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Expected Values of Some Molecular Descriptors in Random Cyclooctane Chains

Zahid Raza [1,*] and Muhammad Imran [2,*]

[1] Department of Mathematics, College of Sciences, University of Sharjah, Sharjah 27272, United Arab Emirates
[2] Department of Mathematical Science, United Arab Emirates University, Al Ain 15551, United Arab Emirates
* Correspondence: zraza@sharjah.ac.ae (Z.R.); m.imran658@uaeu.ac.ae (M.I.)

Abstract: The modified second Zagreb index, symmetric difference index, inverse symmetric index, and augmented Zagreb index are among the molecular descriptors which have good correlations with some physicochemical properties (such as formation heat, total surface area, etc.) of chemical compounds. By a random cyclooctane chain, we mean a molecular graph of a saturated hydrocarbon containing at least two rings such that all rings are cyclooctane, every ring is joint with at most two other rings through a single bond, and exactly two rings are joint with one other ring. In this article, our main purpose is to determine the expected values of the aforementioned molecular descriptors of random cyclooctane chains explicitly. We also make comparisons in the form of explicit formulae and numerical tables consisting of the expected values of the considered descriptors of random cyclooctane chains. Moreover, we outline the graphical profiles of these comparisons among the mentioned descriptors.

Keywords: modified Zagreb index; symmetric difference index; inverse symmetric index; augmented Zagreb index; random cyclooctane chain; cycloalkane; expected values; comparisons; graphical representation

MSC: 05C09; 05C92; 05C90

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Citation: Raza, Z.; Imran, M. Expected Values of Some Molecular Descriptors in Random Cyclooctane Chains. *Symmetry* **2021**, *13*, 2197. https://doi.org/10.3390/sym13112197

Academic Editors: Serge Lawrencenko and Alice Miller

Received: 23 October 2021
Accepted: 12 November 2021
Published: 17 November 2021

1. Introduction

Chemical graph theory is a branch of mathematics which deals with the mathematical modeling of graphs that is also an essential branch of theoretical chemistry. Initial chemical research introduced the theory of chemical graphs. Chemists have confirmed that the physicochemical properties of a compound have been associated with molecular arrangement, with results derived from an enormous number of investigational data. Furthermore, the researchers considered the same topological index based on various chemical properties and applied it to QSR/QSPR learning. Generally, the features of a compound derived by chemical experiments are not very authentic. However, theoretical calculations assume a vital role in many extraordinary cases. There are numerous topological indices in the literature of chemical graph theory. The first of its kind is the Wiener index [1]. After that, the most important topological index is the class of the Zagreb indices and its variants [2]. The family of Adriatic indices was introduced in [3–6]. An especially interesting subclass of these descriptors consists of 148 discrete Adriatic indices. The so-called inverse sum indeg index (ISI) was defined in [4] as a significant predictor of the total surface area of octane isomers. A graph consists of some points (nodes) and lines (edges). Suppose $\Gamma = \Gamma(V, E)$ is a graph of order n with vertex set $V(\Gamma) = \{u_1, u_2, \ldots, u_n\}$ and edge set E. Let u_i be the node of a graph. Then, the degree of a node is the number of edges incident to that vertex and is denoted by d_i. If an edge connects a vertex of degree i and a vertex of degree j in Γ, then we call it an (i, j)-edge. Let $x_{ij}(\Gamma)$ denote the number of (i, j)-edges in the graph Γ.

$$AZI(\Gamma) = \sum_{u_i u_j \in E(\Gamma)} \left(\frac{d_i d_j}{d_i + d_j - 2}\right)^3 \tag{1}$$

$$ISI(\Gamma) = \sum_{u_i u_j \in E(\Gamma)} \frac{d_i d_j}{d_i + d_j} \tag{2}$$

$$SDD(\Gamma) = \sum_{u_i u_j \in E(\Gamma)} \frac{d_i^2 + d_j^2}{d_i d_j} \tag{3}$$

$$aM_2(\Gamma) = \sum_{u_i u_j \in E(\Gamma)} \frac{1}{d_i d_j} \tag{4}$$

Significant efforts have been made to give an explicit formula for the topological indices for a special family of graphs or chemical graphs; see for example the recent papers [7,8].

2. Materials and Methods

A cyclooctane chain is when every node of a cyclooctane system is in an octagon. We obtain a cyclooctane chain by composing an edge joining octagons. Figure 1 shows the unique $\mathcal{RCOC}_m$ for $m = 1, 2$, and Figure 2 shows four $\mathcal{RCOC}_m$ chains for $m = 3$. We termed $\mathcal{RCOC}^1_{m+1}$, $\mathcal{RCOC}^2_{m+1}$, $\mathcal{RCOC}^3_{m+1}$, and $\mathcal{RCOC}^4_{m+1}$ by local adjustment of the cyclooctane chains (see Figure 3). Therefore, $\mathcal{RCOC}_(m; \rho_1, \rho_2, \rho_3)$ can be attained by stepwise addition of a terminal octagon. A random selection $(k = 3, 4, \ldots, m)$ is made at each step from one of the four probable structures:

(i) $\mathcal{RCOC}_{k-1} \to \mathcal{RCOC}^1_k$ with probability ρ_1,
(ii) $\mathcal{RCOC}_{k-1} \to \mathcal{RCOC}^2_k$ with probability ρ_2,
(iii) $\mathcal{RCOC}_{k-1} \to \mathcal{RCOC}^2_k$ with probability ρ_3, or
(iv) $\mathcal{RCOC}_{k-1} \to \mathcal{RCOC}^3_k$ with probability $r = 1 - \rho_1 - \rho_2 - \rho_3$.

