scientific reports

Check for updates

OPEN

Computation of expected values of some connectivity based topological descriptors of random cyclooctane chains

Shamaila Yousaf[1], Zaffar Iqbal[1], Saira Tariq[1], Adnan Aslam[2,3], Fairouz Tchier[4] & Abudulai Issa[5]✉

Cyclooctane is a cycloalkane consisting of carbon and hydrogen atoms arranged in a closed ring structure. Cyclooctane chains can be found in various organic compounds and are significant in the field of organic chemistry due to their diverse reactivity and properties. The atom-bond connectivity index ($\mathcal{ABC}$), the geometric-arithmetic index ($\mathcal{GA}$), the arithmetic–geometric index ($\mathcal{AG}$) and the forgotten index ($\mathcal{F}$) are four well-studied molecular descriptors that have found applications in QSPR and QSAR studies. These topological descriptors have shown significant correlations with different physiochemical properties of octane isomers. In this work, the expected values of four degree based topological descriptors for random cyclooctane chains are calculated. An analytical comparison is given between the expected values of $\mathcal{ABC}$, $\mathcal{GA}$, $\mathcal{AG}$, and $\mathcal{F}$ indices of random cyclooctane chains.

Keywords Chemical graph theory, Topological indices, Cyclooctane chains

A significant branch of mathematics that deals with mathematical models of graphs is called chemical graph theory. It is a branch of mathematics that combines chemistry and graph theory. The physical and chemical properties of molecules correspond with their molecular geometry, which is derived from the vast amount of data used for the analysis. Generally, the characteristics of a molecule obtained through chemical examinations can be efficiently determined by calculating the topological indices. In many cases, theoretical chemistry plays a vital role in chemical graph theory.

Molecular graph theory is a branch of theoretical chemistry that represents chemical compounds, specifically molecules, as graphs. In this context, a graph is a mathematical structure composed of vertices (atoms) and edges (bonds) that connect these vertices. The representation allows for the abstraction and analysis of molecular structures, facilitating the study of various properties and behaviours of chemical compounds. Let $\Pi = \Pi(V, E)$ be a simple, finite connected graph of order n with vertex set $V(\Pi)$ and an edge set $E(\Pi)$. The degree of a vertex u_i is denoted by d_i and is defined as the number of edges incident to it. For undefined notions related to graph theory see[1].

Molecular descriptors are the numerical or categorical representations of the structural and chemical features of a molecule. These molecular descriptors are important in the field of computational chemistry and biology. They provide information about molecular size, chemical composition, shape and other relevant properties of the molecular structure which may be used for designing drug, predicting toxicity and quantitative structure property relationship studies. Numerous molecular descriptors have been introduced by different researchers and are important in studying the characteristics of chemical structures. The first distance based topological index was introduces by H. Wiener[2], while he was working on the boiling point of paraffin. The Zagreb indices and their variants[3] are among the most studied degree based topological indices. They have been used to study branching problem in the early seventeen century. Consider the following general graph invariant

[1]Department of Mathematics, University of Gujrat, Hafiz Hayat Campus, Gujrat, Pakistan. [2]Department of Natural Sciences and Humanities, University of Engineering and Technology, Lahore (RCET), Pakistan. [3]Henan International Joint Laboratory for Multidimensional Topology and Carcinogenic Characteristics Analysis of Atmospheric Particulate Matter PM2.5, Pingdingshan 467000, China. [4]Mathematics Department, College of Science, King Saud University, P.O. Box 22452, 11495 Riyadh, Saudi Arabia. [5]Department of Mathematics, University of Lome, P. O. Box 1515, Lome, Togo. ✉email: issaabudulai13@gmail.com

$$I(\Pi) = \sum_{u_i u_j \epsilon E(\Pi)} f(d_i, d_j).$$

A well-known topological index called the $\mathcal{F}$ index was introduced by Furtula and Gutman[4] in 2015. It is defined as the sum of squares of degrees of the vertices of chemical graphs.

$$\mathcal{F}(\Pi) = \sum_{u_i, u_j \epsilon E(\Pi)} {d_i}^2 + {d_j}^2 \quad (1)$$

It was observed that the predictive ability of $\mathcal{F}$ index and the first Zagreb index is same. The correlation coefficient of $\mathcal{F}$ index for the properties acentric factor and entropy is greater than 0.95.

The Atom-Bond Connectivity index[5] was proposed in 1998 by a Cuban mathematician named Ernesto Estrada. The $\mathcal{ABC}$ index is a helpful predictive index that is used to study the formation of heat in alkanes. It is defined as.

$$\mathcal{ABC}(\Pi) = \sum_{u_i, u_j \epsilon E(\Pi)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}. \quad (2)$$

Vukičević and Furtula[6] introduced a topological index called the geometric-arithmetic index $\mathcal{GA}$. The geometric-arithmetic index is a very useful tool in the investigations of QSAR and QSPR studies. It is defined as

$$\mathcal{GA}(\Pi) = \sum_{u_i, u_j \epsilon E(\Pi)} \frac{2\sqrt{d_i d_j}}{d_i + d_j}. \quad (3)$$

The arithmetic–geometric index $\mathcal{AG}$[7] was recently introduced as a modification of the well-known geometric–arithmetic index $\mathcal{GA}$. This is defined by

$$\mathcal{AG}(\Pi) = \sum_{u_i, u_j \epsilon E(\Pi)} \frac{d_i + d_j}{2\sqrt{d_i d_j}}. \quad (4)$$

For more details on the computations of topological indices for different chemical structures, see[8–11].

In this work, we compute the expected values of four degree based topological indices for the class of random cyclooctane chain: the atom-bond connectivity index, the arithmetic–geometric index, the geometric- arithmetic index, and the forgotten index. An analytical comparison between the expected value of these topological indices with same probability has been given. More precisely, we have proved that the expected value of $\mathcal{ABC}$ index is always less than the expected value of $\mathcal{GA}$ index and that the expected value of $\mathcal{AG}$ index is less than the expected value of forgotten index.

Random cyclooctane chain

A cyclooctane is a cycloalkane which is a type of saturated hydrocarbon with eight carbon atoms arranged in a cycle. It has a chemical formula of C_8H_{16}. Cyclooctane is a stable and nonpolar compound with a simple structure. In organic chemistry, it is used as a reference compound and is part of different organic molecules and reactions. The simple and symmetrical ring structure of cyclooctanes make them ideal model to understand the properties of cyclic hydrocarbons. The study of cyclooctane and its derivatives is important in stereochemistry, particularly when it comes to puckering conformational changes in cycloalkanes. The simple structure and reactivity of cycloocatne make it an important reference point for researchers.

