The Expected Values of Hosoya Index and Merrifield-Simmons Index of Random Octagonal Chains

Chengshan Peng, Xianya Geng

***Abstract*—In this paper, the expectation values of the Hosoya and Merrifield-Simmons exponents for random octagonal chains are obtained by classification and discussion. For the study of polygonal chemicals, some of the indices in the graph theory are shown to be strongly correlated with their physicochemical properties. The exact formulas established in this paper will undoubtedly help to study their corresponding chemical properties.**

***Index Terms*—random octagonal chains, Hosoya index, Merrifield-Simmons index, expected values.**

I. Introduction

The Hosoya indicator was introduced and studied by the Japanese chemist Haruo Hosoya in 1971 in the literature [2], which denotes the number of all matches in the graph G, denoted as $\mu(G)$. This index is closely related to the boiling point, entropy, chemical bonding calculations and chemical structure of substances. The Merrifield-Simmons metric is a chemical topological metric introduced in 1989 by the American chemists Richard E. Merrifield and Howard E. Simmons in the literature [3-6], which represents the number of all independent sets in the graph G, denoted as $\sigma(G)$. This indicator is closely related to the boiling point of a substance.These two topological indicators are of great significance in structural chemistry, and they are often used to characterize the physicochemical and pharmacological properties of organic compounds, which are described in the literature [7-12].

In this paper, we define a graph $G=(V,E)$ with vertex set V and edge set E. If the new graph obtained by removing this vertex from the graph, i.e., $G-v$, has more components than the original graph G, for a vertex $v \in V$, we call this vertex v is a cut vertex of this graph G. A maximal connected branch H of this graph G is called a block if it does not contain cut vertices. It follows that if there is only one cut vertex in G, then the cut vertex is contained in H. A vertex subset $I \subseteq V$ is said to be independent if any pair of vertices in a vertex set I is disjoint in G. Similarly, an edge subset $M \subseteq E$ is said to be matched if any two edges in an edge set M have no common vertices. We use C_k to denote a cycle of length k.

Manuscript received October 16, 2024; revised March 13, 2025.

This work was supported in part by National Science Foundation of China (Grant No. 11671164) and Natural Science Foundation of Anhui Province(Grant No. 2008085MA01)

C. S. Peng is a postgraduate student of the School of Mathematics and Big Data, Anhui University of Science and Technology, Huainan, 232001 China (corresponding author to provide phone: +86-18269875879; fax: +86-18269875879; e-mail: 250192097@qq.com).

X. Y. Geng is a professor of the School of Mathematics and Big Data, Anhui University of Science and Technology, Huainan, 232001 China (e -mail:gengxianya@sina.com).

The randomized helical chains discussed in this paper are composed of cut-points connected by progressively adding octagons; each of his blocks is an octagon, and each octagon has at most two cut-points, with each cut-point shared by exactly two octagons. A regular octagonal chain is a graph that all the blocks are C_8. In this paper, we define for a random octagonal chain $R_n(k_1,k_2,k_3,k_4)$ containing n octagons as follows: for a non-negative integer n, when there exist non-negative real numbers k_1,k_2,k_3,k_4 satisfying $k_1+k_2+k_3+k_4=1$. When $n=0$, it is clear that at this point $R_0(k_1,k_2,k_3,k_4)$ is empty. For $n=1$, $R_1(k_1,k_2,k_3,k_4)$ is an octagon. And when $n=2$, $R_2(k_1,k_2,k_3,k_4)$ consists of two octagons that have one and only one common vertex. When $n \geq 3$, we need to start a discussion based on the different distances between the cut vertexes of octagons.
Here, we consider the graph $R_n(k_1,k_2,k_3,k_4)$ obtained by combining $R_{n-1}(k_1,k_2,k_3,k_4)$ and an octagon O. We label successively along the chain with 1, ... , $n-1$ consecutively labeled with the $(n-1)^{th}$ octagons that make up $R_{n-1}(k_1,k_2,k_3,k_4)$. So, depending on the distance between a vertex of the octagon O and the $(n-1)^{th}$ cut vertex of $R_{n-1}(k_1,k_2,k_3,k_4)$, it can be categorized as follows. When the distance between these two vertexes is 1, the probability of this happening is said to be k_1. When the distance between two vertexes is 2, the probability of this happening is said to be k_2. When the distance between two vertexes is 3, the probability of this happening is k_3. When the distance between two vertexes is 4, the probability of this happening is said to be k_4.

In a related study of the Hosoya index and Merrifield-Simmons index in random chains, Chen et al.[20] gave explicit expressions for the expectation of the Merrifield-Simons index for random phenylene chains and random hexagonal chains. In 2022, Sun et al. found, for random cyclooctene chains containing n octagons, a recursive relationship between the expected values of its Hosoya index and Merrifield-Simmons index.Very recently in 2024,Moe et al. [18] obtained the expected values of these two indices for the random hexagonal cactus and built a generating function by solving the recurrence relation for these indices.In this paper, we would like to solve the problem of the expected value of these indices for random octagonal chains. After categorization and discussion, finally we get the expectation generating functions for these indices.

II. Preliminaries

In this section, to obtain the theorem, we made the following preparations. Firstly, for a non-negative integer n, when there exist four non-negative real numbers k_1,k_2,k_3 and k_4 satisfying $k_1+k_2+k_3+k_4=1$, the graph $R_0(k_1,k_2,k_3,k_4)$ is empty, the graph $R_1(k_1,k_2,k_3,k_4)$ is an octagon and the graph $R_2(k_1,k_2,k_3,k_4)$ consists of two octagons that have one and only one common vertex. For $n \geq 3$, the graph $R_n(k_1,k_2,k_3,k_4)$ is obtained from $R_{n-1}(k_1,k_2,k_3,k_4)$, by identifying different distances between the cut vertex of the $(n-1)^{th}$ octagon and a vertex of O, four possibilities can be classified as k_1,k_2,k_3 and k_4. Figure 1 gives four possible cases of $R_n(k_1,k_2,k_3,k_4)$.

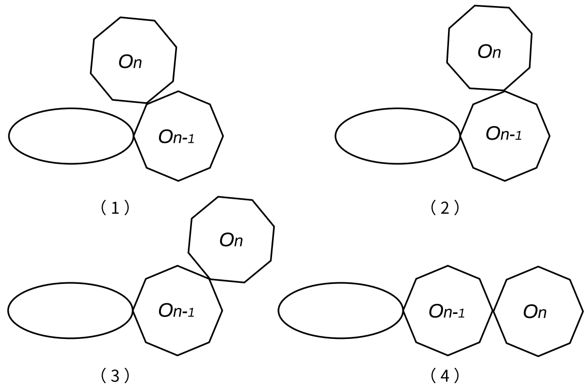

Fig. 1. The graphs $R_n(k_1,k_2,k_3,k_4)$.

From left to right, top to bottom, in the figure 1, depending on the distance between a vertex of the octagon O and the $(n-1)^{th}$ cut vertex of $R_{n-1}(k_1,k_2,k_3,k_4)$, it can be categorized with the probabilities k_1,k_2,k_3 and k_4. Similarly, there are the following definitions.

The graph $R_n^{'}(k_1,k_2,k_3,k_4)$ is obtained from the $R_n(k_1,k_2,k_3,k_4)$ and a path $P_7 = x_1x_2x_3x_4x_5x_6x_7$, by different distances between x_1 of P_7 and the n^{th} cut vertex of $R_n(k_1,k_2,k_3,k_4)$, four possibilities can be classified as k_1,k_2,k_3,k_4. Figure 2 gives four possible cases of $R_n^{'}(k_1,k_2,k_3,k_4)$.

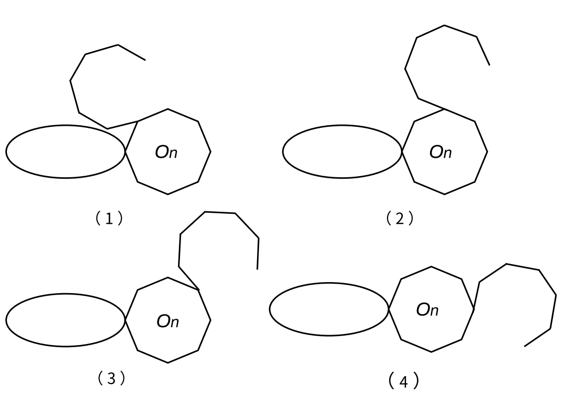

Fig. 2. The graphs $R_n^{'}(k_1,k_2,k_3,k_4)$.

From left to right, top to bottom, in the figure 2,by identifying different distances between x_1 of the path P_7 $=x_1x_2x_3x_4x_5x_6x_7$ and a vertex of the octagon O_n, fo ur possibilities can be classified as k_1,k_2,k_3 and k_4.

The graph $\tilde{R}_n(k_1,k_2,k_3,k_4)$ is obtained from the $R_n(k_1,k_2,k_3,k_4)$ and a path $P_7 = x_1x_2x_3x_4x_5x_6x_7$, by different distances between x_2 of P_7 and the n^{th} cut vertex of $R_n(k_1,k_2,k_3,k_4)$, four possibilities can be classified as k_1,k_2,k_3,k_4. Figure 3 illustrates examples of $\tilde{R}_n(k_1,k_2,k_3,k_4)$.

