})) + p_3E(m(A^3_{n-3})) + p_4E(m(A^4_{n-3})) \\ &= 21p_1E(m(G_{n-3})) + 13p_1E(m(A_{n-4})) + 21p_2E(m(G_{n-3})) + 13p_2E(m(B_{n-4})) \\ &\quad +21p_3E(m(G_{n-3})) + 13p_3E(m(C_{n-4})) + 21p_4E(m(G_{n-3})) + 13p_4E(m(D_{n-4})) \\ &= 21E(m(G_{n-3})) + 13p_1E(m(A_{n-4})) + 13p_2E(m(B_{n-4})) + 13p_3E(m(C_{n-4})) + 13p_4E(m(D_{n-4})). \end{aligned} \tag{5}$$

$$\begin{aligned} E(m(B_{n-3})) &= p_1E(m(B^1_{n-3})) + p_2E(m(B^2_{n-3})) + p_3E(m(B^3_{n-3})) + p_4E(m(B^4_{n-3})) \\ &= 21E(m(G_{n-3})) + 8p_1E(m(A_{n-4})) + 8p_2E(m(B_{n-4})) + 8p_3E(m(C_{n-4})) + 8p_4E(m(D_{n-4})). \end{aligned} \tag{6}$$

$$\begin{aligned} E(m(C_{n-3})) &= p_1E(m(C^1_{n-3})) + p_2E(m(C^2_{n-3})) + p_3E(m(C^3_{n-3})) + p_4E(m(C^4_{n-3})) \\ &= 21E(m(G_{n-3})) + 10p_1E(m(A_{n-4})) + 10p_2E(m(B_{n-4})) + 10p_3E(m(C_{n-4})) + 10p_4E(m(D_{n-4})). \end{aligned} \tag{7}$$

$$\begin{aligned} E(m(D_{n-3})) &= p_1E(m(D^1_{n-3})) + p_2E(m(D^2_{n-3})) + p_3E(m(D^3_{n-3})) + p_4E(m(D^4_{n-3})) \\ &= 21E(m(G_{n-3})) + 9p_1E(m(A_{n-4})) + 9p_2E(m(B_{n-4})) + 9p_3E(m(C_{n-4})) + 9p_4E(m(D_{n-4})). \end{aligned} \tag{8}$$

From Equations (4), (5), (6), (7) and (8), respectively, we have

$$\begin{aligned} &(273p_1^2 + 168p_1p_2 + 210p_1p_3 + 189p_1p_4)E(m(A_{n-3})) \\ =\ & 21(273p_1^2 + 168p_1p_2 + 210p_1p_3 + 189p_1p_4)E(m(G_{n-3})) \\ & +13p_1(273p_1^2 + 168p_1p_2 + 210p_1p_3 + 189p_1p_4)E(m(A_{n-4})) \\ & +13p_2(273p_1^2 + 168p_1p_2 + 210p_1p_3 + 189p_1p_4)E(m(B_{n-4})) \\ & +13p_3(273p_1^2 + 168p_1p_2 + 210p_1p_3 + 189p_1p_4)E(m(C_{n-4})) \\ & +13p_4(273p_1^2 + 168p_1p_2 + 210p_1p_3 + 189p_1p_4)E(m(D_{n-4})) \\ =\ & 21(273p_1^2 + 168p_1p_2 + 210p_1p_3 + 189p_1p_4)E(m(G_{n-3})) \\ & +13p_1(273p_1^2 + 168p_1p_2 + 210p_1p_3 + 189p_1p_4)E(m(A_{n-4})) \\ & +13p_1(273p_1p_2 + 168p_2^2 + 210p_2p_3 + 189p_2p_4)E(m(B_{n-4})) \\ & +13p_1(273p_1p_3 + 168p_2p_3 + 210p_3^2 + 189p_3p_4)E(m(C_{n-4})) \\ & +13p_1(273p_1p_4 + 168p_2p_4 + 210p_3p_4 + 189p_4^2)E(m(D_{n-4})) \\ =\ & 21(273p_1^2 + 168p_1p_2 + 210p_1p_3 + 189p_1p_4)E(m(G_{n-3})) \\ & +13p_1[E(m(G_{n-1})) - 47E(m(G_{n-2})) - 441E(m(G_{n-3}))]. \end{aligned}$$

