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Degree–based topological indices of a general random chain

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Abstract: In this paper, we examine a specific type of random chains and propose a unified approach to studying the degree-based topological indices, including their extreme values. We derive explicit analytical expressions for the expected values and variances of these indices and we establish the asymptotic behavior of the indices. Specifically, we analyze the first Zagreb index, Sombor index, harmonic index, Geometric-Arithmetic index, Inverse Sum Index, and the second Zagreb index for various general random chains, including random phenylene, random polyphenyl, random hexagonal, and linear chains.

Keywords: random chains, topological indices, extreme values, Markov processes.

AMS Subject classification: 05C50, 05C80, 05C35, 60J10, 60J20

1. Introduction

A graph is defined as a pair $G = (V, E)$, where the elements of V are the vertices of the graph G and the elements of E are its edges. The graphs considered in this manuscript are, unless otherwise specified finite, simple and connected. Undoubtedly, graph theory concepts are potentially applicable for many purposes, for instance, a chemical graph is a model of a chemical system, i.e., a graph is used to represent a molecule by considering the atoms as the nodes of the graph and the molecular bonds as the edges.

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The topological indices, on the other hand, quantify the structural information contained in the graph and are independent of the numbering of the nodes and edges. In 1947, Wiener began to use topological indices to study some physico-chemical properties of alkanes, thus giving rise to chemical graph theory [36]. In fact, since then, several topological indices have been introduced and extensively studied to better understand the molecular structure [17, 25, 32]. In particular, Sombor index was recently introduced by Gutman in [12]. Recent papers about Sombor index can be found in [2–5, 19, 20]. Also, Sombor index has several generalizations in the papers [10, 13, 24]. Nowadays, the characterization of molecular structures through topological indices remains a key focus of chemical graph theory, which plays a crucial role in designing molecules with specific physico-chemical or biological properties.

Many important topological indices, specifically degree-based indices, can be defined as

$$TI(G) = \sum_{vu \in E(G)} h(d_v, d_u), \tag{1.1}$$

where h is some function with the property $h(x,y) = h(y,x)$ for $x, y \in \{1, 2, \dots\}$ and d_v is the degree of a node v. In the rest of the manuscript, we will denote $h(x,y)$ as $h_{x,y}$.

In the field of random chains analysis, topological indices have been an evolving research topic for the past two decades [31]. Multiple topological indices have been analyzed for different random chains, such as, random cyclooctane chains ([28],[37]), random polyphenyl chains ([29],[16]), random phenylene chains ([27], [26]), random spiro chains ([15],[35]) and random hexagonal chains ([6],[8]). In the same vein, in [38], Definition 2.1, introduced the concept of a general random chain. In this paper, we adopt this definition with slight modifications.

Definition 1. We say that a graph H is a random chain generated by a graph G if the following conditions hold: H contains $n \in \mathbb{N}$ copies of G (so, we can denote H as G_n), any two copies of G are either adjacent (i.e., they are attached in certain way) or non-adjacent and the adjacent copies induce a path of n vertices. The construction of such a random chain can proceed as follows:

(a) $G_1 = G$ and G_2 consists of two copies of G attached in a specific manner.

(b) For each $n > 2$, G_n is constructed by attaching one copy of G to the last copy of G in G_{n-1} in m ($m \geq 1$) specific ways, resulting in the graphs $G_n^1, G_n^2, \dots, G_n^m$ with probabilities $p_1, p_2, \dots, p_m$ respectively, where $p_i > 0$ and $\sum_{i=1}^m p_i = 1$.

Hence, from now on, we will denote G_n as $G(n, p_1, p_2, \dots, p_m)$.

In addition, the article [38] focused on establishing the distributions of Sombor indices in a general random chain, where explicit analytical expressions for the expected values and variances were derived. Note that, $G(n, p_1, p_2, \dots, p_m)$ is constructed by a zero-order Markov process ($0MP$). At this point, it is important to highligth that random chains play crucial roles in chemistry and material science due to their

unique structural and chemical properties. They are widely used in applications such as conducting polymers, organic electronics, elastomer design, and biocompatible materials ([21],[22]).