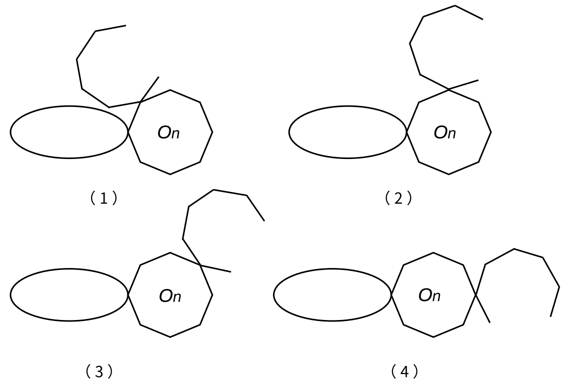

Fig. 3. The graphs $\tilde{R}_n(k_1,k_2,k_3,k_4)$.

From left to right, top to bottom, in the figure 3, by identifying different distances between x_2 of the path P_7 $=x_1x_2x_3x_4x_5x_6x_7$ and a vertex of the octagon O_n, fo ur possibilities can be classified as k_1,k_2,k_3 and k_4.

The graph $\hat{R}_n(k_1,k_2,k_3,k_4)$ is obtained from the $R_n(k_1,k_2,k_3,k_4)$ and a path $P_7 = x_1x_2x_3x_4x_5x_6x_7$, by different distances between x_3 of P_7 and the n^{th} cut vertex of $R_n(k_1,k_2,k_3,k_4)$, four possibilities can be classified as k_1,k_2,k_3,k_4. Figure 4 gives four possible cases of $\hat{R}_n(k_1,k_2,k_3,k_4)$.

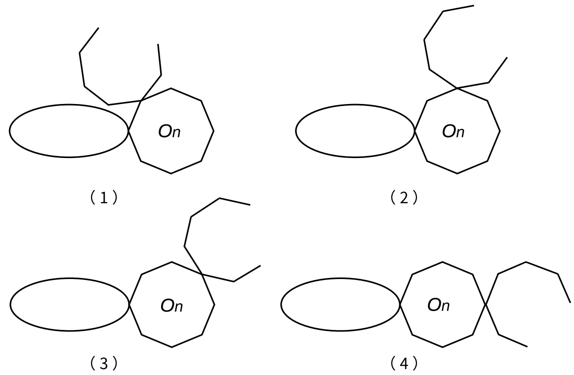

Fig. 4. The graphs $\hat{R}_n(k_1,k_2,k_3,k_4)$.

From left to right, top to bottom, in the figure 4, by identifying different distances between x_3 of the path P_7 $=x_1x_2x_3x_4x_5x_6x_7$ and a vertex of the octagon O_n, fo ur possibilities can be classified as k_1,k_2,k_3,k_4.

The graph $R_n^{*}(k_1,k_2,k_3,k_4)$ is obtained from the $R_n(k_1,k_2,k_3,k_4)$ and a path $P_7 = x_1x_2x_3x_4x_5x_6x_7$, by different distances between x_4 of P_7 and the n^{th} cut vertex of $R_n(k_1,k_2,k_3,k_4)$, four possibilities can be classified as k_1,k_2,k_3 and k_4.Figure 5 illustrates examples of $R_n^{*}(k_1,k_2,k_3,k_4)$.

From left to right, top to bottom, in the figure 5, by identifying different distances between x_5 of the path P_7 $=x_1x_2x_3x_4x_5x_6x_7$ and a vertex of the octagon O_n, fo ur possibilities can be classified as k_1,k_2,k_3,k_4.

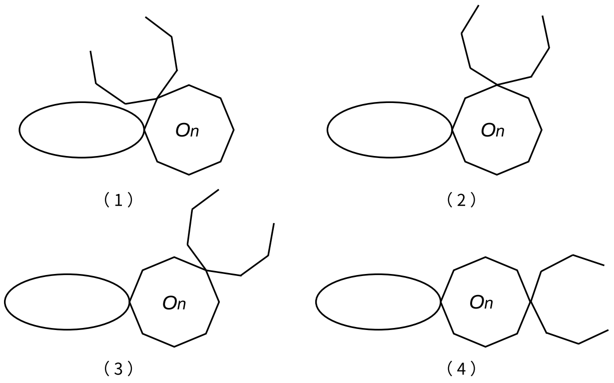

Fig. 5. The graphs $R_n^*(k_1, k_2, k_3, k_4)$.

III. The Expected Values for Hosoya Index of Random Octagonal Chains

Recall that $E(m_n(k_1, k_2, k_3, k_4))$ is the expected value of matches of $R_n(k_1, k_2, k_3, k_4)$, and $M_{k_1,k_2,k_3,k_4}(x)$ is the generating function of $E(m_n(k_1, k_2, k_3, k_4))$. Let $E(m_n)$ and $M(x)$ to denote $E(m_n(k_1, k_2, k_3, k_4))$ and $M_{k_1,k_2,k_3,k_4}(x)$, when there is no danger of confusion, respectively. Therefore,

$$M(x) = \sum_{n=0}^{\infty} E(m_n)x^n$$

Similarly, recall that $E(m_n^{'})$,$E(\tilde{m}_n)$,$E(\hat{m}_n)$ and $E(m_n^*)$ be the expected values of matches of $R_n^{'}(k_1, k_2, k_3, k_4)$, $\tilde{R}_n(k_1, k_2, k_3, k_4)$, $\hat{R}_n(k_1, k_2, k_3, k_4)$ and $R_n^*(k_1, k_2, k_3, k_4)$, respectively. The $M^{'}(x)$, $\tilde{M}(x)$, $\hat{M}(x)$ and $M^*(x)$ is the generating functions of $E(m_n^{'})$,$E(\tilde{m}_n)$,$E(\hat{m}_n)$ and $E(m_n^*)$. Thus,

$$M^{'}(x) = \sum_{n=0}^{\infty} E(m_n^{'})x^n$$

$$\tilde{M}(x) = \sum_{n=0}^{\infty} E(\tilde{m}_n)x^n$$

$$\hat{M}(x) = \sum_{n=0}^{\infty} E(\hat{m}_n)x^n$$

$$M^*(x) = \sum_{n=0}^{\infty} E(m_n^*)x^n$$

Now, for a random octagonal chain, the following equation must be proved in order to obtain the expected value for Hosoya index.

$$\begin{aligned} M(x) = 1 + 26x + 21xM(x) + 26k_1x^2M^{'}(x) \\ +26k_2x^2\tilde{M}(x) + 26k_3x^2\hat{M}(x) + 26k_4x^2M^*(x). \end{aligned} \tag{1}$$

$$\begin{aligned} M^{'}(x) =& 8 + 13M(x) + 8k_1xM^{'}(x) + 8k_2x\tilde{M}(x) \\ &+8k_3x\hat{M}(x) + 8k_4xM^*(x). \end{aligned} \tag{2}$$

$$\begin{aligned} \tilde{M}(x) =& 13 + 8M(x) + 13k_1xM^{'}(x) + 13k_2x\tilde{M}(x) \\ &+13k_3x\hat{M}(x) + 13k_4xM^*(x). \end{aligned} \tag{3}$$

$$\begin{aligned} \hat{M}(x) =& 14 + 7M(x) + 10k_1xM^{'}(x) + 10k_2x\tilde{M}(x) \\ &+10k_3x\hat{M}(x) + 10k_4xM^*(x). \end{aligned} \tag{4}$$

$$\begin{aligned} M^*(x) =& 15 + 6M(x) + 10k_1xM^{'}(x) + 10k_2x\tilde{M}(x) \\ &+10k_3x\hat{M}(x) + 10k_4xM^*(x). \end{aligned} \tag{5}$$

A. Proof of Equation (1).

For the n^{th} octagon O_n of $R_n(k_1, k_2, k_3, k_4)$, we recall the vertices of it in clockwise by $p_1, p_2, ..., p_8$, and the p_1 is the cut vertex of the O_n and the O_{n-1}. Recall that the vertices of O_{n-1} in clockwise by l_1, l_2, ..., l_8, and the l_1 is the cut vertex of the O_{n-1}. Since $R_n(k_1, k_2, k_3, k_4)$ is a chain, $l_1 \neq p_1$. Due to the different distances between p_1 and l_1, it can be classified into four cases.

1) Case 1: The distance between p_1 and l_1 is one.

Therefore, $p_1 = l_2$ or $p_1 = l_8$. Without prejudice to generality, assume that $p_1 = l_2$. The probability that this occurs is k_1. So there are three subcases.

Subcase 1.1: When p_1p_2 is included in the matches. In this subcase,it cannot contain l_1l_2 ,l_2l_3, p_2p_3 and p_1p_8. Therefore, in this instance, this subcase is equivalent to the combination of the path $P_6 = p_3p_4p_5p_6p_7p_8$ and $R_{n-2}^{'}(k_1, k_2, k_3, k_4)$. Since P_6 has 13 matches, there's $13E(m_{n-2}^{'})$.

