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The expected values and variances for degree-based topological indices in three random chains

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Abstract. This article is devoted to obtaining a general method of calculating the expected values and variances for degree-based topological indices in random hexagonal, phenylene and polyphenyl chains. Based on the general method, some important degree-based topological indices are discussed and the explicit analytical expressions of their expected values and variances are presented, in which some known results are included. Besides, the expected values and variances for degree-based topological indices in these random chains are compared. In the end, the extremal values and the average values for degree-based topological indices in these random chains are determined.

1. Introduction

In this paper, we only consider finite simple connected graphs, and refer to Bondy and Murty [1] for the notations and terminologies freely used but not defined here.

Let G be a graph with the vertex set $V(G)$ and the edge set $E(G)$. The degree of $u \in V(G)$ is denoted by $d_G(u)$. If $u, v \in V(G)$ are adjacent, the edge connecting them is labeled by uv.

In the mathematical and chemical literature, several dozens of degree-based topological indices have been introduced and extensively studied [5, 11, 16]. Their general formula is of the form

$$\mathrm{TI}(G) = \sum_{uv \in E(G)} F\left(d_G(u), d_G(v)\right), \tag{1}$$

where F is a binary nonnegative function with the property $F(x, y) = F(y, x)$.

Let m_{ij} denote the number of edges in G with end-vertices of degree i and j. Then we have the following formula used later on:

$$\mathrm{TI}(G) = \sum_{uv \in E(G)} F\left(d_G(u), d_G(v)\right) = \sum_{1 \leqslant i \leqslant j \leqslant n-1} m_{ij} F(i, j). \tag{2}$$

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By selecting different functions $F(x, y)$ in (1), we can obtain different degree-based topological indices. Some important degree-based topological indices mentioned in this paper are listed in Table 1. For more details, see [5, 11, 16] and the references cited therein.

Table 1: Some important degree-based topological indices

name	$F(x, y)$	**name**	$F(x, y)$
first Zagreb index	$x + y$	first Gourava index	$x + y + xy$
second Zagreb index	xy	second Gourava index	$(x + y)xy$
first hyper-Zagreb index	$(x + y)^2$	first hyper-Gourava index	$(x + y + xy)^2$
second hyper-Zagreb index	$(xy)^2$	second hyper-Gourava index	$((x + y)xy)^2$
Randić index (product-connectivity index)	$\frac{1}{\sqrt{xy}}$	product-connectivity Gourava index	$\frac{1}{\sqrt{(x+y)xy}}$
sum-connectivity index	$\frac{1}{\sqrt{x+y}}$	sum-connectivity Gourava index	$\frac{1}{\sqrt{x+y+xy}}$
reciprocal Randić index	$\sqrt{xy}$	Albertson index	$\lvert x - y \rvert$
reciprocal sum-connectivity index	$\sqrt{x+y}$	extended index	$\frac{1}{2}\left(\frac{x}{y} + \frac{y}{x}\right)$
sigma index	$(x - y)^2$	harmonic index	$\frac{2}{x+y}$
atom-bond-connectivity index	$\sqrt{\frac{x+y-2}{xy}}$	forgotten index	$x^2 + y^2$
geometric-arithmetic index	$\frac{2\sqrt{xy}}{x+y}$	inverse degree index	$\frac{1}{x^2} + \frac{1}{y^2}$
inverse sum indeg index	$\frac{xy}{x+y}$	modified first Zagreb index	$\frac{1}{x^3} + \frac{1}{y^3}$
augmented Zagreb index	$\left(\frac{xy}{x+y-2}\right)^3$		

Topological indices play an important role in predicting physicochemical properties of chemical molecules by means of their structures. Currently, many researchers focus on the expected value of some indices in random hexagonal, phenylene and polyphenyl chains. Here are the definitions of these three random chains [21].

The random hexagonal chain $RHC_n = RHC(n, p_1, p_2, p_3)$ with n hexagons is constructured in the following way:

(1) RHC_1 is a hexagon and RHC_2 contains two hexagons, see Figure 1.

(2) For every $n > 2$, RHC_n is constructured in attaching one hexagon to RHC_{n-1} in three ways, resulted in $RHC_n^1, RHC_n^2, RHC_n^3$ with probability p_1, p_2, p_3 respectively, where $p_1 + p_2 + p_3 = 1$, see Figure 2.

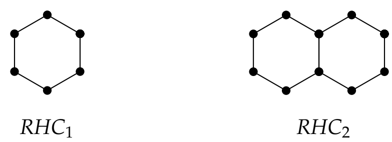
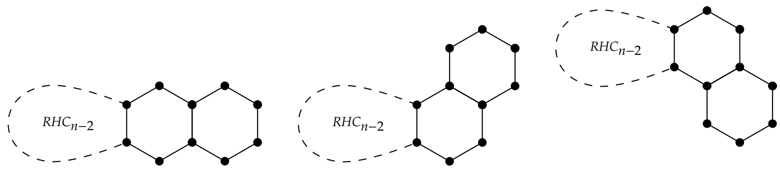


Figure 1: The graphs of RHC_1 and RHC_2



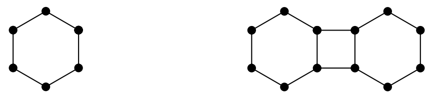
RHC_n^1 RHC_n^2 RHC_n^3

Figure 2: The three link ways for $RHC_n (n > 2)$

The random phenylene chain $RPC_n = RPC(n, p_1, p_2, p_3)$ with n hexagons is constructured in the following way:

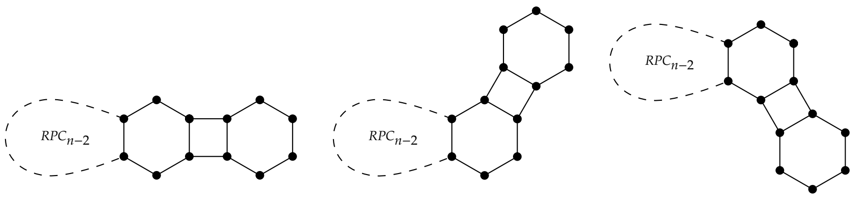
(1) RPC_1 is a hexagon and RPC_2 contains two hexagons, see Figure 3.

(2) For every $n > 2$, RPC_n is constructured in attaching one hexagon to RPC_{n-1} in three ways, resulted in $RPC_n^1, RPC_n^2, RPC_n^3$ with probability p_1, p_2, p_3 respectively, where $p_1 + p_2 + p_3 = 1$, see Figure 4.



RPC_1 RPC_2

Figure 3: The graphs of RPC_1 and RPC_2



RPC_n^1 RPC_n^2 RPC_n^3

Figure 4: The three link ways for $RPC_n (n > 2)$

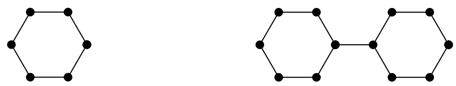
The random polyphenyl chain $PPC_n = PPC(n, p_1, p_2, p_3)$ with n hexagons is constructured in the following way:

(1) PPC_1 is a hexagon and PPC_2 contains two hexagons, see Figure 5.

(2) For every $n > 2$, PPC_n is constructured in attaching one hexagon to PPC_{n-1} in three ways, resulted in $PPC_n^1, PPC_n^2, PPC_n^3$ with probability p_1, p_2, p_3 respectively, where $p_1 + p_2 + p_3 = 1$, see Figure 6.