Given a random chain, let L_i denote the link (attachment) selected at time $i \geq 2$, specifically, L_2 represents the initial link, and for $i \geq 3$, L_i is a random variable with range $\{1, 2, \ldots, m\}$ where, $p_j = \mathbb{P}(L_i = j)$. For us, a random chain generated by a graph G is referred to as a $0MP$-random chain with respect to a topological index TI, if for all $n \geq 3$

$$TI(G(n, p_1, p_2, \ldots, p_m)) - TI(G(n-1, p_1, p_2, \ldots, p_m)) = g(L_n),$$

where $g : \{1, 2, \ldots, m\} \to \mathbb{R}$. In simple terms, for all $n \geq 3$, the change in the calculation of the topological index from time $n - 1$ to n depends solely on the last link, making it independent of the links selected in previous steps.

The primary goal of this manuscript is to derive explicit formulas for the expected value, variance, and asymptotic distribution of a $0MP$-random chain concerning the topological indices defined in Equation (1.1). Furthermore, we show that several well-known random chains, including random phenylene, random polyphenyl, random cyclooctane, and linear chains, fit within this framework, which also allows us to use the same methodology to study the deterministic versions of these chains. As a result, various topological indices are examined for these structures, with several known results emerging as corollaries.

2. Main Result

In this section, we state and prove our main result. First, let $n \geq 2$ and consider the following notation: $TI_n := TI(G(n, p_1, p_2, \ldots, p_m))$, $\alpha := \mathbb{E}(g(X))$ and $\beta := \mathbb{V}(g(X))$, where $X \sim L_i$ for $i \geq 3$. Here, when $m \geq 2$, we use $G(n, p_1, p_2, \ldots, p_{m-1})$ instead of $G(n, p_1, p_2, \ldots, p_m)$ since $\sum_{i=1}^{m} p_i = 1$.

Theorem 1. *Given a $0MP$-random chain with respect to a topological index TI, for $n \geq 2$, we have*

(a) $\mathbb{E}(TI_n) = TI_2 + \alpha(n - 2)$.

(b) $V(TI_n) = \beta(n - 2)$.

(c) As $n \to \infty$, $\frac{TI_n - \alpha n}{\sqrt{\beta n}} \xrightarrow{D} N(0, 1)$.

(d) As $n \to \infty$, $\frac{TI_n}{n} \xrightarrow{a.s} \alpha$.

Proof. It follows by definition that: for all $n \geq 3$,

$$TI_n - TI_{n-1} = g(L_n), \tag{2.1}$$

for some $g : \{1, 2, \ldots, m\} \to \mathbb{R}$. At this point, by using the above recursive relation we have that

$$TI_n = TI_2 + \sum_{i=3}^{n} g(L_i),$$

which directly allows us to obtain the expressions for the expectation and the variance. Likewise, since $\{g(L_i)\}_{i \geq 3}$ are independent and identically distributed (Chapter 2, Theorem 10.4. [11]), due to the the Central Limit Theorem, the Strong Law of Large Number and Theorem 11.4. (Chapter 5, [11]) we can verify (c) and (d), respectively.

$\square$

Remark 1. At this point, it is important to emphasize that, given a $0MP$-random chain with respect to a topological index TI, the following equivalence holds: $TI_n = TI_2 + \alpha(n-2)$ for $n \geq 2$ (a deterministic sequence) if and only if $g(1) = g(2) = \cdots = g(m)$; meaning that, the change remains constant throughout. In particular, when $m = 1$ by vacuity the previous equivalence is verified. Finally, note that, $TI_n = TI_2 + a^T \cdot X$, where $a^T = (g(1), g(2), \ldots, g(m))$ and $X = (X_1, X_2, \ldots, X_m)$ is a multinomial random variable with parameters $n - 2$ and $(p_1, p_2, \ldots, p_m)$. In this context, it is useful to point out that, the approximation given in the previous theorem for the convergence in distribution is identical to the one obtained by using the previous representation and the Central Limit Theorem in the case of random vectors [30].

3.   Application to $0MP$-Random Chains

The purpose of this section is to provide examples of $0MP$-random chains with respect to degree-based topological indices. We will build on the results of the previous section and the following corollaries encapsulate these ideas.