$$\begin{aligned} &(273p_1p_2 + 168p_2^2 + 210p_2p_3 + 189p_2p_4)E(m(B_{n-3})) \\ =\ & 21(273p_1p_2 + 168p_2^2 + 210p_2p_3 + 189p_2p_4)E(m(G_{n-3})) \\ & +8p_2[E(m(G_{n-1})) - 47E(m(G_{n-2})) - 441E(m(G_{n-3}))]. \\ &(273p_1p_3 + 168p_2p_3 + 210p_3^2 + 189p_3p_4)E(m(C_{n-3})) \\ =\ & 21(273p_1p_3 + 168p_2p_3 + 210p_3^2 + 189p_3p_4)E(m(G_{n-3})) \\ & +10p_3[E(m(G_{n-1})) - 47E(m(G_{n-2})) - 441E(m(G_{n-3}))]. \\ &(273p_1p_4 + 168p_2p_4 + 210p_3p_4 + 189p_4^2)E(m(D_{n-3})) \\ =\ & 21(273p_1p_4 + 168p_2p_4 + 210p_3p_4 + 189p_4^2)E(m(G_{n-3})) \\ & +9p_4[E(m(G_{n-1})) - 47E(m(G_{n-2})) - 441E(m(G_{n-3}))]. \end{aligned}$$

Substituting these formulas into Equations (4), we have

$$\begin{aligned} E(m(G_n)) &= 47E(m(G_{n-1})) + 441E(m(G_{n-2})) + [21(273p_1^2 + 168p_1p_2 + 210p_1p_3 + 189p_1p_4) \\ &\quad +21(273p_1p_2 + 168p_2^2 + 210p_2p_3 + 189p_2p_4) + 21(273p_1p_3 + 168p_2p_3 + 210p_3^2 + 189p_3p_4) \\ &\quad +21(273p_1p_4 + 168p_2p_4 + 210p_3p_4 + 189p_4^2)]E(m(D_{n-3})) + (13p_1 + 8p_2 + 10p_3 + 9p_4) \\ &\quad \times[E(m(G_{n-1})) - 47E(m(G_{n-2})) - 441E(m(G_{n-3}))] \\ &= (4p_1 - p_2 + p_3 + 56)E(m(G_{n-1})) - (188p_1 - 47p_2 + 47p_3 - 18)E(m(G_{n-2})). \\ &\quad (since\ p_4 = 1 - p_1 - p_2 - p_3). \end{aligned} \tag{9}$$

A recurrence relation for the expected value of the Hosoya index of a random cyclooctylene chain is obtained

$$E(m(G_n)) = (4p_1 - p_2 + p_3 + 56)E(m(G_{n-1})) - (188p_1 - 47p_2 + 47p_3 - 18)E(m(G_{n-2})).$$

The boundary condition is
$E(m(G_1)) = m(C_8) = 47, \quad E(m(G_2)) = 3150$ (According to the Figure 4).

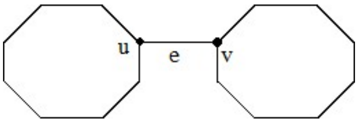

Figure 4. Special graph.

Using the above recurrence relation and the boundary conditions, we have

Theorem 1. *The expected value of the Hosoya index of a random cyclooctylene chain $G_n(p_1, p_2, p_3)$ is*

$$E(m(G_n)) = \frac{-4p_1 + p_2 - p_3 + 38 + \sqrt{(4p_1 - p_2 + p_3 - 38)^2 + 1764}}{2\sqrt{(4p_1 - p_2 + p_3 - 38)^2 + 1764}} \times \left(\frac{4p_1 - p_2 + p_3 + 56 + \sqrt{(4p_1 - p_2 + p_3 - 38)^2 + 1764}}{2}\right)^n + \frac{4p_1 - p_2 + p_3 - 38 + \sqrt{(4p_1 - p_2 + p_3 - 38)^2 + 1764}}{2\sqrt{(4p_1 - p_2 + p_3 - 38)^2 + 1764}} \times \left(\frac{4p_1 - p_2 + p_3 + 56 - \sqrt{(4p_1 - p_2 + p_3 - 38)^2 + 1764}}{2}\right)^n.$$

Let $p_1 = 1, p_2 = 1, p_3 = 1$ and $p_1 = p_2 = p_3 = 0, p_4 = 1$, respectively, we can obtain the Hosoya indices of the ortho-chain O_n, the meta-chain M'_n M''_n and the para-chain L_n from Theorem 1.