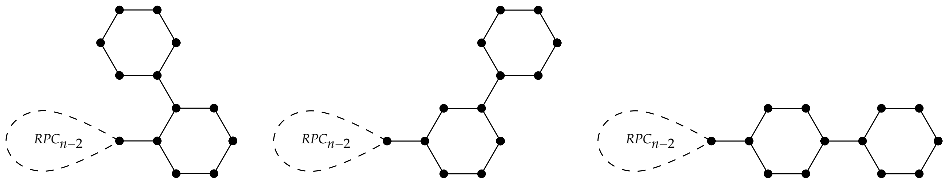
In [6], the expected values of the first Zagreb and Randić indices in random polyphenyl chains are given. In [10, 13], the expected values for atom-bond connectivity and geometric-arithmetic indices in random polyphenyl and phenylene chains are determined. In [14], the expected values of the Harmonic and second Zagreb indices in random polyphenyl and spiro chains are presented. In [19, 20], the expected values and variances for the Gutman index, Schultz index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index in a random polyphenyl chain are presented. In the most recent paper [21], the expected values and variances for Somber indices in a general random chain are discussed. For more related results, we refer the reader to see [2, 4, 7, 12, 17, 18]

Motivated by [6, 10, 13, 14, 19–21], we devote to studying the expected values and variances for degree-based topological indices with the form (1) in random hexagonal, phenylene and polyphenyl chains.



PPC_1 PPC_2

Figure 5: The graphs of PPC_1 and PPC_2



RPC_n^1 RPC_n^2 RPC_n^3

Figure 6: The three link ways for $PPC_n (n > 2)$

This paper is organized as follows. In Section 2, we obtain a general method of calculating the expected values and variances for degree-based topological indices in random hexagonal, phenylene and polyphenyl chains. Based on the general method, the explicit analytical expressions of the expected values and variances for some important degree-based topological indices in these random chains are presented in Appendix. In Section 3 and Section 4, the expected values and the variances for degree-based topological indices in these random chains are compared. In Section 5, the extremal values and the average values of degree-based topological indices in these random chains are determined.

2. A general method

In this section, we obtain a general method of calculating the expected values and variances for degree-based topological indices in random hexagonal, phenylene and polyphenyl chains, see Theorem 2.4. In order to complete the proof of Theorem 2.4, we first briefly recall some of the basic facts from probability theory.

The multinomial distribution $\mathcal{M}(n, \mathbf{p})$ is a distribution with a parameter vector $\mathbf{p}$ in the parameter space

$$\left\{ \mathbf{p} \,\middle|\, \mathbf{p} = (p_1, p_2, \cdots, p_t)^T \in \mathbb{R}^t, p_i \geqslant 0, i = 1, 2, \cdots, t, \text{ and } \sum_{i=1}^{t} p_i = 1 \right\}.$$

The sample space of $\mathcal{M}(n, \mathbf{p})$ is

$$S = \left\{ \mathbf{x} \,\middle|\, \mathbf{x} = (x_1, x_2, \cdots, x_t)^T \in \mathbb{Z}^t, x_i \geqslant 0, i = 1, 2, \cdots, t, \text{ and } \sum_{i=1}^{t} x_i = n \right\}.$$

The probability mass function of $\mathcal{M}(n, \mathbf{p})$ is

$$f(\mathbf{x}) = \binom{n}{\mathbf{x}} \prod_{i=1}^{t} p_i^{x_i}, \mathbf{x} \in S,$$

where

$$\binom{n}{\mathbf{x}} = \frac{n!}{\prod_{i=1}^{t} x_i!}.$$

Let $\mathbf{X}$ be a random vector which follows the multinomial distribution $\mathcal{M}(n, \mathbf{p})$, denoted by $\mathbf{X} \sim \mathcal{M}(n, \mathbf{p})$. Then the expected value and variance of $\mathbf{X}$ is given by

$$\mathbf{E}(\mathbf{X}) = n\mathbf{p}, \mathbf{Var}(\mathbf{X}) = n(\mathbf{diag}(\mathbf{p}) - \mathbf{p}\mathbf{p}^T). \tag{3}$$

In fact, when $n = 1$ and $t = 2$, the multinomial distribution is the Bernoulli distribution, denoted by $\mathcal{B}(p_1)$, when $n > 1$ and $t = 2$, the multinomial distribution is the binomial distribution, denoted by $\mathcal{B}(n, p_1)$, when $n = 1$ and $t > 2$, the multinomial distribution is the categorical distribution, denoted by $\mathcal{C}(\mathbf{p})$.

Here are two important properties of the multinomial distribution.

Proposition 2.1 (Addition Rule [8]). *Let $\mathbf{X}_1, \mathbf{X}_2, \cdots, \mathbf{X}_k$ be independent random vectors and $\mathbf{X}_i \sim \mathcal{M}(n_i, \mathbf{p})$ for each $i = 1, 2, \cdots, k$. Then*

$$\sum_{i=1}^{k} \mathbf{X}_i \sim \mathcal{M}(\sum_{i=1}^{k} n_i, \mathbf{p}).$$

Proposition 2.2 (Marginal Distribution [8]). *Let $\mathbf{X} = (X_1, X_2, \cdots, X_t) \sim \mathcal{M}(n, \mathbf{p})$. Then $X_i \sim \mathcal{B}(n, p_i)$ for each $i = 1, 2, \cdots, t$.*

For more details on the multinomial distributions, we refer the reader to see [3, 8]. The following lemma is frequently used.

Lemma 2.3 ([9]). *Let X be a random variable and $a, b \in \mathbb{R}$. Then*

$$\mathbf{E}(aX + b) = a\mathbf{E}(\mathbf{X}) + b, \mathbf{Var}(aX + b) = a^2\mathbf{Var}(X).$$

Now we present a general method of calculating the expected values and variances for degree-based topological indices in random hexagonal, phenylene and polyphenyl chains.

Theorem 2.4. *Let $n > 2$, $G_n = G(n, p_1, p_2, p_3)$ with $G \in \{RHC, RPC, PPC\}$ be one of the three random chains and X be a random variable which follows the binomial distribution $\mathcal{B}(n-2, p_1)$. Then $\mathrm{TI}(G_n) = AX + B(n-2) + C$ and its expected value and variance are given by*

$$\mathbf{E}\left(\mathrm{TI}(G_n)\right) = \left(p_1 A + B\right)(n-2) + C, \mathbf{Var}\left(\mathrm{TI}(G_n)\right) = A^2(n-2)p_1(1-p_1),$$

where $(A, B, C) = (F(2, 2), F(2, 3), F(3, 3))M$ and

$$M = \begin{cases} \begin{pmatrix} -1 & 1 & 6 \\ 2 & 2 & 4 \\ -1 & 2 & 1 \end{pmatrix}, & \text{if } G = RHC, \\ \begin{pmatrix} -1 & 1 & 6 \\ 2 & 2 & 4 \\ -1 & 5 & 4 \end{pmatrix}, & \text{if } G = RPC, \\ \begin{pmatrix} 1 & 2 & 8 \\ -2 & 4 & 4 \\ 1 & 1 & 1 \end{pmatrix}, & \text{if } G = PPC. \end{cases}$$

Proof. In order to quantify the random variable $\mathrm{TI}(G_n)$, we define a family of 3-dimensional random vectors $\{\mathbf{Z}_k\}_{k=3}^{n}$ as follows:

$$\mathbf{Z}_k = \begin{cases} (1, 0, 0)^T, & \text{if we choice } G_n^1 \text{ in the } k\text{-th step}, \\ (0, 1, 0)^T, & \text{if we choice } G_n^2 \text{ in the } k\text{-th step}, \\ (0, 0, 1)^T, & \text{if we choice } G_n^3 \text{ in the } k\text{-th step}. \end{cases}$$

By the definition of the three random chains, we can check that $\mathbf{Z}_k$ follows the categorical distribution $\mathcal{C}(1, p_1, p_2, p_3)$ and $\mathbf{Z}_3$, $\mathbf{Z}_4$, $\cdots$, $\mathbf{Z}_n$ are independent.