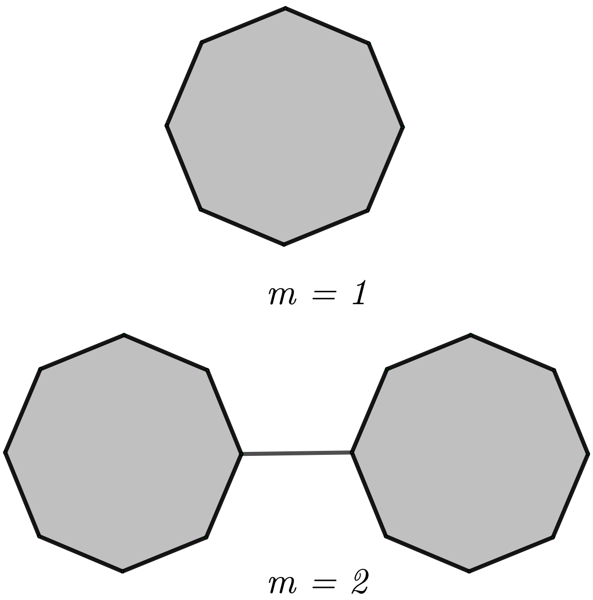

Figure 1. The cyclooctane chains for $m = 1, 2$.

A process is a zeroth-order Markov process if the probabilities ρ_1, ρ_2, ρ_3 are unvarying in step parameter and steady. Several papers are concentrated about random arrangement of graphs. For more details, see [9–15]. The comparison and inequalities among some indices for molecular graphs have been derived in [16,17]. Around one decade before, the coindex versions of these Zagreb indices were introduced. First, two extremum Zagreb indices and coindices of chemical trees were considered in [18]. In degree-based topological indices, many indices depend on the vertex degree of the molecular graph. Some degree-based topological indices are described for pentagonal chains [19]. Bond incident degree (BID) indices for some nanostructures [20,21], tree-like polyphenylene systems, spiro hexagonal systems and polyphenylene dendrimer nanostars [22] are bounds for the general sum-connectivity index of composite graphs [23]. Some vertex-degree-based topological indices are of cacti [24,25]. The Wiener indices of random benzenoid chain was considered by Gutman et al. [26,27]. In 2012, random polyphenyl chains were studied by Yang and Zhang [28].

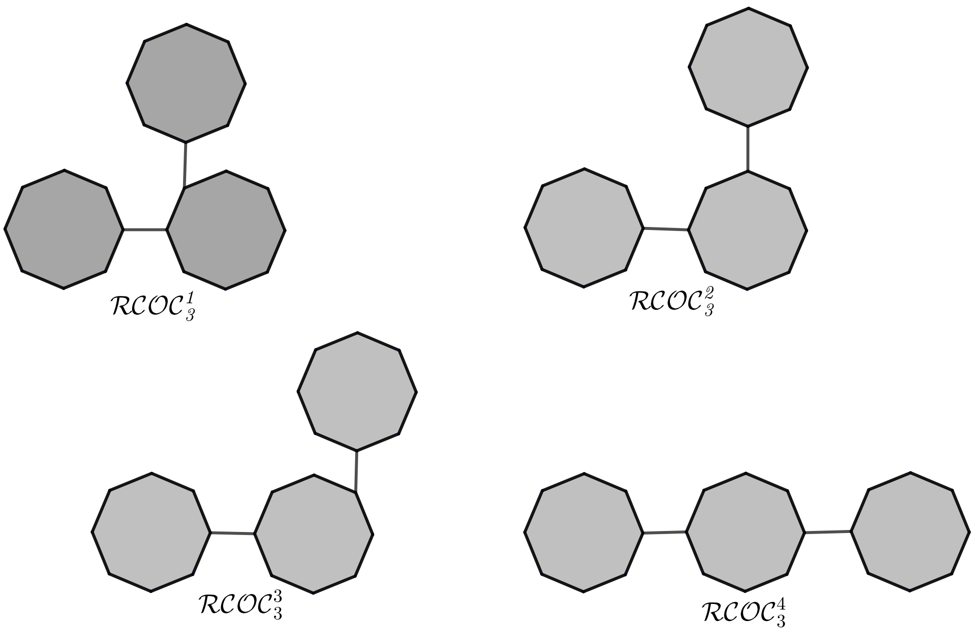

Figure 2. The four types of cyclooctane chains for $m = 3$.

A number of papers are attentive regarding the random arrangement of topological indices [29]. Cyclooctanes are a kind of saturated hydrocarbons. For many years, chemists have paid a lot of attention to their derivatives [30–33]. These derivatives are seen and used in drug synthesis, combustion kinetics, organic synthesis, etc. For example, the osmium-catalysed bis-dihydroxylation of 1,5-cyclooctadiene has utilized cyclooctane $1, 2, 5, 6$ tetrol [33]. Alamdari et al. [30] considered the combination of some cyclooctane-based quinoxaline pyrazines. These molecular-like graphs [34,35] are geometric graphs (finite two-connected) bounded by a quadrangles of side length one and a regular octagon.

Note that a class of polycyclic conjugated hydrocarbons with tree-like octagonal systems is represented in [34]. Some mathematicians were attracted by octagonal graphs [36]. The numbers of isomers in tree-like octagonal graphs were expressed by Brunvoll et al. [34]. Yang and Zhao [35] studied the relationship among the numbers in a class of Hosoya index of the caterpillar trees and octagonal graphs.

In this work, we study the expected values of the modified Zagreb, symmetric difference, inverse symmetric, and augmented Zagreb indices in random cyclooctane chain. Furthermore, we give analytic proofs for comparison, along with numerical and graphical profiles of these indices in a random cyclooctane chain.