Corollary 1.

$$m(O_n) = \frac{17 + \sqrt{730}}{2\sqrt{730}} \times (30 + \sqrt{730})^n + \frac{-17 + \sqrt{730}}{2\sqrt{730}} \times (30 - \sqrt{730})^n;$$

$$m(M'_n) = \frac{13 + \sqrt{365}}{2\sqrt{365}} \times \left(\frac{55 + 3\sqrt{365}}{2}\right)^n + \frac{-13 + \sqrt{365}}{2\sqrt{365}} \times \left(\frac{55 - 3\sqrt{365}}{2}\right)^n;$$

$$m(M''_n) = \frac{37 + \sqrt{3133}}{2\sqrt{3133}} \times \left(\frac{57 + \sqrt{3133}}{2}\right)^n + \frac{-37 + \sqrt{3133}}{2\sqrt{3133}} \times \left(\frac{57 - \sqrt{3133}}{2}\right)^n;$$

$$m(L_n) = \frac{19 + \sqrt{802}}{2\sqrt{802}} \times (28 + \sqrt{802})^n + \frac{-19 + \sqrt{802}}{2\sqrt{802}} \times (28 - \sqrt{802})^n.$$

3. The Expected Value of the Merrifield–Simmons Index of a Random Cyclooctylene Chain

In this section, we will present a simple exact formula of its expected value $E(i(G_n(p_1, p_2, p_3)))$.

(I) If $G_n = G_n^1$ in Figure 2, then by Equations (2) and (3),

$$i(G_n) = i(G_n - v) + i(G_n - N[v]) = i(P_7)i(G_{n-1}) + i(P_5)i(A_{n-2}) = 34i(G_{n-1}) + 13i(A_{n-2}).$$

(i) If $A_{n-2} = A_{n-2}^1$ in Figure 3, then by Equations (2) and (3),

$$i(A_{n-2}) = i(P_6)i(G_{n-2}) + i(P_5)i(A_{n-3}) = 21i(G_{n-2}) + 13i(A_{n-3}).$$

Similarly, we have:

(ii) If $A_{n-2} = A_{n-2}^2$, then

$$i(A_{n-2}) = i(P_6)i(G_{n-2}) + i(P_5)i(B_{n-3}) = 21i(G_{n-2}) + 13i(B_{n-3}).$$

(iii) If $A_{n-2} = A^3_{n-2}$, then
$$i(A_{n-2}) = i(P_6)i(G_{n-2}) + i(P_5)i(C_{n-3}) = 21i(G_{n-2}) + 13i(C_{n-3}).$$
(iv) If $A_{n-2} = A^4_{n-2}$, then
$$i(A_{n-2}) = i(P_6)i(G_{n-2}) + i(P_5)i(D_{n-3}) = 21i(G_{n-2}) + 13i(D_{n-3}).$$
(II) If $G_n = G^2_n$ in Figure 2, then by Equations (2) and (3),
$$i(G_n) = i(G_n - v) + i(G_n - N[v]) = i(P_7)i(G_{n-1}) + i(P_5)i(B_{n-2}) = 34i(G_{n-1}) + 13i(B_{n-2}).$$
(i) If $B_{n-2} = B^1_{n-2}$ in Figure 3, then by Equations (2) and (3),
$$i(B_{n-2}) = i(P_1)i(P_5)i(G_{n-2}) + i(P_4)i(A_{n-3}) = 26i(G_{n-2}) + 8i(A_{n-3}).$$
Similarly, we have:

(ii) If $B_{n-2} = B^2_{n-2}$, then
$$i(B_{n-2}) = i(P_1)i(P_5)i(G_{n-2}) + i(P_4)i(B_{n-3}) = 26i(G_{n-2}) + 8i(B_{n-3}).$$
(iii) If $B_{n-2} = B^3_{n-2}$, then
$$i(B_{n-2}) = i(P_1)i(P_5)i(G_{n-2}) + i(P_4)i(C_{n-3}) = 26i(G_{n-2}) + 8i(C_{n-3}).$$
(iv) If $B_{n-2} = B^4_{n-2}$, then
$$i(B_{n-2}) = i(P_1)i(P_5)i(G_{n-2}) + i(P_4)i(D_{n-3}) = 26i(G_{n-2}) + 8i(D_{n-3}).$$
(III) If $G_n = G^3_n$ in Figure 2, then by Equations (1.2) and (1.3),
$$i(G_n) = i(G_n - v) + i(G_n - N[v]) = i(P_7)i(G_{n-1}) + i(P_5)i(C_{n-2}) = 34i(G_{n-1}) + 13i(C_{n-2}).$$
(i) If $C_{n-2} = C^1_{n-2}$ in Figure 3, then by Equations (2) and (3),
$$i(C_{n-2}) = i(P_2)i(P_4)i(G_{n-2}) + i(P_1)i(P_3)i(A_{n-3}) = 24i(G_{n-2}) + 10i(A_{n-3}).$$
Similarly, we have:

(ii) If $C_{n-2} = C^2_{n-2}$, then
$$i(C_{n-2}) = i(P_2)i(P_4)i(G_{n-2}) + i(P_1)i(P_3)i(B_{n-3}) = 24i(G_{n-2}) + 10i(B_{n-3}).$$
(iii) If $C_{n-2} = C^3_{n-2}$, then
$$i(C_{n-2}) = i(P_2)i(P_4)i(G_{n-2}) + i(P_1)i(P_3)i(C_{n-3}) = 24i(G_{n-2}) + 10i(C_{n-3}).$$
(iv) If $C_{n-2} = C^4_{n-2}$, then
$$i(C_{n-2}) = i(P_2)i(P_4)i(G_{n-2}) + i(P_1)i(P_3)i(D_{n-3}) = 24i(G_{n-2}) + 10i(D_{n-3}).$$
(IV) If $G_n = G^4_n$ in Figure 2, then by Equations (2) and (3),
$$i(G_n) = i(G_n - v) + i(G_n - N[v]) = i(P_7)i(G_{n-1}) + i(P_5)i(D_{n-2}) = 34i(G_{n-1}) + 13i(D_{n-2}).$$
(i) If $D_{n-2} = D^1_{n-2}$ in Figure 3, then by Equations (2) and (3),
$$i(D_{n-2}) = i(P_3)i(P_3)i(G_{n-2}) + i(P_2)i(P_2)i(A_{n-3}) = 25i(G_{n-2}) + 9i(A_{n-3}).$$
Similarly, we have:

(ii) If $D_{n-2} = D^2_{n-2}$, then
$$i(D_{n-2}) = i(P_3)i(P_3)i(G_{n-2}) + i(P_2)i(P_2)i(B_{n-3}) = 25i(G_{n-2}) + 9i(B_{n-3}).$$
(iii) If $D_{n-2} = D^3_{n-2}$, then
$$i(D_{n-2}) = i(P_3)i(P_3)i(G_{n-2}) + i(P_2)i(P_2)i(C_{n-3}) = 25i(G_{n-2}) + 9i(C_{n-3}).$$
(iv) If $D_{n-2} = D^4_{n-2}$, then
$$i(D_{n-2}) = i(P_3)i(P_3)i(G_{n-2}) + i(P_2)i(P_2)i(D_{n-3}) = 25i(G_{n-2}) + 9i(D_{n-3}).$$
Note that $p_1 + p_2 + p_3 + p_4 = 1$, using the formulas in (I) to (IV), we can get the expected value $E(i(G_n)) \ of \ i(G_n)$.

$E(i(G_n)) = p_1E(i(G_n^1)) + p_2E(i(G_n^2)) + p_3E(i(G_n^3)) + p_4E(i(G_n^4))$. Then,

$$\begin{aligned}
E(i(G_n^1)) &= 34E(i(G_{n-1})) + 13[21p_1E(i(G_{n-2})) + 13p_1E(i(A_{n-3})) \\
&\quad +21p_2E(i(G_{n-2})) + 13p_2E(i(B_{n-3})) + 21p_3E(i(G_{n-2})) \\
&\quad +13p_3E(i(C_{n-3})) + 21p_4E(i(G_{n-2})) + 13p_4E(i(D_{n-3}))] \\
&= 34E(i(G_{n-1})) + 273E(i(G_{n-2})) + 169p_1E(i(A_{n-3})) \\
&\quad +169p_2E(i(B_{n-3})) + 169p_3E(i(C_{n-3})) + 169p_4E(i(D_{n-3})). \\
E(i(G_n^2)) &= 34E(i(G_{n-1})) + 13[26p_1E(i(G_{n-2})) + 8p_1E(i(A_{n-3})) \\
&\quad +26p_2E(i(G_{n-2})) + 8p_2E(i(B_{n-3})) + 26p_3E(i(G_{n-2})) \\
&\quad +8p_3E(i(C_{n-3})) + 26p_4E(i(G_{n-2})) + 8p_4E(i(D_{n-3}))] \\
&= 34E(i(G_{n-1})) + 338E(i(G_{n-2})) + 104p_1E(i(A_{n-3})) \\
&\quad +104p_2E(i(B_{n-3})) + 104p_3E(i(C_{n-3})) + 104p_4E(i(D_{n-3})).
\end{aligned}$$