Corollary 1. *Let $RPC_n = RPC(n, p_1, p_2)$ be a random phenylene chain with $n \geq 2$ and TI a degree-based topological index. Then*

(a) $TI_n = AX + Bn + C$,

(b) $\mathbb{E}(TI_n) = (Ap_1 + B)n - 2Ap_1 + C$,

(c) $\mathbb{V}(TI_n) = A^2 p_1 (1 - p_1)(n - 2)$,

(d) As $n \to \infty$, $\frac{TI_n - (Ap_1 + B)n}{A\sqrt{p_1(1-p_1)n}} \xrightarrow{D} N(0, 1)$,

(e) As $n \to \infty$, $\frac{TI_n}{n} \xrightarrow{a.s} Ap_1 + B$,

where $A = 2h_{2,3} - h_{2,2} - h_{3,3}$, $B = h_{2,2} + 2h_{2,3} + 5h_{3,3}$, $C = 4h_{2,2} - 6h_{3,3}$ and $X \sim Binomial(n - 2, p_1)$. In particular, given a phenylene chain pc_n containing n hexagons,

$$TI(pc_n) = An_1 + Bn + C,$$

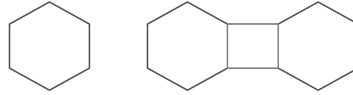*where n_1 represents the number of type-1 links chosen up to the time n.*

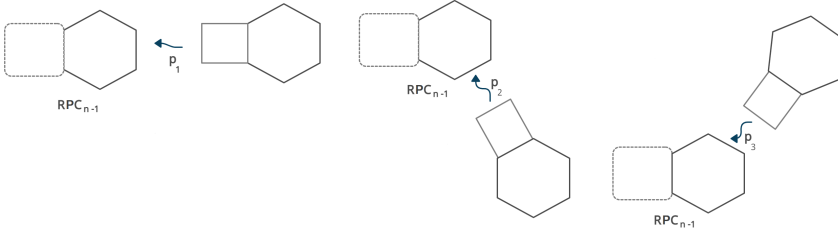**Figure 1.** The graphs of RPC_1 and RPC_2.

Figure 2. RPC_n.

Proof. A random phenylene chain is constructed by the following way: for $n = 1$ and $n = 2$, RPC_n are shown in Figure 1. For $n \geq 3$, the terminal hexagon can be attached in three ways, which results in RPC_n^1, RPC_n^2 and RPC_n^3, respectively, see Figure 2. Given RPC_n, conducting the one-step analysis

$$TI(RPC_n) - TI(RPC_{n-1}) = \sum_{uv \in E_{n,1}} h_n(d_u, d_v) + \sum_{uv \in E_{n,2}} (h_n(d_u, d_v) - h_{n-1}(d_u, d_v)),$$

where $h_k(d_u, d_v) := h(d_u, d_v)$ is calculated within RPC_k, $E_{n,1}$ represents the edges added as we progress from step $n-1$ to n while $E_{n,2}$ are the edges that modify their $h(d_u, d_v)$ during the same transition. By analyzing each sum separately, we find that:

$$\sum_{uv \in E_{n,1}} h_n(d_u, d_v) = 3h_{2,2} + 2h_{2,3} + 3h_{3,3},$$

and

$$\sum_{uv \in E_{n,2}} (h_n(d_u, d_v) - h_{n-1}(d_u, d_v)) = h_{3,3} - 2h_{2,2} + h_{3,3}I_{\{L_n \neq 1\}}$$

$$+ (2h_{2,3} - h_{2,2}) I_{\{L_n = 1\}}.$$

Hence, by definition, a random phenylene chain is a $0MP$-random chain with respect to the degree-based topological index with $g(1) = 4h_{2,3} + 4h_{3,3}$ and $g(2) = g(3) = h_{2,2} + 2h_{2,3} + 5h_{3,3}$. Therefore, by Theorem 1, (b)-(e) have been established. Finally, since $TI_n = TI_2 + (g(1), g(2), g(2)) \cdot X$ for X a multinomial random variable with parameters $n - 2$ and $(p_1, p_2, 1 - p_1 - p_2)$, (a) is completed, and as a consequence, the deterministic formula is proven. □

Corollary 2.   *Let $RPoC_n = RPoC\,(n, p_1, p_2)$ be a random polyphenyl chain with $n \geq 2$ and TI a degree-based topological index. Then*

(a) $TI_n = AX + Bn + C$,

(b) $\mathbb{E}\,(TI_n) = (Ap_1 + B)n - 2Ap_1 + C$,

(c) $\mathbb{V}\,(TI_n) = A^2 p_1\,(1 - p_1)\,(n - 2)$,

(d) As $n \to \infty$, $\dfrac{TI_n - (Ap_1 + B)n}{A\sqrt{p_1(1-p_1)n}} \xrightarrow{D} N(0, 1)$,