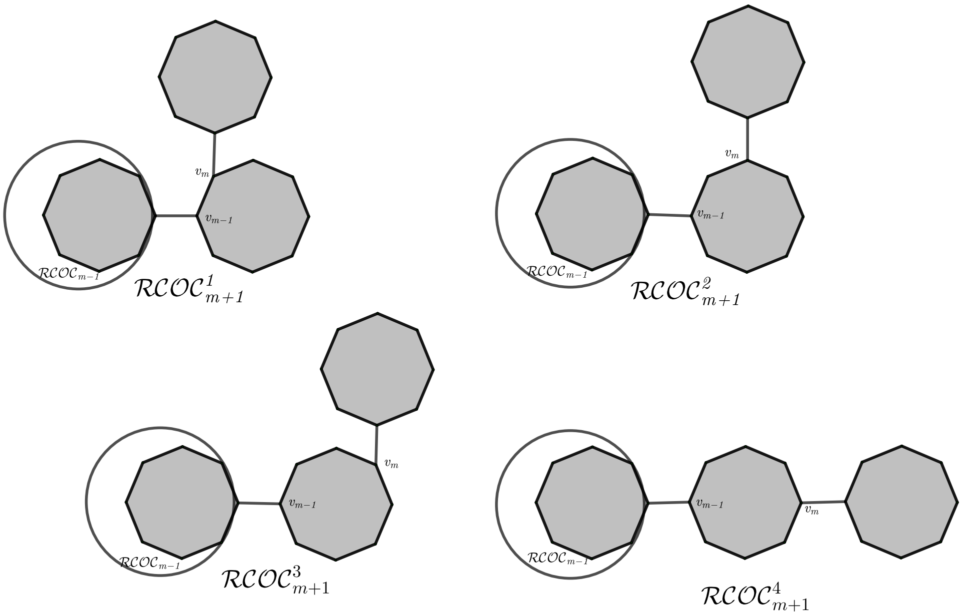

Figure 3. The four types of local arrangements in cyclooctane for $m > 3$.

Here, let us examine the modified Zagreb index, symmetric difference index, inverse symmetric index, and augmented Zagreb index in the chain $\mathcal{RCOC}_m$ with m octagons. Consider $\mathcal{RCOC}_m$ to be the cyclooctane chain obtained from $\mathcal{RCOC}_{m-1}$, as shown in Figure 3. It is easy to see from the structure of the chain $\mathcal{RCOC}_m$ that it contains only $(2,2)$, $(2,3)$, and $(3,3)$-types of edges. Therefore, to calculate these indices for the chain $\mathcal{RCOC}_m$, we need to determine only its edges of types $x_{22}(\mathcal{RCOC}_m)$, $x_{23}(\mathcal{RCOC}_m)$ and $x_{33}(\mathcal{RCOC}_m)$. Hence, from Equations (1)–(4), one can write as:

$$AZI(\mathcal{RCOC}_m) = 8x_{22}(\mathcal{RCOC}_m) + 8x_{23}(\mathcal{RCOC}_m) + \frac{729}{64}x_{33}(\mathcal{RCOC}_m). \tag{5}$$

$$ISI(\mathcal{RCOC}_m) = x_{22}(\mathcal{RCOC}_m) + \frac{6}{5}x_{23}(\mathcal{RCOC}_m) + \frac{3}{2}x_{33}(\mathcal{RCOC}_m). \tag{6}$$

$$SDD(\mathcal{RCOC}_m) = 2x_{22}(\mathcal{RCOC}_m) + \frac{13}{6}x_{23}(\mathcal{RCOC}_m) + 2x_{33}(\mathcal{RCOC}_m). \tag{7}$$

$$aM_2(\mathcal{RCOC}_m) = \frac{1}{4}x_{22}(\mathcal{RCOC}_m) + \frac{1}{6}x_{23}(\mathcal{RCOC}_m) + \frac{1}{9}x_{33}(\mathcal{RCOC}_m). \tag{8}$$

3. Results

Notice that $\mathcal{RCOC}_m$ is a random cyclooctane chain due to its local arrangements. Therefore, $AZI(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))$, $aM_2(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))$, $ISI(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))$ and $SDD(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))$ are the random variables. Now, we will calculate the expected values of these indices in $\mathcal{RCOC}_m$, and denote these as $E^{AZI}_m = E[AZI(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))]$, $E^{aM_2}_m = E[aM_2(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))]$, $E^{ISI}_m = E[ISI(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))]$, $E^{SDD}_m = E[SDD(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))]$, respectively.

Theorem 1. *Let $m \geq 2$ and a random cyclooctane chain $\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3)$. Then*

$$E^{AZI}_m = \frac{m}{64}(4825 + 217\rho_1) - \rho_1\frac{217}{32} - \frac{729}{64}.$$

Proof. Since $E^{AZI}_2 = \frac{8921}{64}$ is correct, then for $m \geq 3$, there are 4 types of probabilities (see Figure 3).

(a). If $\mathcal{RCOC}_{m-1} \to \mathcal{RCOC}^1_m$ with probability ρ_1
$x_{22}(\mathcal{RCOC}^1_m) = x_{22}(\mathcal{RCOC}_{m-1}) + 5$, $x_{23}(\mathcal{RCOC}^1_m) = x_{23}(\mathcal{RCOC}_{m-1}) + 2$ and

$x_{33}(\mathcal{RCOC}_m^1) = x_{33}(\mathcal{RCOC}_{m-1}) + 2$, and from (5), we have
$AZI(\mathcal{RCOC}_m^1) = AZI(\mathcal{RCOC}_{m-1}) + \frac{2521}{32}$.

(b). If $\mathcal{RCOC}_{m-1} \to \mathcal{RCOC}_m^2$ with probability ρ_2, then
$x_{22}(\mathcal{RCOC}_m^2) = x_{22}(\mathcal{RCOC}_{m-1}) + 4, x_{23}(\mathcal{RCOC}_m^2) = x_{23}(\mathcal{RCOC}_{m-1}) + 4$ and
$x_{33}(\mathcal{RCOC}_m^2) = x_{33}(\mathcal{RCOC}_{m-1}) + 1$, and from (5), we have
$AZI(\mathcal{RCOC}_m^2) = AZI(\mathcal{RCOC}_{m-1}) + \frac{4825}{64}$.