$$\begin{aligned}
E(i(G_n^3)) &= 34E(i(G_{n-1})) + 13[24p_1E(i(G_{n-2})) + 10p_1E(i(A_{n-3})) \\
&\quad +24p_2E(i(G_{n-2})) + 10p_2E(i(B_{n-3})) + 24p_3E(i(G_{n-2})) \\
&\quad +10p_3E(i(C_{n-3})) + 24p_4E(i(G_{n-2})) + 10p_4E(i(D_{n-3}))] \\
&= 34E(i(G_{n-1})) + 312E(i(G_{n-2})) + 130p_1E(i(A_{n-3})) \\
&\quad +130p_2E(i(B_{n-3})) + 130p_3E(i(C_{n-3})) + 130p_4E(i(D_{n-3})). \\
E(i(G_n^4)) &= 34E(i(G_{n-1})) + 13[25p_1E(i(G_{n-2})) + 9p_1E(i(A_{n-3})) \\
&\quad +25p_2E(i(G_{n-2})) + 9p_2E(i(B_{n-3})) + 25p_3E(i(G_{n-2})) \\
&\quad +9p_3E(i(C_{n-3})) + 25p_4E(i(G_{n-2})) + 9p_4E(i(D_{n-3}))] \\
&= 34E(i(G_{n-1})) + 325E(i(G_{n-2})) + 117p_1E(i(A_{n-3})) \\
&\quad +117p_2E(i(B_{n-3})) + 117p_3E(i(C_{n-3})) + 117p_4E(i(D_{n-3})).
\end{aligned}$$

$$\begin{aligned}
E(i(G_n)) &= 34E(i(G_{n-1})) + (273p_1 + 338p_2 + 312p_3 + 325p_4)E(i(G_{n-2})) \\
&\quad +(169p_1^2 + 104p_1p_2 + 130p_1p_3 + 117p_1p_4)E(i(A_{n-3})) \\
&\quad +(169p_1p_2 + 104p_2^2 + 130p_2p_3 + 117p_2p_4)E(i(B_{n-3})) \\
&\quad +(169p_1p_3 + 104p_2p_3 + 130p_3^2 + 117p_3p_4)E(i(C_{n-3})) \\
&\quad +(169p_1p_4 + 104p_2p_4 + 130p_3p_4 + 117p_4^2)E(i(D_{n-3})).
\end{aligned} \tag{10}$$

Similarly, we can obtain the expected values $E(i(A_{n-3}))$ of $i(A_{n-3})$, $E(i(B_{n-3}))$ of $i(B_{n-3})$, $E(i(C_{n-3}))$ of $i(C_{n-3})$ and $E(i(D_{n-3}))$ of $i(D_{n-3})$,

$$\begin{aligned}
E(i(A_{n-3})) &= p_1E(i(A_{n-3}^1)) + p_2E(i(A_{n-3}^2)) + p_3E(i(A_{n-3}^3)) + p_4E(i(A_{n-3}^4)) \\
&= p_1[21E(i(G_{n-3})) + 13E(i(A_{n-4}))] + p_2[21E(i(G_{n-3})) + 13E(i(B_{n-4}))] \\
&\quad +p_3[21E(i(G_{n-3})) + 13E(i(C_{n-4}))] + p_4[21E(i(G_{n-3})) + 13E(i(D_{n-4}))] \\
&= 21E(i(G_{n-3})) + 13p_1E(i(A_{n-4})) + 13p_2E(i(B_{n-4})) + 13p_3E(i(C_{n-4})) + 13p_4E(i(D_{n-4})).
\end{aligned} \tag{11}$$

$$\begin{aligned}
E(i(B_{n-3})) &= p_1E(i(B_{n-3}^1)) + p_2E(i(B_{n-3}^2)) + p_3E(i(B_{n-3}^3)) + p_4E(i(B_{n-3}^4)) \\
&= p_1[26E(i(G_{n-3})) + 8E(i(A_{n-4}))] + p_2[26E(i(G_{n-3})) + 8E(i(B_{n-4}))] \\
&\quad +p_3[26E(i(G_{n-3})) + 8E(i(C_{n-4}))] + p_4[26E(i(G_{n-3})) + 8E(i(D_{n-4}))] \\
&= 26E(i(G_{n-3})) + 8p_1E(i(A_{n-4})) + 8p_2E(i(B_{n-4})) + 8p_3E(i(C_{n-4})) + 8p_4E(i(D_{n-4})).
\end{aligned} \tag{12}$$