(e) As $n \to \infty$, $\dfrac{TI_n}{n} \xrightarrow{a.s} Ap_1 + B$,

where $A = h_{2,2} - 2h_{2,3} + h_{3,3}$, $B = 2h_{2,2} + 4h_{2,3} + h_{3,3}$, $C = 4h_{2,2} - 4h_{2,3} - h_{3,3}$ and $X \sim Binomial(n - 2, p_1)$. Moreover, given a polyphenyl chain poc_n containing n hexagons,

$$TI(poc_n) = An_1 + Bn + C,$$

where n_1 represents the number of type-1 links chosen up to the time n.

Figure 3.   The graphs of $RPoC_1$ and $RPoC_2$.
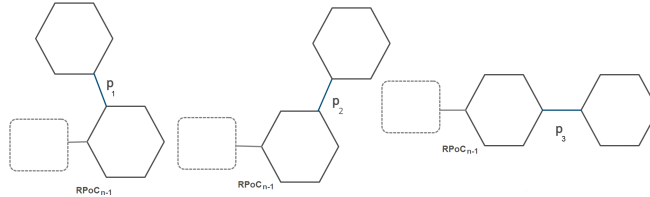

Figure 4. $RPoC_n$.

Proof.   A random polyphenyl chain is constructed as follows: for $n = 1$ and $n = 2$, $RPoC_n$ are illustrated in Figure 3. For $n \geq 3$, the terminal hexagon can be attached in three different ways, resulting in $RPoC_n^1, RPoC_n^2$ and $RPoC_n^3$, respectively, see Figure 4. Following a similar method, we find that a random polyphenyl chain is a $0MP$-random chain with respect to the degree-based topological indices with $g(1) = 2h_{2,2} + 2h_{2,3} + 2h_{3,3}$ and $g(2) = g(3) = 2h_{2,2} + 4h_{2,3} + h_{3,3}$. Therefore, applying the same procedure of the proof of Corollary 1, we complete the proof.   □

Corollary 3.   *Let $RHC_n = RHC\,(n, p_1, p_2)$ be a random hexagonal chain with $n \geq 2$ and TI a degree-based topological index. Then*

(a) $TI_n = AX + Bn + C$,

(b) $\mathbb{E}(TI_n) = (Ap_1 + B)n - 2Ap_1 + C$,

(c) $\mathbb{V}(TI_n) = A^2 p_1 (1 - p_1)(n - 2)$,

(d) As $n \to \infty$, $\frac{TI_n - (Ap_1 + B)n}{A\sqrt{p_1(1-p_1)n}} \xrightarrow{D} N(0, 1)$,

(e) As $n \to \infty$, $\frac{TI_n}{n} \xrightarrow{a.s} Ap_1 + B$,

where $A = -h_{2,2} + 2h_{2,3} - h_{3,3}$, $B = h_{2,2} + 2h_{3,3}$, $C = 4h_{2,2} + 4h_{2,3} - 2h_{3,3}$ and $X \sim Binomial(n - 2, p_1)$. Moreover, given a hexagonal chain hc_n containing n hexagons,

$$TI(hc_n) = An_1 + Bn + C,$$

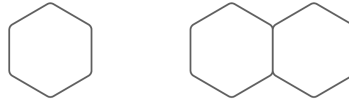where n_1 represents the number of type-1 links chosen up to the time n.

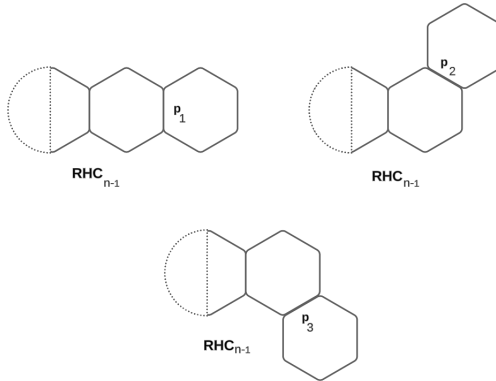**Figure 5.** The graphs of RHC_1 and RHC_2.

Figure 6. RHC_n.