(c). If $\mathcal{RCOC}_{m-1} \to \mathcal{RCOC}_m^2$ with probability ρ_3, then
$x_{22}(\mathcal{RCOC}_m^3) = x_{22}(\mathcal{RCOC}_{m-1}) + 4, x_{23}(\mathcal{RCOC}_m^3) = x_{23}(\mathcal{RCOC}_{m-1}) + 4$ and
$x_{33}(\mathcal{RCOC}_m^3) = x_{33}(\mathcal{RCOC}_{m-1}) + 1$, and from (5), we have
$AZI(\mathcal{RCOC}_m^2) = AZI(\mathcal{RCOC}_{m-1}) + \frac{4825}{64}$.

(d). If $\mathcal{RCOC}_{m-1} \to \mathcal{RCOC}_m^3$ with probability $1-\rho_1-\rho_2-\rho_3$, then
$x_{22}(\mathcal{RCOC}_m^4) = x_{22}(\mathcal{RCOC}_{m-1}) + 4, x_{23}(\mathcal{RCOC}_m^4) = x_{23}(\mathcal{RCOC}_{m-1}) + 4$ and
$x_{33}(\mathcal{RCOC}_m^4) = x_{33}(\mathcal{RCOC}_{m-1}) + 1$, and from (5), we have
$AZI(\mathcal{RCOC}_m^3) = AZI(\mathcal{RCOC}_{m-1}) + \frac{4825}{64}$.

Thus, we obtain

$$\begin{aligned} E_m^{AZI} &= \rho_1 AZI(\mathcal{RCOC}_m^1) + \rho_2 AZI(\mathcal{RCOC}_m^2) + \rho_3 AZI(\mathcal{RCOC}_m^3) \\ &+ (1-\rho_1-\rho_2-\rho_3)AZI(\mathcal{RCOC}_m^4) \\ &= \rho_1[AZI(\mathcal{RCOC}_m + \frac{2521}{32})] + \rho_2[AZI(\mathcal{RCOC}_m + \frac{4825}{64})] \\ &+ \rho_3[AZI(\mathcal{RCOC}_m + \frac{4825}{64})] + (1-\rho_1-\rho_2-\rho_3)[AZI(\mathcal{RCOC}_m) + \frac{4825}{64}] \\ &= AZI(\mathcal{RCOC}_{m-1}) + \rho_1\frac{217}{64} + \frac{4825}{64}. \end{aligned}$$

$$E_m^{AZI} = AZI(\mathcal{RCOC}_{m-1}) + \rho_1\frac{217}{64} + \frac{4825}{64}. \tag{9}$$

However, $E[E_m^{AZI}] = E_m^{AZI}$; thus, applying the operator E on (9), we obtain

$$E_m^{AZI} = E_{m-1}^{AZI} + \rho_1\frac{217}{64} + \frac{4825}{64}, \quad m > 2, \tag{10}$$

and by the recurrence relation (10) using initial conditions, we get

$$E_m^{AZI} = \frac{m}{64}(4825 + 217\rho_1) - \rho_1\frac{217}{32} - \frac{729}{64}.$$

□

Theorem 2. *Let $m \geq 2$ and a random cyclooctane chain $\mathcal{RCOC}(m; \rho_1, \rho_2, \rho_3)$. Then*

$$E_m^{ISI} = \frac{m}{10}(\rho_1 + 103) - \frac{23}{10} - \frac{\rho_1}{5}.$$

Proof. Since $E_2^R = \frac{183}{10}$ is correct, then for $m \geq 3$, there are 4 types of probabilities (see Figure 3).

(a). If $\mathcal{RCOC}_{m-1} \to \mathcal{RCOC}_m^1$ with probability ρ_1
$x_{22}(\mathcal{RCOC}_m^1) = x_{22}(\mathcal{RCOC}_{m-1}) + 5, x_{23}(\mathcal{RCOC}_m^1) = x_{23}(\mathcal{RCOC}_{m-1}) + 2$ and
$x_{33}(\mathcal{RCOC}_m^1) = x_{33}(\mathcal{RCOC}_{m-1}) + 2$, and from (6), we have
$ISI(\mathcal{RCOC}_m^1) = ISI(\mathcal{RCOC}_{m-1}) + \frac{52}{5}$.

(b). If $\mathcal{RCOC}_{m-1} \to \mathcal{RCOC}_m^2$ with probability ρ_2, then
$x_{22}(\mathcal{RCOC}_m^2) = x_{22}(\mathcal{RCOC}_{m-1}) + 4, x_{23}(\mathcal{RCOC}_m^2) = x_{23}(\mathcal{RCOC}_{m-1}) + 4$ and
$x_{33}(\mathcal{RCOC}_m^2) = x_{33}(\mathcal{RCOC}_{m-1}) + 1$, and from (6), we have
$ISI(\mathcal{RCOC}_m^2) = ISI(\mathcal{RCOC}_{m-1}) + \frac{103}{10}$.

(c). If $\mathcal{RCOC}_{m-1} \rightarrow \mathcal{RCOC}_m^2$ with probability ρ_3, then
$x_{22}(\mathcal{RCOC}_m^3) = x_{22}(\mathcal{RCOC}_{m-1}) + 4, x_{23}(\mathcal{RCOC}_m^3) = x_{23}(\mathcal{RCOC}_{m-1}) + 4$ and
$x_{33}(\mathcal{RCOC}_m^3) = x_{33}(\mathcal{RCOC}_{m-1}) + 1$, and from (6), we have
$ISI(\mathcal{RCOC}_m^2) = ISI(\mathcal{RCOC}_{m-1}) + \frac{103}{10}$.

(d). If $\mathcal{RCOC}_{m-1} \rightarrow \mathcal{RCOC}_m^3$ with probability $1 - \rho_1 - \rho_2 - \rho_3$, then
$x_{22}(\mathcal{RCOC}_m^4) = x_{22}(\mathcal{RCOC}_{m-1}) + 4, x_{23}(\mathcal{RCOC}_m^4) = x_{23}(\mathcal{RCOC}_{m-1}) + 4$ and
$x_{33}(\mathcal{RCOC}_m^4) = x_{33}(\mathcal{RCOC}_{m-1}) + 1$, and from (6), we have
$ISI(\mathcal{RCOC}_m^3) = ISI(\mathcal{RCOC}_{m-1}) + \frac{103}{10}$.