$$\begin{aligned}
E(i(C_{n-3})) &= p_1E(i(C_{n-3}^1)) + p_2E(i(C_{n-3}^2)) + p_3E(i(C_{n-3}^3)) + p_4E(i(C_{n-3}^4)) \\
&= p_1[24E(i(G_{n-3})) + 10E(i(A_{n-4}))] + p_2[24E(i(G_{n-3})) + 10E(i(B_{n-4}))] \\
&\quad +p_3[24E(i(G_{n-3})) + 10E(i(C_{n-4}))] + p_4[24E(i(G_{n-3})) + 10E(i(D_{n-4}))] \\
&= 24E(i(G_{n-3})) + 10p_1E(i(A_{n-4})) + 10p_2E(i(B_{n-4})) + 10p_3E(i(C_{n-4})) + 10p_4E(i(D_{n-4})).
\end{aligned} \tag{13}$$

$$\begin{aligned}
E(i(D_{n-3})) &= p_1E(i(D_{n-3}^1)) + p_2E(i(D_{n-3}^2)) + p_3E(i(D_{n-3}^3)) + p_4E(i(D_{n-3}^4)) \\
&= p_1[25E(i(G_{n-3})) + 9E(i(A_{n-4}))] + p_2[25E(i(G_{n-3})) + 9E(i(B_{n-4}))] \\
&\quad +p_3[25E(i(G_{n-3})) + 9E(i(C_{n-4}))] + p_4[25E(i(G_{n-3})) + 9E(i(D_{n-4}))] \\
&= 25E(i(G_{n-3})) + 9p_1E(i(A_{n-4})) + 9p_2E(i(B_{n-4})) + 9p_3E(i(C_{n-4})) + 9p_4E(i(D_{n-4})).
\end{aligned} \tag{14}$$

From Equations (10), (11), (12), (13) and (14), respectively, we have

$$
\begin{aligned}
&(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)E(i(A_{n-3}))\\
=\ & 21(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)E(i(G_{n-3}))\\
&+13p_1(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)E(i(A_{n-4}))\\
&+13p_2(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)E(i(B_{n-4}))\\
&+13p_3(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)E(i(C_{n-4}))\\
&+13p_4(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)E(i(D_{n-4}))\\
=\ & 21(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)E(i(G_{n-3}))\\
&+13p_1(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)E(i(A_{n-4}))\\
&+13p_1(169p_1p_2+104p_2^2+130p_2p_3+117p_2p_4)E(i(B_{n-4}))\\
&+13p_1(169p_1p_3+104p_2p_3+130p_3^2+117p_3p_4)E(i(C_{n-4}))\\
&+13p_1(169p_1p_4+104p_2p_4+130p_3p_4+117p_4^2)E(i(D_{n-4})).
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
&(169p_1p_2+104p_2^2+130p_2p_3+117p_2p_4)E(i(B_{n-3}))\\
=\ & 26(169p_1p_2+104p_2^2+130p_2p_3+117p_2p_4)E(i(G_{n-3}))\\
&+8p_2(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)E(i(A_{n-4}))\\
&+8p_2(169p_1p_2+104p_2^2+130p_2p_3+117p_2p_4)E(i(B_{n-4}))\\
&+8p_2(169p_1p_3+104p_2p_3+130p_3^2+117p_3p_4)E(i(C_{n-4}))\\
&+8p_2(169p_1p_4+104p_2p_4+130p_3p_4+117p_4^2)E(i(D_{n-4})).
\end{aligned}
$$

$$
\begin{aligned}
&(169p_1p_3+104p_2p_3+130p_3^2+117p_3p_4)E(i(C_{n-3}))\\
=\ & 24(169p_1p_3+104p_2p_3+130p_3^2+117p_3p_4)E(i(G_{n-3}))\\
&+10p_3(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)E(i(A_{n-4}))\\
&+10p_3(169p_1p_2+104p_2^2+130p_2p_3+117p_2p_4)E(i(B_{n-4}))\\
&+10p_3(169p_1p_3+104p_2p_3+130p_3^2+117p_3p_4)E(i(C_{n-4}))\\
&+10p_3(169p_1p_4+104p_2p_4+130p_3p_4+117p_4^2)E(i(D_{n-4})).\\
&(169p_1p_4+104p_2p_4+130p_3p_4+117p_4^2)E(i(D_{n-3}))\\
=\ & 25(169p_1p_4+104p_2p_4+130p_3p_4+117p_4^2)E(i(G_{n-3}))\\
&+9p_4(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)E(i(A_{n-4}))\\
&+9p_4(169p_1p_2+104p_2^2+130p_2p_3+117p_2p_4)E(i(B_{n-4}))\\
&+9p_4(169p_1p_3+104p_2p_3+130p_3^2+117p_3p_4)E(i(C_{n-4}))\\
&+9p_4(169p_1p_4+104p_2p_4+130p_3p_4+117p_4^2)E(i(D_{n-4})).
\end{aligned}
$$