For a long time, chemists gave more attention to the derivatives of saturated hydrocarbons, which are used in drug synthesis, kinetic combustion, and organic synthesis etc. For example, they are used as reagents, synthetic organics. They are also used in the production of adhesives, coatings, and many other purposes. Some scientists got interested in octagonal graphs[12]. Brunvoll et al.[1] studied the number of isomers in octagonal graphs. Many scientists showed their interest in the topological indices of cyclooctanes. Shouliu Wei et. al.[13] calculated the Wiener indices of cyclooctanes. Three types of Kirchoff indices of cyclooctanes have been determined by Yoy Linhua et. al. in[14]. Jia-Bao Liu et. al.[15] calculated the Gutman index and Schultz index of the cyclooctane chains. Recently, Zahid Raza et. al.[16] calculated some topological index such as harmonic index and sum-connectivity index of cyclooctane chains. Liu H. et. al. have computed some expected values of sombor indices of hexagonal chains, phenylene graphs[17]. For more details, see[8–11,18–30].

Materials and methods

The topological indices of the molecular structures that have been derived from their corresponding chemical graphs are called the molecular descriptors. There are many topological indices that have some applications in structural chemistry, especially in QSPR/QSAR research. The cyclooctanes have distinctive physicochemical properties due to saturated and unsaturated hydrocarbons. The cyclooctane chains are made up of a specific arrangement of eight-membered rings. A random cyclooctane chain is an arrangement of octagons such that any two consecutive octagons are attached by an edge in a random way. We use the notation $\mathcal{RCOC}_{\text{m}}$ to denote a cyclooctane chain with m number of octagons. For $\varkappa = 1, 2$, Fig. 1 represents the unique arrangement in $\mathcal{RCOC}_{\text{m}}$. For $\varkappa = 3$, we get four $\mathcal{RCOC}_{\text{m}}$ chains as shown in Fig. 2. The four types of cyclooctane chains are denoted by $\mathcal{RCOC}^1_{z+1}$, $\mathcal{RCOC}^2_{z+1}$, $\mathcal{RCOC}^3_{z+1}$ and $\mathcal{RCOC}^4_{z+1}$(see Fig. 3). Therefore, $\mathcal{RCOC}$ (m; ρ_1, ρ_2, ρ_3) can be attained

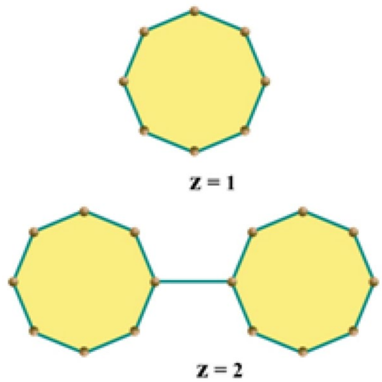

Figure 1. The cyclooctane chains for $z = 1, 2$.

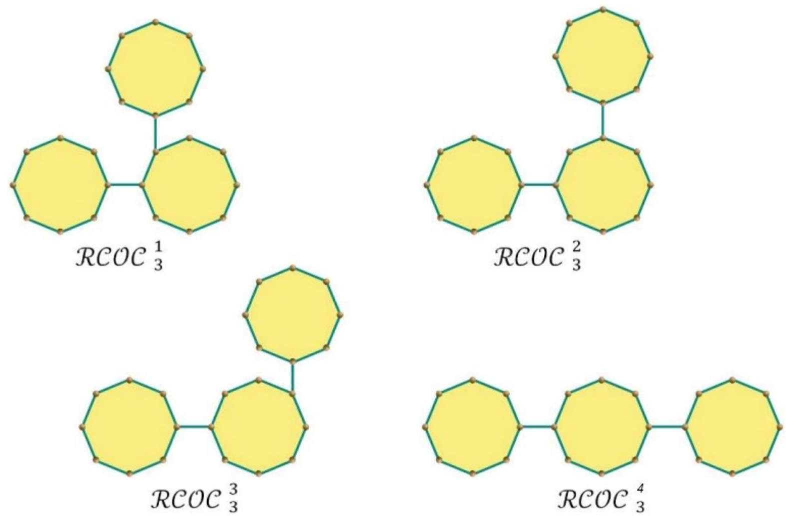

Figure 2. The four type of cyclooctane chains for $z = 3$.

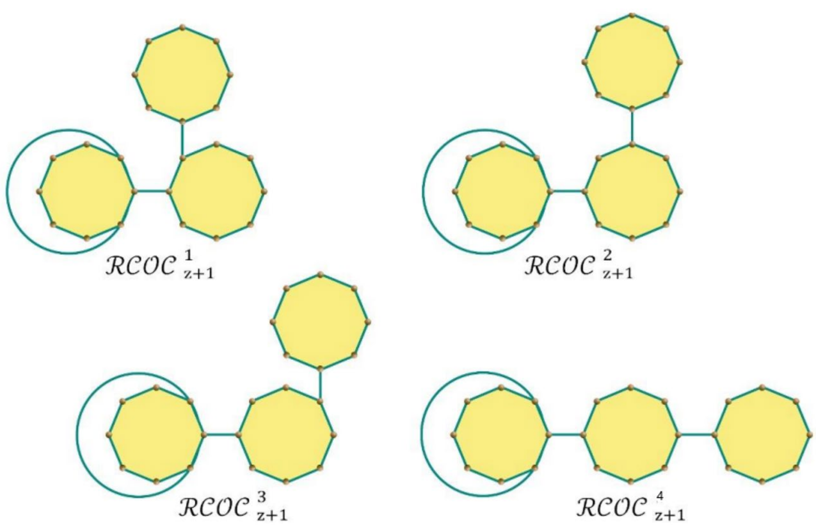

Figure 3. Four types of local arrangements in cyclooctane chains for $z > 3$.

by stepwise addition of a terminal octagon. The possible four structures that can be made at each step from a random selection (z = 3, 4,…,k) are

