

DEGREE-BASED TOPOLOGICAL INDICES IN RANDOM POLYGONAL AND SPIRO CHAINS

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(Received: Sep. 23, 2024 Accepted: Jul. 18, 2025 Published: Aug. 30, 2025)

Abstract: A topological descriptors is a numerical quantity associated with the chemical structures which play an essential role in the chemical graph theory. In this work, we state and prove the expected values of the degree- based topological indices and generalized $ISI_{(\alpha,\beta)}$ index for the random l -polygonal chain and random l -polygonal spiro chain. Based on the results above, we present the average values of the TIs with respect to the set of all polygonal and spiro polygonal chains with n polygons. As applications, we apply the affiliated formulae to obtain the expected values of the TIs of some special polygonal chains and spiro polygonal chains. Furthermore, we present diverse representations of graph that highlights the correlations between expected mean of indices and structural parameters.

Keywords and Phrases: Topological indices, Generalized ISI index, Random polygonal chain, Random polygonal spiro chain, Expected value, Average value.

2020 Mathematics Subject Classification: 05C09, 05C80, 05C90, 05C92.

1. Introduction

Chemical graph theory [32] is an essential branch of mathematics and theoretical chemistry which model graphs mathematically. A topological index or molecular descriptor [14, 25, 31] correlate each molecular structure with a numerical value. It helps to predict different kind of physico-chemical properties and biological activity associated with the structure of the compounds. These indices are extensively used

in the QSPR and QSAR studies, pharmaceutical drug designing, isomer discrimination etc. The topological indices of Random molecular graphs are very much important in theoretical chemistry. The study of random arrangement of topological indices has received an ample amount of attention of researchers from various fields of Mathematical and Chemical Sciences [6, 11, 15, 26, 33].

A polygonal chain of n cycles (polygons) is obtained from a sequence of polygons O_1, O_2, \dots, O_n , by adjoining a cut edge to each pair of consecutive cycles. This polygonal chain is an l -polygonal chain (of length n) if all the cycles are l -cycles and is denoted as PC_n . The O_i cycle is called the i^{th} -polygon of PC_n , $1 \leq i \leq n$. For $n = 1, 2$, the polygonal chains are unique as shown in Figure 1 [38]. But PC_n is not unique when $n \geq 3$. Let $O_{n-1} = x_1x_2\dots x_lx_1$ in PC_{n-1} for $n \geq 3$. There is a cut edge connecting x_1 and v_{n-2} which is a vertex in O_{n-2} . Let PC_n^i be obtained by local adjustment of the l -polygonal chains (see Figure 2) [38], where $1 \leq i \leq m$. Let $m = \lfloor \frac{l}{2} \rfloor$. By symmetry, there are m ways to adjoin a cut edge between the $(n-1)^{th}$ cycle O_{n-1} of PC_{n-1} to the terminal l -cycle O_n [38].

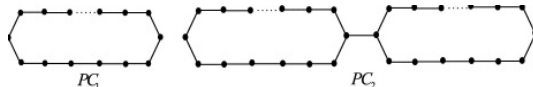


Figure 1: The polygonal chains for $n = 1$ and $n = 2$.

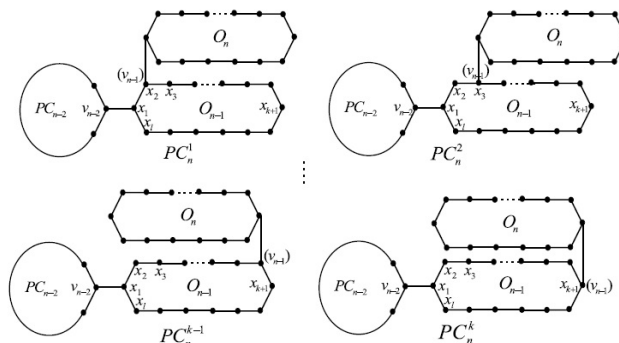


Figure 2: k types of local arrangements in an l -polygonal chain

Similarly, a l -polygonal spiro chain of length n , denoted by SPC_n , can be obtained from a l -polygonal chain PC_n by contracting each cut edge between each pair of l -cycles in PC_n . Figure 3 [20] shows the unique l -polygonal spiro chains for $n = 1, 2$. SPC_n is also not unique when $n \geq 3$ and has m types of local arrangements which are denoted as SPC_n^i , where $1 \leq i \leq m$ (see Figure 4) [20].

Therefore, PC_n^i can be attained by stepwise addition of a terminal l -polygonal chain to PC_{n-1} and also SPC_n^i can be attained by stepwise addition of a terminal l -polygonal spiro chain to SPC_{n-1} which are random in nature with probability p_i and $\sum_{i=1}^m p_i = 1$. We also assume that the probabilities p_1, p_2, \dots, p_m , are constants and independent of n , that is, the process described is a zeroth-order Markov process. After associating probabilities, such an l -polygonal chain is called a random l -polygonal chain and denoted by $PC(n; p_1, p_2, \dots, p_m)$. Also, l -polygonal spiro chain known as random l -polygonal spiro chain, denoted by $SPC(n; p_1, p_2, \dots, p_m)$.

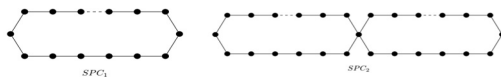


Figure 3: The polygonal spiro chains for $n = 1$ and $n = 2$.

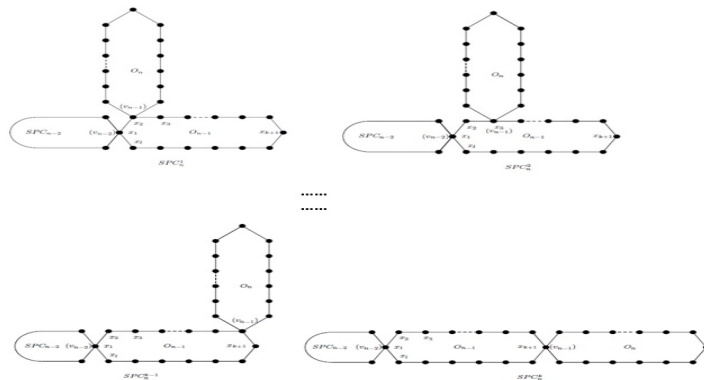


Figure 4: k types of local arrangements in an l -polygonal spiro chain

Brunvoll et al. [2] expressed the number of isomers in tree-like octagonal graphs. Wang et al. [34] obtained the Wiener indices of random pentagonal chains (i.e., 5-polygonal chains) in 2013. Recently, Wei et al. [37] obtained simple formulae for the expected values of the Wiener indices of random generalized polyomino chain graphs (i.e., 4-polygonal chains) and random cyclooctane chain graphs (i.e., 8-polygonal chains). For more detailed survey on the chemical applications and the mathematical literature of the indices of random chains, see [1, 8, 16, 19, 21, 23, 27-29, 41] and the references cited therein.

In recent year, random arrangement of various kind of polygonal chains and polygonal spiro chains attracted many researchers in the field of mathematical physics,

statistics, environmental chemistry etc [1, 18, 24, 35, 40, 45]. Polyomino system is a polycyclic hydrocarbons extensively studied in organic chemistry. The compounds like polyphenylenes, cyclooctanes are a kind of unbranched saturated hydrocarbons and their derivatives attracted many chemists and researchers for many years due to their excellent properties. They are used in synthesis of drug, exchange of heat, synthesis of organic chemicals and petrochemicals, combustion kinetics etc.

In this paper, we consider the general form of degree - based topological indices which is :

$$TI(G) = \sum_{u_i u_j \in E(G)} f(d_i, d_j) \quad (1.1)$$

where, f is a real valued function, u_i is the vertex of the graph G , d_i is the degree of the vertex u_i .

There are legion of topological indices in the literature. In 2020, Buragohain et al. [3] proposed a generalized topological index which is defined as

$$ISI_{(\alpha, \beta)}(G) = \sum_{u_i u_j \in E(G)} (d_i d_j)^\alpha (d_i + d_j)^\beta.$$

Most of the molecular descriptors are the special cases of this generalized index. Table 1 shows the connection of $ISI_{(\alpha, \beta)}$ - index with the molecular descriptors by assigning values to the parameters α and β . For more details of the index, refer to [9, 10, 12, 13, 25, 30, 39, 42-44].

