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Research article

The expected values of the total numbers of independent edge sets and independent sets in random alpha-type pentagonal chains [☆]

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ABSTRACT

A independent edge set of G containing mutually independent edges is also called a matching of G. The total numbers of matchings and independent sets of a graph G, namely, the Hosoya index and the Merrifield-Simmons index, respectively, are two important topological indices. We compute the average total numbers of independent edge sets and independent sets in random alpha-type pentagonal chains.

1. Introduction

Hosoya first proposed a topological descriptor in 1971, named Hosoya index (abbreviated H index), which also can be used to computing the total number of independent edge sets of graphs in mathematics. Hosoya and the authors also demonstrated strongly relations between the index and various topological properties of saturated hydrocarbons in some papers [1–5], and theory indicated that the index have many applications in organic chemistry [6–8].

In 1980, the chemists Merrifield and Simmoms sought to describe molecular structures through finite-set topology. Ultimately, their theory failed, however, the corresponding results attracted extensively attention of researchers, and the Merrifield-Simmons index (abbreviated MS index) was put forward [9], which also can be used to computing the total number of independent sets of graphs in mathematics. Some other results for the index can refer to subsequent papers [10–13].

The H and MS indices are very popular used in mathematical chemistry. Due to the interesting combinatorial properties of them, a lot of works have been done on the two topological descriptor in recent years. Concerning on research methods and results of the two indices refer to Wagner and Gutman [14], and for others recent works see [15–17]. In subsequent studies, for the extremal problems of the two indices, all kinds of chemical graphs are considered. Such as spiro hexagonal chains [18], random polyphenylene chain [19], polyphenyl chains [22,23], random spiro chain [24]; and including other topological indices, such as Wiener indices [20] and Kirchhoff indices [21] of spiro and polyphenyl hexagonal chains, respectively. In 2022, the Hosoya properties of the power graph formed by a finite group are investigated [25]. Recently, the topological invariants had been used for analyzing properties of new drugs of COVID-19, one can see [26–31].

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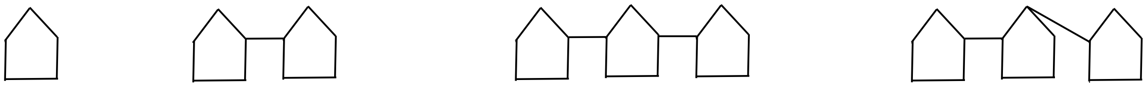

Fig. 1. Alpha-pentagonal chains with one, two, and three pentagons.

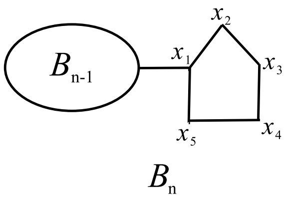

Fig. 2. An alpha-pentagonal chain with n pentagons.

Pentagonal chains are an important class of unbranched conjugated hydrocarbons, which possess great research being of chemical synthesis. Motivated by the work [32], we compute the average total numbers of independent edge sets and independent sets in random alpha-type pentagonal chains in this paper.

Suppose that $G = (V, E)$ is a simple connected graph, u is a vertex of G. We denote by $G - u$ the graph obtained by deleting u and the edges incident with u. $G - e$ (or $G\backslash e$, respectively) represents the subgraph of G by deleting e (or by deleting e and both its end-vertices, respectively), where e is an edge of G. $N(u)$ is the set of vertices adjacent with u in G, and $N[u] = N(u) \bigcup \{u\}$.