Thus, we get

$$\begin{aligned}
E_m^{ISI} &= \rho_1 ISI(\mathcal{RCOC}_m^1) + \rho_2 ISI(\mathcal{RCOC}_m^2) + \rho_3 ISI(\mathcal{RCOC}_m^3) \\
&+ (1 - \rho_1 - \rho_2 - \rho_3) ISI(\mathcal{RCOC}_m^4) \\
&= \rho_1[ISI(\mathcal{RCOC}_m) + \frac{52}{5}] + \rho_2[ISI(\mathcal{RCOC}_m)) + \frac{103}{10}] \\
&+ \rho_3[ISI(\mathcal{RCOC}_m) + \frac{103}{10}] + (1 - \rho_1 - \rho_2 - \rho_3)[ISI(\mathcal{RCOC}_m)) + \frac{103}{10}]
\end{aligned}$$

$$E_m^{ISI} = ISI(\mathcal{RCOC}_{m-1}) + \rho_1 \frac{1}{10} + \frac{103}{10}. \tag{11}$$

However, $E[E_m]^H = E_m^H$; thus, applying the operator E on (11), we obtain

$$E_m^{ISI} = E_{m-1}^{ISI} + \rho_1 \frac{1}{10} + \frac{103}{10}. \quad m > 2, \tag{12}$$

and by the recurrence relation (12) using initial conditions, we get

$$E_m^{ISI} = \frac{m}{10}(\rho_1 + 103) - \frac{23}{10} - \rho_1 \frac{1}{5}.$$

□

Theorem 3. *Let $m \geq 2$ and a random cyclooctane chain $\mathcal{RCOC}(m; \rho_1, \rho_2, \rho_3)$. Then*

$$E_m^{SDD} = \frac{1}{3}[m(56 - \rho_1) + 2\rho_1 - 8].$$

Proof. Since $E_2^R = \frac{104}{3}$ is correct, then for $m \geq 3$, there are 4 types of probabilities (see Figure 3). Thus, from (7) we get the following:

$$\begin{aligned}
E_m^{SDD} &= \rho_1 SDD(\mathcal{RCOC}_m^1) + \rho_2 SDD(\mathcal{RCOC}_m^2) + \rho_3 SDD(\mathcal{RCOC}_m^3) \\
&+ (1 - \rho_1 - \rho_2 - \rho_3) SDD(\mathcal{RCOC}_m^4) \\
&= \rho_1[SDD(\mathcal{RCOC}_m) + \frac{55}{3}] + \rho_2[SDD(\mathcal{RCOC}_m)) + \frac{56}{3}] \\
&+ \rho_3[SDD(\mathcal{RCOC}_m) + \frac{56}{3}] + (1 - \rho_1 - \rho_2 - \rho_3)[SDD(\mathcal{RCOC}_m)) + \frac{56}{3}]
\end{aligned}$$

$$E_m^{SDD} = SDD(\mathcal{RCOC}_{m-1}) - \rho_1 \frac{1}{3} + \frac{56}{3}. \tag{13}$$

However, $E[E_m]^{SDD} = E_m^{SDD}$; thus, applying the operator E on (13), we obtain

$$E_m^{SDD} = E_{m-1}^{SDD} - \rho_1 \frac{1}{3} + \frac{56}{3}. \quad m > 2, \tag{14}$$

and by the recurrence relation (16) using initial conditions, we get

$$E_m^{SDD} = \frac{1}{3}[m(56 - \rho_1) + 2\rho_1 - 8].$$

□

Theorem 4. *Let $m \geq 2$ and a random cyclooctane chain $\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3)$. Then*

$$E_m^{aM_2} = m[\frac{16}{9} + \frac{\rho_1}{36}] - \frac{\rho_1}{18} + \frac{2}{9}.$$

Proof. Since $E_2^{aM_2} = \frac{34}{9}$ is correct, then for $m \geq 3$, there are 4 types of probabilities (see Figure 3). Thus, from (8), we get the following:

$$\begin{aligned} E_m^{aM_2} &= \rho_1 aM_2(\mathcal{RCOC}_m^1) + \rho_2 aM_2(\mathcal{RCOC}_m^2) + \rho_3 aM_2(\mathcal{RCOC}_m^3) \\ &+ (1-\rho_1-\rho_2-\rho_3)aM_2(\mathcal{RCOC}_m^4) \\ &= \rho_1[aM_2(\mathcal{RCOC}_m) + \frac{65}{36}] + \rho_2[aM_2(\mathcal{RCOC}_m)) + \frac{16}{9}] \\ &+ \rho_3[aM_2(\mathcal{RCOC}_m) + \frac{16}{9}] + (1-\rho_1-\rho_2-\rho_3)[aM_2(\mathcal{RCOC}_m)) + \frac{16}{9}] \end{aligned}$$

$$E_m^{aM_2} = aM_2(\mathcal{RCOC}_{m-1}) + \rho_1\frac{1}{36} + \frac{16}{9}. \tag{15}$$

However, $E[E_m]^{aM_2} = E_m^{aM_2}$; thus, applying the operator E on (15), we obtain

$$E_m^{aM_2} = E_{m-1}^{aM_2} + \rho_1\frac{1}{36} + \frac{16}{9}. \quad m > 2, \tag{16}$$

and by the recurrence relation (16) using initial conditions, we get

$$E_m^{aM_2} = m[\frac{16}{9} + \frac{\rho_1}{36}] - \frac{\rho_1}{18} + \frac{2}{9}.$$

□

We now turn our attention to the special cyclooctane chains $\mathcal{CO}_m, \mathcal{CZ}_m, \mathcal{CM}_m$ and $\mathcal{CL}_m$, as shown in Figure 4. These chains can also be obtained as $\mathcal{CO}_m = \mathcal{RCOC}(m;1,0,0)$, $\mathcal{CM}_m = \mathcal{RCOC}(m;0,1,0)$, $\mathcal{CZ}_m = \mathcal{RCOC}(m;0,0,1)$, and $\mathcal{CL}_m = \mathcal{RCOC}(m;0,0,0)$. Then, we can easily calculate these indices for these four special chains by using Theorems 1–4.