For each $k = 3, 4, \cdots, n$, $\mathrm{TI}(G_k)$ can be quantified as

$$\mathrm{TI}(G_k) = (\mathrm{TI}(G_k^1), \mathrm{TI}(G_k^2), \mathrm{TI}(G_k^3))\mathbf{Z}_k. \tag{4}$$

By the definition of degree-based topological indices, we have

$$\mathrm{TI}(G_k^i) - \mathrm{TI}(G_{k-1}) = \mathrm{TI}(G_3^i) - \mathrm{TI}(G_2), \text{ for each } k = 3, 4, \cdots, n \text{ and } i = 1, 2, 3.$$

We denote $A_i = \mathrm{TI}(G_3^i) - \mathrm{TI}(G_2)$, $i = 1, 2, 3$. Then

$$\mathrm{TI}(G_k^i) = \mathrm{TI}(G_{k-1}) + A_i, i = 1, 2, 3. \tag{5}$$

Associated (4) with (5), we obtain the following recurrence relation:

$$\mathrm{TI}(G_k) = \mathrm{TI}(G_{k-1}) + (A_1, A_2, A_3)\mathbf{Z}_k. \tag{6}$$

Solving the recurrence relation with the boundary condition $\mathrm{TI}(G_2)$, we obtain

$$\mathrm{TI}(G_n) = (A_1, A_2, A_3)\mathbf{X} + \mathrm{TI}(G_2), \mathbf{X} = (X_1, X_2, X_3)^T = \sum_{k=3}^{n} \mathbf{Z}_k. \tag{7}$$

By Proposition 2.1, $\mathbf{X} = \sum_{k=3}^{n} \mathbf{Z}_k$ follows the Multinomial distribution $\mathcal{M}(n-2, p_1, p_2, p_3)$.

By (2), we have

$$(A_1, A_2, A_3) = \begin{cases} (F(2,2), F(2,3), F(3,3)) \begin{pmatrix} 0 & 1 & 1 \\ 4 & 2 & 2 \\ 1 & 2 & 2 \end{pmatrix}, & \text{if } G = RHC, \\ (F(2,2), F(2,3), F(3,3)) \begin{pmatrix} 0 & 1 & 1 \\ 4 & 2 & 2 \\ 4 & 5 & 5 \end{pmatrix}, & \text{if } G = RPC, \\ (F(2,2), F(2,3), F(3,3)) \begin{pmatrix} 3 & 2 & 2 \\ 2 & 4 & 4 \\ 2 & 1 & 1 \end{pmatrix}, & \text{if } G = PPC. \end{cases}$$

Therefore, $A_2 = A_3$. By (7), we have

$$\begin{aligned} \mathrm{TI}(G_n) =& (A_1, A_2, A_2)\mathbf{X} + \mathrm{TI}(G_2) \\ =& (A_1 - A_2)(1, 0, 0)\mathbf{X} + A_2(1, 1, 1)\mathbf{X} + \mathrm{TI}(G_2), \\ =& (A_1 - A_2)X_1 + A_2(n-2) + \mathrm{TI}(G_2). \end{aligned} \tag{8}$$

By Proposition 2.2, we have X_1 follows the binomial distribution $\mathcal{B}(n-2, p_1)$.

Put $A = A_1 - A_2$, $B = A_2$, $C = \mathrm{TI}(G_2)$, then

$$(A, B, C) = \begin{cases} (F(2,2), F(2,3), F(3,3)) \begin{pmatrix} -1 & 1 & 1 \\ 2 & 2 & 2 \\ -1 & 2 & 2 \end{pmatrix}, & \text{if } G = RHC, \\ (F(2,2), F(2,3), F(3,3)) \begin{pmatrix} -1 & 1 & 1 \\ 2 & 2 & 2 \\ -1 & 5 & 5 \end{pmatrix}, & \text{if } G = RPC, \\ (F(2,2), F(2,3), F(3,3)) \begin{pmatrix} 1 & 2 & 2 \\ -2 & 4 & 4 \\ 1 & 1 & 1 \end{pmatrix}, & \text{if } G = PPC. \end{cases}$$

Therefore, the proof of the first part is completed.

Applying Lemma 2.3 in (8), we obtain

$$\mathbf{E}\left(\mathrm{TI}(G_n)\right) = \left(p_1 A + B\right)(n-2) + C, \mathbf{Var}\left(\mathrm{TI}(G_n)\right) = A^2(n-2)p_1(1-p_1).$$

This completes the proof. □

In fact, Theorem 2.4 obtains a general method of calculating the expected values and variances for degree-based topological indices in random hexagonal, phenylene and polyphenyl chains. The vector $(F(2,2), F(2,3), F(3,3))$ and three matrices in Theorem 2.4 play an important role in calculation. For the sake of simplifying presentation, we denote $\mathbf{t}_F = (F(2,2), F(2,3), F(3,3))$ and

$$M_{RHC} = \begin{pmatrix} -1 & 1 & 6 \\ 2 & 2 & 4 \\ -1 & 2 & 1 \end{pmatrix}, M_{RPC} = \begin{pmatrix} -1 & 1 & 6 \\ 2 & 2 & 4 \\ -1 & 5 & 4 \end{pmatrix}, M_{PPC} = \begin{pmatrix} 1 & 2 & 8 \\ -2 & 4 & 4 \\ 1 & 1 & 1 \end{pmatrix}.$$

In the following, an important value Δ_F is used frequently, denoted by

$$\Delta_F = 2F(2,3) - F(2,2) - F(3,3).$$

By applying Theorem 2.4, we can easily obtain the explicit analytical expressions of the expected values and variances for some important degree-based topological indices listed in Table 1.

In Appendix, Table 2 shows the values of the vectors $\mathbf{t}_F$ and Δ_F. And the explicit analytical expressions of the expected values and variances are demonstrated in Tables 3 – 6.

Remark 2.5. *Tables 3 – 5 include some known results. For example, the expected values of the first Zagreb and Randić indices in random polyphenyl chains [6], the expected values for atom-bond connectivity and geometric-arithmetic indices in random polyphenyl and phenylene chains [10, 13] and the expected values of the Harmonic and second Zagreb indices in random polyphenyl chains [14] are obtained in Tables 3–5.*

3. Comparisons of the expected values

In this section, we make comparisons of the expected values for degree-based topological indices in random hexagonal, phenylene and polyphenyl chains.

Let $n > 2$, $G_n = G(n, p_1, p_2, p_3)$ with $G \in \{RHC, RPC, PPC\}$ be a random chain. The following Propositions 3.1–3.2 show that $\mathrm{TI}(G_n)$ increases or decreases monotonically with increasing p_1.

Proposition 3.1. *Let $n > 2$, $G_n = G(n, p_1, p_2, p_3)$, $G'_n = G(n, p'_1, p'_2, p'_3)$ be two random chains with $p_1 < p'_1$ and $G \in \{RHC, RPC\}$. Then the following statements hold.*

(1) *If $\Delta_F = 0$, then $\mathbf{E}(\mathrm{TI}(G_n)) = \mathbf{E}(\mathrm{TI}(G'_n))$.*

(2) *If $\Delta_F > 0$, then $\mathbf{E}(\mathrm{TI}(G_n)) < \mathbf{E}(\mathrm{TI}(G'_n))$.*

(3) *If $\Delta_F < 0$, then $\mathbf{E}(\mathrm{TI}(G_n)) > \mathbf{E}(\mathrm{TI}(G'_n))$.*

Proof. By Theorem 2.4, we have

$$\mathbf{E}(\mathrm{TI}(G_n)) = (p_1\Delta_F + B)(n-2) + C, \mathbf{E}(\mathrm{TI}(G'_n)) = (p'_1\Delta_F + B)(n-2) + C,$$

where

$$(\Delta_F, B, C) = \begin{cases} \mathbf{t}_F M_{RHC}, & \text{if } G = RHC, \\ \mathbf{t}_F M_{RPC}, & \text{if } G = RPC. \end{cases}$$

Let $f(x) = (x\Delta_F + B)(n-2) + C$, $0 < x < 1$. When $\Delta_F = 0$, we have

$$\mathbf{E}(\mathrm{TI}(G_n)) = f(p_1) = B(n-2) + C = f(p'_1) = \mathbf{E}(\mathrm{TI}(G'_n)).$$