A subset M of E is called a matching (or independent edge set) in G if its elements are edges and no two are adjacent in G, and k-matching of G if $|M| = k$, where $|M|$ is the size of M. If we denote by $m_k(G)$ is the number of k-matchings in G, then $m_0(G) = 1$, $m_1(G)$ is the number of edges in G, and $m(G) = \sum_{k\geq 0} m_k(G)$ is the total number of matchings in G. A subset S of V satisfying with the condition that no two vertices of S are adjacent in G, is called an independent set of G, and k-independent set of G if $|S| = k$. If we denote $i_k(G)$ by the number of k-independent sets in G, easy to see that $i_0(G) = 1$, $i_1(G)$ is the number of vertices in G, and $i(G) = \sum_{k\geq 0} i_k(G)$ is the total number of independent sets in G. It is known that $m(G)$ and $i(G)$ represent H index and MS index of G in chemical literature, respectively.

Recall that P_n (or C_n) is a path (or a cycle) with n vertices. The following three formulae (due to Gutman and Polansky [7]) will be used in the rest of the computations in this paper.

Let G be a graph with components $G_1, G_2, \ldots, G_k$, and e (or v) an edge (or a vertex) of G. Then we have

$$m(G) = m(G - e) + m(G\backslash e); \tag{1}$$

$$i(G) = i(G - v) + i(G - N[v]); \tag{2}$$

$$m(G) = \prod_{i=1}^{k} m(G_i), i(G) = \prod_{i=1}^{k} i(G_i); \tag{3}$$

Obviously, the values of H index and MS index for few vertices of path and cycle easily obtained.

The following Fig. 1 illustrated short alpha-pentagonal chains for $n = 1, 2$ and 3. An alpha-pentagonal chain B_n with n pentagons obtained from an alpha-pentagonal chain B_{n-1} with $n - 1$ pentagons by addition of a new terminal pentagon as shown in Fig. 2. However, for $n \geq 2$ the terminal pentagon can be attached in two local arrangements we describe as B_n^1 and B_n^2 illustrated in Fig. 3.

A random alpha-pentagonal chain $B_n(p, 1 - p)$ with n pentagons is a pentagonal chain obtained by stepwise addition of terminal pentagon. At each step k ($k \geq 3$), a random selection is made from one of the two possible constructions:

(i) $B_{k-1} \to B_k^1$ with probability p;
(ii) $B_{k-1} \to B_k^2$ with probability $1 - p$; where $p\,(0 \leq p < 1)$ is constant, irrelative to parameter k.

2. H index of random alpha-type pentagonal chains

A random alpha-pentagonal chain $B_n(p, 1 - p)$ can be viewed as at random by attaching B_{n-1} a terminal pentagon in two local arrangements. It is clear that the Hosoya index can be viewed as a random variable. In this section, we will present exact formulae of its expected values $E(m(B_n))$ in terms of auxiliary graphs, and two type auxiliary graphs A_k, C_k as shown in Fig. 4, where $A_k \in \{A_k^1, A_k^2\}$, $C_k \in \{C_k^1, C_k^2\}$.

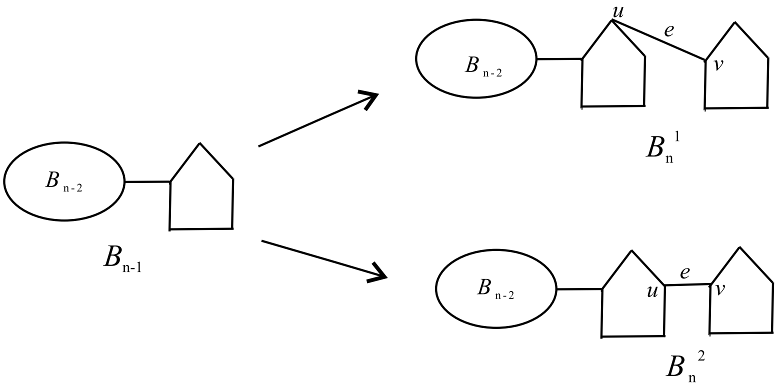

Fig. 3. The two types of local arrangement in alpha-pentagonal chains.