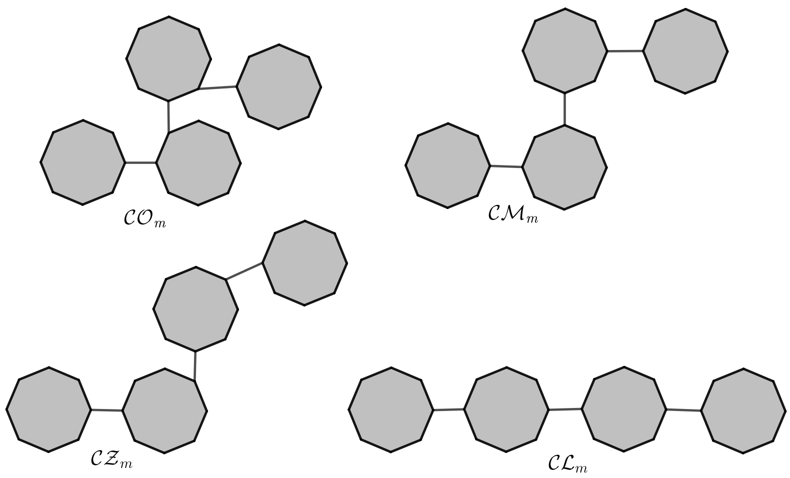

Figure 4. Four special cyclooctain chains with m octagons.

Corollary 1. *For $m \geq 2$, we have the following:*

1. • $AZI(\mathcal{CO}_m) = \frac{2521}{32}m - \frac{1163}{64}.$;
   • $ISI(\mathcal{CO}_m) = \frac{52}{5}m - \frac{5}{2}$;

- $SDD(\mathcal{CO}_m) = \frac{1}{3}[55m - 6]$;
- $aM_2(\mathcal{CO}_m) = \frac{65}{36}m + \frac{1}{6}$.

2.
- $AZI(\mathcal{CZ}_m) = AZI(\mathcal{CL}_m) = AZI(\mathcal{CM}_m) = \frac{1}{64}[4825m - 729]$;
- $ISI(\mathcal{CM}_m) = ISI(\mathcal{CZ}_m) = ISI(\mathcal{CL}_m) = \frac{103}{10}m - \frac{23}{10}.$;
- $SDD(\mathcal{CM}_m) = SDD(\mathcal{CZ}_m) = SDD(\mathcal{CL}_m) = \frac{1}{3}[56m - 8]$;
- $aM_2(\mathcal{CM}_m) = aM_2(\mathcal{CZ}_m) = aM_2(\mathcal{CL}_m) = \frac{1}{9}[16m + 2]$.

4. Discussion and Conclusions

In this section, we are going to provide an expository comparison between the expected values for the modified Zagreb, symmetric difference, inverse symmetric, and augmented Zagreb indices for arbitrary cyclooctane chains with the same probabilities. At that point, the comparison between the expected values of these indices for diverse values of the probability ρ_1 is given in Tables 1–4. The augmented Zagreb index is continuously more noteworthy than the other three indices, specifically the modified Zagreb, symmetric difference, and inverse symmetric indices. The graphical profile of the comparison between two indices is given in Figure 5, which recommends that the augmented Zagreb index is always greater than the symmetric difference index. From Figure 6, one can see that the symmetric difference index is continuously greater than the inverse symmetric index, and Figure 7 proposes that the inverse symmetric index is continuously more prominent than the modified Zagreb index. The graphical profile of the comparison between all four indices is given in Figure 8, which suggests that the augmented Zagreb index is always greater than the other indices.

Table 1. Expected values of indices for $p_1 = 1$.

m	E^{AZI}	E^{SDD}	E^{ISI}	E^{aM_2}
4	296.953125	71.33333333	39.1	7.333333333
5	375.734375	89.66666667	49.5	9.138888889
6	454.515625	108	59.9	10.94444444
7	533.296875	126.3333333	70.3	12.75
8	612.078125	144.6666667	80.7	14.55555556
9	690.859375	163	91.1	16.36111111
10	769.640625	181.3333333	101.5	18.16666667
11	848.421875	199.6666667	111.9	19.97222222
12	927.203125	218	122.3	21.77777778
13	1005.984375	236.3333333	132.7	23.58333333

Table 2. Expected values of indices for $p_1 = 0$.

m	E^{AZI}	E^{SDD}	E^{ISI}	E^{aM_2}
4	290.171875	72	38.9	7.333333333
5	365.5625	90.66666667	49.2	9.111111111
6	440.953125	109.3333333	59.5	10.88888889
7	516.34375	128	69.8	12.66666667
8	591.734375	146.6666667	80.1	14.44444444
9	667.125	165.3333333	90.4	16.22222222
10	742.515625	184	100.7	18
11	817.90625	202.6666667	111	19.77777778
12	893.296875	221.3333333	121.3	21.55555556
13	968.6875	240	131.6	23.33333333

Table 3. Expected values of indices for $p_1 = 1/2$.

m	E^{AZI}	E^{SDD}	E^{ISI}	E^{aM_2}
4	293.5625	71.66666667	39	7.361111111
5	370.6484375	90.16666667	49.35	9.152777778
6	447.734375	108.6666667	59.7	10.94444444
7	524.8203125	127.1666667	70.05	12.73611111
8	601.90625	145.6666667	80.4	14.52777778
9	678.9921875	164.1666667	90.75	16.31944444
10	756.078125	182.6666667	101.1	18.11111111
11	833.1640625	201.1666667	111.45	19.90277778
12	910.25	219.6666667	121.8	21.69444444
13	987.3359375	238.1666667	132.15	23.48611111