When $\Delta_F > 0$, by the increased monotonicity of $f(x)$, we have

$$\mathbf{E}(\mathrm{TI}(G_n)) = f(p_1) < f(p'_1) = \mathbf{E}(\mathrm{TI}(G'_n)).$$

When $\Delta_F < 0$, by the decreased monotonicity of $f(x)$, we have

$$\mathbf{E}(\mathrm{TI}(G_n)) = f(p_1) > f(p'_1) = \mathbf{E}(\mathrm{TI}(G'_n)).$$

This completes the proof. □

Proposition 3.2. *Let $n > 2$, $PPC_n = PPC(n, p_1, p_2, p_3)$, $PPC'_n = PPC'(n, p'_1, p'_2, p'_3)$ be two random polyphenyl chains with $p_1 < p'_1$. Then the following statements hold.*

(1) *If $\Delta_F = 0$, then $\mathbf{E}(\mathrm{TI}(PPC_n)) = \mathbf{E}(\mathrm{TI}(PPC'_n))$.*

(2) *If $\Delta_F > 0$, then $\mathbf{E}(\mathrm{TI}(PPC_n)) > \mathbf{E}(\mathrm{TI}(PPC'_n))$.*

(3) *If $\Delta_F < 0$, then $\mathbf{E}(\mathrm{TI}(PPC_n)) < \mathbf{E}(\mathrm{TI}(PPC'_n))$.*

Proof. By Theorem 2.4, we have

$$\mathbf{E}(\mathrm{TI}(PPC_n)) = (-p_1\Delta_F + B)(n-2) + C, \mathbf{E}(\mathrm{TI}(PPC'_n)) = (-p'_1\Delta_F + B)(n-2) + C,$$

where $(-\Delta_F, B, C) = \mathbf{t}_F M_{PPC}$.

Let $f(x) = (-x\Delta_F + B)(n-2) + C$, $0 < x < 1$. When $\Delta_F = 0$, we have

$$\mathbf{E}(\mathrm{TI}(PPC_n)) = f(p_1) = B(n-2) + C = f(p'_1) = \mathbf{E}(\mathrm{TI}(PPC'_n)).$$

When $\Delta_F > 0$, by the decreased monotonicity of $f(x)$, we have

$$\mathbf{E}(\mathrm{TI}(PPC_n)) = f(p_1) > f(p'_1) = \mathbf{E}(\mathrm{TI}(PPC'_n)).$$

When $\Delta_F < 0$, by the increased monotonicity of $f(x)$, we have

$$\mathbf{E}(\mathrm{TI}(PPC_n)) = f(p_1) < f(p'_1) = \mathbf{E}(\mathrm{TI}(PPC'_n)).$$

This completes the proof. □

For a graph G, let $\mathrm{TI}'(G)$ be another degree-based topological index defined as

$$\mathrm{TI}'(G) = \sum_{uv\in E(G)} F'\left(d_G(u), d_G(v)\right),$$

where F' is another binary nonnegative function with the property $F'(x, y) = F'(y, x)$. We denote $\mathbf{t}_{F'} = (F'(2,2), F'(2,3), F'(3,3))$ and $\Delta_{F'} = 2F'(2,3) - F'(2,2) - F'(3,3)$.

For $\mathrm{TI}(G)$ and $\mathrm{TI}'(G)$, we write $\mathbf{t}_F < \mathbf{t}_{F'}$ if $F(2,2) \leqslant F'(2,2)$, $F(2,3) \leqslant F'(2,3)$, $F(3,3) \leqslant F'(3,3)$ and $\mathbf{t}_F \neq \mathbf{t}_{F'}$. The following Proposition 3.3 gives an effective sufficient condition for comparing the expected values for different degree-based topological indices in the same random chains.

Proposition 3.3. *Let $n > 2$, $G_n = G(n, p_1, p_2, p_3)$ with $G \in \{RHC, RPC, PPC\}$ be a random chain and $\mathrm{TI}(G_n)$, $\mathrm{TI}'(G_n)$ be two degree-based topological indices with $\mathbf{t}_F < \mathbf{t}_{F'}$. Then $\mathbf{E}(\mathrm{TI}(G_n)) < \mathbf{E}(\mathrm{TI}'(G_n))$.*

Proof. By Theorem 2.4, we have

$$\mathbf{E}(\mathrm{TI}(G_n)) = (p_1 A + B)(n-2) + C, \mathbf{E}(\mathrm{TI}'(G_n)) = (p_1 A' + B')(n-2) + C',$$

where $(A, B, C) = \mathbf{t}_F M$ and $(A', B', C') = \mathbf{t}_{F'} M$.

Note that

$$\begin{aligned}
&\mathbf{E}(\mathrm{TI}'(G_n)) - \mathbf{E}(\mathrm{TI}(G_n))\\
=&(p_1(A'-A) + (B'-B))(n-2) + (C'-C)\\
=&(A'-A, B'-B, C'-C)(p_1(n-2), n-2, 1)^T\\
=&(\mathbf{t}_{F'} - \mathbf{t}_F)M(p_1(n-2), n-2, 1)^T\\
=&\begin{cases} (\mathbf{t}_{F'} - \mathbf{t}_F)M_{RHC}(p_1(n-2), n-2, 1)^T, & \text{if } G_n = RHC_n,\\ (\mathbf{t}_{F'} - \mathbf{t}_F)M_{RPC}(p_1(n-2), n-2, 1)^T, & \text{if } G_n = RPC_n,\\ (\mathbf{t}_{F'} - \mathbf{t}_F)M_{PPC}(p_1(n-2), n-2, 1)^T, & \text{if } G_n = PPC_n,\end{cases}\\
=&\begin{cases} (\mathbf{t}_{F'} - \mathbf{t}_F)((1-p_1)(n-2) + 6, (2+2p_1)(n-2) + 4, (2-p_1)(n-2) + 1)^T > 0,\\ (\mathbf{t}_{F'} - \mathbf{t}_F)((1-p_1)(n-2) + 6, (2+2p_1)(n-2) + 4, (5-p_1)(n-2) + 4)^T > 0,\\ (\mathbf{t}_{F'} - \mathbf{t}_F)((2+p_1)(n-2) + 8, (4-2p_1)(n-2) + 4, (1+p_1)(n-2) + 1)^T > 0.\end{cases}
\end{aligned}$$

Therefore, $\mathbf{E}(\mathrm{TI}(G_n)) < \mathbf{E}(\mathrm{TI}'(G_n))$. □

According to Proposition 3.3 and the values of $\mathbf{t}_F$ in Table 2, we can order the expected values for the indices listed in Table 1.

The following Propositions 3.4–3.6 give some effective sufficient conditions for comparing the expected values for the same degree-based topological indices in different random chains.

Proposition 3.4. *Let $n > 2$, $RHC_n = RHC(n, p_1, p_2, p_3)$ be a random hexagonal chain and $RPC_n = RPC(n, p_1, p_2, p_3)$ be a random phenylene chain. Then $\mathbf{E}(\mathrm{TI}(RHC_n)) \leqslant \mathbf{E}(\mathrm{TI}(RPC_n))$ with equality if and only if $F(3,3) = 0$.*

Proof. By Theorem 2.4, we have

$$\mathbf{E}(\mathrm{TI}(RHC_n)) = (p_1A + B)(n-2) + C, \mathbf{E}(\mathrm{TI}(RPC_n)) = (p_1A' + B')(n-2) + C',$$

where $(A, B, C) = \mathbf{t}_F M_{RHC}$ and $(A', B', C') = \mathbf{t}_F M_{RPC}$.