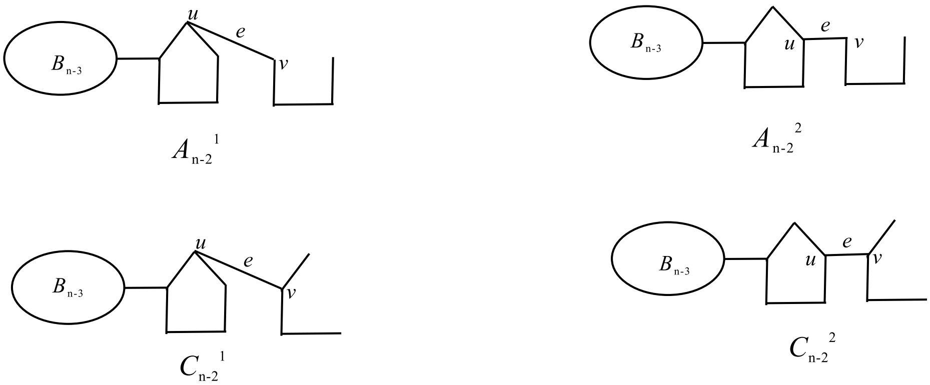

Fig. 4. Auxiliary graphs A^1_{n-2}, A^2_{n-2} and C^1_{n-2}, C^2_{n-2}.

If $B_n = B_n^1$ is as shown in Fig. 3, according to Eqs. (1)-(3), then we have

$$\begin{aligned} m(B_n) &= m(B_n - e) + m(B_n \backslash e) \\ &= m(C_5)m(B_{n-1}) + m(P_4)m(A_{n-2}) \\ &= 11m(B_{n-1}) + 5m(A_{n-2}). \end{aligned} \tag{4}$$

Similarly, if $B_n = B_n^2$,

$$\begin{aligned} m(B_n) &= m(B_n - e) + m(B_n \backslash e) \\ &= m(C_5)m(B_{n-1}) + m(P_4)m(C_{n-2}) \\ &= 11m(B_{n-1}) + 5m(C_{n-2}). \end{aligned} \tag{5}$$

In case of auxiliary graphs A_{n-2} and C_{n-2}. Similarly,
If $A_{n-2} = A^1_{n-2}$, then

$$\begin{aligned} m(A_{n-2}) &= m(P_4)m(B_{n-2}) + m(P_3)m(A_{n-3}) \\ &= 5m(B_{n-2}) + 3m(A_{n-3}). \end{aligned} \tag{6}$$

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

$$\begin{aligned} m(A_{n-2}) &= m(P_4)m(B_{n-2}) + m(P_3)m(C_{n-3}) \\ &= 5m(B_{n-2}) + 3m(C_{n-3}). \end{aligned} \tag{7}$$

If $C_{n-2} = C^1_{n-2}$, then we have

$$\begin{aligned} m(C_{n-2}) &= m(P_4)m(B_{n-2}) + m(P_2)m(A_{n-3}) \\ &= 5m(B_{n-2}) + 2m(A_{n-3}). \end{aligned} \tag{8}$$

If $C_{n-2} = C^2_{n-2}$, then

$$\begin{aligned} m(C_{n-2}) &= m(P_4)m(B_{n-2}) + m(P_2)m(C_{n-3}) \\ &= 5m(B_{n-2}) + 2m(C_{n-3}). \end{aligned} \tag{9}$$

So we can get the values of $E(m(B_n))$, $E(m(A_{n-2}))$ and $E(m(C_{n-2}))$ of $m(B_n)$, $m(A_{n-2})$ and $m(C_{n-2})$ respectively. From Eqs. (4)-(9) we have

$$\begin{aligned} E(m(B_n)) =& pE(m(B^1_n)) + (1-p)E(m(B^2_n)) \\ =& pE(11m(B_{n-1}) + 5m(A_{n-2})) + (1-p)E(11m(B_{n-1}) + 5m(C_{n-2})) \\ =& 11E(m(B_{n-1})) + 5pE(m(A_{n-2})) + 5(1-p)E(m(C_{n-2})). \end{aligned} \tag{10}$$