(i) $\mathcal{RCOC}_{z-1} \rightarrow \mathcal{RCOC}_z^1$ with probability m_1,
(ii) $\mathcal{RCOC}_{z-1} \rightarrow \mathcal{RCOC}_z^2$ with probability m_2,
(iii) $\mathcal{RCOC}_{z-1} \rightarrow \mathcal{RCOC}_z^3$ with probability m_3,
(iv) $\mathcal{RCOC}_{z-1} \rightarrow \mathcal{RCOC}_z^4$ with probability $r = 1 - m_1 - m_2 - m_3$

If we assume that the probabilities are constant and independent of the step parameter, then this process is a zeroth-order Markov process. In order to compute the atom-bond connectivity index, the arithmetic–geometric, geometric-arithmetic, and forgotten index of $\mathcal{RCOC}_z$, we need to find the edge partition of $\mathcal{RCOC}_z$ depending on the degree of end vertices of each edge. It is easy to see that it contains only (2, 2), (2, 3), and (3, 3)-types of edges. Therefore, the mathematical expression of $\mathcal{ABC}$, $\mathcal{GA}$, $\mathcal{AG}$, and $\mathcal{F}$ indices can be written as:

$$\mathcal{F}(\mathcal{RCOC}_z) = 8x_{22}(\mathcal{RCOC}_z) + 13x_{23}(\mathcal{RCOC}_z) + 18x_{33}(\mathcal{RCOC}_z) \tag{5}$$

$$\mathcal{ABC}(\mathcal{RCOC}_z) = \frac{1}{\sqrt{2}}x_{22}(\mathcal{RCOC}_z) + \frac{1}{\sqrt{2}}x_{23}(\mathcal{RCOC}_z) + \frac{2}{3}x_{33}(\mathcal{RCOC}_z). \tag{6}$$

$$\mathcal{GA}(\mathcal{RCOC}_z) = x_{22}(\mathcal{RCOC}_z) + \frac{2\sqrt{6}}{5}x_{23}(\mathcal{RCOC}_z) + x_{33}(\mathcal{RCOC}_z). \tag{7}$$

$$\mathcal{AG}(\mathcal{RCOC}_z) = x_{22}(\mathcal{RCOC}_z) + \frac{5}{2\sqrt{6}}x_{23}(\mathcal{RCOC}_z) + x_{33}(\mathcal{RCOC}_z). \tag{8}$$

Results

A random cyclooctane chain $\mathcal{RCOC}_z$ is a local arrangement. Hence, $\mathcal{F}(\mathcal{RCOC}(z; m_1, m_2, m_3))$, $\mathcal{ABC}(\mathcal{RCOC}(z; m_1, m_2, m_3))$, $\mathcal{GA}(\mathcal{RCOC}(z; m_1, m_2, m_3))$, and $\mathcal{AG}(\mathcal{RCOC}(z; m_1, m_2, m_3))$ are the random variables. We use the notation $E_z^{\mathcal{F}} = E[\mathcal{F}(\mathcal{RCOC}(z; m_1, m_2, m_3))]$, $E_z^{ABC} = E[\mathcal{ABC}(\mathcal{RCOC}(z; m_1, m_2, m_3))]$,$E_z^{\mathcal{GA}} = E[\mathcal{GA}(\mathcal{RCOC}(z; m_1, m_2, m_3))]$, and $E_z^{\mathcal{AG}} = E[\mathcal{AG}(\mathcal{RCOC}(z; m_1, m_2, m_3))]$ to denote the expected values of the forgotten, the atom bond connectivity, the geometric arithmetic and the arithmetic geometric indices of $\mathcal{RCOC}_z$ respectively.

Theorem 1 *Let $\mathcal{RCOC}(z; m_1, m_2, m_3)$ be the random cyclooctane and $z \geq 2$. Then*

$$E_z^{\mathcal{F}} = z[102] - 38$$

Proof It is easy to see that $E_2^{\mathcal{F}} = 166$, which is indeed true. For z ≥ 3, there are four possibilities:

(i) If $\mathcal{RCOC}_{z-1} \rightarrow \mathcal{RCOC}_z^1$ with probability m_1, then
$x_{22}\left(\mathcal{RCOC}_z^1\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 5$, $x_{23}\left(\mathcal{RCOC}_z^1\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 2$, $x_{33}(\mathcal{RCOC}) = x_{33}(\mathcal{RCOC}_{z-1}) + 2$,
From Eq. (5), we have $\mathcal{F}\left(\mathcal{RCOC}_z^1\right) = \mathcal{F}(\mathcal{RCOC}_{z-1}) + 102$.
(ii) If $\mathcal{RCOC}_{z-1} \rightarrow \mathcal{RCOC}_z^2$ with probability m_2, then
$x_{22}\left(\mathcal{RCOC}_z^2\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 4$, $x_{23}\left(\mathcal{RCOC}_z^2\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 4$, $x_{33}\left(\mathcal{RCOC}_z^2\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 1$,
From Eq. (5), we have $\mathcal{F}\left(\mathcal{RCOC}_z^2\right) = \mathcal{F}(\mathcal{RCOC}_{z-1}) + 102$.
(iii) If $\mathcal{RCOC}_{z-1} \rightarrow \mathcal{RCOC}_z^3$ with probability m_3, then
$x_{22}\left(\mathcal{RCOC}_z^3\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 4$, $x_{23}\left(\mathcal{RCOC}_z^3\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 4$, $x_{33}\left(\mathcal{RCOC}_z^3\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 1$,
From Eq. (5), we have $\mathcal{F}\left(\mathcal{RCOC}_z^3\right) = \mathcal{F}(\mathcal{RCOC}_{z-1}) + 102$.
(iv) If $\mathcal{RCOC}_{z-1} \rightarrow \mathcal{RCOC}_z^4$ with probability $1 - m_1 - m_2 - m_3$, then
$x_{22}\left(\mathcal{RCOC}_z^4\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 4$, $x_{23}\left(\mathcal{RCOC}_z^4\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 1$, $x_{33}\left(\mathcal{RCOC}_z^4\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 1$,