Topological index	Corresponding $ISI_{(\alpha, \beta)}$ - index
First Zagreb index, $M_1(G)$	$ISI_{(0,1)}(G)$
Second Zagreb index, $M_2(G)$	$ISI_{(1,0)}(G)$
Second modified Zagreb index, $\bar{M}_2(G)$	$ISI_{(-1,0)}(G)$
Redefined third Zagreb index, $ReZG_3(G)$	$ISI_{(1,1)}(G)$
Inverse sum indeg index, $ISI(G)$	$ISI_{(1,-1)}(G)$
Harmonic index, $H(G)$	$2ISI_{(0,-1)}(G)$
Hyper-Zagreb index, $HM(G)$	$ISI_{(0,2)}(G)$
Randić index, $R(G)$	$ISI_{(-\frac{1}{2},0)}(G)$
Sum connectivity index, $SCI(G)$	$ISI_{(0,-\frac{1}{2})}(G)$
Geometric- Arithmetic Mean index, $GA(G)$	$2ISI_{(\frac{1}{2},-1)}(G)$
First Generalized Randić index, $R_\alpha(G)$	$ISI_{(\alpha,0)}(G)$
General sum - connectivity index, $\chi_\alpha(G)$	$ISI_{(0,\alpha)}(G)$

Table 1: Relation of $ISI_{(\alpha, \beta)}$ - index with other molecular descriptors

2. Some Preliminaries

Let G be graph and (i, j) - edge denote the edge connecting a vertex of degree i and j in G . Let $x_{ij}(G)$ denote the number of (i, j) -edges in the graph G .

2.1. Random polygonal chain

The $m = \lfloor \frac{l}{2} \rfloor$ local arrangements of the l - polygonal chains with probability p_k is denoted by PC_n^k . From the structure of the chain PC_n , one can see that there are $(2, 2)$, $(2, 3)$ and $(3, 3)$ types of edges only.

We define

$$\gamma_{(i,j)}^{(k)} = x_{ij}(PC_n^k) - x_{ij}(PC_{n-1}),$$

where $1 \leq k \leq m$. For $n \geq 3$, there are m probable structures of l - polygonal chain of length n which is constructed as

$$PC_{n-1} \rightarrow PC_n^k$$

with probability p_k , where p_k are steady and independent of the parameter k and $\sum_{k=1}^m p_k = 1$. Then,
For $k = 1$,

$$\begin{aligned}\gamma_{(2,2)}^{(1)} &= x_{22}(PC_n^1) - x_{22}(PC_{n-1}) = l - 3, \\ \gamma_{(2,3)}^{(1)} &= x_{23}(PC_n^1) - x_{23}(PC_{n-1}) = 2, \\ \gamma_{(3,3)}^{(1)} &= x_{33}(PC_n^1) - x_{33}(PC_{n-1}) = 2.\end{aligned}$$

For $2 \leq k \leq \lfloor \frac{l}{2} \rfloor$,

$$\begin{aligned}\gamma_{(2,2)}^{(k)} &= x_{22}(PC_n^k) - x_{22}(PC_{n-1}) = l - 4, \\ \gamma_{(2,3)}^{(k)} &= x_{23}(PC_n^k) - x_{23}(PC_{n-1}) = 4, \\ \gamma_{(3,3)}^{(k)} &= x_{33}(PC_n^k) - x_{33}(PC_{n-1}) = 1.\end{aligned}$$

We also define

$$\gamma = \sum_{k=1}^m \sum_{(i,j) \in E(G)} p_k \gamma_{(i,j)}^{(k)} f(d_i, d_j), \quad i \leq j. \quad (2.1)$$

2.2. Random l -polygonal spiro chain

The $m = \lfloor \frac{l}{2} \rfloor$ local arrangements of the l - polygonal spiro chains with probability p_k is denoted by SPC_n^k . From the structure of the chain SPC_n , one can see that

there are only $(2, 2)$, $(2, 4)$ and $(4, 4)$ types of edges.

We define

$$\delta_{(i,j)}^{(k)} = x_{ij}(SPC_n^k) - x_{ij}(SPC_{n-1}),$$

where $1 \leq k \leq m$. For $n \geq 3$, there are m probable structures of l - polygonal spiro chain of length n which is constructed as

$$SPC_{n-1} \rightarrow SPC_n^k$$

with probability p_k , where p_k are steady and independent of the parameter k and $\sum_{k=1}^m p_k = 1$. Then,
For $k = 1$,

$$\begin{aligned}\delta_{(2,2)}^{(1)} &= x_{22}(SPC_n^1) - x_{22}(SPC_{n-1}) = l - 3, \\ \delta_{(2,4)}^{(1)} &= x_{24}(SPC_n^1) - x_{24}(SPC_{n-1}) = 2, \\ \delta_{(4,4)}^{(1)} &= x_{44}(SPC_n^1) - x_{44}(SPC_{n-1}) = 1.\end{aligned}$$

For $2 \leq k \leq \lfloor \frac{l}{2} \rfloor$,

$$\begin{aligned}\delta_{(2,2)}^{(k)} &= x_{22}(SPC_n^k) - x_{22}(SPC_{n-1}) = l - 4, \\ \delta_{(2,4)}^{(k)} &= x_{24}(SPC_n^k) - x_{24}(SPC_{n-1}) = 4, \\ \delta_{(4,4)}^{(k)} &= x_{44}(SPC_n^k) - x_{44}(SPC_{n-1}) = 0.\end{aligned}$$

We also define

$$\delta = \sum_{k=1}^m \sum_{(i,j) \in E(G)} p_k \delta_{(i,j)}^{(k)} f(d_i, d_j), \quad i \leq j. \quad (2.2)$$

3. Main Results

In this section, we state and prove the explicit formulas of expected mean of random l - polygonal chain and random l - polygonal spiro chain alongwith their generalized *ISI* index.

3.1. Random l - polygonal chain

Notice that PC_n is a random l - polygonal chain due to its local arrangements and $TI(PC(n; p_1, p_2, \dots, p_m))$ is the random variable. Denote the expected value of the topological descriptors as $E_n^{TI} = E[TI(PC(n; p_1, p_2, \dots, p_m))]$.

Theorem 3.1. Let $n \geq 2$ and $l \geq 4$, and a random l - polygonal chain $PC(n; p_1, p_2, \dots, p_m)$ of length n . Then

$$E_n^{TI} = E_2^{TI} + \gamma(n-2),$$

where

$$E_2^{TI} = \sum_{(i,j) \in E(G)} f(d_i, d_j) x_{ij}(PC_2), \quad i \leq j.$$

Proof. For $n \geq 3$, there are $m = \lfloor \frac{l}{2} \rfloor$ types of probabilities (see Figure 2) [38]. Therefore, we have

$$\begin{aligned} E_n^{TI} &= p_1 TI(PC_n^1) + p_2 TI(PC_n^2) + \dots + p_m TI(PC_n^m) \\ &= p_1 (TI(PC_{n-1}) + (l-3)f(d_2, d_2) + 2f(d_2, d_3) + 2f(d_3, d_3)) \\ &\quad + p_2 (TI(PC_{n-1}) + (l-4)f(d_2, d_2) + 4f(d_2, d_3) + 1f(d_3, d_3)) + \dots \\ &\quad + p_m (TI(PC_{n-1}) + (l-4)f(d_2, d_2) + 4f(d_2, d_3) + 1f(d_3, d_3)) \\ &= p_1 (TI(PC_{n-1}) + \sum_{(i,j) \in E(G)} \gamma_{(i,j)}^{(1)} f(d_i, d_j)) + p_2 (TI(PC_{n-1}) \\ &\quad + \sum_{(i,j) \in E(G)} \gamma_{(i,j)}^{(2)} f(d_i, d_j)) + \dots + p_m (TI(PC_{n-1}) + \sum_{(i,j) \in E(G)} \gamma_{(i,j)}^{(m)} f(d_i, d_j)) \\ &= \sum_{k=1}^m p_k (TI(PC_{n-1}) + \sum_{(i,j) \in E(G)} \gamma_{(i,j)}^k f(d_i, d_j)) \\ &= TI(PC_{n-1}) + \sum_{k=1}^m \sum_{(i,j) \in E(G)} p_k \gamma_{(i,j)}^k f(d_i, d_j) \end{aligned} \tag{3.1}$$

However, $E[E_n^{TI}] = E_n^{TI}$, Eq. (3.1) gives

$$\begin{aligned} E_n^{TI} &= E_{n-1}^{TI} + \sum_{k=1}^m \sum_{(i,j) \in E(G)} p_k \gamma_{(i,j)}^{(k)} f(d_i, d_j) \\ E_n^{TI} &= E_{n-1}^{TI} + \gamma, \quad n > 2 \end{aligned} \quad [From \text{ Eq. (2.1)}]$$

Using recurrence relation and using initial conditions, we get

$$E_n^{TI} = E_2^{TI} + \gamma(n-2).$$

Hence, proved.