Similarly, we have

$$\begin{aligned} E(m(A_{n-2})) =& pE(m(A^1_{n-2})) + (1-p)E(m(A^2_{n-2})) \\ =& 5E(m(B_{n-2})) + 3pE(m(A_{n-3})) + 3(1-p)E(m(C_{n-3})), \end{aligned} \tag{11}$$

and

$$\begin{aligned} E(m(C_{n-2})) =& pE(m(C^1_{n-2})) + (1-p)E(m(C^2_{n-2})) \\ =& 5E(m(B_{n-2})) + 2pE(m(A_{n-3})) + 2(1-p)E(m(C_{n-3})), \end{aligned} \tag{12}$$

then from Eqs. (10)-(12) we have

$$\begin{aligned} E(m(B_n)) =& 11E(m(B_{n-1})) + 25E(m(B_{n-2})) \\ &+ (10p + 5p^2)E(m(A_{n-3})) + (10 - 5p - 5p^2)E(m(C_{n-3})). \end{aligned}$$

With the same method, from Eqs. (11), (12) we have

$$\begin{aligned} &(10p + 5p^2)E(m(A_{n-3})) + (10 - 5p - 5p^2)E(m(C_{n-3})) \\ =&(10p + 5p^2)\Big(pE\big(m(A^1_{n-3})\big) + (1-p)E\big(m(A^2_{n-3})\big)\Big) \\ &+ (10 - 5p - 5p^2)\Big(pE\big(m(C^1_{n-3})\big) + (1-p)E\big(m(C^2_{n-3})\big)\Big) \\ =&(50 + 25p)E(m(B_{n-3}) + (20p + 20p^2 + 5p^3)E(m(A_{n-4})) + (20 - 15p - 5p^3)E(m(C_{n-4})) \\ =&(2+p)\Big(25E\big(m(B_{n-3})\big) + (10p + 5p^2)E\big(m(A_{n-4})\big) + (10 - 5p - 5p^2)E\big(m(C_{n-4})\big)\Big) \\ =&(2+p)\Big(E\big(m(B_{n-1})\big) - 11E\big(m(B_{n-2})\big)\Big). \end{aligned} \tag{13}$$

From above, we have

$$\begin{aligned} E(m(B_n)) =& 11E(m(B_{n-1})) + 25E(m(B_{n-2})) + (2+p)\Big(E\big(m(B_{n-1})\big) - 11E\big(m(B_{n-2})\big)\Big) \\ =& (13+p)E(m(B_{n-1})) + (3 - 11p)E(m(B_{n-2})). \end{aligned} \tag{14}$$

Theorem 1. *Let $B_n(p, 1-p)$ be a random alpha-type pentagonal chain with n pentagons. Then*

$$\begin{aligned} E(m(B_n)) =& \frac{149 - 11p + 11\sqrt{p^2 - 18p + 181}}{p^2 - 18p + 181 + (13+p)\sqrt{p^2 - 18p + 181}} \, \frac{(13 + p + \sqrt{p^2 - 18p + 181})^n}{2^n} \\ &+ \frac{149 - 11p - 11\sqrt{p^2 - 18p + 181}}{p^2 - 18p + 181 - (13+p)\sqrt{p^2 - 18p + 181}} \, \frac{(13 + p - \sqrt{p^2 - 18p + 181})^n}{2^n}. \end{aligned} \tag{15}$$

Proof. From (14) we know that

$$E(m(B_n)) = (13+p)E(m(B_{n-1})) + (3 - 11p)E(m(B_{n-2})),$$

and

$$E(m(B_1)) = 11, \qquad E(m(B_2)) = 146.$$

The characteristic equation of the above recursive relationship is $x^2-(13+p)x+(11p-3)=0$, and whose characteristic roots are

$$q_1=\frac{13+p+\sqrt{p^2-18p+181}}{2},\quad q_2=\frac{13+p-\sqrt{p^2-18p+181}}{2}.$$