Table 4. Expected values of indices for $p_1 = 1/4$.

m	E^{AZI}	E^{SDD}	E^{ISI}	E^{aM_2}
4	291.8671875	71.83333333	38.95	7.347222222
5	368.1054688	90.41666667	49.275	9.131944444
6	444.34375	109	59.6	10.91666667
7	520.5820313	127.5833333	69.925	12.70138889
8	596.8203125	146.1666667	80.25	14.48611111
9	673.0585938	164.75	90.575	16.27083333
10	749.296875	183.3333333	100.9	18.05555556
11	825.5351563	201.9166667	111.225	19.84027778
12	901.7734375	220.5	121.55	21.625
13	978.0117188	239.0833333	131.875	23.40972222

Theorem 5. *If $m \geq 2$, then*

$$E[AZI(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))] > E[SDD(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))].$$

Proof. It is true for $m = 2$. Now, let us solve it for $m > 2$; by using Theorems 1 and 3, we have

$$E[AZI(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))] - E[SDD(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))]$$

$$\begin{aligned} &= \frac{m}{64}(4825+217\rho_1) - \rho_1\frac{217}{32} - \frac{729}{64} \\ &- \frac{1}{3}[m(56-\rho_1)+2\rho_1-8] \\ &= (m-2)[\frac{10891}{192}+\rho_1\frac{715}{192}] + \frac{20107}{192} \\ &= \frac{(m-2)}{192}[10891+715\rho_1] + \frac{20107}{192} \\ &> 0 \qquad \because m > 2 \ and \ 0 \leq \rho_1 \leq 1. \end{aligned}$$

□

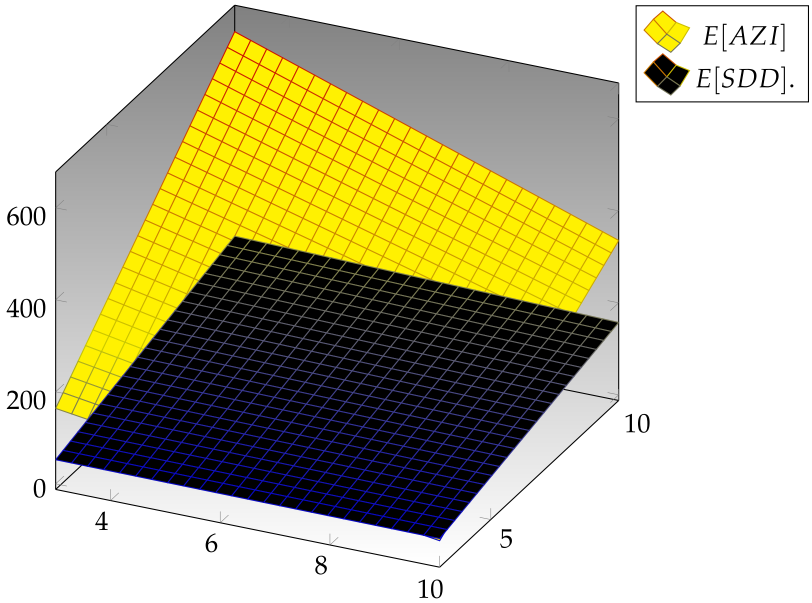

Figure 5. Difference between $E[AZI]$ and $E[SDD]$.

Theorem 6. *If $m \geq 2$, then*

$$E[SDD(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))] > E[ISI(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))].$$

Proof. It is true for $m = 2$. Now, let us solve it for $m > 2$; by using Theorems 2 and 3, we have

$$E[SDD(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))] - E[ISI(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))]$$

$$\begin{aligned}
&= \frac{1}{3}[m(56-\rho_1)+2\rho_1-8] \\
&- [\frac{m}{10}(\rho_1+103)-\frac{23}{10}-\frac{\rho_1}{5}] \\
&= (m-2)[\frac{251}{30}-\rho_1\frac{13}{30}]+\frac{491}{30} \\
&= \frac{(m-2)}{30}[251-13\rho_1]+\frac{491}{30} \\
&> 0 \qquad \because 251-13\rho_1 > 0,\ m > 2 \textit{ and } 0 \leq \rho_1 \leq 1.
\end{aligned}$$

□

Theorem 7. *If $m \geq 2$, then*

$$E[ISI(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))] > E[aM_2(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))].$$

Proof. It is true for $m = 2$. Now, let us solve it for $m > 2$; by using Theorems 3 and 4, we have

$$E[ISI(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))] - E[aM_2(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))]$$

$$
\begin{aligned}
&= \frac{m}{10}(\rho_1 + 103) - \frac{23}{10} - \frac{\rho_1}{5} \\
&- m[\frac{16}{9} + \frac{\rho_1}{36}] + \frac{\rho_1}{18} - \frac{2}{9} \\
&= (m-2)[\frac{767}{90} + \rho_1\frac{13}{180}] + \frac{1307}{90} \\
&= \frac{(m-2)}{180}[1534 + 13\rho_1] + \frac{1307}{90} \\
&> 0 \qquad \because m > 2 \text{ and } 0 \leq \rho_1 \leq 1.
\end{aligned}
$$