Subcase 1.2: When p_1p_8 is included in the matches. This instance is similar to subcase 1.1. Therefore, there's $13E(m_{n-2}^{'})$.

Subcase 1.3: When neither p_1p_2 nor p_1p_8 is included in the matches. Therefore, in this instance, this subcase is equivalent to the combination of the path $P_7 = p_2p_3p_4p_5p_6p_7p_8$ and $R_{n-1}(k_1, k_2, k_3, k_4)$. Since P_7 has 21 matches, there's $21E(m_{n-1})$.

Thus, there's $26k_1E(m_{n-2}^{'})$+$21k_1E(m_{n-1})$ from the above subcases.

2) Case 2: The distance between p_1 and l_1 is two.

Therefore, $p_1 = l_3$ or $p_1 = l_7$. Without prejudice to generality, assume that $p_1 = l_3$. The probability that this occurs is k_2. So there are three subcases.

Subcase2.1: When p_1p_2 is included in the matches. In this subcase, it cannot contain l_2l_3, l_3l_4, p_2p_3 and p_1p_8. Therefore, in this instance, this subcase is equivalent to the combination of the path $P_6 = p_3p_4p_5p_6p_7p_8$ and $\tilde{R}_{n-2}(k_1, k_2, k_3, k_4)$. Since P_6 has 13 matches, there's $13E(\tilde{m}_{n-2})$.

Subcase 2.2: When p_1p_8 is included in the matches.This instance is similar to subcase 2.1. Therefore, there's $13E(\tilde{m}_{n-2})$.

Subcase 2.3: When neither p_1p_2 nor p_1p_8 is included in the matches. Therefore, in this instance, this subcase is equivalent to the combination of the path $P_7 = p_2p_3p_4p_5p_6p_7p_8$ and $R_{n-1}(k_1, k_2, k_3, k_4)$.Since P_7 has 21 matches, there's $21E(m_{n-1})$.

Thus, there's $26k_2E(\tilde{m}_{n-2})$+$21k_2E(m_{n-1})$ from the above subcases.

3) Case 3: The distance between p_1 and l_1 is three.

Therefore, $p_1 = l_4$ or $p_1 = l_6$. Without prejudice to generality, assume that $p_1 = l_4$. The probability that this occurs is k_3. So there are three subcases.

Subcase 3.1: When p_1p_2 is included in the matches. In this subcase, it cannot contain l_3l_4, l_4l_5, p_2p_3 and p_1p_8. Therefore, This instance is equivalent to the combination of the path $P_6 = p_3p_4p_5p_6p_7p_8$ and $\hat{R}_{n-2}(k_1, k_2, k_3, k_4)$. Since P_6 has 13 matches, there's $13E(\hat{m}_{n-2})$.

Subcase 3.2: When p_1p_8 is included in the matches. This instance is similar to subcase 3.1. Therefore, there's $13E(\hat{m}_{n-2})$.

Subcase 3.3: When neither p_1p_2 nor p_1p_8 is included in the matches. Therefore, in this instance, this subcase is equivalent to the combination of the path $P_7 = p_2p_3p_4p_5p_6p_7p_8$ and $R_{n-1}(k_1, k_2, k_3, k_4)$. Since P_7 has 21 matches, there's $21E(m_{n-1})$.

Thus, there's $26k_3E(\hat{m}_{n-2})$+$21k_3E(m_{n-1})$ from the above subcases.

4) Case 4: The distance between p_1 and l_1 is four.

Therefore, $p_1 = l_5$. The probability that this occurs is k_4. So there are three subcases.

Subcase 4.1: When p_1p_2 is included in the matches. In this subcase, it cannot contain l_4l_5, l_5l_6, p_2p_3 and p_1p_8.Therefore, This instance is equivalent to the combination of the path $P_6 = p_3p_4p_5p_6p_7p_8$ and $R^*_{n-2}(k_1, k_2, k_3, k_4)$. Since P_6 has 13 matches, there's $13E(m^*_{n-2})$.

Subcase 4.2: When p_1p_8 is included in the matches. This instance is similar to subcase 4.1. Therefore, there's $13E(m^*_{n-2})$.

Subcase 4.3: When neither p_1p_2 nor p_1p_8 is included in the matches. Therefore, in this instance, this subcase is equivalent to the combination of the path $P_7 = p_2p_3p_4p_5p_6p_7p_8$ and $R_{n-1}(k_1, k_2, k_3, k_4)$. Since P_7 has 21 matches, there's $21E(m_{n-1})$.

Thus, there's $26k_4E(m^*_{n-2})$+$21k_4E(m_{n-1})$ from the above subcases.

Thus, the following results can be derived from Cases 1, 2, 3 and 4.

$$\begin{aligned} E(m_n) =& 26k_1E(m'_{n-2}) + 21k_1E(m_{n-1}) + 26k_2E(\tilde{m}_{n-2}) \\ &+21k_2E(m_{n-1}) + 26k_3E(\hat{m}_{n-2}) + 21k_3E(m_{n-1}) \\ &+26k_4E(m^*_{n-2}) + 21k_4E(m_{n-1}) \\ =& 21(k_1 + k_2 + k_3 + k_4)E(m_{n-1}) + 26k_1E(m'_{n-2}) \\ &+26k_2E(\tilde{m}_{n-2}) + 26k_3E(\hat{m}_{n-2}) + 26k_4E(m^*_{n-2}) \\ =& 21E(m_{n-1}) + 26k_1E(m'_{n-2}) + 26k_2E(\tilde{m}_{n-2}) \\ &+26k_3E(\hat{m}_{n-2}) + 26k_4E(m^*_{n-2}). \end{aligned}$$

When $n \geq 2$, we can obtain that

$$\begin{aligned} \sum_{n=2}^{\infty} E(m_n)x^n =& \sum_{n=2}^{\infty} 21E(m_{n-1})x^n + 26k_1 \sum_{n=2}^{\infty} E(m'_{n-2})x^n \\ &+26k_2 \sum_{n=2}^{\infty} E(\tilde{m}_{n-2}x^n) + 26k_3 \sum_{n=2}^{\infty} E(\hat{m}_{n-1})x^n \\ &+26k_4 \sum_{n=2}^{\infty} E(m^*_{n-2})x^n \end{aligned}$$

which implies that

$$\begin{aligned} M(x) - E(m_0) - E(m_1)x = & 21x(M(x) - E(m_0)) \\ &+26k_1x^2M'(x) + 26k_2x^2\tilde{M}(x) \\ &+21k_3x^2\hat{M}(x) + 26k_4x^2M^*(x). \end{aligned}$$

Note that $E(m_0)$ is the number of matches of size 0, the empty set of the empty graph, thus, $E(m_0) = 1$. Since $E(m_1)$ is the number of matches of one octagon, $E(m_1) = 47$. Therefore,

$$\begin{aligned} M(x) =& 1 + 26x + 21xM(x) + 26k_1x^2M'(x) \\ &+26k_2x^2\tilde{M}(x) + 26k_3x^2\hat{M}(x) + 26k_4x^2M^*(x). \end{aligned}$$

Equation (1) can be proved from the above.

B. Proof of Equation (2).

The graph $R'_n(k_1, k_2, k_3, k_4)$ is a combination of $R_n(k_1, k_2, k_3, k_4)$ and a path $P_7 = x_1x_2x_3x_4x_5x_6x_7$. At the same time, x_1 is a vertex of the n^{th} octagon of $R_n(k_1, k_2, k_3, k_4)$. For the n^{th} octagon O_n of $R'_n(k_1, k_2, k_3, k_4)$, we recall that the vertices of it in clockwise direction by p_1, p_2, ..., p_8, and the p_1 is the cut vertex of the O_n and the O_{n-1}. It is clear that $x_1 \neq p_1$.Due to the different distances between x_1 and p_1, it can be classified into four cases.

1) Case 1: The distance between x_1 and p_1 is one.

Therefore, $x_1 = p_2$ or $x_1 = p_8$. Without prejudice to generality, assume that $x_1 = p_2$. The probability that this occurs is k_1. So there are two subcases.

Subcase 1.1: When x_1x_2 is included in the matches. In this subcase, it cannot contain x_2x_3, p_1p_2 and p_2p_3. Therefore, this subcase is equivalent to the combination of the $R'_{n-1}(k_1, k_2, k_3, k_4)$ and the path $P_5 = x_3x_4x_5x_6x_7$. Since P_5 has 8 matches, there's $8E(m'_{n-1})$.

Subcase 1.2: When x_1x_2 is not included in the matches. Therefore, this subcase is equivalent to the combination of the $R_n(k_1, k_2, k_3, k_4)$ and the path $P_6 = x_2x_3x_4x_5x_6x_7$. Since P_6 has 13 matches, there's $13E(m_n)$.

Thus, there's $8k_1E(m'_{n-1})$+$13k_1E(m_n)$ from the above subcases.

2) Case 2: The distance between x_1 and p_1 is two.

Therefore, $x_1 = p_3$ or $x_1 = p_7$. Without prejudice to generality, assume that $x_1 = p_3$. The probability that this occurs is k_2. So there are two subcases.