Theorem 3.2. Let $n \geq 2$ and $l \geq 4$, and a random l - polygonal chain $PC(n; p_1, p_2, \dots, p_m)$ of length n . Then

$$E_n^{ISI(\alpha, \beta)} = n[(l-4).4^{\alpha+\beta} + 4.6^\alpha.5^\beta + 3^{2\alpha+\beta}.2^\beta] + p_1(4^{\alpha+\beta} - 2.6^\alpha.5^\beta + 3^{2\alpha+\beta}.2^\beta) \\ - 2p_1(4^{\alpha+\beta} - 2.6^\alpha.5^\beta + 3^{2\alpha+\beta}.2^\beta) + (4^{\alpha+\beta+1} - 4.6^\alpha.5^\beta - 3^{2\alpha+\beta}.2^\beta).$$

Proof. For $n = 2$,

$$x_{22}(PC_2) = 2l - 4, x_{23}(PC_2) = 4, x_{33}(PC_2) = 1.$$

$$E_2^{ISI(\alpha, \beta)} = (2l - 4).4^{\alpha+\beta} + 4.6^\alpha.5^\beta + 9^\alpha.6^\beta.$$

For $n \geq 3$,

$$\gamma = p_1[(l-3).4^\alpha.4^\beta + 2.6^\alpha.5^\beta + 2.9^\alpha.6^\beta] + p_2[(l-4).4^\alpha.4^\beta + 4.6^\alpha.5^\beta + 1.9^\alpha.6^\beta] \\ + \dots + p_m[(l-4).4^\alpha.4^\beta + 4.6^\alpha.5^\beta + 1.9^\alpha.6^\beta] \\ = ((l-4).4^{\alpha+\beta} + 4.6^\alpha.5^\beta + 9^\alpha.6^\beta) + p_1(4^{\alpha+\beta} - 2.6^\alpha.5^\beta + 9^\alpha.6^\beta).$$

Therefore,

$$E_n^{ISI(\alpha, \beta)} = (2l - 4).4^{\alpha+\beta} + 4.6^\alpha.5^\beta + 9^\alpha.6^\beta + [(l-4).4^{\alpha+\beta} + 4.6^\alpha.5^\beta + 9^\alpha.6^\beta] \\ + p_1(4^{\alpha+\beta} - 2.6^\alpha.5^\beta + 9^\alpha.6^\beta)(n-2) \\ = n[(l-4).4^{\alpha+\beta} + 4.6^\alpha.5^\beta + 3^{2\alpha+\beta}.2^\beta] + p_1(4^{\alpha+\beta} - 2.6^\alpha.5^\beta + 3^{2\alpha+\beta}.2^\beta) \\ - 2p_1(4^{\alpha+\beta} - 2.6^\alpha.5^\beta + 3^{2\alpha+\beta}.2^\beta) + (4^{\alpha+\beta+1} - 4.6^\alpha.5^\beta - 3^{2\alpha+\beta}.2^\beta).$$

3.2. Random l - polygonal spiro chain

Notice that SPC_n is a random l - polygonal spiro chain due to its local arrangements and $TI(SPC(n; p_1, p_2, \dots, p_m))$ is the random variable. Denote the expected value of the topological descriptors as $E_n^{TI} = E[TI(SPC(n; p_1, p_2, \dots, p_m))]$.

Theorem 3.3. Let $n \geq 2$ and $l \geq 4$ a random l - polygonal spiro chain $SPC(n; p_1, p_2, \dots, p_m)$ of length n . Then

$$E_n^{TI} = E_2^{TI} + \delta(n-2),$$

where

$$E_2^{TI} = \sum_{(i,j) \in E(G)} f(d_i, d_j) x_{ij}(SPC_2), \quad i \leq j.$$

Proof. For $n \geq 3$, there are $m = \lfloor \frac{l}{2} \rfloor$ possible constructions (see Figure 4) [20]. Therefore, we have

$$\begin{aligned}
E_n^{TI} &= p_1 TI(RPC_n^1) + p_2 TI(RPC_n^2) + p_3 TI(RPC_n^3) \\
&= p_1 (TI(RPC_{n-1}) + \sum_{(i,j) \in E(G)} \delta_{(i,j)}^{(1)} f(d_i, d_j)) + p_2 (TI(RPC_{n-1}) \\
&\quad + \sum_{(i,j) \in E(G)} \delta_{(i,j)}^{(2)} f(d_i, d_j)) + p_3 (TI(RPC_{n-1}) + \sum_{(i,j) \in E(G)} \gamma_{(i,j)}^{(3)} f(d_i, d_j)) \\
&= \sum_{k=1}^3 p_k (TI(RPC_{n-1}) + \sum_{(i,j) \in E(G)} \delta_{(i,j)}^k f(d_i, d_j)) \\
&= TI(RPC_{n-1}) + \sum_{k=1}^3 \sum_{(i,j) \in E(G)} p_k \delta_{(i,j)}^k f(d_i, d_j) \tag{3.2}
\end{aligned}$$

However, $E[E_n^{TI}] = E_n^{TI}$, Eq. (3.2) gives

$$\begin{aligned}
E_n^{TI} &= E_{n-1}^{TI} + \sum_{k=1}^3 \sum_{(i,j) \in E(G)} p_k \delta_{(i,j)}^k f(d_i, d_j) \\
E_{TI}^n &= E_{TI}^{n-1} + \delta, \quad n > 2 \quad [From \text{ Eq. (2.2)}]
\end{aligned}$$

Using recurrence relation and using initial conditions, we get

$$E_{TI}^n = E_{TI}^2 + \delta (n - 2).$$

Hence, proved.

Theorem 3.4. Let $n \geq 2$ and $l \geq 4$, and a random l - polygonal spiro chain $SPC(n; p_1, p_2, \dots, p_m)$ of length n . Then

$$\begin{aligned}
E_n^{ISI(\alpha, \beta)} &= n[(l-4).4^{\alpha+\beta} + 4.8^\alpha.6^\beta + p_1(4^{\alpha+\beta} - 2.8^\alpha.6^\beta + 16^\alpha.8^\beta)] \\
&\quad - 2p_1(4^{\alpha+\beta} - 2.8^\alpha.6^\beta + 16^\alpha.8^\beta) + (4^{\alpha+\beta+1} - 4.8^\alpha.6^\beta).
\end{aligned}$$

Proof. For $n = 2$,

$$x_{22}(SPC_2) = 2l - 4, x_{24}(SPC_2) = 4, x_{44}(SPC_2) = 0.$$

$$E_2^{ISI(\alpha, \beta)} = (2l - 4).4^{\alpha+\beta} + 4.8^\alpha.6^\beta.$$

For $n \geq 3$,

$$\begin{aligned}\delta &= p_1[(l-3).4^\alpha.4^\beta + 2.8^\alpha.6^\beta + 1.16^\alpha.8^\beta] + p_2[(l-4).4^\alpha.4^\beta + 4.8^\alpha.6^\beta + 0.16^\alpha.8^\beta] \\ &\quad + \dots + p_m[(l-4).4^\alpha.4^\beta + 4.8^\alpha.6^\beta + 0.16^\alpha.8^\beta] \\ &= (l-4).4^{\alpha+\beta} + 4.8^\alpha.6^\beta + p_1(4^{\alpha+\beta} - 2.8^\alpha.6^\beta + 1.16^\alpha.8^\beta).\end{aligned}$$

Therefore,

$$\begin{aligned}E_n^{ISI(\alpha,\beta)} &= ((2l-4).4^{\alpha+\beta} + 4.8^\alpha.6^\beta) + [(l-4).4^{\alpha+\beta} + 4.8^\alpha.6^\beta] \\ &\quad + p_1(4^{\alpha+\beta} - 2.8^\alpha.6^\beta + 16^\alpha.8^\beta)](n-2) \\ &= n[(l-4).4^{\alpha+\beta} + 4.8^\alpha.6^\beta + p_1(4^{\alpha+\beta} - 2.8^\alpha.6^\beta + 16^\alpha.8^\beta)] \\ &\quad - 2p_1(4^{\alpha+\beta} - 2.8^\alpha.6^\beta + 16^\alpha.8^\beta) + (4^{\alpha+\beta+1} - 4.8^\alpha.6^\beta).\end{aligned}$$

4. Some special results based on the derived results

In this section, we present the average values of the molecular descriptors with respect to the set of all l - polygonal chains and set of all l - polygonal spiro chains with n polygons. Also, we give attention to the special l - polygonal chains and l - polygonal spiro chains.