Let

$$E(m(G_n))=Aq_1^n+Bq_2^n.$$

We know that

$$E(m(B_1))=Aq_1+Bq_2=11,\qquad E(m(B_2))=Aq_1^2+Bq_2^2=146,$$

then

$$A=\frac{149-11p+11\sqrt{p^2-18p+181}}{p^2-18p+181+(13+p)\sqrt{p^2-18p+181}},$$
$$B=\frac{149-11p-11\sqrt{p^2-18p+181}}{p^2-18p+181-(13+p)\sqrt{p^2-18p+181}}.$$

The result can be obtained by the simplified method. □

Let B_n be a random alpha-type pentagonal chain, and if each step B_k $(3\le k\le n)$, $B_k=B_k^2$, we call B_n be a linear random alpha-type pentagonal chain, if each step B_k $(3\le k\le n)$, $B_k=B_k^1$, we call B_n be a non-linear random alpha-type pentagonal chain.

Corollary 1. *Let B_n be linear alpha-type pentagonal chain with n pentagons. Then*

$$E(m(B_n))=\frac{149+11\sqrt{181}}{181+13\sqrt{181}}\frac{(13+\sqrt{181})^n}{2^n}+\frac{149-11\sqrt{181}}{181-13\sqrt{181}}\frac{(13-\sqrt{181})^n}{2^n},\tag{16}$$

and if B_n is non-linear alpha-type pentagonal chain with n pentagons. Then

$$E(m(B_n))=\frac{138+11\sqrt{164}}{164+14\sqrt{164}}\frac{(14+\sqrt{164})^n}{2^n}+\frac{138-11\sqrt{164}}{164-14\sqrt{164}}\frac{(14-\sqrt{164})^n}{2^n}.\tag{17}$$

Proof. From Theorem 1, we can complete the proof for $p=0$ and $p=1$, respectively. □

3. MS index of random alpha-type pentagonal chains

In this section, we will give a simple exact formula of its excepted value $E(i(B_n))$.

If $B_n=B_n^1$, then by Eqs. (2) and (3) we have

$$\begin{aligned}i(B_n)&=i(B_n-v)+i(B_n-N[v])\\&=i(P_4)i(B_{n-1})+i(P_2)i(A_{n-2})\\&=8i(B_{n-1})+3i(A_{n-2}),\end{aligned}\tag{18}$$

similarly, if $B_n=B_n^2$,

$$\begin{aligned}i(B_n)&=i(B_n-v)+i(B_n-N[v])\\&=i(P_4)i(B_{n-1})+i(P_2)i(C_{n-2})\\&=8i(B_{n-1})+3i(C_{n-2}).\end{aligned}\tag{19}$$

Now we search the case of auxiliary graphs A_{n-2} and C_{n-2}.

If $A_{n-2}=A_{n-2}^1$

$$\begin{aligned}i(A_{n-2})&=i(P_3)i(B_{n-2})+i(P_2)i(A_{n-3})\\&=5i(B_{n-2})+3i(A_{n-3}).\end{aligned}\tag{20}$$

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

$$\begin{aligned}i(A_{n-2})&=i(P_3)i(B_{n-2})+i(P_2)i(C_{n-3})\\&=5i(B_{n-2})+3i(C_{n-3}).\end{aligned}\tag{21}$$

If $C_{n-2} = C^1_{n-2}$, then

$$\begin{aligned} i(C_{n-2}) &= i(P_1)i(P_2)i(B_{n-2}) + i(P_1)i(A_{n-3}) \\ &= 6i(B_{n-2}) + 2i(A_{n-3}). \end{aligned} \tag{22}$$