Subcase 2.1: When x_1x_2 is included in the matches. In this subcase, it cannot contain x_2x_3, p_2p_3 and p_3p_4. Therefore, this subcase is equivalent to the combination of the $\tilde{R}_{n-1}(k_1, k_2, k_3, k_4)$ and the path $P_5 = x_3x_4x_5x_6x_7$. Since P_5 has 8 matches, there's $8E(\tilde{m}_{n-1})$.

Subcase 2.2: When x_1x_2 is not included in the matches. Therefore, in this subcase, this subcase is equivalent to the combination of the $R_n(k_1, k_2, k_3, k_4)$ and the path $P_6 = x_2x_3x_4x_5x_6x_7$. Since P_6 has 13 matches, there's $13E(m_n)$.

Thus, there's $8k_2E(\tilde{m}_{n-1})$+$13k_2E(m_n)$ from the above subcases.

3) Case 3: The distance between x_1 and p_1 is three.

Therefore, $x_1 = p_4$ or $x_1 = p_6$. Without prejudice to generality, assume that $x_1 = p_4$. The probability that this occurs is k_3. So there are two subcases.

Subcase 3.1: When x_1x_2 is included in the matches. In this subcase, it cannot contain x_2x_3, p_3p_4 and p_4p_5. Therefore, this subcase is equivalent to the combination of the $\hat{R}_{n-1}(k_1, k_2, k_3, k_4)$ and the path $P_5 = x_3x_4x_5x_6x_7$. Since P_5 has 8 matches, there's $8E(\hat{m}_{n-1})$.

Subcase 3.2: When x_1x_2 is not included in the matches. Therefore, in this subcase, this subcase is equivalent to the combination of the $R_n(k_1, k_2, k_3, k_4)$ and the path $P_6 = x_2x_3x_4x_5x_6x_7$. Since P_6 has 13 matches, there's $13E(m_n)$.

Thus, there's $8k_3E(\hat{m}_{n-1})$+$13k_3E(m_n)$ from the above subcases.

4) Case 4: The distance between x_1 and p_1 is four.

Therefore, $x_1 = p_5$. The probability that this occurs is k_4. So there are two subcases.

Subcase 4.1: When x_1x_2 is included in the matches. In this subcase, it cannot contain x_2x_3, p_4p_5 and p_5p_6. Therefore, this subcase is equivalent to the combination of the $R^*_{n-1}(k_1,k_2,k_3,k_4)$ and the path $P_5 = x_3x_4x_5x_6x_7$. Since P_5 has 8 matches, there's $8E(m^*_{n-1})$.

Subcase 4.2: When x_1x_2 is not included in the matches. Therefore, in this subcase, this subcase is equivalent to the combination of the $R_n(k_1,k_2,k_3,k_4)$ and the path $P_6 = x_2x_3x_4x_5x_6x_7$. Since P_6 has 13 matches, there's $13E(m_n)$.

Thus, there's $8k_4E(m^*_{n-1})$+$13k_4E(m_n)$ from the above subcases.

Thus, the following results can be derived from Cases 1, 2, 3 and 4.

$$\begin{aligned}E(m_n^{'}) =&8k_1E(m_{n-1}^{'}) + 13k_1E(m_n) + 8k_2E(\tilde{m}_{n-1})\\&+13k_2E(m_n) + 8k_3E(\hat{m}_{n-1}) + 13k_3E(m_n)\\&+8k_4E(m^*_{n-1}) + 13k_4E(m_n)\\=&13(k_1+k_2+k_3+k_4)E(m_n) + 8k_1E(m_{n-1}^{'})\\&+8k_2E(\tilde{m}_{n-1}) + 8k_3E(\hat{m}_{n-1}) + 8k_4E(m^*_{n-1})\\=&13E(m_n) + 8k_1E(m_{n-1}^{'}) + 8k_2E(\tilde{m}_{n-1})\\&+8k_3E(\hat{m}_{n-1}) + 8k_4E(m^*_{n-1}).\end{aligned}$$

When $n \geq 1$, we can obtain that

$$\begin{aligned}\sum_{n=1}^{\infty}E(m_n^{'})x^n =&\sum_{n=1}^{\infty}13E(m_n)x^n + 8k_1\sum_{n=1}^{\infty}E(m_{n-1}^{'})x^n\\&+8k_2\sum_{n=1}^{\infty}E(\tilde{m}_{n-1}x^n) + 8k_3\sum_{n=1}^{\infty}E(\hat{m}_{n-1})x^n\\&+8k_4\sum_{n=1}^{\infty}E(m^*_{n-1})x^n\end{aligned}$$

which implies that

$$\begin{aligned}M^{'}(x) - E(m_0^{'}) =&13(M(x) - E(m_0)) + 8k_1xM^{'}(x)\\&+8k_2x\tilde{M}(x) + 8k_3x\hat{M}(x) + 8k_4xM^*(x).\end{aligned}$$

Note that $E(m_0^{'})$ is the number of matches of path of 7 vertices, thus, $E(m_0^{'}) = 21$. The $E(m_0) = 1$. Therefore,

$$\begin{aligned}M^{'}(x) =&8 + 13M(x) + 8k_1xM^{'}(x) + 8k_2x\tilde{M}(x)\\&+8k_3x\hat{M}(x) + 8k_4xM^*(x).\end{aligned}$$

Equation (2) can be proved from the above.

C. Proof of Equation (3).

The graph $\tilde{R}_n(k_1,k_2,k_3,k_4)$ is a combination of $R_n(k_1,k_2,k_3,k_4)$ and a path $P_7 = x_1x_2x_3x_4x_5x_6x_7$. At the same time, x_2 is a vertex of the n^{th} octagon of $R_n(k_1,k_2,k_3,k_4)$. For the n^{th} octagon O_n of $\tilde{R}_n(k_1,k_2,k_3,k_4)$, we recall that the vertices of it in clockwise by p_1, p_2, ..., p_8, and p_1 is the cut vertex of the O_n and the O_{n-1}. It is clear that $x_2 \neq p_1$. Due to the different distances between x_2 and p_1, it can be classified into four cases.

1) Case 1: The distance between x_2 and p_1 is one.

Therefore, $x_2 = p_2$ or $x_2 = p_8$. Without prejudice to generality, assume that $x_2 = p_2$. The probability that this occurs is k_1. So there are three subcases.

Subcase 1.1: When x_1x_2 is included in the matches. In this subcase, it cannot contain x_2x_3, p_1p_2 and p_2p_3. Therefore, this subcase is equivalent to the combination of the $R_{n-1}^{'}(k_1,k_2,k_3,k_4)$ and $P_5 = x_3x_4x_5x_6x_7$. Since P_5 has 8 matches, there's $8E(m_{n-1}^{'})$.

Subcase 1.2: When x_2x_3 is included in the matches. In this subcase, x_1x_2, x_3x_4, p_1p_2 and p_2p_3 are not included. Therefore, this subcase is equivalent to the combination of the path $P_4 = x_4x_5x_6x_7$ and the $R_{n-1}^{'}(a,b,c,d)$. Since P_4 has 5 matches, there's $5E(m_{n-1}^{'})$.

Subcase 1.3: When neither x_1x_2 nor x_2x_3 is included in the matches. Therefore, in this subcase, this subcase is equivalent to the combination of the $R_n(k_1,k_2,k_3,k_4)$ and the path $P_5 = x_3x_4x_5x_6x_7$. Since P_5 has 8 matches, there's $8E(m_n)$.

Thus, there's $13k_1E(m_{n-1}^{'})$+$8k_1E(m_n)$ from the above subcases.

2) Case 2: The distance between x_2 and p_1 is two.

Therefore, $x_2 = p_3$ or $x_2 = p_7$. Without prejudice to generality, assume that $x_2 = p_3$. The probability that this occurs is k_2. So there are three subcases.

Subcase 2.1: When x_1x_2 is included in the matches. In this subcase, it cannot contain x_2x_3, p_2p_3 and p_3p_4. Therefore, this subcase is equivalent to the combination of the $\tilde{R}_{n-1}(k_1,k_2,k_3,k_4)$ and the path $P_5 = x_3x_4x_5x_6x_7$. Since P_5 has 8 matches, there's $8E(\tilde{m}_{n-1})$.

Subcase 2.2: When x_2x_3 is included in the matches. In this subcase, it cannot contain x_1x_2, x_3x_4, p_2p_3 and p_3p_4. Therefore, this subcase is equivalent to the combination of the $\tilde{R}_{n-1}(k_1,k_2,k_3,k_4)$, the vertex x_1 and the path $P_4 = x_4x_5x_6x_7$. Since P_4 has 5 matches, there's $5E(\tilde{m}_{n-1})$.

Subcase 2.3: When neither x_1x_2 nor x_2x_3 is included in the matches. Therefore, in this subcase, this subcase is equivalent to the combination of the $R_n(k_1,k_2,k_3,k_4)$ and the path $P_5 = x_3x_4x_5x_6x_7$. Since P_5 has 8 matches, there's $8E(m_n)$.

Thus, there's $13k_2E(\tilde{m}_{n-1})$+$8k_2E(m_n)$ from the above subcases.

3) Case 3: The distance between x_2 and p_1 is three.