Let \mathbb{PC}_n and \mathbb{SPC}_n be the sets of all l - polygonal chains and all l - polygonal spiro chains with n polygons. The average values of the TIs of \mathbb{PC}_n and \mathbb{SPC}_n are defined by

$$TI_{avg}(\mathbb{PC}_n) = \frac{1}{|\mathbb{PC}_n|} \sum_{G \in \mathbb{PC}_n} TI(G)$$

and

$$TI_{avg}(\mathbb{SPC}_n) = \frac{1}{|\mathbb{SPC}_n|} \sum_{G \in \mathbb{SPC}_n} TI(G),$$

respectively. In fact, average value is the population mean of the topological indices of all elements in \mathbb{PC}_n and also in \mathbb{SPC}_n . Since every element occurring in \mathbb{PC}_n and \mathbb{SPC}_n has the same probability, we have $p_1 = p_2 = \dots = p_m$, where $m = \lfloor \frac{l}{2} \rfloor$. Thus, we can apply Theorem 3.1 and 3.3 by putting $p_1 = p_2 = \dots = p_m = \frac{1}{m}$ and obtain the following results.

Theorem 4.1. *The average value of the TIs with respect to \mathbb{PC}_n is*

$$\begin{aligned}TI_{avg}(\mathbb{PC}_n) &= E_2^{TI} + (n-2) \cdot \frac{1}{m} [(ml - 4m + 1)f(d_2, d_2) + (4m - 2)f(d_2, d_3) \\ &\quad + (m + 1)f(d_3, d_3)].\end{aligned}$$

Proof. By substituting $p_k = \frac{1}{m}$ for $1 \leq k \leq m$ in Eq.(2.1), we have

$$\begin{aligned}
\gamma &= \frac{1}{m} \sum_{k=1}^m \sum_{\substack{(i,j) \in E(G) \\ i \leq j}} \gamma_{(i,j)}^{(k)} f(d_i, d_j) \\
&= \frac{1}{m} [(l-3)f(d_2, d_2) + 2f(d_2, d_3) + 2f(d_3, d_3) + (l-4)f(d_2, d_2) \\
&\quad + 4f(d_2, d_3) + 1f(d_3, d_3) + \dots] \\
&= \frac{1}{m} [f(d_2, d_2)\{(l-3) + (m-1)(l-4)\} + f(d_2, d_3)\{2 + (m-1)4\} \\
&\quad + f(d_3, d_3)\{2 + (m-1)\}] \\
&= \frac{1}{m} [(ml-4m+1)f(d_2, d_2) + (4m-2)f(d_2, d_3) + (m+1)f(d_3, d_3)]
\end{aligned}$$

From Theorem 3.1,

$$\begin{aligned}
TI_{avg}(\mathbb{PC}_n) &= E[TI(PC(n; \frac{1}{m}, \frac{1}{m}, \dots, \frac{1}{m}))] \\
&= E_2^{TI} + (n-2) \cdot \frac{1}{m} [(ml-4m+1)f(d_2, d_2) \\
&\quad + (4m-2)f(d_2, d_3) + (m+1)f(d_3, d_3)].
\end{aligned}$$

Theorem 4.2. The average value of the TIs with respect to \mathbb{SPC}_n is

$$TI_{avg}(\mathbb{SPC}_n) = E_2^{TI} + (n-2) \cdot \frac{1}{m} [(ml-4m+1)f(d_2, d_2) + (4m-2)f(d_2, d_4) + f(d_4, d_4)].$$

Proof. The theorem is obtained by substituting $p_k = \frac{1}{m}$ for $1 \leq k \leq m$ in Eq.(2.2) and using Theorem 3.3.

Now, we turn our attention to the m special l - polygonal chains and l - polygonal spiro chains when setting $p_k = 1$ and $p_q = 0$ where $1 \leq q \leq m$ and $q \neq k$.

Corollary 4.1. For $n \geq 2$, we have the following:

$$\begin{aligned}
1. TI(PC(n; 1, 0, 0, \dots, 0)) &= E_2^{TI} + (n-2) [\sum_{\substack{(i,j) \in E(G) \\ i \leq j}} \gamma_{(i,j)}^{(1)} f(d_i, d_j)]. \\
2. TI(SPC(n; 1, 0, 0, \dots, 0)) &= E_2^{TI} + (n-2) [\sum_{\substack{(i,j) \in E(G) \\ i \leq j}} \delta_{(i,j)}^{(1)} f(d_i, d_j)].
\end{aligned}$$

Fix $p_1 = 0$, and setting as above for all $(m-1)$ cases, we have

$$\begin{aligned}
3. TI(PC(n; 0, 1, 0, \dots, 0)) &= E_2^{TI} + (n-2) [\sum_{\substack{(i,j) \in E(G) \\ i \leq j}} \gamma_{(i,j)}^{(k)} f(d_i, d_j)]. \\
4. TI(SPC(n; 0, 1, 0, \dots, 0)) &= E_2^{TI} + (n-2) [\sum_{\substack{(i,j) \in E(G) \\ i \leq j}} \delta_{(i,j)}^{(k)} f(d_i, d_j)].
\end{aligned}$$

5. Applications

In Section 3, we have provided some derivation for the expected values of the molecular descriptors alongwith the generalized $ISI_{(\alpha,\beta)}$ index in a random l -polygonal chain and random l -polygonal spiro chain. In this section, we apply them to obtain the expected values of the topological indices of some class of random polygonal chains and random polygonal spiro chains such as the random 4-polygonal, random 5-polygonal, random 6-polygonal, random 8-polygonal chain and its spiro chain which were highly correlated with the mathematical physics, organic chemistry, pharmaceutical sciences etc.

The random 4-polygonal chain $PC(n; p_1, 1 - p_1)$ of length n is a random generalized polyomino chain with n square cells each joined by an edge and is denoted by $GPC_n(p_1)$. The random 4-polygonal spiro chain $SPC(n; p_1, 1 - p_1)$ of length n is a random generalized polyomino spiro chain with n square cells obtained from $GPC_n(p_1)$ by contracting each cut edge between each square cells and is denoted by $SGPC_n(p_1)$. At the present time, these graphs have attracted many researchers from various fields. Polyomino systems is a polycyclic aromatic compounds widely studied in organic chemistry. Some recent works on the polyomino chains includes [5, 17, 22] rook polynomial, extremal problems, perfect matchings etc. According to the definition of random l -polygonal and random l -polygonal spiro chain, there are two probable local arrangements in $GPC_n(p_1)$ and $SGPC_n(p_1)$.

Corollary 5.1. Take $l = 4$ and $m = \lfloor \frac{4}{2} \rfloor = 2$ in Eq.(2.1) and using Theorem 3.1, we get the expected value of the TIs of $GPC_n(p_1)$.

Corollary 5.2. Take $l = 4$ and using Theorem 3.2, we get the expected value of generalized $ISI_{(\alpha,\beta)}$ index of $GPC_n(p_1)$.

Corollary 5.3. Take $l = 4$ and $m = \lfloor \frac{4}{2} \rfloor = 2$ in Eq.(2.2) and using Theorem 3.3, we get the expected value of the TIs of $SGPC_n(p_1)$.

Corollary 5.4. Take $l = 4$ and using Theorem 3.4, we get the expected value of generalized $ISI_{(\alpha,\beta)}$ index of $SGPC_n(p_1)$.

The random 5-polygonal chain $PC(n; p_1, 1 - p_1)$ of length n is a random pentagonal chain with n pentagons connected with an edge and is denoted by $P_n^\alpha(p_1)$. The random 5-polygonal spiro chain $SPC(n; p_1, 1 - p_1)$ of length n is a random pentagonal spiro chain with n pentagons obtained from $P_n^\alpha(p_1)$ by contracting each cut edge between each pentagons and is denoted by $SP_n^\alpha(p_1)$. According to the definition of random l -polygonal and random l -polygonal spiro chain, there are two probable local arrangements in $P_n^\alpha(p_1)$ and $SP_n^\alpha(p_1)$ [34].