□

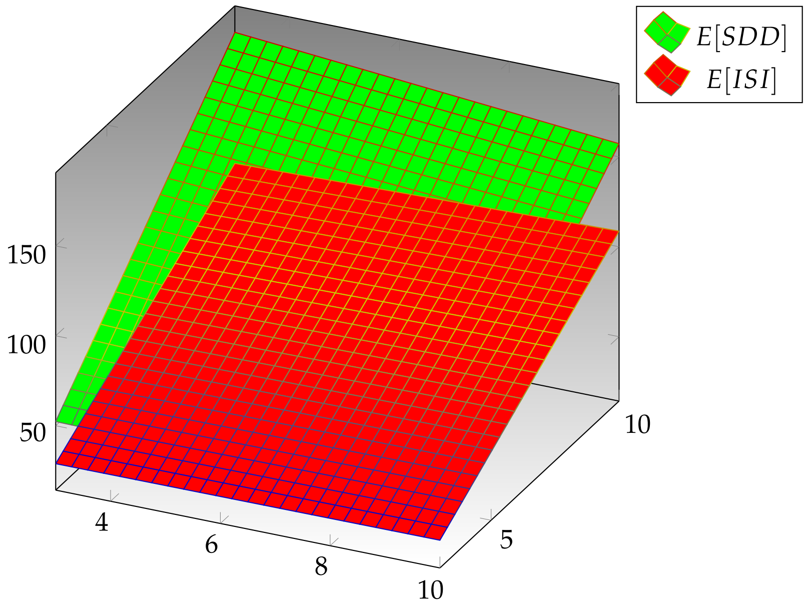

Figure 6. Difference between $E[SDD]$ and $E[ISI]$.

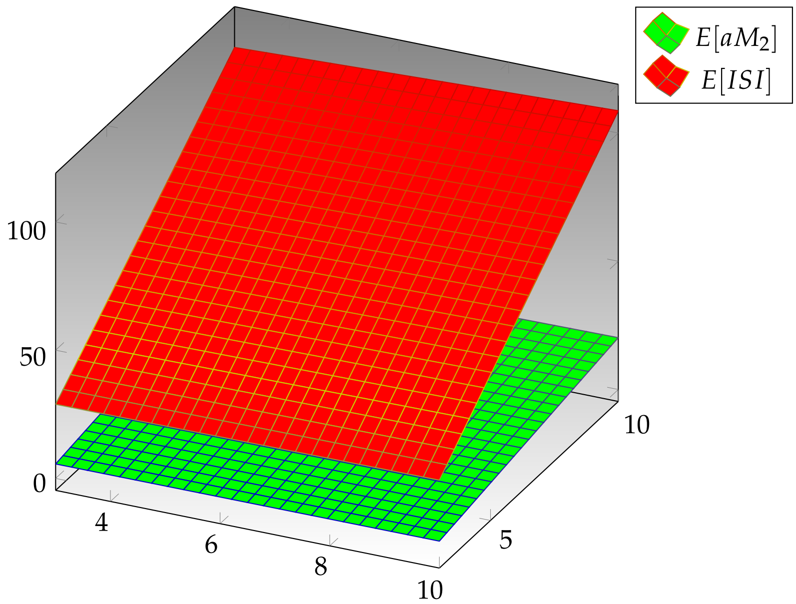

Figure 7. Difference between $E[aM_2]$ and $E[ISI]$.

Theorem 8. *If $m \geq 2$, then*

$$E[AZI(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))] > E[SDD(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))]$$
$$> E[ISI(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))] > E[aM_2(\mathcal{RCOC}(m;\rho_1,\rho_2,\rho_3))].$$

Proof. We may prove this result with the help of Theorems 5–7. □

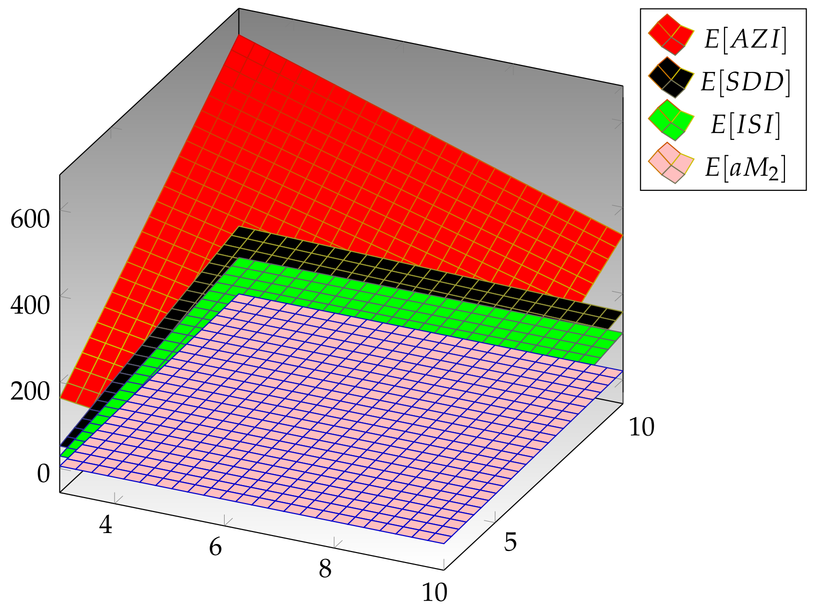

Figure 8. Difference between $E[AZI]$, $E[SDD]$, $E[ISI]$ and, $E[aM_2]$.

In this work, we study the expected values of the modified Zagreb, symmetric difference, inverse symmetric, and augmented Zagreb indices in a random cyclooctane chain. Furthermore, we give analytic proofs for comparisons, along with numerical and graphical profiles of these indices in random cyclooctane chains. More precisely, the numerical tables and graphical profiles suggest that the augmented Zagreb index is continuously more noteworthy than the other three indices, specifically the modified Zagreb, symmetric difference, and inverse symmetric indices.

Author Contributions: Conceptualization, Z.R.; methodology, Z.R.; validation, Z.R.; investigation, Z.R. and M.I.; resources, M.I. and Z.R.; writing—original draft preparation, Z.R.; writing—review and editing, Z.R. and M.I.; supervision, Z.R.; funding acquisition, M.I. and Z.R. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Acknowledgments: Muhammad Imran has been supported during the work on this paper by the University program of Advanced Research (UPAR) and UAEU-AUA grants of United Arab Emirates University (UAEU) via Grant No. G00003271 and Grant No. G00003461. Zahid Raza has been supported during the work on this paper by the University of Sharjah under Projects #2102144098 and #1802144068 and MASEP Research Group.

Conflicts of Interest: The authors declare no conflict of interest.

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