Substituting these formulas into Equations (10), we have

$$
\begin{aligned}
E(i(G_n)) =\ & 34E(i(G_{n-1}))+(273p_1+338p_2+312p_3+325p_4)E(i(G_{n-2}))\\
&+[21(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)\\
&+26(169p_1p_2+104p_2^2+130p_2p_3+117p_2p_4)\\
&+24(169p_1p_3+104p_2p_3+130p_3^2+117p_3p_4)\\
&+25(169p_1p_4+104p_2p_4+130p_3p_4+117p_4^2)]E(i(D_{n-3}))\\
&+(13p_1+8p_2+10p_3+9p_4)[(169p_1^2+104p_1p_2+130p_1p_3+117p_1p_4)E(i(A_{n-4}))\\
&+(169p_1p_2+104p_2^2+130p_2p_3+117p_2p_4)E(i(B_{n-4}))\\
&+(169p_1p_3+104p_2p_3+130p_3^2+117p_3p_4)E(i(C_{n-4}))\\
&+(169p_1p_4+104p_2p_4+130p_3p_4+117p_4^2)E(i(D_{n-4}))]\\
=\ & (13p_1+8p_2+10p_3+9p_4+34)E(i(G_{n-1}))-(169p_1-66p_2+28p_3-19p_4)E(i(G_{n-2}))\\
=\ & (4p_1-p_2+p_3+43)E(i(G_{n-1}))-(188p_1-47p_2+47p_3-19)E(i(G_{n-2})).\\
& (since\ p_4=1-p_1-p_2-p_3).
\end{aligned}
$$

A recurrence relation for the expected value of the Merrifield–Simmons index of a random cyclooctylene chain is obtained

$E(i(G_n))=(4p_1-p_2+p_3+43)E(i(G_{n-1}))-(188p_1-47p_2+47p_3-19)E(i(G_{n-2}))$.

The boundary condition is

$E(i(G_1))=i(C_8)=47$, $\quad E(i(G_2))=2040$ (According to the Figure 4)

Using the above recurrence relation and the boundary conditions, we have

Theorem 2. *The expected value of the Merrifield–Simmons index of a random cyclooctylene chain $G_n(p_1, p_2, p_3)$ is*

$$\begin{aligned} E(i(G_n)) = & \frac{-4p_1 + p_2 - p_3 + 51 + \sqrt{(4p_1 - p_2 + p_3 - 51)^2 - 676}}{2\sqrt{(4p_1 - p_2 + p_3 - 51)^2 - 676}} \\ & \times (\frac{4p_1 - p_2 + p_3 + 43 + \sqrt{(4p_1 - p_2 + p_3 - 51)^2 - 676}}{2})^n \\ & + \frac{4p_1 - p_2 + p_3 - 51 + \sqrt{(4p_1 - p_2 + p_3 - 51)^2 - 676}}{2\sqrt{(4p_1 - p_2 + p_3 - 51)^2 - 676}} \\ & \times (\frac{4p_1 - p_2 + p_3 + 43 - \sqrt{(4p_1 - p_2 + p_3 - 51)^2 - 676}}{2})^n. \end{aligned}$$

Let $p_1 = 1, p_2 = 1, p_3 = 1$ and $p_1 = p_2 = p_3 = 0, p_4 = 1$, respectively, we can obtain the Merrifieid–Simmons indices of the ortho-chain O_n, the meta-chain M'_n M''_n and the para-chain L_n from Theorem 2.