Corollary 5.5. Take $l = 5$ and $m = \lfloor \frac{5}{2} \rfloor = 2$ in Eq.(2.1) and using Theorem 3.1,

we get the expected value of the TIs of $P_n^\alpha(p_1)$.

Corollary 5.6. Take $l = 5$ and using Theorem 3.2, we get the expected value of generalized $ISI_{(\alpha,\beta)}$ index of $P_n^\alpha(p_1)$.

Corollary 5.7. Take $l = 5$ and $m = \lfloor \frac{5}{2} \rfloor = 2$ in Eq.(2.2) and using Theorem 3.3, we get the expected value of the TIs of $SP_n^\alpha(p_1)$.

Corollary 5.8. Take $l = 5$ and using Theorem 3.4, we get the expected value of generalized $ISI_{(\alpha,\beta)}$ index of $SP_n^\alpha(p_1)$.

The random 6-polygonal chain $PC(n; p_1, p_2, 1 - p_1 - p_2)$ of length n is a random polyphenyl chain with n hexagons connected with an edge and is denoted by $PPC_n(p_1, p_2)$. The random 6-polygonal spiro chain $SPC(n; p_1, p_2, 1 - p_1 - p_2)$ of length n is a random polyphenyl spiro chain with n hexagons obtained from $PPC_n(p_1, p_2)$ by contracting each cut edge between each hexagons and is denoted by $SPPC_n(p_1, p_2)$. Polyphenyl chains are a class of unbranched polycyclic aromatic compounds, and their derivatives have attracted many chemists and researchers for many years as they are used in drug synthesis, petrochemicals, heat exchangers etc. For more results, interested readers can see [4, 7, 11, 36]. According to the definition of random l -polygonal and random l -polygonal spiro chain, there are three probable local arrangements in $PPC_n(p_1, p_2)$ and $SPPC_n(p_1, p_2)$.

Corollary 5.9. Take $l = 6$ and $m = \lfloor \frac{6}{2} \rfloor = 3$ in Eq.(2.1) and using Theorem 3.1, we get the expected value of the TIs of $PPC_n(p_1, p_2)$.

Corollary 5.10. Take $l = 6$ and using Theorem 3.2, we get the expected value of generalized $ISI_{(\alpha,\beta)}$ index of $PPC_n(p_1, p_2)$.

Corollary 5.11. Take $l = 6$ and $m = \lfloor \frac{6}{2} \rfloor = 3$ in Eq.(2.2) and using Theorem 3.3, we get the expected value of the TIs of $SPPC_n(p_1, p_2)$.

Corollary 5.12. Take $l = 6$ and using Theorem 3.4, we get the expected value of generalized $ISI_{(\alpha,\beta)}$ index of $SPPC_n(p_1, p_2)$.

The random 8-polygonal chain $PC(n; p_1, p_2, p_3, 1 - p_1 - p_2 - p_3)$ of length n is a random cyclooctane chain with n octagons connected with an edge and is denoted by $COC_n(p_1, p_2, p_3)$. The random 8-polygonal spiro chain $SPC(n; p_1, p_2, p_3, 1 - p_1 - p_2 - p_3)$ of length n is a random cyclooctane spiro chain with n octagons obtained from $COC_n(p_1, p_2, p_3)$ by contracting each cut edge between each octagons and is denoted by $SCOC_n(p_1, p_2, p_3)$. Cyclooctanes are a kind of saturated hydrocarbons and their derivatives are essential in drug discovery, heat exchangers, synthesis of organic chemicals and petrochemicals etc. For more results, interested readers can see [1, 2, 29, 37]. According to the definition of random l -polygonal

and random l -polygonal spiro chain, there are four probable local arrangements in $COC_n(p_1, p_2, p_3)$ and $SCOC_n(p_1, p_2, p_3)$.

Corollary 5.13. Take $l = 8$ and $m = \lfloor \frac{8}{2} \rfloor = 4$ in Eq.(2.1) and using Theorem 3.1, we get the expected value of the TIs of $COC_n(p_1, p_2, p_3)$.

Corollary 5.14. Take $l = 8$ and using Theorem 3.2, we get the expected value of generalized $ISI_{(\alpha, \beta)}$ index of $COC_n(p_1, p_2, p_3)$.

Corollary 5.15. Take $l = 8$ and $m = \lfloor \frac{8}{2} \rfloor = 4$ in Eq.(2.2) and using Theorem 3.3, we get the expected value of the TIs of $SCOC_n(p_1, p_2, p_3)$.

Corollary 5.16. Take $l = 8$ and using Theorem 3.4, we get the expected value of generalized $ISI_{(\alpha, \beta)}$ index of $SCOC_n(p_1, p_2, p_3)$.

The explicit formulas of expected mean are stated for random l - polygonal chain and random l - polygonal spiro chain alongwith their generalized ISI index in Section 3. To verify the behavior of expected mean of indices for random l - polygonal chain such as random generalized polyomino chain, random pentachain, random polyphenyl chain, and random cyclooctane chain, different values of n are considered with $p_1 = 0$ and $p_1 = 1$. It is noticed from Table 2-9 (see Appendix) that the values of expected mean of TIs increases as the n value increases. The obtained E_n^{TI} are represented using graphs for the distinct values of n as shown in Figure 5-8 (see Appendix). Among all cases, it is observed that $E[ReZG_3] > E[HM] > E[M_2] > E[M_1] > E[ISI] > E[GA] > E[SCI] > E[R] > E[H] > E[\bar{M}_2]$. In addition, we compare the logarithmic values of $E[R_\alpha]$ and $E[\chi_\alpha]$ for different random l - polygonal chains at $n = 4$ and $p_1 = 1$ in Figure 9 (see Appendix). Notice that $E[R_\alpha] > E[\chi_\alpha]$.

6. Conclusion

Nowadays, topological indices are extending over a large area in research field of chemical graph theory due to its application in physico-chemical properties and biological activities of chemical compounds. In this discussion, we derive the formula to find the expected value of degree-based topological indices of random l -polygonal chain and random l - polygonal spiro chain. Moreover, from the derived results generalized $ISI_{(\alpha, \beta)}$ index for random polygonal chains and spiro chains were also obtained. Further, by assigning specific values to the parameter α and β , expected mean for some of the existing topological indices of the random polygonal chains and spiro chains can also be obtained as a special case. We also present the average values and m - special cases of TIs for the polygonal and spiro polygonal chains. We have also implemented the derived results to some polygonal chains which have applications for the future chemical research. We also provide some

numerical comparison and graphical representation of the expected values of the *TIs*. All indices are increases with respect to the increase of graph parameters. $ReZG_3$ has the highest expected value and \bar{M}_2 has the lowest. These assists to predict different properties and activities of the molecular compounds. Higher value corresponds to exaggerate stability and reacts less, while lower value reveals potential reactivity sites. These topological index has important applications as they are the foundations of chemical prediction and modeling software. Finding results for other statistical parameters can be a challenging task for near future.

References

- [1] Bharadwaj, R. K., Conformational properties of cyclooctane: A molecular dynamics simulation study, *Mol. Phys.*, 98, (2000), 211-218.
- [2] Brunvoll, J., Cyvin, S. J., Cyvin, B. N., Enumeration of tree-like octagonal systems, *J. Math. Chem.*, 21, (1997), 193-196.
- [3] Buragohain, J., Deka, B., Bharali, A., A Generalized ISI index of some chemical structures, *Journal of Molecular Structure*, 1208, (2020), 127843.
- [4] Chen, A., Zhang, F., Wiener index and perfect matchings in random phenylene chains, *MATCH Commun. Math. Comput. Chem.*, 61, (2009), 623-630.
- [5] Chen, R., Perfect matchings of generalized polyomino graphs, *Graphs Combin.*, 21, (2005), 515-529.
- [6] Chunsong, B., Naeem, A., Yousaf, S., Aslam, A., Tchier, F., Issa, A., Exploring expected values of topological indices of random cyclodecane chains for chemical insights, *Scientific Reports*, 14, (2024), 10065.
- [7] Deng, H. Y., Wiener indices of spiro and polyphenyl hexagonal chains, *Math. Comput. Model.*, 55, (2012), 634-644.
- [8] Došlić, T., Møølø, F., Chain hexagonal cacti: Matchings and independent sets, *Discrete Math.*, 310, (2010), 1676-1690.
- [9] Gutman, I., Das, K., The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.*, 50, (2004), 83-92.
- [10] Gutman, I., Furtula, B., (Eds.) Recent Results in Theory of Randić Index, *Mathematical Chemistry Monographs*, 2008.