Note that

$$\begin{aligned}
&\mathbf{E}(\mathrm{TI}(RPC_n)) - \mathbf{E}(\mathrm{TI}(RHC_n))\\
=&(p_1(A'-A) + (B'-B))(n-2) + (C'-C)\\
=&(A'-A, B'-B, C'-C)(p_1(n-2), n-2, 1)^T\\
=&\mathbf{t}_F(M_{RPC} - M_{RHC})(p_1(n-2), n-2, 1)^T\\
=&(3n-3)F(3,3)\\
\geqslant&0.
\end{aligned}$$

Therefore, $\mathbf{E}(\mathrm{TI}(RHC_n)) \leqslant \mathbf{E}(\mathrm{TI}(RPC_n))$ with equality if and only if $F(3,3) = 0$. □

Proposition 3.5. *Let $n > 2$, $RHC_n = RHC(n, p_1, p_2, p_3)$ be a random hexagonal chain, $PPC_n = PPC(n, p_1, p_2, p_3)$ be a random polyphenyl chain and $(1 - 2p_1)\Delta_F \geqslant 0$. Then $\mathbf{E}(\mathrm{TI}(RHC_n)) \leqslant \mathbf{E}(\mathrm{TI}(PPC_n))$.*

Proof. By Theorem 2.4, we have

$$\mathbf{E}(\mathrm{TI}(RHC_n)) = (p_1A + B)(n-2) + C, \mathbf{E}(\mathrm{TI}(PPC_n)) = (p_1A' + B')(n-2) + C',$$

where $(A, B, C) = \mathbf{t}_F M_{RHC}$ and $(A', B', C') = \mathbf{t}_F M_{PPC}$.

Note that

$$\begin{aligned}
&\mathbf{E}(\mathrm{TI}(PPC_n)) - \mathbf{E}(\mathrm{TI}(RHC_n))\\
=&(p_1(A'-A) + (B'-B))(n-2) + (C'-C)\\
=&(A'-A, B'-B, C'-C)(p_1(n-2), n-2, 1)^T\\
=&\mathbf{t}_F(M_{PPC} - M_{RHC})(p_1(n-2), n-2, 1)^T\\
=&\mathbf{t}_F((1+2p_1)(n-2) + 2, (2-4p_1)(n-2), (-1+2p_1)(n-2))^T\\
=&(1-2p_1)\Delta_F(n-2) + (2n-2)F(2,2)\\
\geqslant&0.
\end{aligned}$$

Therefore, $\mathbf{E}(\mathrm{TI}(RHC_n)) \leqslant \mathbf{E}(\mathrm{TI}(PPC_n))$. □

Proposition 3.6. *Let $n > 2$, $RPC_n = RPC(n, p_1, p_2, p_3)$ be a random phenylene chain and $PPC_n = PPC(n, p_1, p_2, p_3)$ be a random polyphenyl chain. Then*

(1) *If $(1 - 2p_1)\Delta_F \geqslant 0$ and $2F(2,2) \geqslant 3F(3,3)$, then $\mathbf{E}(\mathrm{TI}(RPC_n)) \leqslant \mathbf{E}(\mathrm{TI}(PPC_n))$.*

(2) *If $(1 - 2p_1)\Delta_F \leqslant 0$ and $2F(2,2) \leqslant 3F(3,3)$, then $\mathbf{E}(\mathrm{TI}(PPC_n)) \leqslant \mathbf{E}(\mathrm{TI}(RPC_n))$.*

Proof. By Theorem 2.4, we have

$$\mathbf{E}(\mathrm{TI}(RPC_n)) = (p_1A + B)(n-2) + C, \mathbf{E}(\mathrm{TI}(PPC_n)) = (p_1A' + B')(n-2) + C',$$

where $(A, B, C) = \mathbf{t}_F M_{RPC}$ and $(A', B', C') = \mathbf{t}_F M_{PPC}$.

Note that

$$\begin{aligned}
&\mathbf{E}(\mathrm{TI}(PPC_n)) - \mathbf{E}(\mathrm{TI}(RPC_n)) \\
=&(p_1(A' - A) + (B' - B))(n-2) + (C' - C) \\
=&(A' - A, B' - B, C' - C)(p_1(n-2), n-2, 1)^T \\
=&\mathbf{t}_F(M_{PPC} - M_{RPC})(p_1(n-2), n-2, 1)^T \\
=&\mathbf{t}_F((1 + 2p_1)(n-2) + 2, (2 - 4p_1)(n-2), (-4 + 2p_1)(n-2))^T \\
=&(1 - 2p_1)\Delta_F(n-2) + (2F(2,2) - 3F(3,3))(n-1).
\end{aligned}$$

Therefore, if $(1 - 2p_1)\Delta_F \geqslant 0$ and $2F(2,2) \geqslant 3F(3,3)$, then $\mathbf{E}(\mathrm{TI}(RPC_n)) \leqslant \mathbf{E}(\mathrm{TI}(PPC_n))$. If $(1 - 2p_1)\Delta_F \leqslant 0$ and $2F(2,2) \leqslant 3F(3,3)$, then $\mathbf{E}(\mathrm{TI}(PPC_n)) \leqslant \mathbf{E}(\mathrm{TI}(RPC_n))$. □

4. Comparisons of the variances

In this section, we make comparisons of the variances for degree-based topological indices in random hexagonal, phenylene and polyphenyl chains.

Let $n > 2$, $G_n = G(n, p_1, p_2, p_3)$ be a random chain and $G \in \{RHC, RPC, PPC\}$, by Theorem 2.4, we have

$$\mathbf{Var}(\mathrm{TI}(G_n)) = (\Delta_F)^2(n-2)p_1(1-p_1). \tag{9}$$

It is obvious that (9) implies $\mathbf{Var}(\mathrm{TI}(RHC_n)) = \mathbf{Var}(\mathrm{TI}(RPC_n)) = \mathbf{Var}(\mathrm{TI}(PPC_n))$.

By (9), we can easily obtain Propositions 4.1–4.3.

Proposition 4.1. *Let $n > 2$, $G_n = G(n, p_1, p_2, p_3)$ be a random chain with $0 < p_1 < 1$, $G \in \{RHC, RPC, PPC\}$. Then $\mathbf{Var}(\mathrm{TI}(G_n)) = 0$ if and only if $\Delta_F = 0$.*

Proposition 4.2. *Let $n > 2$, $G_n = G(n, p_1, p_2, p_3)$ be a random chain with $0 < p_1 < 1$, $G \in \{RHC, RPC, PPC\}$ and $\Delta_F \neq 0$. Then*

$$0 < \mathbf{Var}(\mathrm{TI}(G_n)) \leqslant \frac{n-2}{4}(\Delta_F)^2,$$

with equality if and only if $p_1 = \frac{1}{2}$.

Proof. By Theorem 2.4, we have

$$\mathbf{Var}(\mathrm{TI}(G_n)) = (\Delta_F)^2(n-2)p_1(1-p_1) = (\Delta_F)^2(n-2)\left(-(p_1 - \frac{1}{2})^2 + \frac{1}{4}\right) \leqslant \frac{n-2}{4}(\Delta_F)^2,$$

with equality if and only if $p_1 = \frac{1}{2}$. □

Proposition 4.3. *Let $n > 2$, $G_n = G(n, p_1, p_2, p_3)$ be a random chain with $0 < p_1 < 1$, $G \in \{RHC, RPC, PPC\}$ and $\mathrm{TI}(G_n)$, $\mathrm{TI}'(G_n)$ be two degree-based topological indices of G_n. Then the following statements hold.*

(1) *If $|\Delta_F| = |\Delta_{F'}|$, then $\mathbf{Var}(\mathrm{TI}(G_n)) = \mathbf{Var}(\mathrm{TI}'(G_n))$.*

(2) *If $|\Delta_F| < |\Delta_{F'}|$, then $\mathbf{Var}(\mathrm{TI}(G_n)) < \mathbf{Var}(\mathrm{TI}'(G_n))$.*

(3) *If* $|\Delta_F| > |\Delta_{F'}|$, *then* $\mathbf{Var}(\mathrm{TI}(G_n)) > \mathbf{Var}(\mathrm{TI}'(G_n))$.