From Eq. (5), we have $\mathcal{F}\left(\mathcal{RCOC}_z^4\right) = \mathcal{F}(\mathcal{RCOC}_{z-1}) + 102$
Thus, we get

$$E_z^{\mathcal{F}} = m_1\mathcal{F}\left(\mathcal{RCOC}_z^1\right) + m_2\mathcal{F}\left(\mathcal{RCOC}_z^2\right) + m_3\mathcal{F}\left(\mathcal{RCOC}_z^3\right) + (1 - m_1 - m_2 - m_3)\mathcal{F}\left(\mathcal{RCOC}_z^4\right)$$

$$= m_1[\mathcal{F}(\mathcal{RCOC}_z + 102)] + m_2[\mathcal{F}(\mathcal{RCOC}_z + 102)] + m_3[\mathcal{F}(\mathcal{RCOC}_z + 102)] + (1 - m_1 - m_2 - m_3)[\mathcal{F}(\mathcal{RCOC}_z + 102)]$$

$$E_z^{\mathcal{F}} = \mathcal{F}(\mathcal{RCOC}_{z-1}) + 102 \tag{9}$$

Since $E[E_z^{\mathcal{F}}] = E_z^{\mathcal{F}}$, by applying operator on Eq. (9), we obtain

$$E_z^{\mathcal{F}} = E_{z-1}^{\mathcal{F}} + 102, \quad m > 2 \tag{10}$$

Using the initial conditions and solving recurrence relation, we get

$$E_z^{\mathcal{F}} = z[102] - 38.$$

Theorem 2 *Let $\mathcal{RCOC}(z; m_1, m_2, m_3)$ be the random cyclooctane and $z \geq 2$. Then*

$$E_z^{\mathcal{ABC}} = z\left[\left(\frac{4-3\sqrt{2}}{6}\right)m_1 + \frac{2+12\sqrt{2}}{3}\right] - \left(\frac{4-3\sqrt{2}}{3}\right)m_1 - \frac{2}{3}$$

Proof It is easy to calculate that $E_2^{\mathcal{ABC}} = \frac{2+24\sqrt{2}}{3}$, which is indeed true. For z$\geq$ 3, we have four possibilities:

(a) If $\mathcal{RCOC}_{z-1} \to \mathcal{RCOC}_z^1$ with probability m_1, then
$x_{22}\left(\mathcal{RCOC}_z^1\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 5$, $x_{23}\left(\mathcal{RCOC}_z^1\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 2$, $x_{33}\left(\mathcal{RCOC}_z^1\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 2$,
From Eq. (6), we have $\mathcal{ABC}\left(\mathcal{RCOC}_z^1\right) = \mathcal{ABC}(\mathcal{RCOC}_{z-1}) + \frac{8+21\sqrt{2}}{6}$.

(b) If $\mathcal{RCOC}_{z-1} \to \mathcal{RCOC}_z^2$ with probability m_2, then
$x_{22}\left(\mathcal{RCOC}_z^2\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 4$, $x_{23}\left(\mathcal{RCOC}_z^2\right) = x_{23}(R\mathcal{RCOC}_{z-1}) + 4$, $x_{33}\left(\mathcal{RCOC}_z^2\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 1$,
From Eq. (6), we have $\mathcal{ABC}\left(\mathcal{RCOC}_z^2\right) = \mathcal{ABC}(\mathcal{RCOC}_{z-1}) + \frac{2+12\sqrt{2}}{3}$.

(c) If $\mathcal{RCOC}_{z-1} \to \mathcal{RCOC}_z^3$ with probability m_3, then
$x_{22}\left(\mathcal{RCOC}_z^3\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 4$, $x_{23}\left(\mathcal{RCOC}_z^3\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 4$, $x_{33}\left(\mathcal{RCOC}_z^3\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 1$,
From Eq. (6), we have $\mathcal{ABC}\left(\mathcal{RCOC}_z^3\right) = \mathcal{ABC}(\mathcal{RCOC}_{z-1}) + \frac{2+12\sqrt{2}}{3}$.

(d) If $\mathcal{RCOC}_{z-1} \to \mathcal{RCOC}_z^4$ with probability $1 - m_1 - m_2 - m_3$, then
$x_{22}\left(\mathcal{RCOC}_z^4\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 4$, $x_{23}\left(\mathcal{RCOC}_z^4\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 1$, $x_{33}\left(\mathcal{RCOC}_z^4\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 1$,
From Eq. (6), we have $\mathcal{ABC}\left(\mathcal{RCOC}_z^4\right) = \mathcal{ABC}(\mathcal{RCOC}_{z-1}) + \frac{2+12\sqrt{2}}{3}$.

Thus, we get

$$E_z^{\mathcal{ABC}} = m_1\mathcal{ABC}\left(\mathcal{RCOC}_z^1\right) + m_2\mathcal{ABC}\left(\mathcal{RCOC}_z^2\right) + m_3\mathcal{ABC}\left(\mathcal{RCOC}_z^3\right) + (1 - m_1 - m_2 - m_3)\mathcal{ABC}\left(\mathcal{RCOC}_z^4\right)$$

$$= m_1\left[\mathcal{ABC}\left(\mathcal{RCOC}_z + \frac{8+21\sqrt{2}}{6}\right)\right] + m_2\left[\mathcal{ABC}\left(\mathcal{RCOC}_z + \frac{2+12\sqrt{2}}{3}\right)\right] + m_3\left[\mathcal{ABC}\left(\mathcal{RCOC}_z + \frac{2+12\sqrt{2}}{3}\right)\right] + (1 - m_1 - m_2 - m_3)\left[\mathcal{ABC}\left(\mathcal{RCOC}_z + \frac{2+12\sqrt{2}}{3}\right)\right]$$

$$E_z^{\mathcal{ABC}} = \mathcal{ABC}(\mathcal{RCOC}_{z-1}) + \left(\frac{4-3\sqrt{2}}{6}\right)m_1 + \frac{2+12\sqrt{2}}{3} \tag{11}$$

Since $E[E_z^{\mathcal{ABC}}] = E_z^{\mathcal{ABC}}$, by applying operator on Eq. (11), we obtain

$$E_z^{\mathcal{ABC}} = E_{z-1}^{\mathcal{ABC}} + \left(\frac{4-3\sqrt{2}}{6}\right)m_1 + \frac{2+12\sqrt{2}}{3}, m > 2 \tag{12}$$

Using the initial conditions and solving the recurrence relation, we get

$$E_z^{\mathcal{ABC}} = z\left[\left(\frac{4-3\sqrt{2}}{6}\right)m_1 + \frac{2+12\sqrt{2}}{3}\right] - \left(\frac{4-3\sqrt{2}}{3}\right)m_1 - \frac{2}{3}.$$