Corollary 2.

$$\begin{aligned} i(O_n) &= \frac{1}{\sqrt{1533}}[(\frac{47 + \sqrt{1533}}{2})^{n+1} - (\frac{47 - \sqrt{1533}}{2})^{n+1}]; \\ i(M'_n) &= \frac{26 + \sqrt{507}}{2\sqrt{507}} \times (21 + \sqrt{507})^n + \frac{-26 + \sqrt{507}}{2\sqrt{507}} \times (21 - \sqrt{507})^n; \\ i(M''_n) &= \frac{25 + 2\sqrt{114}}{4\sqrt{114}} \times (22 + 2\sqrt{114})^n + \frac{-25 + 2\sqrt{114}}{4\sqrt{114}} \times (22 - 2\sqrt{114})^n; \\ i(L_n) &= \frac{51 + 5\sqrt{77}}{10\sqrt{77}} \times (\frac{43 + 5\sqrt{77}}{2})^n + \frac{-51 + 5\sqrt{77}}{10\sqrt{77}} \times (\frac{43 - 5\sqrt{77}}{2})^n. \end{aligned}$$

4. The Average Value of Hosoya Index and Merrifield–Simmons Index

Let ζ_n be the set of all cyclooctylene chains with n octagons. The average values of the Hosoya index and the Merrifield–Simmons index with respect to ζ_n are

$$m_{avr}(\zeta_n) = \frac{1}{|\zeta_n|} \sum_{G \in \zeta_n} m(G) \text{ and } i_{avr}(\zeta_n) = \frac{1}{|\zeta_n|} \sum_{G \in \zeta_n} i(G).$$

In order to obtain the average values $m_{avr}(\zeta_n)$ *and* $i_{avr}(\zeta_n)$, we only need to take $p_1 = p_2 = p_3 = p_4 = \frac{1}{4}$ in the expected values $E(m(G_n))$ *and* $E(i(G_n))$. From Theorems 1 and 2, we have

Theorem 3. *The average value of the Hosoya index and the Merrifield–Simmons index with respect to ζ_n are*

$$\begin{aligned} m_{avr}(\zeta_n) &= \frac{37 + \sqrt{3133}}{2\sqrt{3133}} \times (\frac{57 + \sqrt{3133}}{2})^n + \frac{-37 + \sqrt{3133}}{2\sqrt{3133}} \times (\frac{57 - \sqrt{3133}}{2})^n; \\ i_{avr}(\zeta_n) &= \frac{25 + 2\sqrt{114}}{4\sqrt{114}} \times (22 + 2\sqrt{114})^n + \frac{-25 + 2\sqrt{114}}{4\sqrt{114}} \times (22 - 2\sqrt{114})^n. \end{aligned}$$

Surprisingly, Theorem 3. shows that the average values of the Hosoya index and the Merrifield–Simmons index with respect to ζ_n are just the expected values of the Hosoya index and the Merrifield–Simmons index of the metachain M''_n.

5. Discussion

Previously, many people have analyzed and studied the Hosoya index $m(G_n)$ and Merrifield–Simmons index $i(G_n)$, for example, similar contents to the ones in this paper have been studied in the random polyethylene chains, that is, studying the two indexes of connectting the hexagonal chemical chain at the end, and obtaining the index expectation of different connection modes at the end according to the relevant known conclusions, on the basis of obtaining the probability of different connection modes of the terminal hexagon, the exponential problem of three different chains is further solved.

According to the relevant contents of the hexagon introduced before, in this article, we further push down and obtain the end connected octagon. Firstly, a series of exact formulas to push the Hosoya index and the Merrifield–Simmons index are presented, and the two indexes of the simple graph used in the later research process are calculated. Then, the corresponding chemical diagrams in the calculation process are depicted by drawing software through different connection methods. Finally, different formulas and corresponding graphs are combined to obtain the expected values of the two indexes of the random cyclooctylene chain with n octagons; it is inferred that four different probabilities represent different connection modes of terminal octagons, which means that there are accurate values of the Hosoya index and the Merrifield–Simmons index of four chemical chains, meanwhile, we also obtain the average value with respect to the set of all the random cyclooctylene chains.

6. Concluding Remarks

There are still some limitations and problems for further study in this paper. Firstly, for the graphs studied by Hosoya index and Merrifield–Simmons index, they are all finite simple and directional graphs with special restriction conditions. Therefore, there are many problems related to different graphs that have not been solved for later discussion and study. Secondly, the exact formula given in the process of research expectation is only one research method. There are many different ways to solve the two indices, and different ways have different advantages and disadvantages. Finally, there are still many questions about the different indices of different chemical chains that require further study and characterization. This paper only presents the Hosoya index and Merrifield–Simmons index of random cyclooctylene chains, cyclooctylene and their derivatives have attracted a lot of attention, and their composition and structure are also being studied in the direction of graph theory.

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