Proof. A random hexagonal chain is constructed by the following way: for $n = 1$ and $n = 2$, RHC_n are shown in Figure 5. For $n \geq 3$, the terminal octagon can be attached in three ways, which results in RHC_n^1 and RHC_n^2 respectively, see Figure 6. By following a similar method, we have that a random hexagonal chain is a $0MP$-random chain with respect to the degree-based topological indices with $g(1) = 2h_{2,3} + h_{3,3}$ and $g(2) = g(3) = h_{2,2} + 2h_{3,3}$. Therefore, applying the same procedure of the proof of Corollary 1, we complete the proof. □

Remark 2. By Remark 1, we know that a degree-based topological index on the above random chains will be deterministic if and only if the corresponding A's are 0; which also is aligned with the expressions found in the previous corollaries. Likewise, since $A_{RHC_n} = A_{RPoC_n} = -A_{RPC_n}$, it follows that: a fixed degree-based topological index is deterministic for RHC_n, $RPoC_n$ and RPC_n if and only if

$$h_{2,2} + h_{3,3} = 2h_{2,3}. \tag{3.1}$$

In particular, when $h(x,y) = x^a + y^a$ with $a \in \mathbb{R}$, i.e., we are working with the Generalized Zagreb Index, Equation (3.1) holds. Remember that, $TI_n = Bn + C = \sum_{v \in V(G)} (d_v)^{a+1}$, due to the identity [7]

$$\sum_{vu \in E(G)} (d_v)^a + (d_u)^a = \sum_{v \in V(G)} (d_v)^{a+1}.$$

It is worth noting that a similar argument may be used to demonstrate that random cyclooctane and random spiro chains [35] are also $0MP$-random chains with respect to the degree-based topological indices.

Remark 3. Given the definition of a $0MP$-random chain with respect to a topological index (TI), analyzing the extreme values of the function g, which is determined by the recursive formula (2.1), could enables us to identify the extreme values of the topological index over the random chains with a fixed n. The analysis of the previously studied random chains ultimately reduces to a comparison between $g(1)$ and $g(2)$. If $g(1) < g(2)$, then the minimum and maximum values of TI_n are achieved in Ch_1 and $Ch_{2,3}$, respectively. Conversely, if $g(1) > g(2)$, the minimum and maximum values of TI_n are attained in $Ch_{2,3}$ and Ch_1, respectively. Here, given a fixed n, Ch_1 denotes the chain where all the selected links are of type-1, while $Ch_{2,3}$ represents any chain where none of the selected links are of type-1.

The authors in works such as ([1], [23], [18], [14], [9]) examined several well-known topological indices within the context of a polyomino chain. A random polyomino chain at time $n \geq 1$ denoted as $RSC_n = RSC(n, p_1)$ can be constructed as follows: for $n = 1$ and $n = 2$, the configurations of RSC_n are illustrated in Figure 7. For $n \geq 3$, the terminal square can be attached in two ways, resulting in RSC_n^1 and RSC_n^2 respectively, see Figure 8. If $L_n = 2$ for all $n \geq 3$ then $RSC_n = Z_n$ (a zigzag chain) whereas if $L_n = 1$ for all $n \geq 3$ then $RSC_n = Li_n$ (a linear chain). Note that, in general, a random polyomino chain is not a $0MP$-random chain with respect to any degree-based topological index. For example, the change between $R(Z_2)$ and $R(Z_3)$ differs from the change between $R(Z_4)$ and $R(Z_5)$ where R represents the Randić index. In contrast, a linear chain is classified as a $0MP$-random chain concerning degree-based topological indices, so, we can directly obtain the next corollary, which is aligned with Remark 1. By the way, both zigzag and linear chains represent examples of general random chains with $m = 1$; however, while linear chain qualifies as a $0MP$-random chain regarding degree-based topological indices, zigzag chain does not.
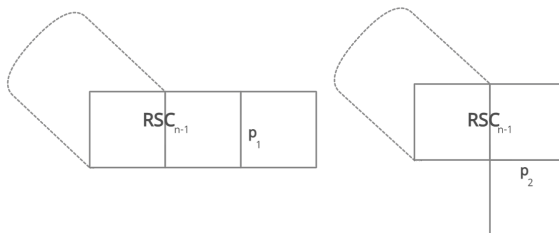
Figure 7. The graphs of RSC_1 and RSC_2.

Figure 8. RSC_n.

Corollary 4. *Let Li_n be a linear chain with $n \geq 2$. Then*

$$TI_n = An + B,$$

where $A = 3h_{3,3}$ and $B = 2h_{2,2} + 4h_{2,3} - 5h_{3,3}$.