Theorem 3 *Let $\mathcal{RCOC}(z; m_1, m_2, m_3)$ be the random cyclooctane and $z \geq 2$. Then*

$$E_z^{\mathcal{GA}} = z\left[\left(\frac{10-4\sqrt{6}}{5}\right)m_1 + \frac{25+8\sqrt{6}}{5}\right] - \left(\frac{20-8\sqrt{6}}{5}\right)m_1 + \frac{15-8\sqrt{6}}{5}$$

Proof Observe that $E_2^{\mathcal{GA}} = \frac{65+8\sqrt{6}}{5}$, which is indeed true.. For z$\geq$ 3, we have four possibilities:

(a) If $\mathcal{RCOC}_{z-1} \to \mathcal{RCOC}_z^1$ with probability m_1, then
$x_{22}\left(\mathcal{RCOC}_z^1\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 5, x_{23}\left(\mathcal{RCOC}_z^1\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 2, x_{33}\left(\mathcal{RCOC}_z^1\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 2,$
From Eq. (7), we have $\mathcal{GA}\left(\mathcal{RCOC}_z^1\right) = \mathcal{GA}(\mathcal{RCOC}_{z-1}) + \frac{35+4\sqrt{6}}{5}$.

(b) If $\mathcal{RCOC}_{z-1} \to \mathcal{RCOC}_z^2$ with probability m_2, then
$x_{22}\left(\mathcal{RCOC}_z^2\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 4, x_{23}\left(\mathcal{RCOC}_z^2\right) = x_{23}(R\mathcal{RCOC}_{z-1}) + 4, x_{33}\left(\mathcal{RCOC}_z^2\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 1,$
From Eq. (7), we have $\mathcal{GA}\left(\mathcal{RCOC}_z^2\right) = \mathcal{GA}(\mathcal{RCOC}_{z-1}) + \frac{25+8\sqrt{6}}{5}$.

(iii) If $\mathcal{RCOC}_{z-1} \to \mathcal{RCOC}_z^3$ with probability m_3, then
$x_{22}\left(\mathcal{RCOC}_z^3\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 4, x_{23}\left(\mathcal{RCOC}_z^3\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 4, x_{33}\left(\mathcal{RCOC}_z^3\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 1,$
From Eq. (7), we have $\mathcal{GA}\left(\mathcal{RCOC}_z^3\right) = \mathcal{GA}(\mathcal{RCOC}_{z-1}) + \frac{25+8\sqrt{6}}{5}$.

(iv) If $\mathcal{RCOC}_{z-1} \to \mathcal{RCOC}_z^4$ with probability $1 - m_1 - m_2 - m_3$, then
$x_{22}\left(\mathcal{RCOC}_z^4\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 4, x_{23}\left(\mathcal{RCOC}_z^4\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 1, x_{33}\left(\mathcal{RCOC}_z^4\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 1,$
From Eq. (7), we have $\mathcal{GA}\left(\mathcal{RCOC}_z^4\right) = \mathcal{GA}(\mathcal{RCOC}_{z-1}) + \frac{25+8\sqrt{6}}{5}$.

Thus, we get

$$E_z^{\mathcal{GA}} = m_1\mathcal{GA}\left(\mathcal{RCOC}_z^1\right) + m_2\mathcal{GA}\left(\mathcal{RCOC}_z^2\right) + m_3\mathcal{GA}\left(\mathcal{RCOC}_z^3\right) + (1 - m_1 - m_2 - m_3)\mathcal{GA}\left(\mathcal{RCOC}_z^4\right)$$

$$= m_1\left[\mathcal{GA}\left(\mathcal{RCOC}_z + \frac{35+4\sqrt{6}}{5}\right)\right] + m_2\left[\mathcal{GA}\left(\mathcal{RCOC}_z + \frac{25+8\sqrt{6}}{5}\right)\right]$$
$$+ m_3\left[\mathcal{GA}\left(\mathcal{RCOC}_z + \frac{25+8\sqrt{6}}{5}\right)\right] + (1 - m_1 - m_2 - m_3)\left[\mathcal{GA}\left(\mathcal{RCOC}_z + \frac{25+8\sqrt{6}}{5}\right)\right]$$

$$E_z^{\mathcal{GA}} = \mathcal{GA}(\mathcal{RCOC}_{z-1}) + \left(\frac{10-4\sqrt{6}}{5}\right)m_1 + \frac{25+8\sqrt{6}}{5} \tag{13}$$

Since $E[E_z^{\mathcal{GA}}] = E_z^{\mathcal{GA}}$, by applying operator on Eq. (13), we obtain

$$E_z^{\mathcal{GA}} = E_{z-1}^{\mathcal{GA}} + \left(\frac{10-4\sqrt{6}}{5}\right)m_1 + \frac{25+8\sqrt{6}}{5}, m > 2 \tag{14}$$

Using the initial conditions and solving recurrence relation, we get

$$E_z^{\mathcal{GA}} = z\left[\left(\frac{10-4\sqrt{6}}{5}\right)m_1 + \frac{25+8\sqrt{6}}{5}\right] - \left(\frac{20-8\sqrt{6}}{5}\right)m_1 + \frac{15-8\sqrt{6}}{5}$$

Theorem 4 *Let $\mathcal{RCOC}(z; m_1, m_2, m_3)$ be the random cyclooctane and $z \geq 2$. Then*

$$E_z^{\mathcal{AG}} = z\left[\left(\frac{12-5\sqrt{6}}{6}\right)m_1 + \frac{15+5\sqrt{6}}{3}\right] - \left(\frac{12-5\sqrt{6}}{3}\right)m_1 + \frac{9-5\sqrt{6}}{3}$$

Proof It is easy to see that $E_2^{\mathcal{AG}} = \frac{39+5\sqrt{6}}{3}$ which is indeed true. For z$\geq$ 3, we have four possibilities:

(a) If $\mathcal{RCOC}_{z-1} \to \mathcal{RCOC}_z^1$ with probability m_1, then
$x_{22}\left(\mathcal{RCOC}_z^1\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 5, x_{23}\left(\mathcal{RCOC}_z^1\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 2, x_{33}\left(\mathcal{RCOC}_z^1\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 2,$
From Eq. (8), we have $\mathcal{AG}\left(\mathcal{RCOC}_z^1\right) = \mathcal{AG}(\mathcal{RCOC}_{z-1}) + \frac{42+5\sqrt{6}}{6}$.