Proof. By Theorem 2.4, we have

$$\mathbf{Var}(\mathrm{TI}(G_n)) = (\Delta_F)^2(n-2)p_1(1-p_1), \mathbf{Var}(\mathrm{TI}'(G_n)) = (\Delta_{F'})^2(n-2)p_1(1-p_1).$$

Therefore, if $|\Delta_F| = |\Delta_{F'}|$, then $\mathbf{Var}(\mathrm{TI}(G_n)) = \mathbf{Var}(\mathrm{TI}'(G_n))$. If $|\Delta_F| < |\Delta_{F'}|$, then $\mathbf{Var}(\mathrm{TI}(G_n)) < \mathbf{Var}(\mathrm{TI}'(G_n))$. If $|\Delta_F| > |\Delta_{F'}|$, then $\mathbf{Var}(\mathrm{TI}(G_n)) > \mathbf{Var}(\mathrm{TI}'(G_n))$. □

According to Proposition 4.3 and the values of Δ_F in Table 2, we can order the variances for the indices listed in Table 1.

The following Proposition 4.4 shows that the variances change with increasing p_1.

Proposition 4.4. *Let* $n > 2$, $G_n = G(n, p_1, p_2, p_3)$, $G'_n = G(n, p'_1, p'_2, p'_3)$ *be two random chains with* $0 < p_1 < p'_1 < 1$, $G \in \{RHC, RPC, PPC\}$ *and* $\Delta_F \neq 0$. *Then the following statements hold.*

(1) *If* $p_1 + p'_1 = 1$, *then* $\mathbf{Var}(\mathrm{TI}(G_n)) = \mathbf{Var}(\mathrm{TI}(G'_n))$.

(2) *If* $p_1 + p'_1 < 1$, *then* $\mathbf{Var}(\mathrm{TI}(G_n)) < \mathbf{Var}(\mathrm{TI}(G'_n))$.

(3) *If* $p_1 + p'_1 > 1$, *then* $\mathbf{Var}(\mathrm{TI}(G_n)) > \mathbf{Var}(\mathrm{TI}(G'_n))$.

Proof. By Theorem 2.4, we have

$$\mathbf{Var}(\mathrm{TI}(G_n)) = (\Delta_F)^2(n-2)p_1(1-p_1), \mathbf{Var}(\mathrm{TI}(G'_n)) = (\Delta_F)^2(n-2)p'_1(1-p'_1).$$

Note that $\mathbf{Var}(\mathrm{TI}(G'_n)) - \mathbf{Var}(\mathrm{TI}(G_n)) = (\Delta_F)^2(n-2)(p'_1 - p_1)(p_1 + p'_1 - 1)$ and $p_1 < p'_1$. Therefore, if $p_1 + p'_1 = 1$, then $\mathbf{Var}(\mathrm{TI}(G_n)) = \mathbf{Var}(\mathrm{TI}(G'_n))$. If $p_1 + p'_1 < 1$, then $\mathbf{Var}(\mathrm{TI}(G_n)) < \mathbf{Var}(\mathrm{TI}(G'_n))$. If $p_1 + p'_1 > 1$, then $\mathbf{Var}(\mathrm{TI}(G_n)) > \mathbf{Var}(\mathrm{TI}(G'_n))$. □

5. Extremal values and average values

In this section, we determine the extremal values and the average values for degree-based topological indices in random hexagonal, phenylene and polyphenyl chains.

Proposition 5.1. *Let* $n > 2$, $G_n = G(n, p_1, p_2, p_3)$ *with* $G \in \{RHC, RPC, PPC\}$ *be a random chain. Then*

$$\mathrm{TI}_{\max}(G_n) = \max\{B(n-2) + C, (A+B)(n-2) + C\},$$

$$\mathrm{TI}_{\min}(G_n) = \min\{B(n-2) + C, (A+B)(n-2) + C\},$$

where

$$(A, B, C) = \begin{cases} \mathbf{t}_F M_{RHC}, & \text{if } G_n = RHC_n, \\ \mathbf{t}_F M_{RPC}, & \text{if } G_n = RPC_n, \\ \mathbf{t}_F M_{PPC}, & \text{if } G_n = PPC_n. \end{cases}$$

Proof. By Theorem 2.4, put $X = 0$ and $X = n - 2$, then the proof is completed. □

Denote by $\mathcal{HC}_n$ the set of all hexagonal chains with n hexagons, $\mathcal{PC}_n$ the set of all phenylene chains with n hexagons and $\mathcal{PPC}_n$ the set of all polyphenyl chains with n hexagons. The average value of degree-based topological indices among $\mathcal{HC}_n$, $\mathcal{PC}_n$ and $\mathcal{PPC}_n$ are defined as follows:

$$\mathrm{TI}_{\mathrm{avr}}(RHC_n) = \frac{1}{|\mathcal{HC}_n|} \sum_{G_n \in \mathcal{HC}_n} \mathrm{TI}(G_n),$$

$$\mathrm{TI}_{\mathrm{avr}}(RPC_n) = \frac{1}{|\mathcal{P}C_n|}\sum_{G_n\in\mathcal{P}C_n}\mathrm{TI}(G_n),$$

$$\mathrm{TI}_{\mathrm{avr}}(PPC_n) = \frac{1}{|\mathcal{P}\mathcal{P}C_n|}\sum_{G_n\in\mathcal{P}\mathcal{P}C_n}\mathrm{TI}(G_n).$$

By Theorem 2.4, put $p_1 = \frac{1}{3}$, then we have the following Proposition 5.2.

Proposition 5.2. *Let $n > 2$, $G_n = G(n, p_1, p_2, p_3)$ with $G \in \{RHC, RPC, PPC\}$ be a random chain. Then*

$$\mathrm{TI}_{\mathrm{avr}}(G_n) = \left(\frac{A}{3} + B\right)(n-2) + C,$$

where

$$(A, B, C) = \begin{cases} \mathbf{t}_F M_{RHC}, & \text{if } G_n = RHC_n, \\ \mathbf{t}_F M_{RPC}, & \text{if } G_n = RPC_n, \\ \mathbf{t}_F M_{PPC}, & \text{if } G_n = PPC_n. \end{cases}$$

Appying Propositions 3.4-3.6 with $p_1 = \frac{1}{3}$, we have the following Propositions 5.3-5.5.

Proposition 5.3. *Let RHC_n be a random hexagonal chain and RPC_n be a random phenylene chain. Then* $\mathrm{TI}_{\mathrm{avr}}(RHC_n) \leqslant \mathrm{TI}_{\mathrm{avr}}(RPC_n)$ *with equality if and only if $F(3,3) = 0$.*

Proposition 5.4. *Let RPC_n be a random phenylene chain, PPC_n be a random polyphenyl chain and $\Delta_F \geqslant 0$. Then* $\mathrm{TI}_{\mathrm{avr}}(RPC_n) \leqslant \mathrm{TI}_{\mathrm{avr}}(PPC_n)$.

Proposition 5.5. *Let RPC_n be a random phenylene chain and PPC_n be a random polyphenyl chain. Then*

(1) *If $\Delta_F \geqslant 0$ and $2F(2,2) \geqslant 3F(3,3)$, then* $\mathrm{TI}_{\mathrm{avr}}(RPC_n) \leqslant \mathrm{TI}_{\mathrm{avr}}(PPC_n)$.

(2) *If $\Delta_F \leqslant 0$ and $2F(2,2) \leqslant 3F(3,3)$, then* $\mathrm{TI}_{\mathrm{avr}}(PPC_n) \leqslant \mathrm{TI}_{\mathrm{avr}}(RPC_n)$.

6. Conclusion

In this paper, we obtain a general method of calculating the expected values and variances for degree-based topological indices in random hexagonal, phenylene and polyphenyl chains, see Theorem 2.4. As applications, we obtain the explicit analytical expressions of the expected values and variances for some important degree-based topological indices, see Tables 3 – 6, in which some known results are included, see Remark 2.5. Besides, we make comparisons of the expected values in Section 3 and the variances in Section 4. In Section 5, we determine the extremal values and the average values for degree-based topological indices in these three random chains.