- [11] Gutman, I., Kennedy, J. W., Quintas, L. V., Wiener numbers of random benzenoid chains, *Chem. Phys. Lett.*, 173(4), (1990), 403-408.
- [12] Gutman, I., Lepović, M., Choosing the Exponent in the Definition of Connectivity Index, *J. Serb. Chem. Soc.*, 66(9), (2001), 605-611.
- [13] Gutman, I., Milovanović, E., Milovanović, I., Beyond the Zagreb Indices, *AKCE International Journal of Graphs and Combinatorics*, 17(1), (2020), 74-85.
- [14] Gutman, I., Trinajstić, N., Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, 17, (1972), 535-538.
- [15] Havare, Ö. C., Topological indices and QSPR modeling of some novel drugs used in the cancer treatment, *International Journal of Quantum Chemistry*, 121(24), (2021), e26813.
- [16] Huang, G. H., Kuang, M. J., Deng, H. Y., The expected values of Kirchhoff indices in the random polyphenyl and spiro chains, *Ars Math. Contemp.*, 9, (2013), 207-217.
- [17] John, P., Sachs, H., Zerntic, H., Counting perfect matchings in polyominoes with applications to the dimer problem, *Zastos. Mat. (Appl. Math.)*, 19, (1987), 465-477.
- [18] Li, S., Shi, L., Gao, W., Topological indices computing on random chain structures, *International Journal of Quantum Chemistry*, 121(8), (2020), e26589.
- [19] Li, X. Y., Wang, G. P., Bian, H., Hu, R. W., The Hosoya polynomial decomposition for polyphenyl chains, *MATCH Commun. Math. Comput. Chem.*, 67, (2012), 357.
- [20] Liu, X., Liang, X., Geng, X., Expected Value of Multiplicative Degree-Kirchhoff Index in Random Polygonal Chains, *Mathematical Biosciences and Engineering*, 20(1), (2022), 707-719.
- [21] Loksha, V., Manjunath, M., Deepika, T., Cevik, A. S., Cangul, I. N., Adriatic indices of some derived graphs of Triglyceride, *South East Asian J. of Mathematics and Mathematical Sciences*, 17(3), (2021), 213-222.

- [22] Motoyama, A., Hosoya, H., King and domino polyominals for polyomino graphs, *J. Math. Phys.*, 18, (1997), 1485-1490.
- [23] Narendra, V. H., Mahalakshmi, P., Deepika, T., Lokesha, V., VL-Multiplicative total eccentricity index and VL-Multiplicative hyper total eccentricity index of some standard graphs, *South East Asian J. of Mathematics and Mathematical Sciences*, 20(3), (2024), 01-14.
- [24] Qi, J., Ni, J., Geng, X., The expected values for the Kirchhoff indices in the random cyclooctatetraene and spiro chains, *Discrete Applied Mathematics*, 321, (2022), 240-249.
- [25] Randić, M., On characterization of molecular branching, *J. Am. Chem. Soc.*, 97, (1975), 6609-6615.
- [26] Ranjini, P. S., Lokesha, V., Usha, A., Relation between phenylene and hexagonal squeeze using harmonic index, *Int. J. Graph Theory*, 1(4), (2013), 116-121.
- [27] Raza, Z., The expected values of some indices in random phenylene chains, *Eur. Phys. J. Plus*, 136, (2021), 1-15.
- [28] Raza, Z., The harmonic and second Zagreb indices in random polyphenyl and spiro chains, *Polycycl. Aromat. Compd.*, (2020), 1-10.
- [29] Salamci, E., Ustabaay, R., Aoruh, U., Yavuz, M., Vazquez-Lopez, E. M., Cyclooctane-1, 2, 5, 6-tetrayl tetraacetate, *Acta Crystallogr. Sect. E: Struct. Rep. Online*, 62, (2006), 02401-02402.
- [30] Shirdel, G. H., Rezapour, H., Sayadi, A. M., The Hyper-Zagreb Index of Graph Operations, *Iran. J. Math. Chem.*, 4, (2013), 213-220.
- [31] Todeschini, R., Consonni, V., *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim, 2009.
- [32] Trinajstić, N., *Chemical Graph Theory*, CRC Press, Boca Raton, 1983.
- [33] Vukičević, D., Furtula, B., Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.*, 46, (2009), 1369-1376.
- [34] Wang, H., Qin, J., Gutman, I., Wiener numbers of random pentagonal chains, *Iran. J. Math. Chem.*, 4(1), (2013), 59-76.

- [35] Wei, S., Ke, X., Lin, F., Perfect matchings in random polyomino chain graphs, *J. Math Chem*, 54, (2016), 690-697.
- [36] Wei, S. L., Ke, X. L., Hao, G. L., Comparing the expected values of atom-bond connectivity and geometric-arithmetic indices in random spiro chains, *J. Inequalities Appl.*, 2018, (2018), 45.
- [37] Wei, S., Ke, X., Wang, Y., Wiener indices in random cyclooctane chains, *Wuhan Univ. J. Nat. Sci.*, 23(2018), 498-502.
- [38] Wei, S., and Shiu, W. C., Enumeration of Wiener indices in random polygonal chains, *J. Math. Anal. Appl.*, 469(2), (2019), 537-548.
- [39] Wiener, H., Structure determination of paraffin boiling points, *J. Math. Chem. Soc.*, 69, (1947), 17-20.
- [40] Wu, T., Lü, H., Zhang, X., Extremal Matching Energy of Random Polyomino Chains, *Entropy*, 19(12), (2017), 684.
- [41] Yang, X., Zhao, B., Kekulic Structures of Octagonal Chains and the Hosoya Index of Caterpillar Trees, *J. Xinjiang Univ. (Nat. Sci. Ed.)*, 3, (2013), 1-5.
- [42] Zhang, L., The Harmonic Index for Graphs, *Appl. Math. Lett.*, 25, (2012), 561-566.
- [43] Zhou, B., Trinajstić, N., On a Novel Connectivity Index, *J. Math. Chem.*, 46, (2009), 1252-1270.
- [44] Zhou, B., Trinajstić, N., On General Sum-Connectivity Index, *J. Math. Chem.*, 47, (2010), 210-218.
- [45] Zhu, W., Geng, X, Enumeration of the Multiplicative Degree-Kirchhoff Index in the Random Polygonal Chains, *Molecules*, 27(17), (2022), 5669.

Appendix

[n]	$E[M_1]$	$E[M_2]$	$E[M_2]$	$E[ReZG_3]$	E[ISI]	E[H]	E[HM]	E[R]	E[SCI]	E[GA]
3	68	82	2.55	412	16.6	5.86	336	5.93	6.39	13.83
4	94	115	3.33	586	22.9	7.8	472	7.89	8.59	18.75
5	120	148	4.11	760	29.2	9.73	608	9.86	10.78	23.67
6	146	181	4.88	934	35.5	11.66	744	11.83	12.98	28.59
7	172	214	5.66	1108	41.8	13.6	880	13.79	15.18	33.51
8	198	247	6.44	1282	48.1	15.53	1016	15.76	17.37	38.43
9	224	280	7.22	1456	54.4	17.46	1152	17.73	19.57	43.35
10	250	313	8	1630	60.7	19.4	1288	19.69	21.77	48.27
11	276	346	8.77	1804	67	21.33	1424	21.66	23.97	53.19
12	302	379	9.55	1978	73.3	23.26	1560	23.62	26.16	58.11
13	328	412	10.33	2152	79.6	25.2	1696	25.59	28.36	63.03

Table 2: Numerical comparison of expected value of degree-based indices of random generalized polyomino chain at $p_1 = 0$ for $n = 3$ to 13

[n]	$E[M_1]$	$E[M_2]$	$E[M_2]$	$E[ReZG_3]$	E[ISI]	E[H]	E[HM]	E[R]	E[SCI]	E[GA]
3	68	83	2.58	422	16.7	5.9	338	5.94	6.35	13.87
4	94	117	3.38	606	23.1	7.86	476	7.93	8.56	18.83
5	120	151	4.19	790	29.5	9.83	614	9.91	10.77	23.79
6	146	185	5	974	35.9	11.8	752	11.89	12.99	28.75
7	172	219	5.80	1158	42.3	13.76	890	13.88	15.20	33.71
8	198	253	6.61	1342	48.7	15.73	1028	15.86	17.41	38.67
9	224	287	7.41	1526	55.1	17.7	1166	17.84	19.62	43.63
10	250	321	8.22	1710	61.5	19.66	1304	19.83	21.83	48.59
11	276	355	9.02	1894	67.9	21.63	1442	21.81	24.04	53.55
12	302	389	9.83	2078	74.3	23.6	1580	23.79	26.25	58.51
13	328	423	10.63	2262	80.7	25.56	1718	25.78	28.46	63.47