(b) If $\mathcal{RCOC}_{z-1} \to \mathcal{RCOC}_z^2$ with probability m_2, then
$x_{22}\left(\mathcal{RCOC}_z^2\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 4, x_{23}\left(\mathcal{RCOC}_z^2\right) = x_{23}(R\mathcal{RCOC}_{z-1}) + 4, x_{33}\left(\mathcal{RCOC}_z^2\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 1,$
From Eq. (8), we have $\mathcal{AG}\left(\mathcal{RCOC}_z^2\right) = \mathcal{AG}(\mathcal{RCOC}_{z-1}) + \frac{15+5\sqrt{6}}{3}$.

(c) If $\mathcal{RCOC}_{z-1} \rightarrow \mathcal{RCOC}_z^3$ with probability m_3, then
$x_{22}\left(\mathcal{RCOC}_z^3\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 4, x_{23}\left(\mathcal{RCOC}_z^3\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 4, x_{33}\left(\mathcal{RCOC}_z^3\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 1,$
From Eq. (8), we have $\mathcal{AG}\left(\mathcal{RCOC}_z^3\right) = \mathcal{AG}(\mathcal{RCOC}_{z-1}) + \frac{15+5\sqrt{6}}{3}$

(d) If $\mathcal{RCOC}_{z-1} \rightarrow \mathcal{RCOC}_z^4$ with probability $1 - m_1 - m_2 - m_3$, then
$x_{22}\left(\mathcal{RCOC}_z^4\right) = x_{22}(\mathcal{RCOC}_{z-1}) + 4, x_{23}\left(\mathcal{RCOC}_z^4\right) = x_{23}(\mathcal{RCOC}_{z-1}) + 1, x_{33}\left(\mathcal{RCOC}_z^4\right) = x_{33}(\mathcal{RCOC}_{z-1}) + 1,$
From Eq. (8), we have $\mathcal{AG}\left(\mathcal{RCOC}_z^4\right) = \mathcal{AG}(\mathcal{RCOC}_{z-1}) + \frac{15+5\sqrt{6}}{3}$.

Thus, we get

$$E_z^{\mathcal{AG}} = m_1\mathcal{AG}\left(\mathcal{RCOC}_z^1\right) + m_2\mathcal{AG}\left(\mathcal{RCOC}_z^2\right) + m_3\mathcal{AG}\left(\mathcal{RCOC}_z^3\right) + (1 - m_1 - m_2 - m_3)\mathcal{AG}\left(\mathcal{RCOC}_z^4\right)$$

$$= m_1\left[\mathcal{AG}\left(\mathcal{RCOC}_z + \frac{42+5\sqrt{6}}{6}\right)\right] + m_2\left[\mathcal{AG}\left(\mathcal{RCOC}_z + \frac{15+5\sqrt{6}}{3}\right)\right]$$
$$+ m_3\left[\mathcal{AG}\left(\mathcal{RCOC}_z + \frac{15+5\sqrt{6}}{3}\right)\right] + (1 - m_1 - m_2 - m_3)\left[\mathcal{AG}\left(\mathcal{RCOC}_z + \frac{15+5\sqrt{6}}{3}\right)\right]$$

$$E_z^{\mathcal{AG}} = \mathcal{AG}(\mathcal{RCOC}_{z-1}) + \left(\frac{12-5\sqrt{6}}{6}\right)m_1 + \frac{15+5\sqrt{6}}{3} \tag{15}$$

Since, $E[E_z^{\mathcal{AG}}] = E_z^{\mathcal{AG}}$, by applying operator on Eq. (15), we obtain

$$E_z^{\mathcal{AG}} = E_{z-1}^{\mathcal{AG}} + \left(\frac{12-5\sqrt{6}}{6}\right)m_1 + \frac{15+5\sqrt{6}}{3}, m > 2 \tag{16}$$

Using the initial conditions and solving the recurrence relation, we get

$$E_z^{\mathcal{AG}} = z\left[\left(\frac{12-5\sqrt{6}}{6}\right)m_1 + \frac{15+5\sqrt{6}}{3}\right] - \left(\frac{12-5\sqrt{6}}{3}\right)m_1 + \frac{9-5\sqrt{6}}{3}$$

Now our focus is the special cyclooctanes such as $\mathcal{CZ}_m, \mathcal{CL}_m, \mathcal{CO}_m$, and $\mathcal{CM}_m$, which are shown in Fig. 4. Such cyclooctane chains can be obtained as: $\mathcal{CZ}_m = \mathcal{RCOC}(m; 1, 0, 0), \mathcal{CL}_m = \mathcal{RCOC}(m; 0, 1, 0), \mathcal{CO}_m = \mathcal{RCOC}(m; 0, 0, 1)$, and $\mathcal{CM}_m = \mathcal{RCOC}(m; 0, 0, 0)$. With the help of Theorems 1–4, we can calculate the expected value of these special type of cyclooctane chains.

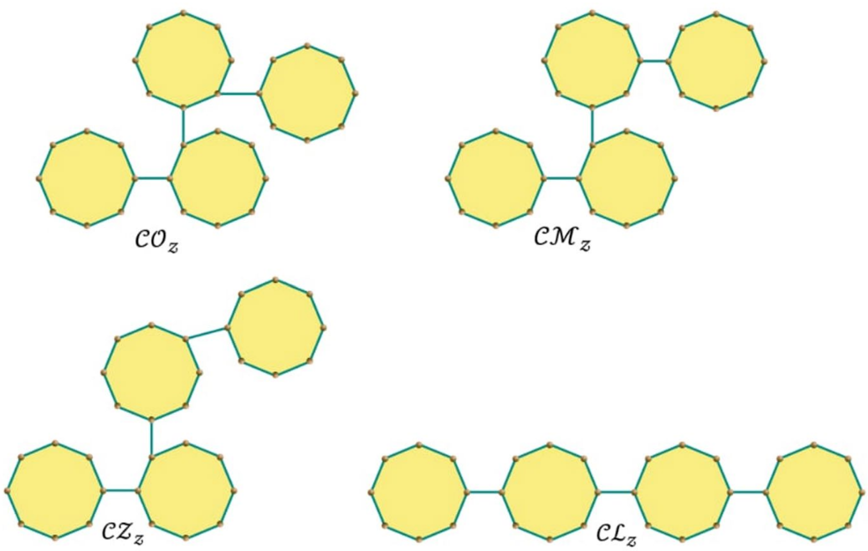

Figure 4. Four special types of cyclooctane chains with z octagons.

z	$E^{\mathcal{F}}$	$E^{\mathcal{ABC}}$	$E^{\mathcal{GA}}$	$E^{\mathcal{AG}}$
4	370	24.5465	34.8388	35.1649
5	472	30.8296	43.7979	44.2062
6	574	37.1126	52.7575	53.2474
7	676	43.3950	61.7171	62.2888
8	778	49.6788	70.6767	71.3299
9	880	55.9615	79.6363	80.3711
10	982	62.2450	88.5959	89.4124
11	1084	68.5280	97.5555	98.4532
12	1186	74.8111	106.5150	107.4948
13	1288	81.0942	115.4746	116.5361

Table 1. Expected values of topological indices for $m_1 = 1$.