If $C_{n-2} = C^2_{n-2}$, then

$$\begin{aligned} i(C_{n-2}) &= i(P_1)i(P_2)i(B_{n-2}) + i(P_1)i(C_{n-3}) \\ &= 6i(B_{n-2}) + 2i(C_{n-3}). \end{aligned} \tag{23}$$

From above, we can get the expected values $E(i(B_n))$, $E(i(A_{n-2}))$ and $E(i(C_{n-2}))$ of $i(B_n)$, $i(A_{n-2})$ and $i(C_{n-2})$ respectively. From Eqs. (18)-(23) we have

$$\begin{aligned} E(i(B_n)) &= pE(i(B^1_n)) + (1-p)E(i(B^2_n)) \\ &= 8E(i(B_{n-1})) + 3pE(i(A_{n-2})) + 3(1-p)E(i(C_{n-2})). \end{aligned} \tag{24}$$

Similarly, we have

$$\begin{aligned} E(i(A_{n-2})) &= pE(i(A^1_{n-2})) + (1-p)E(i(A^2_{n-2})) \\ &= 5E(i(B_{n-2})) + 3pE(i(A_{n-3})) + 3(1-p)E(i(C_{n-3})), \end{aligned} \tag{25}$$

and

$$\begin{aligned} E(i(C_{n-2})) &= pE(i(C^1_{n-2})) + (1-p)E(i(C^2_{n-2})) \\ &= 6E(i(B_{n-2})) + 2pE(i(A_{n-3})) + 2(1-p)E(i(C_{n-3})). \end{aligned} \tag{26}$$

From (24)-(26) we have

$$\begin{aligned} E(i(B_n)) &= 8E(i(B_{n-1})) + 3pE(i(A_{n-2})) + 3(1-p)E(i(C_{n-2})) \\ &= 8E(i(B_{n-1})) + (18-3p)E(i(B_{n-2})) + (6p+3p^2)E(i(A_{n-3})) \\ &\quad + (6-3p-3p^2)E(i(C_{n-3})). \end{aligned} \tag{27}$$

With the same method, we have

$$\begin{aligned} &(6p+3p^2)E(i(A_{n-3})) + (6-3p-3p^2)E(i(C_{n-3})) \\ =&(6p+3p^2)\Big(pE\big(i(A^1_{n-3})\big) + (1-p)E\big(i(A^2_{n-3})\big)\Big) \\ &+ (6-3p-3p^2)\Big(pE\big(i(C^1_{n-3})\big) + (1-p)E\big(i(C^2_{n-3})\big)\Big) \\ =&(36+12p-3p^2)E\big(i(B_{n-3})\big) + (12p+12p^2+3p^3)E\big(i(A_{n-4})\big) + (12-9p^2-3p^3)E\big(i(C_{n-4})\big) \\ =&(2+p)\Big((18-3p)E\big(i(B_{n-3})\big) + (6p+3p^2)E\big(i(A_{n-4})\big) + (6-3p-3p^2)E\big(i(C_{n-4})\big)\Big) \\ =&(2+p)\Big(E\big(i(B_{n-1})\big) - 8E\big(i(B_{n-2})\big)\Big). \end{aligned} \tag{28}$$

From above, then

$$\begin{aligned} E(i(B_n)) &= 8E(i(B_{n-1})) + (18-3p)E(i(B_{n-2})) + (2+p)(E(i(B_{n-1})) - 8E(i(B_{n-2}))) \\ &= (10+p)E(i(B_{n-1})) + (2-11p)E(i(B_{n-2})). \end{aligned} \tag{29}$$

Theorem 2. *If $B_n(p, 1-p)$ is a random alpha-type pentagonal chain with n pentagons. Then*

$$\begin{aligned} E(i(B_n)) = &\frac{114 - 11p + 11\sqrt{p^2-24p+108}}{p^2-24p+108+(10+p)\sqrt{p^2-24p+108}} \frac{(10+p+\sqrt{p^2-24p+108})^n}{2^n} \\ &+ \frac{114 - 11p - 11\sqrt{p^2-24p+108}}{p^2-24p+108-(10+p)\sqrt{p^2-24p+108}} \frac{(10+p-\sqrt{p^2-24p+108})^n}{2^n}. \end{aligned} \tag{30}$$