Appendix

In Appendix, Table 2 shows the values of the vector $\mathbf{t}_F$ and Δ_F. Tables 3 – 6 show the explicit analytical expressions of the expected values and variances for the indices listed in Table 1 in random hexagonal, phenylene and polyphenyl chains.

Table 2: The vector $\mathbf{t}_F$ and Δ_F of some important degree-based topological indices

name	$F(x,y)$	$\mathbf{t}_F$	Δ_F
first Zagreb index	$x+y$	$(4,5,6)$	0
second Zagreb index	xy	$(4,6,9)$	-1
first hyper-Zagreb index	$(x+y)^2$	$(16,25,36)$	-2
second hyper-Zagreb index	$(xy)^2$	$(16,36,81)$	-25
Randić index (product-connectivity index)	$\frac{1}{\sqrt{xy}}$	$\left(\frac{1}{2},\frac{1}{\sqrt{6}},\frac{1}{3}\right)$	$\frac{2}{\sqrt{6}}-\frac{1}{2}-\frac{1}{3}$
sum-connectivity index	$\frac{1}{\sqrt{x+y}}$	$\left(\frac{1}{2},\frac{1}{\sqrt{5}},\frac{1}{\sqrt{6}}\right)$	$\frac{2}{\sqrt{5}}-\frac{1}{2}-\frac{1}{\sqrt{6}}$
reciprocal Randić index	$\sqrt{xy}$	$(2,\sqrt{6},3)$	$2\sqrt{6}-5$
reciprocal sum-connectivity index	$\sqrt{x+y}$	$\left(2,\sqrt{5},\sqrt{6}\right)$	$2\sqrt{5}-2-\sqrt{6}$
first Gourava index	$x+y+xy$	$(8,11,15)$	-1
second Gourava index	$(x+y)xy$	$(16,30,54)$	-10
first hyper-Gourava index	$(x+y+xy)^2$	$(64,121,225)$	-47
second hyper-Gourava index	$((x+y)xy)^2$	$(256,900,2916)$	-1372
product-connectivity Gourava index	$\frac{1}{\sqrt{(x+y)xy}}$	$\left(\frac{1}{4},\frac{1}{\sqrt{30}},\frac{1}{\sqrt{54}}\right)$	$\frac{2}{\sqrt{30}}-\frac{1}{4}-\frac{1}{\sqrt{54}}$
sum-connectivity Gourava index	$\frac{1}{\sqrt{x+y+xy}}$	$\left(\frac{1}{\sqrt{8}},\frac{1}{\sqrt{11}},\frac{1}{\sqrt{15}}\right)$	$\frac{2}{\sqrt{11}}-\frac{1}{\sqrt{8}}-\frac{1}{\sqrt{15}}$
Albertson index	$\lvert x-y\rvert$	$(0,1,0)$	2
extended index	$\frac{1}{2}\left(\frac{x}{y}+\frac{y}{x}\right)$	$\left(1,\frac{13}{12},1\right)$	$\frac{1}{6}$
sigma index	$(x-y)^2$	$(0,1,0)$	2
harmonic index	$\frac{2}{x+y}$	$\left(\frac{1}{2},\frac{2}{5},\frac{1}{3}\right)$	$-\frac{1}{30}$
atom-bond-connectivity index	$\sqrt{\frac{x+y-2}{xy}}$	$\left(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},\frac{2}{3}\right)$	$\frac{1}{\sqrt{2}}-\frac{2}{3}$
geometric-arithmetic index	$\frac{2\sqrt{xy}}{x+y}$	$\left(1,\frac{2\sqrt{6}}{5},1\right)$	$\frac{4\sqrt{6}}{5}-2$
forgotten index	x^2+y^2	$(8,13,18)$	0
inverse degree index	$\frac{1}{x^2}+\frac{1}{y^2}$	$\left(\frac{1}{2},\frac{13}{36},\frac{2}{9}\right)$	0
inverse sum indeg index	$\frac{xy}{x+y}$	$\left(1,\frac{6}{5},\frac{3}{2}\right)$	$-\frac{1}{10}$
modified first Zagreb index	$\frac{1}{x^3}+\frac{1}{y^3}$	$\left(\frac{1}{4},\frac{35}{216},\frac{2}{27}\right)$	0
augmented Zagreb index	$\left(\frac{xy}{x+y-2}\right)^3$	$\left(8,8,\frac{729}{64}\right)$	$-\frac{217}{64}$

Table 3: The expected values for some indices in $RHC_n (n > 2)$

name	**Expected values**
first Zagreb index	$26(n-2)+50$
second Zagreb index	$(-p_1+34)(n-2)+57$
first hyper-Zagreb index	$(-2p_1+138)(n-2)+232$
second hyper-Zagreb index	$(-25p_1+250)(n-2)+321$
Randić index (product-connectivity index)	$\left((-5+2\sqrt{6})p_1/6 + (7+2\sqrt{6})/6\right)(n-2) + (10+2\sqrt{6})/3$
sum-connectivity index	$((-1/2+2/\sqrt{5}-1/\sqrt{6})p_1 + (1/2+2/\sqrt{5} +2/\sqrt{6}))(n-2) + \left(3+4/\sqrt{5}+1/\sqrt{6}\right)$
reciprocal Randić index	$\left((-5+2\sqrt{6})p_1+(8+2\sqrt{6})\right)(n-2)+(15+4\sqrt{6})$
reciprocal sum-connectivity index	$\left((-2+2\sqrt{5}-\sqrt{6})p_1 + (2+2\sqrt{5}+2\sqrt{6})\right)(n-2) + (12+4\sqrt{5}+\sqrt{6})$
first Gourava index	$(-p_1+60)(n-2)+107$
second Gourava index	$(-10p_1+184)(n-2)+270$
first hyper-Gourava index	$(-47p_1+756)(n-2)+1093$
second hyper-Gourava index	$(-1372p_1+7888)(n-2)+8052$
product-connectivity Gourava index	$((-1/4+\sqrt{30}/15-\sqrt{6}/18)p_1 + (1/4+\sqrt{30}/15 +\sqrt{6}/9))(n-2) + (3/2+2\sqrt{30}/15+\sqrt{6}/18)$
sum-connectivity Gourava index	$((-1\sqrt{8}+2/\sqrt{11}-1/\sqrt{15})p_1 + (1/\sqrt{8}+2/\sqrt{11} +2/\sqrt{15}))(n-2) + (3/\sqrt{2}+4/\sqrt{11}+1/\sqrt{15})$
Albertson index	$(2p_1+2)(n-2)+4$
extended index	$(p_1/6+31/6)+34/3$
sigma index	$(2p_1+2)(n-2)+4$
harmonic index	$(-p_1/30+59/30)(n-2)+74/15$
atom-bond-connectivity index	$\left((1/\sqrt{2}-2/3)p_1 + (3/\sqrt{2}+4/3)\right)(n-2) + (10/\sqrt{2}+2/3)$
geometric-arithmetic index	$\left((-10+4\sqrt{6})p_1/5 + (15+4\sqrt{6})/5\right)(n-2) + (35+8\sqrt{6})/5$
forgotten index	$70(n-2)+118$
inverse degree index	$5(n-2)/3+14/3$
inverse sum indeg index	$(-p_1/10+32/5)(n-2)+123/10$
modified first Zagreb index	$13(n-2)/18+20/9$
augmented Zagreb index	$(-217p_1/64+1497/32)(n-2)+5849/64$