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

1. $\mathcal{F}(\mathcal{CO}_m) = 102z - 38$

$$\mathcal{ABC}(\mathcal{CO}_m) = \left(\frac{8 + 21\sqrt{2}}{6}\right)z - (2 - \sqrt{2})$$

z	$E^{\mathcal{F}}$	$E^{\mathcal{ABC}}$	$E^{\mathcal{GA}}$	$E^{\mathcal{AG}}$
4	370	24.627	34.757	35.247
5	472	30.950	43.676	44.329
6	574	37.247	52.5959	53.412
7	676	43.597	61.515	62.4948
8	778	49.921	70.434	71.577
9	880	56.245	79.353	80659
10	982	62.5685	88.272	89.6598
11	1084	68.892	97.191	98.824
12	1186	75.215	106.111	107.907
13	1288	81.539	115.030	116.984

Table 2. Expected values of topological indices for $m_1 = 0$.

z	$E^{\mathcal{F}}$	$E^{\mathcal{ABC}}$	$E^{\mathcal{GA}}$	$E^{\mathcal{AG}}$
4	370	24.586	34.797	35.206
5	472	30.890	43.737	44.268
6	574	37.193	52.676	53.329
7	676	43.395	61.616	62.391
8	778	49.802	70.555	71.453
9	880	56.103	79.494	80.575
10	982	62.406	88.434	89.515
11	1084	68.710	97.373	98.639
12	1186	75.013	106.313	107.701
13	1288	81.316	115.252	116.762

Table 3. Expected values of topological indices for $m_1 = \frac{1}{2}$.

z	$E^{\mathcal{F}}$	$E^{\mathcal{ABC}}$	$E^{\mathcal{GA}}$	$E^{\mathcal{AG}}$
4	370	24.6071	34.777	35.226
5	472	30.920	43.707	44.299
6	574	37.234	52.636	53.371
7	676	43.547	61.565	62.443
8	778	49.860	70.494	71.515
9	880	56.174	79.424	80.587
10	982	62.487	88.353	89.659
11	1084	68.801	97.282	98.732
12	1186	75.114	106.212	107.804
13	1288	81.427	115.141	116.876

Table 4. Expected values of indices for $m_1 = \frac{1}{4}$.

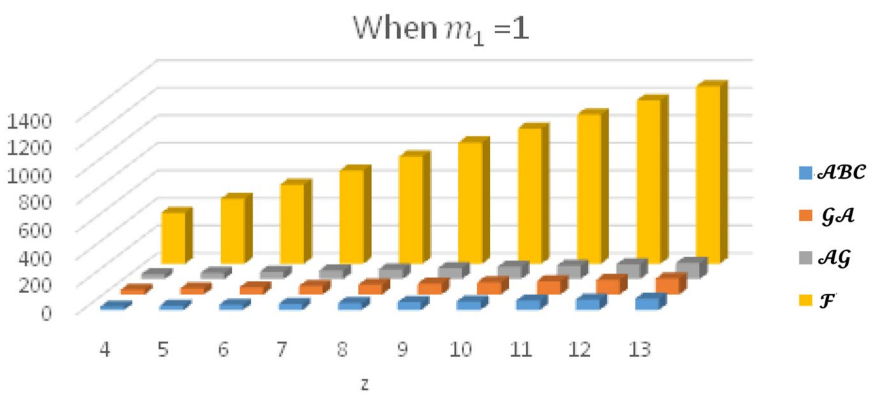

Figure 5. Plot of expected values of topological indices $m_1 = 1$.

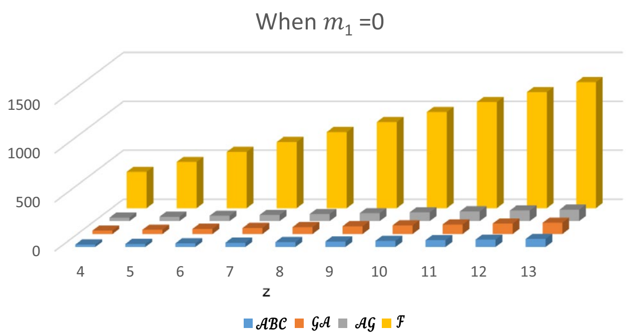

Figure 6. Plot of expected values of topological indices for $m_1 = 0$.

$$\mathcal{GA}(\mathcal{CO}_m) = \left(\frac{35 + 4\sqrt{6}}{5}\right)z - 1$$

$$\mathcal{AG}(\mathcal{CO}_m) = \left(\frac{42 + 5\sqrt{6}}{6}\right)z - 1$$

2. $\mathcal{ABC}(\mathcal{CM}_m) = \mathcal{ABC}(\mathcal{CZ}_m) = \mathcal{ABC}(\mathcal{CL}_m) = \left(\frac{2+12\sqrt{2}}{3}\right)z - \frac{2}{3}$

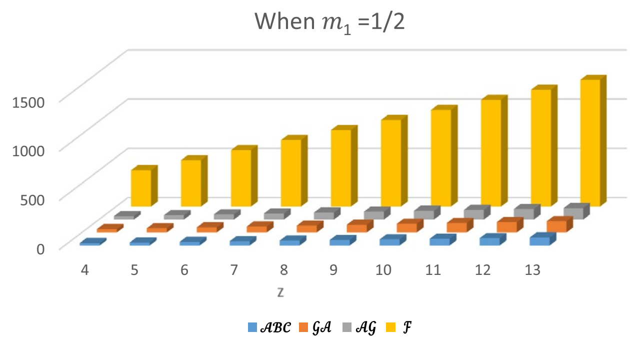

Figure 7. Plot of expected values of topological indices $m_1 = \frac{1}{2}$.