Table 3: Numerical comparison of expected value of degree-based indices of random generalized polyomino chain at $p_1 = 1$ for $n = 3$ to 13

[n]	$E[M_1]$	$E[M_2]$	$E[M_2]$	$E[ReZG_3]$	E[ISI]	E[H]	E[HM]	E[R]	E[SCI]	E[GA]
3	80	94	3.30	460	19.6	7.36	384	7.43	7.89	16.83
4	110	131	4.33	650	26.9	9.8	536	9.89	10.59	22.75
5	140	168	5.36	840	34.2	12.23	688	12.36	13.28	28.67
6	170	205	6.38	1030	41.5	14.66	840	14.83	15.98	34.59
7	200	242	7.41	1220	48.8	17.1	992	17.29	18.68	40.51
8	230	279	8.44	1410	56.1	19.53	1144	19.76	21.37	46.43
9	260	316	9.47	1600	63.4	21.96	1296	22.23	24.07	52.35
10	290	353	10.5	1790	70.7	24.4	1448	24.69	26.77	58.27
11	320	390	11.52	1980	78	26.83	1600	27.16	29.47	64.19
12	350	427	12.55	2170	85.3	29.26	1752	29.62	32.16	70.11
13	380	464	13.58	2360	92.6	31.7	1904	32.09	34.86	76.03

Table 4: Numerical comparison of expected value of degree-based indices of random pentachain at $p_1 = 0$ for $n = 3$ to 13

[n]	$E[M_1]$	$E[M_2]$	$E[M_2]$	$E[ReZG_3]$	E[ISI]	E[H]	E[HM]	E[R]	E[SCI]	E[GA]
3	80	95	3.33	470	19.7	7.4	386	7.44	7.85	16.87
4	110	133	4.38	670	27.1	9.86	540	9.93	10.56	22.83
5	140	171	5.44	870	34.5	12.33	694	12.41	13.27	28.79
6	170	209	6.5	1070	41.9	14.8	848	14.89	15.99	34.75
7	200	247	7.55	1270	49.3	17.26	1002	17.38	18.70	40.71
8	230	285	8.61	1470	56.7	19.73	1156	19.86	21.41	46.67
9	260	323	9.66	1670	64.1	22.2	1310	22.34	24.12	52.63
10	290	361	10.72	1870	71.5	24.66	1464	24.83	26.83	58.59
11	320	399	11.77	2070	78.9	27.13	1618	27.31	29.54	64.55
12	350	437	12.83	2270	86.3	29.6	1772	29.79	32.25	70.51
13	380	475	13.88	2470	93.7	32.06	1926	32.28	34.96	76.47

Table 5: Numerical comparison of expected value of degree-based indices of random generalized pentachain at $p_1 = 1$ for $n = 3$ to 13

[n]	$E[M_1]$	$E[M_2]$	$E[M_2]$	$E[ReZG_3]$	E[ISI]	E[H]	E[HM]	E[R]	E[SCI]	E[GA]
3	92	106	4.05	508	22.6	8.86	432	8.93	9.39	19.83
4	126	147	5.33	714	30.9	11.8	600	11.89	12.59	26.75
5	160	188	6.61	920	39.2	14.73	768	14.86	15.78	33.67
6	194	229	7.88	1126	47.5	17.66	936	17.83	18.98	40.59
7	228	270	9.16	1332	55.8	20.6	1104	20.79	22.18	47.51
8	262	311	10.44	1538	64.1	23.53	1272	23.76	25.37	54.43
9	296	352	11.72	1744	72.4	26.46	1440	26.73	28.57	61.35
10	330	393	13	1950	80.7	29.4	1608	29.69	31.77	68.27
11	364	434	14.27	2156	89	32.33	1776	32.66	34.97	75.19
12	398	475	15.55	2362	97.3	35.26	1944	35.62	38.16	82.11
13	432	516	16.83	2568	105.6	38.2	2112	38.59	41.36	89.03

Table 6: Numerical comparison of expected value of degree-based indices of random polyphenyl chain at $p_1 = 0$ for $n = 3$ to 13

[n]	$E[M_1]$	$E[M_2]$	$E[M_2]$	$E[ReZG_3]$	$E[ISI]$	$E[H]$	$E[HM]$	$E[R]$	$E[SCI]$	$E[GA]$
3	92	107	4.08	518	22.7	8.9	434	8.94	9.35	19.87
4	126	149	5.38	734	31.1	11.86	604	11.93	12.56	26.83
5	160	191	6.69	950	39.5	14.83	774	14.91	15.77	33.79
6	194	233	8	1166	47.9	17.8	944	17.89	18.99	40.75
7	228	275	9.30	1382	56.3	20.76	1114	20.88	22.20	47.71
8	262	317	10.61	1598	64.7	23.73	1284	23.86	25.41	54.67
9	296	359	11.91	1814	73.1	26.7	1454	26.84	28.62	61.63
10	330	401	13.22	2030	81.5	29.66	1624	29.83	31.83	68.59
11	364	443	14.52	2246	89.9	32.63	1794	32.81	35.04	75.55
12	398	485	15.83	2462	98.3	35.6	1964	35.79	38.25	82.51
13	432	527	17.13	2678	106.7	38.56	2134	38.78	41.46	89.47

Table 7: Numerical comparison of expected value of degree-based indices of random polyphenyl chain at $p_1 = 1$ for $n = 3$ to 13

[n]	$E[M_1]$	$E[M_2]$	$E[M_2]$	$E[ReZG_3]$	$E[ISI]$	$E[H]$	$E[HM]$	$E[R]$	$E[SCI]$	$E[GA]$
3	116	118	5.55	604	28.6	11.86	528	11.93	12.39	25.83
4	158	163	7.33	842	38.9	15.8	728	15.89	16.59	34.75
5	200	208	9.11	1080	49.2	19.73	928	19.86	20.78	43.67
6	242	253	10.88	1318	59.5	23.66	1128	23.83	24.98	52.59
7	284	298	12.66	1556	69.8	27.6	1328	27.79	29.18	61.51
8	326	343	14.44	1794	80.1	31.53	1528	31.76	33.37	70.43
9	368	388	16.22	2032	90.4	35.46	1728	35.73	37.57	79.35
10	410	433	18	2270	100.7	39.4	1928	39.69	41.77	88.27
11	452	478	19.77	2508	111	43.33	2128	43.66	45.97	97.19
12	494	523	21.55	2746	121.3	47.26	2328	47.62	50.16	106.11
13	536	568	23.33	2984	131.6	51.2	2528	51.59	54.36	115.03

Table 8: Numerical comparison of expected value of degree-based indices of random cyclooctane chain at $p_1 = 0$ for $n = 3$ to 13

[n]	$E[M_1]$	$E[M_2]$	$E[M_2]$	$E[ReZG_3]$	$E[ISI]$	$E[H]$	$E[HM]$	$E[R]$	$E[SCI]$	$E[GA]$
3	116	119	5.58	614	28.7	11.9	530	11.94	12.35	25.87
4	158	165	7.38	862	39.1	15.86	732	15.93	16.56	34.83
5	200	211	9.19	1110	49.5	19.83	934	19.91	20.77	43.79
6	242	257	11	1358	59.9	23.8	1136	23.89	24.99	52.75
7	284	303	12.80	1606	70.3	27.76	1338	27.88	29.20	61.71
8	326	349	14.61	1854	80.7	31.73	1540	31.86	33.41	70.67
9	368	395	16.41	2102	91.1	35.7	1742	35.84	37.62	79.63
10	410	441	18.22	2350	101.5	39.66	1944	39.83	41.83	88.59
11	452	487	20.02	2598	111.9	43.63	2146	43.81	46.04	97.55
12	494	533	21.83	2846	122.3	47.6	2348	47.79	50.25	106.51
13	536	579	23.63	3094	132.7	51.56	2550	51.78	54.46	115.47