Therefore, $x_2 = p_4$ or $x_2 = p_6$. Without prejudice to generality, assume that $x_2 = p_4$. The probability that this occurs is k_3. So there are three subcases. *Subcase 3.1:* When x_1x_2 is included in the matches. In this subcase, it cannot contain x_2x_3, p_3p_4 and p_4p_5. Therefore, this subcase is equivalent to the combination of the path $P_5 = x_3x_4x_5x_6x_7$ and the $\hat{R}_{n-1}(a,b,c,d)$. Since P_5 has 8 matches, there's $8E(\hat{m}_{n-1})$.

Subcase 3.2: When x_2x_3 is included in the matches. In this subcase, x_1x_2, x_3x_4, p_3p_4 and p_4p_5 are not included. Therefore, this subcase is equivalent to the combination of the path $P_4 = x_4x_5x_6x_7$ and the $\hat{R}_{n-1}(k_1,k_2,k_3,k_4)$. Since P_4 has 5 matches, there's $5E(\hat{m}_{n-1})$.

Subcase 3.3: When neither x_1x_2 nor x_2x_3 is included in the matches. Therefore, this subcase is equivalent to the combination of the $R_n(k_1,k_2,k_3,k_4)$ and the path $P_5 = x_3x_4x_5x_6x_7$. Since P_5 has 8 matches, there's $8E(m_n)$.

Thus, there's $13k_3E(\hat{m}_{n-1})$+$8k_3E(m_n)$ from the above subcases.

4) Case 4: The distance between x_2 and p_1 is four.

Therefore, $x_2 = p_5$. The probability that this occurs is k_4. So there are three subcases.

Subcase 4.1: When x_1x_2 is included in the matches. In this subcase, it cannot contain x_2x_3, p_4p_5 and p_5p_6. Therefore, this subcase is equivalent to the combination of the $R^*_{n-1}(k_1, k_2, k_3, k_4)$ and the path $P_5 = x_3x_4x_5x_6x_7$. Since P_5 has 8 matches, there's $8E(m^*_{n-1})$.

Subcase 4.2: When x_2x_3 is included in the matches. In this subcase, it cannot contain x_1x_2, x_3x_4, p_4p_5 and p_5p_6. Therefore, this subcase is equivalent to the combination of the $R^*_{n-1}(k_1, k_2, k_3, k_4)$ and the path $P_4 = x_4x_5x_6x_7$. Since P_4 has 5 matches, there's $5E(m^*_{n-1})$.

Subcase 4.3: When neither x_1x_2 nor x_2x_3 is included in the matches. Therefore, in this subcase, this subcase is equivalent to the combination of the $R_n(k_1, k_2, k_3, k_4)$ and the path $P_5 = x_3x_4x_5x_6x_7$. Since P_5 has 8 matches, there's $8E(m_n)$.

Thus, there's $13k_4E(m^*_{n-1})$+$8k_4E(m_n)$ from the above subcases.

Thus, the following results can be derived from Cases 1, 2, 3 and 4.

$$\begin{aligned}
E(\tilde{m}_n) =& 13k_1E(m^{'}_{n-1}) + 8k_1E(m_n) + 13k_2E(\tilde{m}_{n-1}) \\
&+8k_2E(m_n) + 13k_3E(\hat{m}_{n-1}) + 8k_3E(m_n) \\
&+13k_4E(m^*_{n-1}) + 8k_4E(m_n) \\
=& 8(k_1 + k_2 + k_2 + k_4)E(m_n) + 13k_1E(m^{'}_{n-1}) \\
&+13k_2E(\tilde{m}_{n-1}) + 13k_3E(\hat{m}_{n-1}) + 13k_4E(m^*_{n-1}) \\
=& 8E(m_n) + 13k_1E(m^{'}_{n-1}) + 13k_2E(\tilde{m}_{n-1}) \\
&+13k_3E(\hat{m}_{n-1}) + 13k_4E(m^*_{n-1}).
\end{aligned}$$

When $n \geq 1$, we can obtain that

$$\begin{aligned}
\sum_{n=1}^{\infty} E(\tilde{m}_n)x^n =& \sum_{n=1}^{\infty} 8E(m_n)x^n + 13k_1 \sum_{n=1}^{\infty} E(m^{'}_{n-1})x^n \\
&+13k_2 \sum_{n=1}^{\infty} E(\tilde{m}_{n-1})x^n + 13k_3 \sum_{n=1}^{\infty} E(\hat{m}_{n-1})x^n \\
&+13k_4 \sum_{n=1}^{\infty} E(m^*_{n-1})x^n
\end{aligned}$$

which implies that

$$\begin{aligned}
\tilde{M}(x) - E(\tilde{m}_0) =& 8(M(x) - E(m_0)) + 13k_1xM^{'}(x) \\
&+13k_2x\tilde{M}(x) + 13k_3x\hat{M}(x) + 13k_4xM^*(x).
\end{aligned}$$

Note that $E(\tilde{m}_0)$ is the number of matches of path of 7 vertices, $E\tilde{m}_0) = 21$. $E(m_0)$ is the number of matches of size 0,the empty set of the empty graph. Thus, $E(m_0) = 1$. Therefore,

$$\begin{aligned}
\tilde{M}(x) =& 13 + 8M(x) + 13k_1xM^{'}(x) + 13k_2x\tilde{M}(x) \\
&+13k_3x\hat{M}(x) + 13k_4xM^*(x).
\end{aligned}$$

Equation (3) can be proved from the above.

D. Proof of Equation (4).

The graph $\hat{R}_n(k_1, k_2, k_3, k_4)$ is a combination of $R_n(k_1, k_2, k_3, k_4)$ and a path $P_7 = x_1x_2x_3x_4x_5x_6x_7$. At the same time, x_3 is a vertex of the n^{th} octagon of $R_n(k_1, k_2, k_3, k_4)$. For the n^{th} octagon O_n) of $\hat{R}_n(k_1, k_2, k_3, k_4)$, we recall that the vertices of it in clockwise by p_1, p_2, ..., p_8, and the p_1 is the cut vertex of the O_n and the O_{n-1}. It is clear that $x_3 \neq p_1$. Due to the different distances between x_3 and p_1, it can be classified into four cases.

1) Case 1: The distance between x_3 and p_1 is one.

Therefore, $x_3 = p_2$ or $x_3 = p_8$. Without prejudice to generality, assume that $x_3 = p_2$. The probability that this occurs is k_1. So there are three subcases. *Subcase 1.1:* When x_2x_3 is included in the matches. In this subcase, it cannot contain x_1x_2, x_3x_4, p_1p_2 and p_2p_3. Therefore, this subcase is equivalent to the combination of the $R^{'}_{n-1}(k_1, k_2, k_3, k_4)$ and the path $P_4 = x_4x_5x_6x_7$. Since P_4 has 5 matches, there's $5E(m^{'}_{n-1})$.

Subcase 1.2: When x_3x_4 is included in the matches. In this subcase, it cannot contain x_2x_3, x_4x_5, p_1p_2 and p_2p_3. Therefore, this subcase is equivalent to the combination of the $R^{'}_{n-1}(k_1, k_2, k_3, k_4)$, the paths $P_2 = x_1x_2$ and $P_3 = x_5x_6x_7$. Since P_2 and P_3 have 5 matches, there's $5E(m^{'}_{n-1})$.

Subcase 1.3: When neither x_2x_3 nor x_3x_4 is included in the matches. Therefore, this subcase is equivalent to the combination of the $R_n(k_1, k_2, k_3, k_4)$, the paths $P_2 = x_1x_2$ and $P_4 = x_4x_5x_6x_7$. Since P_2 and P_4 have 7 matches, there's $7E(m_n)$.

Thus, there's $10k_1E(m^{'}_{n-1})$+$7k_1E(m_n)$. from the above subcases.

2) Case 2: The distance between x_3 and p_1 is two.

Therefore, $x_3 = p_3$ or $x_3 = p_7$. Without prejudice to generality, assume that $x_3 = p_3$. The probability that this occurs is k_2. So there are three subcases.

Subcase 2.1: When x_2x_3 is included in the matches. In this subcase, x_1x_2, x_3x_4, p_2p_3 and p_3p_4 are not included. Therefore, this subcase is equivalent to the combination of the $\tilde{R}_{n-1}(k_1, k_2, k_3, k_4)$, the vertex x_1 and the path $P_4 = x_4x_5x_6x_7$. Since P_4 has 5 matches, there's $5E(\tilde{m}_{n-1})$.

Subcase 2.2: When x_3x_4 is included in the matches. In this subcase, x_2x_3, x_4x_5, p_2p_3 and p_3p_4 are not included. Therefore, this subcase is equivalent to the combination of the $\tilde{R}_{n-1}(k_1, k_2, k_3, k_4)$, the paths $P_2 = x_1x_2$ and $P_3 = x_5x_6x_7$. Since P_2 and P_3 have 5 matches, there's $5E(\tilde{m}_{n-1})$.

Subcase 2.3: When neither x_2x_3 nor x_3x_4 is included in the matches. Therefore, this subcase is equivalent to the combination of the $R_n(k_1, k_2, k_3, k_4)$, the paths $P_2 = x_1x_2$ and $P_4 = x_4x_5x_6x_7$. Since P_2 and P_4 have 7 matches, there's $7E(m_n)$.