Indeed, Corollary 4 is established in [1]. This analysis raises a natural question: Could a similar procedure be applied to specific types of topological indices in random polyomino chains? This question is explored in [33, 34].

Finally, Tables 1, 2, 3, and 4 display the form of the first Zagreb index (M_1), Sombor index (S), harmonic index (H), geometric-arithmetic index (GA), inverse sum indeg index (ISI), and second Zagreb index (M_2) for the random chains analyzed in this section. Note that the results align with Remark 2 for M_1. Additionally, in light of Remark 3, for a fixed n, these tables emphasize the chains where the extreme values of the topological indices are attained. In particular, for these random chains, the extreme values can be directly computed as a consequence of the deterministic part of Corollaries 1, 2, and 3.

By way of summary, in this paper, we present a unified approach to studying degree-based topological indices in general random chains. We have derived the expected value, variance, and distribution of these indices. Additionally, we explored the asymptotic behavior and extreme values of the topological indices. Specifically, we focus on the Sombor, harmonic, geometric-arithmetic, and inverse sum indeg indices for various general random chains, including random phenylene and random polyphenyl. Finally, we believe the proposed method could be utilized in future research to explore additional properties of both similar and distinct random chains, extending its application to a wider variety of topological indices beyond those solely dependent on degree.

TI	RPC_n
M_1	(0,44,-20)
S	(0.14,31.25,-14.4) [38], $(RPC(Ch_1), RPC(Ch_{2,3}))$
H	(-1/30,89/30,0) [27], $(RPC(Ch_{2,3}), RPC(Ch_1))$
GA	$(-0.04, 7.96, -2)$, $(RPC(Ch_1), RPC(Ch_{2,3}))$ [26]
ISI	(-0.1,10.9,-5), $(RPC(Ch_1), RPC(Ch_{2,3}))$
M_2	(-1,61,-38), $(RPC(Ch_1), RPC(Ch_{2,3}))$

Table 1. The relevant information associated with each topological index on RPC_n is presented in the structure $\approx (A, B, C)$. The minimum and maximum values are respectively given in an ordered pair.

TI	$RPoC_n$
M_1	(0, 34, -10)
S	(-0.14, 24.32, -7.35) [38], [29], $(RPoC(Ch_1), RPoC(Ch_{2,3}))$
H	(0.03,2.93,0.07), $(RPoC(Ch_{2,3}), RPoC(Ch_1))$
GA	$(2 - 4\sqrt{6}/5, 3 + 8\sqrt{6}/5, 3 - 8\sqrt{6}/5)$ [16], $(RPoC(Ch_{2,3}), RPoC(Ch_1))$
ISI	(0.1,8.3,-2.3), $(RPoC(Ch_{2,3}), RPoC(Ch_1))$
M_2	(1,41,-17), $(RPoC(Ch_{2,3}), RPoC(Ch_1))$

Table 2. The relevant information associated with each topological index on $RPoC_n$ is presented in the structure $\approx (A, B, C)$. The minimum and maximum values are respectively given in an ordered pair.

TI	Li_n
M_1	(18,-2) [23], [18]
S	(12.73,-1.13)
H	(1,14/15) [23], [18]
GA	$(3, \frac{8\sqrt{6}}{5} - 3)$ [23]
ISI	(4.5,-0.7) [23], [18]
M_2	(27,-13) [23], [18]

Table 3. The information of interest associated with each topological index on Li_n is exposed with the structure $\approx (A, B)$.

TI	RHC_n
M_1	(0,16,24)
S	(0.14, 11.31, 17.25), $(RHC(Ch_{2,3}), RHC(Ch_1))$ [8]
H	(-0.03, 1.167, 2.93), $(RHC(Ch_1), RHC(Ch_{2,3}))$
GA	(-0.04, 3, 5.92), $(RHC(Ch_1), RHC(Ch_{2,3}))$
ISI	(-0.1, 4, 5.8), $(RHC(Ch_1), RHC(Ch_{2,3}))$
M_2	(-1,22,22), $(RHC(Ch_1), RHC(Ch_{2,3}))$

Table 4. The relevant information associated with each topological index on RHC_n is presented in the structure $\approx (A, B, C)$. The minimum and maximum values are respectively given in an ordered pair.

Conflict of Interest: The authors declare that they have no conflict of interest.

Data Availability: Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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