Table 4: The expected values for some indices in $RPC_n(n > 2)$

name	**Expected values**
first Zagreb index	$44(n-2)+68$
second Zagreb index	$(-p_1+61)(n-2)+84$
first hyper-Zagreb index	$(-2p_1+246)(n-2)+340$
second hyper-Zagreb index	$(-25p_1+493)(n-2)+564$
Randić index (product-connectivity index)	$\left((-5+2\sqrt{6})p_1/6 + (13+2\sqrt{6})/6\right)(n-2) + (13+2\sqrt{6})/3$
sum-connectivity index	$((-1/2+2/\sqrt{5}-1/\sqrt{6})p_1+(1/2+2/\sqrt{5} +5/\sqrt{6}))(n-2)+(3+4/\sqrt{5}+4/\sqrt{6})$
reciprocal Randić index	$\left((-5+2\sqrt{6})p_1+(17+2\sqrt{6})\right)(n-2)+(24+4\sqrt{6})$
reciprocal sum-connectivity index	$\left((-2+2\sqrt{5}-\sqrt{6})p_1 + (2+2\sqrt{5}+5\sqrt{6})\right)(n-2) + (12+4\sqrt{5}+4\sqrt{6})$
first Gourava index	$(-p_1+105)(n-2)+152$
second Gourava index	$(-10p_1+346)(n-2)+432$
first hyper-Gourava index	$(-47p_1+1431)(n-2)+1768$
second hyper-Gourava index	$(-1372p_1+16636)(n-2)+16800$
product-connectivity Gourava index	$((-1/4+\sqrt{30}/15-\sqrt{6}/18)p_1+(1/4+\sqrt{30}/15 +5\sqrt{6}/18))(n-2)+(3/2+2\sqrt{30}/15+2\sqrt{6}/9)$
sum-connectivity Gourava index	$((-1/\sqrt{8}+2/\sqrt{11}-1/\sqrt{15})p_1+(1/\sqrt{8}+2/\sqrt{11} +5/\sqrt{15}))(n-2)+(3/\sqrt{2}+4/\sqrt{11}+4/\sqrt{15})$
Albertson index	$(2p_1+2)(n-2)+4$
extended index	$(p_1/6+49/6)+43/3$
sigma index	$(2p_1+2)(n-2)+4$
harmonic index	$(-p_1/30+89/30)+89/15$
atom-bond-connectivity index	$\left((1/\sqrt{2}-2/3)p_1 + (3/\sqrt{2}+10/3)\right)(n-2) + (10/\sqrt{2}+8/3)$
geometric-arithmetic index	$\left((-10+4\sqrt{6})p_1/5+(30+4\sqrt{6})/5\right)+(50+8\sqrt{6})/5$
forgotten index	$124(n-2)+172$
inverse degree index	$7(n-2)/3+16/3$
inverse sum indeg index	$(-p_1/10+109/10)(n-2)+84/5$
modified first Zagreb index	$17(n-2)/18+22/9$
augmented Zagreb index	$(-217p_1/64+5181/64)(n-2)+2009/16$

Table 5: The expected values for some indices in $PPC_n (n > 2)$

name	Expected values
first Zagreb index	$34(n-2)+58$
second Zagreb index	$(p_1+41)(n-2)+65$
first hyper-Zagreb index	$(2p_1+168)(n-2)+264$
second hyper-Zagreb index	$(25p_1+257)(n-2)+353$
Randić index (product-connectivity index)	$\left((5-2\sqrt{6})p_1/6+(4+2\sqrt{6})/3\right)(n-2)+(13+2\sqrt{6})/3$
sum-connectivity index	$\left((1/2-2/\sqrt{5}+1/\sqrt{6})p_1 + (1+4/\sqrt{5}+1/\sqrt{6})\right)(n-2) + (4+4/\sqrt{5}+1/\sqrt{6})$
reciprocal Randić index	$\left((5-2\sqrt{6})p_1+(7+4\sqrt{6})\right)(n-2)+(19+4\sqrt{6})$
reciprocal sum-connectivity index	$\left((2-2\sqrt{5}+\sqrt{6})p_1 + (4+4\sqrt{5}+\sqrt{6})\right)(n-2) + (16+4\sqrt{5}+\sqrt{6})$
first Gourava index	$(p_1+75)(n-2)+123$
second Gourava index	$(10p_1+206)(n-2)+302$
first hyper-Gourava index	$(47p_1+837)(n-2)+1221$
second hyper-Gourava index	$(1372p_1+7028)(n-2)+8564$
product-connectivity Gourava index	$((1/4-\sqrt{30}/15+\sqrt{6}/18)p_1+(1/2+2\sqrt{30}/15 + \sqrt{6}/18)\big)(n-2)+(2+2\sqrt{30}/15+\sqrt{6}/18)$
sum-connectivity Gourava index	$((1/\sqrt{8}-2/\sqrt{11}+1/\sqrt{15})p_1+(1/\sqrt{2}+4/\sqrt{11} + 1/\sqrt{15})\big)(n-2)+(4/\sqrt{2}+4/\sqrt{11}+1/\sqrt{15})$
Albertson index	$(-2p_1+4)(n-2)+4$
extended index	$(-p_1/6+22/3)+40/3$
sigma index	$(-2p_1+4)(n-2)+4$
harmonic index	$(p_1/30+44/15)+89/15$
atom-bond-connectivity index	$\left((-1/\sqrt{2}+2/3)p_1 + (6/\sqrt{2}+2/3)\right)(n-2) + (12/\sqrt{2}+2/3)$
geometric-arithmetic index	$\left((10-4\sqrt{6})p_1/5+(15+8\sqrt{6})/5\right)+(45+8\sqrt{6})/5$
forgotten index	$86(n-2)+134$
inverse degree index	$8(n-2)/3+17/3$
inverse sum indeg index	$(p_1/10+83/10)(n-2)+143/10$
modified first Zagreb index	$11(n-2)/9+49/18$
augmented Zagreb index	$(217p_1/64+3801/64)(n-2)+6873/64$

Table 6: The variances for some indices in RHC_n, RPC_n and $PPC_n (n > 2)$

name	**Variances**
first Zagreb index	0
second Zagreb index	$(n-2)p_1(1-p_1)$
first hyper-Zagreb index	$4(n-2)p_1(1-p_1)$
second hyper-Zagreb index	$625(n-2)p_1(1-p_1)$
Randić index (product-connectivity index)	$\frac{49-20\sqrt{6}}{36}(n-2)p_1(1-p_1)$
sum-connectivity index	$\frac{73-24\sqrt{5}+10\sqrt{6}-8\sqrt{30}}{60}(n-2)p_1(1-p_1)$
reciprocal Randić index	$(49-20\sqrt{6})(n-2)p_1(1-p_1)$
reciprocal sum-connectivity index	$\left(30-8\sqrt{5}-4\sqrt{6}-4\sqrt{30}\right)(n-2)p_1(1-p_1)$
first Gourava index	$(n-2)p_1(1-p_1)$
second Gourava index	$100(n-2)p_1(1-p_1)$
first hyper-Gourava index	$2209(n-2)p_1(1-p_1)$
second hyper-Gourava index	$1882384(n-2)p_1(1-p_1)$
product-connectivity Gourava index	$\frac{463-96\sqrt{5}+60\sqrt{6}-72\sqrt{30}}{2160}(n-2)p_1(1-p_1)$
sum-connectivity Gourava index	$\frac{733-120\sqrt{22}+44\sqrt{30}-32\sqrt{165}}{1320}(n-2)p_1(1-p_1)$
Albertson index	$4(n-2)p_1(1-p_1)$
extended index	$\frac{1}{36}(n-2)p_1(1-p_1)$
sigma index	$4(n-2)p_1(1-p_1)$
harmonic index	$\frac{1}{900}(n-2)p_1(1-p_1)$
atom-bond-connectivity index	$\frac{17-6\sqrt{2}}{18}(n-2)p_1(1-p_1)$
geometric-arithmetic index	$\frac{196-80\sqrt{6}}{25}(n-2)p_1(1-p_1)$
forgotten index	0
inverse degree index	0
inverse sum indeg index	$\frac{1}{100}(n-2)p_1(1-p_1)$
modified first Zagreb index	0
augmented Zagreb index	$\frac{47089}{4096}(n-2)p_1(1-p_1)$

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