Thus, there's $10k_2E(\tilde{m}_{n-1})$+$7k_2E(m_n)$ from the above subcases.

3) Case 3: The distance between x_3 and p_1 is three.

Therefore, $x_3 = p_4$ or $x_3 = p_6$. Without prejudice to generality, assume that $x_3 = p_4$. The probability that this occurs is k_3. So there are three subcases.

Subcase 3.1: When x_2x_3 is included in the matches. In this subcase, it cannot contain x_1x_2, x_3x_4, p_3p_4 and p_4p_5. Therefore, this subcase is equivalent to the combination of the path $P_4 = x_4x_5x_6x_7$ and the $\hat{R}_{n-1}(k_1, k_2, k_3, k_4)$. Since

P_4 has 5 matches, there's $5E(\hat{m}_{n-1})$.

Subcase 3.2: When x_3x_4 is included in the matches. In this subcase, it cannot contain x_2x_3, x_4x_5, p_3p_4 and p_4p_5. Therefore, this subcase is equivalent to the combination of the $\hat{R}_{n-1}(k_1, k_2, k_3, k_4)$, the paths $P_2 = x_1x_2$ and $P_3 = x_5x_6x_7$. Since P_2 and P_3 have 5 matches, there's $5E(\hat{m}_{n-1})$.

Subcase 3.3: When neither x_2x_3 nor x_3x_4 is included in the matches. Therefore, this subcase is equivalent to the combination of the $R_n(k_1, k_2, k_3, k_4)$, the paths $P_2 = x_1x_2$ and $P_4 = x_4x_5x_6x_7$. Since P_2 and P_4 have 7 matches, there's $7E(m_n)$.

Thus, there's $10k_3E(\hat{m}_{n-1})$+$7k_3E(m_n)$ from the above subcases.

4) Case 4: The distance between x_3 and p_1 is four.

Therefore, $x_3 = p_5$. The probability that this occurs is k_4. So there are three subcases.

Subcase 4.1: When x_2x_3 is included in the matches. In this subcase, it cannot contain x_1x_2, x_3x_4, p_4p_5 and p_5p_6. Therefore, this subcase is equivalent to the combination of the path $P_4 = x_4x_5x_6x_7$ and the $R^*_{n-1}(k_1, k_2, k_3, k_4)$. Since P_4 has 5 matches, there's $5E(m^*_{n-1})$.

Subcase 4.2: When x_3x_4 is included in the matches. In this subcase, it cannot contain x_2x_3, x_4x_5, p_4p_5 and p_5p_6. Therefore, this subcase is equivalent to the combination of the $R^*_{n-1}(k_1, k_2, k_3, k_4)$, the paths $P_2 = x_1x_2$ and $P_3 = x_5x_6x_7$. Since P_2 and P_3 have 5 matches, there's $5E(m^*_{n-1})$.

Subcase 4.3: When neither x_2x_3 nor x_3x_4 is included in the matches. Therefore, this subcase is equivalent to the combination of the $R_n(k_1, k_2, k_3, k_4)$, the paths $P_2 = x_1x_2$ and $P_4 = x_4x_5x_6x_7$. Since P_2 and P_4 have 7 matches, there's $7E(m_n)$.

Thus, there's $10k_4E(m^*_{n-1})$+$7k_4E(m_n)$. from the above subcases.

Thus, the following results can be derived from Cases 1, 2, 3 and 4.

$$
\begin{aligned}
E(\hat{m}_n) =& 10k_1E(m^{'}_{n-1}) + 7k_1E(m_n) + 10k_2E(\tilde{m}_{n-1}) \\
&+7k_2E(m_n) + 10k_3E(\hat{m}_{n-1}) + 7k_3E(m_n) \\
&+10k_4E(m^*_{n-1}) + 7k_4E(m_n) \\
=& 7(k_1 + k_2 + k_3 + k_4)E(m_n) + 10k_1E(m^{'}_{n-1}) \\
&+10k_2E(\tilde{m}_{n-1}) + 10k_3E(\hat{m}_{n-1}) + 10k_4E(m^*_{n-1}) \\
=& 7E(m_n) + 10k_1E(m^{'}_{n-1}) + 10k_2E(\tilde{m}_{n-1}) \\
&+10k_3E(\hat{m}_{n-1}) + 10k_4E(m^*_{n-1}).
\end{aligned}
$$

When $n \geq 1$, we can obtain that

$$
\begin{aligned}
\sum_{n=1}^{\infty} E(\hat{m}_n)x^n =& \sum_{n=1}^{\infty} 7E(m_n)x^n + 10k_1 \sum_{n=1}^{\infty} E(m^{'}_{n-1})x^n \\
&+10k_2 \sum_{n=1}^{\infty} E(\tilde{m}_{n-1})x^n + 10k_3 \sum_{n=1}^{\infty} E(\hat{m}_{n-1})x^n \\
&+10k_4 \sum_{n=1}^{\infty} E(m^*_{n-1})x^n
\end{aligned}
$$

which implies that

$$
\begin{aligned}
\hat{M}(x) - E(\hat{m}_0) =& 7(M(x) - E(m_0)) \\
&+10k_1xM^{'}(x) + 10k_2x\tilde{M}(x) \\
&+10k_3x\hat{M}(x) + 10k_4xM^*(x).
\end{aligned}
$$

Note that $E(\hat{m}_0)$ is the number of matches of path of 7 vertices, so $E(\hat{m}_0) = 21$. While $E(m_0)$ is the number of matching of size 0,the empty set of the empty graph, thus, $E(m_0) = 1$. Therefore,

$$
\begin{aligned}
\hat{M}(x) =& 14 + 7M(x) + 10k_1xM^{'}(x) + 10k_2x\tilde{M}(x) \\
&+10k_3x\hat{M}(x) + 10k_4xM^*(x).
\end{aligned}
$$

Equation (4) can be proved from the above.

E. Proof of Equation (5).

The graph $R^*_n(k_1, k_2, k_3, k_4)$ is a combination of $R_n(k_1, k_2, k_3, k_4)$ and a path $P_7 = x_1x_2x_3x_4x_5x_6x_7$. At the same time, x_4 is a vertex of the n^{th} octagon of $R_n(k_1, k_2, k_3, k_4)$. For the n^{th} octagon O_n of $R^*_n(k_1, k_2, k_3, k_4)$, we recall that the vertices of it in clockwise by p_1, p_2, ..., p_8, and the p_1 is the cut vertex of the $O_n$and the O_{n-1}. It is clear that $x_4 \neq p_1$. Due to the different distances between x_4 and p_1, it can be classified into four cases.

1) Case 1: The distance between x_4 and p_1 is one.

Therefore, $x_4 = p_2$ or $x_4 = p_8$. Without prejudice to generality, assume that $x_4 = p_2$. The probability that this occurs is k_1. So there are three subcases.

Subcase 1.1: When x_3x_4 is included in the matches. In this subcase, it cannot contain x_2x_3, x_4x_5, p_1p_2 and p_2p_3.Therefore, this subcase is equivalent to the combination of the $R^{'}_{n-1}(k_1, k_2, k_3, k_4)$, the paths $P_2 = x_1x_2$ and $P_3 = x_5x_6x_7$. Since P_2 and P_3 have 5 matches, there's $5E(m^{'}_{n-1})$.

Subcase 1.2: When x_4x_5 is included in the matches. In this subcase, it cannot contain x_3x_4, x_5x_6, p_1p_2 and p_2p_3. Therefore, this subcase is equivalent to the combination of the $R^{'}_{n-1}(k_1, k_2, k_3, k_4)$, the paths $P_3 = x_1x_2x_3$ and $P_2 = x_6x_7$. Since P_3 and P_2 have 5 matches, there's $5E(m^{'}_{n-1})$.

Subcase 1.3: When neither x_3x_4 nor x_4x_5 is included in the matches. Therefore, this subcase is equivalent to the combination of the $R_n(k_1, k_2, k_3, k_4)$, the paths $P_3 = x_1x_2x_3$ and $P_3 = x_5x_6x_7$. Since P_3 and P_3 have 6 matches, there's $6E(m_n)$.

Thus, there's $10k_1E(m^{'}_{n-1})$+$6k_1E(m_n)$. from the above subcases.

2) Case 2: The distance between x_4 and p_1 is two.

Therefore, $x_4 = p_3$ or $x_4 = p_7$. Without prejudice to generality, assume that $x_4 = p_3$. The probability that this occurs is k_2. So there are three subcases.

Subcase 2.1: When x_3x_4 is included in the matches. In this subcase, it cannot contain x_2x_3, x_4x_5, p_2p_3 and p_3p_4. Therefore, this subcase is equivalent to the combination of the $\tilde{R}_{n-1}(k_1, k_2, k_3, k_4)$, the paths $P_2 = x_1x_2$ and $P_3 = x_5x_6x_7$. Since P_2 and P_3 have 5 matches, there's $5E(\tilde{m}_{n-1})$.