Proof. We know that

$$E(i(B_n)) = (10+p)E(i(B_{n-1})) + (2-11p)E(i(B_{n-2})),$$

and

$$E(i(B_1)) = 11, \qquad E(i(B_2)) = 112.$$

The characteristic equation of the above recursive relationship is $x^2 - (10+p)x + (11p-2) = 0$, and whose characteristic roots are:

$$q_1 = \frac{10+p+\sqrt{p^2-24p+108}}{2}, \quad q_2 = \frac{10+p-\sqrt{p^2-24p+108}}{2}.$$

Let

$$E(i(B_n)) = Aq_1^n + Bq_2^n.$$

We know that

$$E(i(B_1)) = Aq_1 + Bq_2 = 11, \qquad E(i(B_2)) = Aq_1^2 + Bq_2^2 = 112,$$

then

$$A = \frac{114 - 11p + 11\sqrt{p^2-24p+108}}{p^2-24p+108+(10+p)\sqrt{p^2-24p+108}},$$
$$B = \frac{114 - 11p - 11\sqrt{p^2-24p+108}}{p^2-24p+108-(10+p)\sqrt{p^2-24p+108}}.$$

The result can be obtained by the simplified method. □

Corollary 2. *If B_n is a linear alpha-type pentagonal chain with n pentagons. Then*

$$E(i(B_n)) = \frac{114+11\sqrt{108}}{108+10\sqrt{108}}\frac{(10+\sqrt{108})^n}{2^n} + \frac{114-11\sqrt{108}}{108-10\sqrt{108}}\frac{(10-\sqrt{108})^n}{2^n}, \tag{31}$$

and if B_n is a non-linear alpha-type pentagonal chain with n pentagons. Then

$$E(i(B_n)) = \frac{103+11\sqrt{85}}{85+11\sqrt{85}}\frac{(11+\sqrt{85})^n}{2^n} + \frac{103-11\sqrt{85}}{85-11\sqrt{85}}\frac{(11-\sqrt{85})^n}{2^n}. \tag{32}$$

Proof. Easily obtained from Theorem 2, for $p = 0$ and $p = 1$, respectively. □

4. The average values of H index and MS index of random alpha-type pentagonal chains

Suppose that $\mathcal{B}_n$ is the set of all alpha-type pentagonal chains with n pentagons. Then we have the following results.

$$M_{avr}(\mathcal{B}_n) = \frac{1}{|\mathcal{B}_n|}\sum_{B_n \in \mathcal{B}_n} m(B_n),$$
$$i_{avr}(\mathcal{B}_n) = \frac{1}{|\mathcal{B}_n|}\sum_{B_n \in \mathcal{B}_n} i(B_n).$$

The values of $m_{avr}(\mathcal{B}_n)$ and $i_{avr}(\mathcal{B}_n)$ are obtained, we only need to take $p = \frac{1}{2}$ in the values of $E(m(B_n))$ and $E(i(B_n))$. According to Theorems 1 and 2, we have

Theorem 3. *If $\mathcal{B}_n$ is the set of all alpha-type pentagonal chains with n pentagons. Then*

$$\begin{aligned} m_{avr}(\mathcal{B}_n) &= \frac{574+22\sqrt{689}}{689+27\sqrt{689}}\left(\frac{27+\sqrt{689}}{4}\right)^n + \frac{574-22\sqrt{689}}{689-27\sqrt{689}}\left(\frac{27-\sqrt{689}}{4}\right)^n, \\ i_{avr}(\mathcal{B}_n) &= \frac{434+22\sqrt{385}}{385+21\sqrt{385}}\left(\frac{21+\sqrt{385}}{4}\right)^n + \frac{434-22\sqrt{385}}{385-21\sqrt{385}}\left(\frac{21-\sqrt{385}}{4}\right)^n. \end{aligned} \tag{33}$$