Table 9: Numerical comparison of expected value of degree-based indices of random cyclooctane chain at $p_1 = 1$ for $n = 3$ to 13

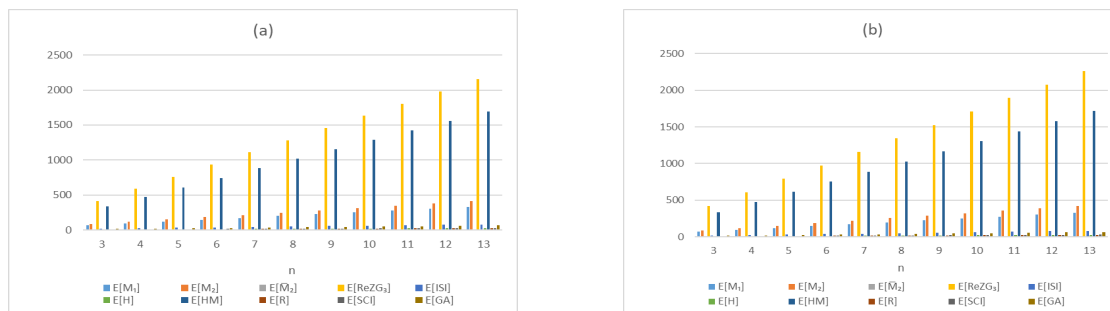


Figure 5: Graphical representation of expected value of degree-based TIs for random generalized polyomino chain for (a) $p_1 = 0$ and (b) $p_1 = 1$.

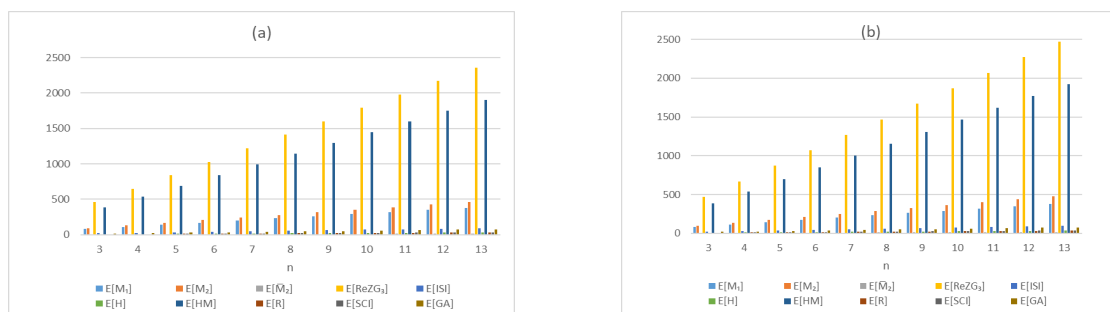


Figure 6: Graphical representation of expected value of degree-based TIs for random pentachain for (a) $p_1 = 0$ and (b) $p_1 = 1$.

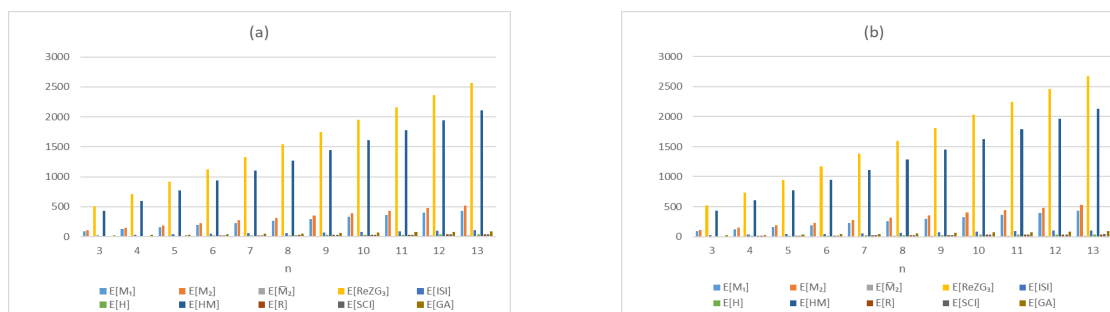


Figure 7: Graphical representation of expected value of degree-based TIs for random polyphenyl chain for (a) $p_1 = 0$ and (b) $p_1 = 1$.

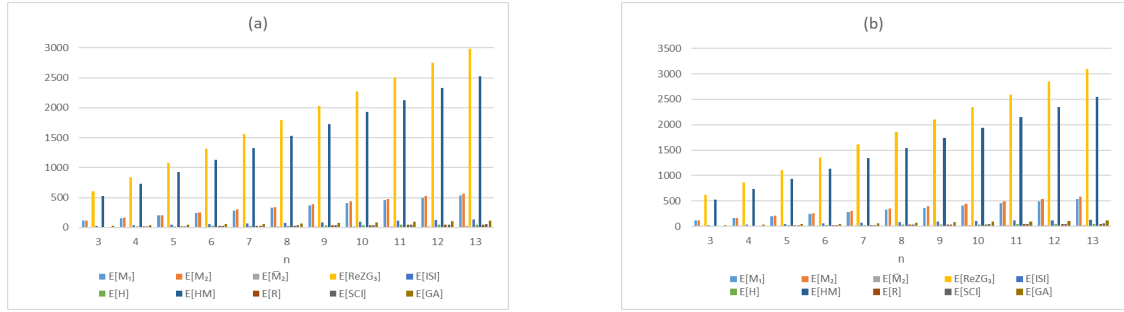


Figure 8: Graphical representation of expected value of degree-based TIs for random cyclooctane chain for (a) $p_1 = 0$ and (b) $p_1 = 1$.

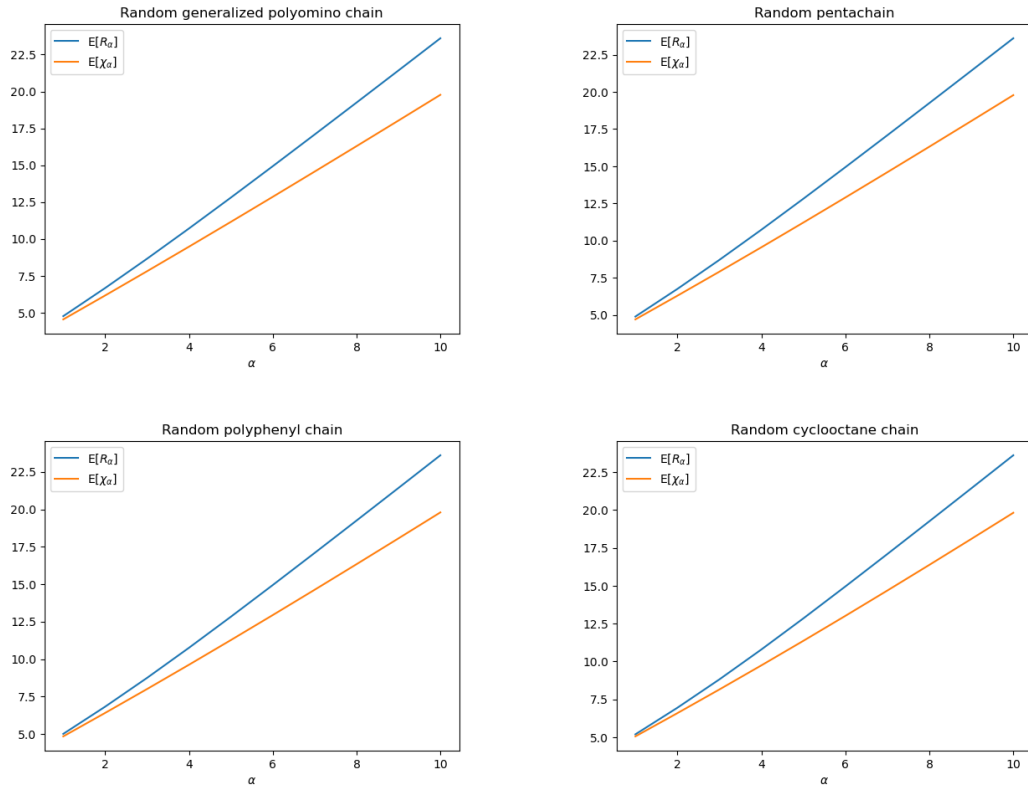


Figure 9: Plotting of $E[R_\alpha]$ and $E[\chi_\alpha]$ for different random l - polygonal chains at $n = 4$ and $p_1 = 1$. In vertical axis, logarithmic values of expected mean of indices are considered to show the comparison clearly.

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