Subcase 2.2: When x_4x_5 is included in the matches. In this subcase, it cannot contain x_2x_3, x_4x_5, p_2p_3 and p_3p_4. Therefore, this subcase is equivalent to the combination of the $\tilde{R}_{n-1}(k_1, k_2, k_3, k_4)$, the paths $P_3 = x_1x_2x_3$ and $P_2 = x_6x_7$. Since P_3 and P_2 have 5 matches, there's $5E(\tilde{m}_{n-1})$.

Subcase 2.3: When neither x_3x_4 nor x_4x_5 is included in the matches. Therefore, this subcase is equivalent to the combination of the $R_n(k_1, k_2, k_3, k_4)$, the paths $P_3 = x_1x_2x_3$ and $P_3 = x_5x_6x_7$. Since P_3 and P_3 have 6 matches, there's $6E(m_n)$.

Thus, there's $10k_2E(\tilde{m}_{n-1})$+$6k_2E(m_n)$ from the above subcases.

3) Case 3: The distance between x_4 and p_1 is three.

Therefore, $x_4 = p_4$ or $x_4 = p_6$. Without prejudice to generality, assume that $x_4 = p_4$. The probability that this occurs is k_3. So there are three subcases.

Subcase 3.1: When x_3x_4 is included in the matches. In this subcase, it cannot contain x_2x_3, x_4x_5, p_3p_4 and p_4p_5. Therefore, this subcase is equivalent to the combination of the $\hat{R}_{n-1}(k_1, k_2, k_3, k_4)$, the paths $P_2 = x_1x_2$ and $P_3 = x_5x_6x_7$. Since P_2 and P_3 have 5 matches, there's $5E(\hat{m}_{n-1})$.

Subcase 3.2: When x_4x_5 is included in the matches. In this subcase, it cannot contain x_3x_4, x_5x_6, p_3p_4 and p_4p_5. Therefore, this subcase is equivalent to the combination of the $\hat{R}_{n-1}(k_1, k_2, k_3, k_4)$, the paths $P_3 = x_1x_2x_3$ and $P_2 = x_6x_7$. Since P_3 and P_2 have 5 matches, there's $5E(\hat{m}_{n-1})$.

Subcase 3.3: When neither x_3x_4 nor x_4x_5 is included in the matches. Therefore, this subcase is equivalent to the combination of the $R_n(k_1, k_2, k_3, k_4)$,the paths $P_3 = x_1x_2x_3$ and $P_3 = x_5x_6x_7$. Since P_3 and P_3 have 6 matches, there's $6E(m_n)$.

Thus, there's $10k_3E(\hat{m}_{n-1})$+$6k_3E(m_n)$ from the above subcases.

4) Case 4: The distance between x_4 and p_1 is four.

Therefore, $x_4 = p_5$. The probability that this occurs is k_4. So there are three subcases.

Subcase 4.1: When x_3x_4 is included in the matches. In this subcase, it cannot contain x_2x_3, x_4x_5, p_4p_5 and p_5p_6. Therefore, this subcase is equivalent to the combination of the $R^*_{n-1}(k_1, k_2, k_3, k_4)$,the paths $P_2 = x_1x_2$ and $P_3 = x_5x_6x_7$. Since P_2 and P_3 have 5 matches, there's $5E(m^*_{n-1})$.

Subcase 4.2: When x_4x_5 is included in the matches. In this subcase, it cannot contain x_3x_4, x_5x_6, p_4p_5 and p_5p_6. Therefore, this subcase is equivalent to the combination of the $R^*_{n-1}(k_1, k_2, k_3, k_4)$, the paths $P_3 = x_1x_2x_3$ and $P_2 = x_6x_7$. Since P_3 and P_2 have 5 matches, there's $5E(m^*_{n-1})$.

Subcase 4.3: When neither x_3x_4 nor x_4x_5 is included in the matches. Therefore, this subcase is equivalent to the combination of the $R_n(k_1, k_2, k_3, k_4)$, the paths $P_3 = x_1x_2x_3$ and $P_3 = x_5x_6x_7$. Since P_3 and P_3 have 6 matches, there's $6E(m_n)$.

Thus, there's $10k_4E(m^*_{n-1})$+$6k_4E(m_n)$ from the above subcases.

Thus, the following results can be derived from Cases 1, 2, 3 and 4.

$$\begin{aligned}E(m^*_n) =&10k_1E(m'_{n-1}) + 6k_1E(m_n) + 10k_2E(\tilde{m}_{n-1})\\&+6k_2E(m_n) + 10k_3E(\hat{m}_{n-1}) + 6k_3E(m_n)\\&+10k_4E(m^*_{n-1}) + 6k_4E(m_n)\\=&6(k_1 + k_2 + k_3 + k_4)E(m_n) + 10k_1E(m'_{n-1})\\&+10k_2E(\tilde{m}_{n-1}) + 10k_3E(\hat{m}_{n-1})\\&+10k_4E(m^*_{n-1})\\=&6E(m_n) + 10k_1E(m'_{n-1}) + 10k_2E(\tilde{m}_{n-1})\\&+10k_3E(\hat{m}_{n-1}) + 10k_4E(m^*_{n-1}).\end{aligned}$$

When $n \geq 1$, we can obtain that

$$\begin{aligned}\sum_{n=1}^{\infty} E(m^*_n)x^n = &\sum_{n=1}^{\infty} 6E(m_n)x^n + 10k_1\sum_{n=1}^{\infty} E(m'_{n-1})x^n\\&+10k_2\sum_{n=1}^{\infty} E(\tilde{m}_{n-1})x^n + 10k_3\sum_{n=1}^{\infty} E(\hat{m}_{n-1})x^n\\&+10k_4\sum_{n=1}^{\infty} E(m^*_{n-1})x^n\end{aligned}$$

which implies that

$$\begin{aligned}M^*(x) - E(m^*_0) =&6(M(x) - E(m_0))\\&+10k_1xM'(x) + 10k_2x\tilde{M}(x)\\&+10k_3x\hat{M}(x) + 10k_4xM^*(x).\end{aligned}$$

Note that $E(m^*_0)$ is the number of matches of path of 7 vertices while $E(m_0)$ is the number of matching of size 0,the empty set of the empty graph.Thus, $E(m_0) = 1$ and $E(m^*_0) = 21$. Therefore,

$$\begin{aligned}M^*(x) =&15 + 6M(x) + 10k_1xM'(x) + 10k_2x\tilde{M}(x)\\&+10k_3x\hat{M}(x) + 10k_4xM^*(x).\end{aligned}$$

Equation (5) can be proved from the above.

According to Equations (1), (2), (3), (4) and (5), the final result of random octagonal chains of the expected values for Hosoya index is about to be obtained.

IV. The expected values for Merrifield-Simmons index of random octagonal chains

In this subsection, to obtain the expected values of random octagonal chains for Merrifield-Simmons index, the following preparations have to be done.

The expected value of $R_n(k_1, k_2, k_3, k_4)$ of the number of independent sets is denoted as $E(i_n(k_1, k_2, k_3, k_4))$.And the generating function of $E(i_n(k_1, k_2, k_3, k_4)$ is denoted as $I_{k_1,k_2,k_3,k_4}(x)$. Normally, $E(i_n)$ and $I(x)$ can be used to denote $E(i_n(k_1, k_2, k_3, k_4))$ and $I_{k_1,k_2,k_3,k_4}(x)$. Therefore,

$$I(x) = \sum_{n=0}^{\infty} E(i_n)x^n$$

For the expected values of the number of independent sets of the $R'_n(k_1, k_2, k_3, k_4)$, the $\tilde{R}_n(k_1, k_2, k_3, k_4)$, the $\hat{R}_n(k_1, k_2, k_3, k_4)$ and the $R^*_n(k_1, k_2, k_3, k_4)$, the $E(i'_n)$,$E(\tilde{i}_n)$,$E(\hat{i}_n)$ and $E(i^*_n)$ are used to denote, respectively. Meanwhile, the generating functions can be denoted by $I'(x)$, $\tilde{I}(x)$, $\hat{I}(x)$ and $I^*(x)$, respectively. Thus,

$$I'(x) = \sum_{n=0}^{\infty} E(i'_n)x^n$$

$$\tilde{I}(x) = \sum_{n=0}^{\infty} E(\tilde{i}_n)x^n$$

$$\hat{I}(x) = \sum_{n=0}^{\infty} E(\hat{i}_n)x^n$$

$$I^*(x) = \sum_{n=0}^{\infty} E(i_n^*)x^n$$

Now, for a random octagonal chain, the following equation must be proved in order to obtain the expected value for Merrifield-Simmons index.

$$I(x) = 1{+}35x + 13xI(x) + 21k_1x^2I^{'}(x) + 21k_2x^2\tilde{I}(x) + 21k_3x^2\hat{I}(x) + 21k_4x^2I^*(x). \tag{6}$$

$$I^{'}(x) = 21 + 13I(x) + 8k_1xI^{'}(x) + 8k_2x\tilde{I}(x) + 8k_3x\hat{I}(x) + 8k_4xI^*(x). \tag{7}$$

$$\tilde{I}(x) = 26 + 8I(x) + 18k_1xI^{'}(x) + 18k_2x\tilde{I}(x) + 18k_3x\hat{I}(x) + 18k_4xI^*(x). \tag{8}$$

$$\hat{I}(x) = 26 + 10I(x) + 14k_1xI^{'}(x) + 14k_2x\tilde{I}(x) + 14k_3x\hat{I}(x) + 14k_4xI^*(x). \tag{9}$$

$$I^*(x) = 25 + 9I(x) + 16k_1xI^{'}(x) + 16k_2x\tilde{I}(x) + 16k_3x\hat{I}(x) + 16k_4xI^*(x). \tag{10}$$

Because we can prove Equations (6) - (10) by similar arguments as Equations (1) - (5), we omit the proofs of these equations. By Equations (6),(7),(8),(9)and (10), the final result of random octagonal chains of the expected values for Merrifield-Simmons index is about to be obtained.