In order to better study the two expected values of H index and MS index of linear or non-linear alpha-type pentagonal chains, and we will present the relationship between them by using corresponding table and scatter diagram, which shows that these two expected values are exponential function, and the corresponding values will be very large, so we can study relations between them by taking the logarithm of expressions of them. Let x, y, z, w be the logarithm of the two expected values of H index and MS index of linear alpha-type pentagonal chains and non-linear alpha-type pentagonal chains, respectively. Through matlab software, we will get the final table and scatter diagram, one can see Table 1 and Fig. 5, the value of each logarithm of expected value will keep two decimal.

Table 1
Logarithms of expected values.

n	1	2	3	4	5	6	7	8	9	10	11	12
x	2.40	4.98	7.57	10.15	12.73	15.31	17.89	20.48	23.06	25.64	28.22	30.81
y	2.40	4.98	7.58	10.17	12.77	15.37	17.96	20.56	23.15	25.75	28.34	30.94
z	2.40	4.72	7.04	9.36	11.68	14.01	16.33	18.65	20.97	23.29	25.62	27.94
w	2.40	4.72	7.03	9.35	11.66	13.97	16.29	18.60	20.91	23.23	25.54	27.85

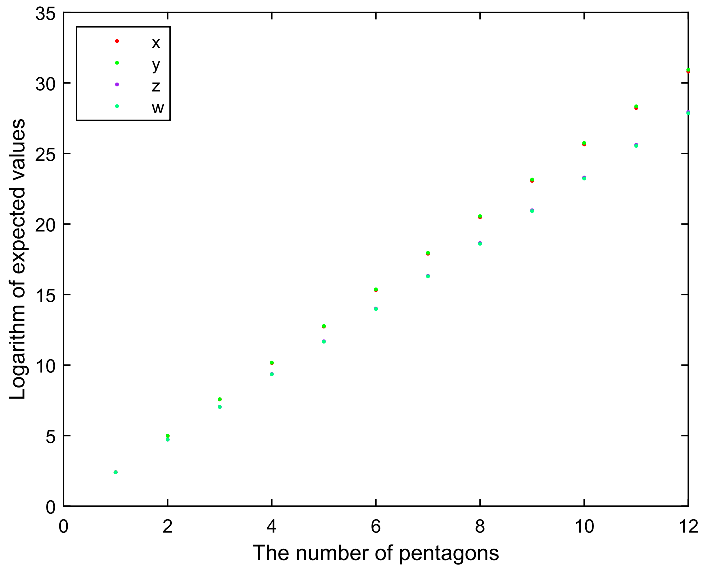

Fig. 5. The scatter diagram of Logarithms of expected values.

By using of Matlab, we obtain the above table and scatter diagram. We found that when $n = 1$, we have $x = y = z = w$, when $n = 2$, we have $x = y$, $z = w$. As n increases, x and y are greater than z and w, and y is greater than x, and z is greater than w. So the corresponding expected values have the same relationships.

5. Conclusion

Topological descriptor of molecular structure has extensively applications in QSPR and QSAR studies. In this paper, we determine that the explicit formulae for the expected values of H index and MS index of random alpha-type pentagonal chains, and analyzed relationships in these expected values by taking the logarithm of expressions of them in matlab software. Moreover, we also present accurate average values of H index and MS index in all alpha-type pentagonal chains with n pentagons.

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CRediT authorship contribution statement

Lina Wei: Contributed reagents, materials, analysis tools or data; Wrote the paper.
Hong Bian: Conceived and designed the experiments.
Haizheng Yu: Performed the experiments; Analyzed and interpreted the data.

Declaration of competing interest

The authors declare no conflict of interest.

Data availability

Data included in article/supp. material/referenced in article.

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