V. Numerical results

The specific conclusions drawn in this paper are as follows:

Theorems 1. For a non-negative integer n ,when there exist four non-negative real numbers k_1,k_2,k_3 and k_4 satisfying $k_1 + k_2 + k_3 + k_4 = 1$, let $R_n(k_1, k_2, k_3, k_4)$ be a random octagonal chain with n octagons. The expected value of the number of matches of $R_n(k_1, k_2, k_3, k_4)$ can be denoted by $E(m_n(k_1, k_2, k_3, k_4))$. And $M_{k_1,k_2,k_3,k_4}(x)$ is the generating function of $E(m_n(k_1, k_2, k_3, k_4))$.Then

$$M(x) = 1 + 26x + 21xM(x) + 26ax^2M^{'}(x) + 26bx^2\tilde{M}(x) + 26cx^2\hat{M}(x) + 26dx^2M^*(x).$$

$$M^{'}(x) = 8 + 13M(x) + 8axM^{'}(x) + 8bx\tilde{M}(x) + 8cx\hat{M}(x) + 8dxM^*(x).$$

$$\tilde{M}(x) = 13 + 8M(x) + 13axM^{'}(x) + 13bx\tilde{M}(x) + 13cx\hat{M}(x) + 13dxM^*(x).$$

$$\hat{M}(x) = 14 + 7M(x) + 10axM^{'}(x) + 10bx\tilde{M}(x) + 10cx\hat{M}(x) + 10dxM^*(x).$$

$$M^*(x) = 15 + 6M(x) + 10axM^{'}(x) + 10bx\tilde{M}(x) + 10cx\hat{M}(x) + 10dxM^*(x).$$

Theorems 2. For a non-negative integer n, when there exist four non-negative real numbers k_1,k_2,k_3 and k_4 satisfying $k_1 + k_2 + k_3 + k_4 = 1$, $R_n(k_1, k_2, k_3, k_4)$ is a random octagonal chain with n octagons. The expected value of the number of matches of $R_n(k_1, k_2, k_3, k_4)$ can be denoted by $E(i_n(k_1, k_2, k_3, k_4))$. And $I_{k_1,k_2,k_3,k_4}(x)$ is the generating function of $E(i_n(k_1, k_2, k_3, k_4))$. Then

$$I(x) = 1{+}35x + 13xI(x) + 21ax^2I^{'}(x) + 21bx^2\tilde{I}(x) + 21cx^2\hat{I}(x) + 21dx^2I^*(x).$$

$$I^{'}(x) = 21 + 13I(x) + 8axI^{'}(x) + 8bx\tilde{I}(x) + 8cx\hat{I}(x) + 8dxI^*(x).$$

$$\tilde{I}(x) = 26 + 8I(x) + 18axI^{'}(x) + 18bx\tilde{I}(x) + 18cx\hat{I}(x) + 18dxI^*(x).$$

$$\hat{I}(x) = 26 + 10I(x) + 14axI^{'}(x) + 14bx\tilde{I}(x) + 14cx\hat{I}(x) + 14dxI^*(x).$$

$$I^*(x) = 25 + 9I(x) + 16axI^{'}(x) + 16bx\tilde{I}(x) + 16cx\hat{I}(x) + 16dxI^*(x).$$

VI. Conclusions

In this paper, in order to obtain the expressions of the expected values of the Hosoya index and the Merrifield-Simmons index for random octagonal chains, we solve the problem by classification and discussion. The precise formulas established in this paper will undoubtedly help in the study of their corresponding chemical properties.

References

[1] J.A. Bondy, U.S.R. Murty, "Graph Theory," *Springer,* New York, 2008.

[2] H. Hosoya, "Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons," *Bull. Chem. Soc. Jpn.* 44 (1971) 2332–2339.

[3] R. M. Merrifield, H. E. Simmons, "The structure of molecular topological spaces," *Theor. Chim. Acta.* 55 (1980) 55–75.

[4] R. M. Merrifield, H. E. Simmons, "Enumeration of structure-sensitive graphical subsets: Theory," *Proc. Natl. Acad. Sci.* 78 (1981) 692–695.

[5] R. M. Merrifield, H. E. Simmons, "Enumeration of structure-sensitive graphical subsets: Calculations", *Proc. Natl. Acad. Sci.* 78 (1981)1329–1332.

[6] R. M. Merrifield, H. E. Simmons, "Mathematical description of molecular Structure: Molecular topology," *Proc. Natl. Acad. Sci.* 78 (1981)2616–2619.

[7] I. Gutman, D. Vidovi´c, H. Hosoya, "The relation between the eigenvalue sum and the topological index Z revisited," *Bull. Chem. Soc.Jpn.* 75 (1986) 1723–1727.

[8] A.L. Chen, F.J. Zhang, "Wiener index and perfect matches in random phenylene chains," *MATCH Commun. Math. Comput. Chem.* 61 (2009) 623-630.

[9] E. J. Farrell, "Matching in hexagonal cacti," *Int. J. Math. Math. Sci.* 10 (1987) 321–338.

[10] R.C. Entringer, D.E. Jackson, D.A. Snyder, "Distance in graphs," *Czechoslovak Math. J.* 26 (1976) 283-296.

[11] M. S. Oz, I. N. Cangul, "Computing the Hosoya and the Merrifield-Simmons indices of two special benzenoid systems," *Iran. J. Math.Chem.* 12 (2021) 161–174.

[12] I. Gutman, F. Zhang, "On the ordering of graphs with respect to their matching numbers," *Discr. Appl. Math.* 15 (1986) 25–33.

[13] S. Gupta, M. Singh, A.K. Madan, "Eccentric distance sum: A novel graph invariant for predicting biological and physical properties," *J. Math. Anal. Appl.* 275 (2002) 386-401.

[14] I. Gutman, L. Feng, G. Yu, "Degree resistance distance of unicyclic graphs," *Trans. Comb.* 1 (2) (2012) 27-40.

[15] S. Wagner, I. Gutman, "Maxima and minima of Hosoya index and Merrifield-Simmons index," *Acta Appl. Math.* 112 (2010) 323–346.

[16] M. S. Oz, I. N. Cangul, "Computing the Merrifield-Simmons indices of benzenoid chains and double benzenoid chains," *J. Appl. Math. Comput.* 68 (2021) 3263–3293.

[17] G. Huang, M. Kuang, H. Deng, "The expected values of Hosoya index and Merrifield–Simmons index in a random polyphenylene chain," *J.Comb. Optim.* 32 (2016) 550–562.

[18] M. M. Oo, N. W, N. Klamsakul, "The expected values of Hosoya index and Merrifield–Simmons index of random hexagonal cactus chains," *MATCH Commun. Math. Comput. Chem.* 91 (2024) 683–707.

[19] Y. Sun, X. Geng, "The expected value of Hosoya index and Merrifield–Simmons index in a random cyclooctylene chain," *Axioms* 11(2022) 261.

[20] A. Chen, "Merrifield-Simmons index in random phenylene chains and random hexagon chains," *Discr. Dyn. Nat. Soc.* 2015 (2015) 568926.

[21] Ryan J. Schwamm, Mathew D. Anker, Matthias Lein, Reduction vs. "Addition: The Reaction of an Aluminyl Anion with 1,3,5,7-Cyclooctatetraene," *J. Chem.* 58 (5) 2019 1489-1493.

[22] S.C. Li, W. Wei, "Some edge-grafting transformations on the eccentricity resistance-distance sum and their applications," *Discrete Appl. Math.* 211 (2016) 130-142.

[23] G. Luthe, J.A. Jacobus, L.W. Robertson, " Receptor interactions by polybrominated diphenyl ethers versus polychlorinated biphenyls: a theoretical structure-activity assessment," *Environ. Toxicol. Pharm.* 25 (2008) 202-210.

[24] Nicholas Milas, John Nolan, Jr., Petrus H.L. Otto, "Notes-Ozonization of Cyclooctatetraene," *J. Org. Chem.* 23 (4) (1958) 624-625.

[25] M. Somodi, "On the Ihara zeta function and resistance distance-based indices," *Linear Algebra Appl.* 513 (2017) 201-209.

[26] M. Tang, C.E. Priebe, "Limit theorems for eigenvectors of the normalized Laplacian for random graphs," *Ann. Statist.* 46 (5) (2018) 2360-2415.

[27] H. Wiener, "Structrual determination of paraffin boiling points," *J. Am. Chem. Soc.* 69 (1947) 17-20.