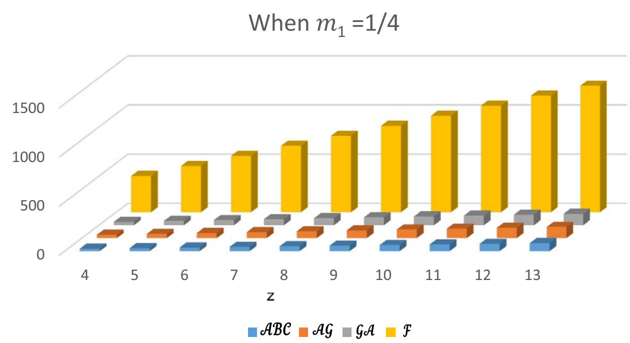

Figure 8. Plot of expected values of topological indices $m_1 = \frac{1}{4}$.

$$\mathcal{GA}(\mathcal{CM}_{m}) = \mathcal{GA}(\mathcal{CZ}_{m}) = \mathcal{GA}(\mathcal{CL}_{m}) = \left(\frac{25+8\sqrt{6}}{5}\right)z + \frac{15-8\sqrt{6}}{5}$$

$$\mathcal{AG}(\mathcal{CM}_{m}) = \mathcal{AG}(\mathcal{CZ}_{m}) = \mathcal{AG}(\mathcal{CL}_{m}) = \left(\frac{12+5\sqrt{6}}{3}\right)z + \frac{9-5\sqrt{6}}{3}$$

Comparison between the expected values of topological indices

In this section, the expected values of the forgotten index, the arithmetic–geometric index, the geometric-arithmetic index, and the atom-bond connectivity index are analyzed and compared. In Tables 1, 2, 3 and 4, we have computed the expected values of these indices for different values of m_1. Observe that the value of forgotten index is always greater than the expected values of other topological indices. The graphical comparison between the forgotten index, arithmetic–geometric index, geometric-arithmetic index and atom-bond connectivity index for the cyclooctane chains with the same probabilities is shown in Figs. 5, 6, 7 and 8. One can see that the expected value of the forgotten index is always greater than the expected value of arithmetic–geometric index and the expected value of arithmetic–geometric index is always greater than the expected value of geometric-arithmetic index and the expected value of geometric-arithmetic index is greater than the expected value of atom-bond connectivity index. We give an analytical proof of this fact in the next theorems.

Theorem 5 *Let $z \geq 2$, then*

$$E[\mathcal{F}(\mathcal{RCOC}(z; m_1, m_2, m_3))] > E[\mathcal{AG}(\mathcal{RCOC}(z; m_1, m_2, m_3))].$$

Proof It is true for $z = 2$. Now, let $z > 2$, by using Theorem 1 and 2, we have

$$E[\mathcal{F}(\mathcal{RCOC}(z; m_1, m_2, m_3))] - E[\mathcal{AG}(\mathcal{RCOC}(z; m_1, m_2, m_3))]$$

$$= z[102] - 38 - \left[z\left[\left(\frac{12-5\sqrt{6}}{6}\right)m_1 + \frac{15+5\sqrt{6}}{3}\right] - \left(\frac{12-5\sqrt{6}}{3}\right)m_1 + \frac{9-5\sqrt{6}}{3}\right]$$

$$= (z-2)\left[\frac{321+5\sqrt{6}}{3}+\left(\frac{12-5\sqrt{6}}{6}\right)m_1\right]+179+5\sqrt{6}$$

$$= \frac{(z-2)}{3}\left[321+5\sqrt{6}+\left(\frac{12-5\sqrt{6}}{2}\right)m_1\right]+179+5\sqrt{6}$$

$$> 0$$

$$\because z \geq 2 \text{ and } 0 \leq m_1 \leq 1.$$

Theorem 6 *If* $z \geq 2$, *then*

$$E[\mathcal{AG}(\mathcal{RCOC}(z;m_1,m_2,m_3))] > E[\mathcal{GA}(\mathcal{RCOC}(z;m_1,m_2,m_3))].$$

Proof It is true for $z = 2$. Let $z > 2$, by using Theorem 2 and 3, we have.

$$E[\mathcal{AG}(\mathcal{RCOC}(z;m_1,m_2,m_3))] - E[\mathcal{GA}(\mathcal{RCOC}(z;m_1,m_2,m_3))]$$

$$= \left[z\left[\left(\frac{12-5\sqrt{6}}{6}\right)m_1+\frac{15+5\sqrt{6}}{3}\right]-\left(\frac{12-5\sqrt{6}}{3}\right)m_1+\frac{9-5\sqrt{6}}{3}\right]$$
$$- \left[z\left[\left(\frac{10-4\sqrt{6}}{5}\right)m_1+\frac{25+8\sqrt{6}}{5}\right]-\left(\frac{20-8\sqrt{6}}{5}\right)m_1+\frac{15-8\sqrt{6}}{5}\right]$$

$$= (z-2)\left[\frac{\sqrt{6}}{15}+\left(\frac{\sqrt{6}}{30}\right)m_1\right]+\frac{\sqrt{6}}{15}$$

$$= \frac{(z-2)}{15}\left[\sqrt{6}+\left(\frac{\sqrt{6}}{2}\right)m_1\right]+\frac{\sqrt{6}}{15}$$

$$> 0$$

$$\because z \geq 2 \text{ and } 0 \leq m_1 \leq 1.$$

Theorem 7. $E[F(\mathcal{RCOC}(z;m_1,m_2,m_3))] > E[\mathcal{AG}(\mathcal{RCOC}(z;m_1,m_2,m_3))] > E[\mathcal{GA}(\mathcal{RCOC}(z;m_1,m_2,m_3))] > E[\mathcal{ABC}(\mathcal{RCOC}(z;m_1,m_2,m_3))]$.

Data availability

All data generated or analysed during this study are included in this published article [and its supplementary information files].

Received: 18 November 2023; Accepted: 14 March 2024
Published online: 02 April 2024

References

1. Brunvoll, J., Cyvin, S. J. & Cyvin, B. N. Enumeration of tree-like octagonal systems. *J. Math. Chem.* **21**, 193–196 (1997).
2. Wiener, H. Structural determination of paraffin boiling points. *J. Am. Chem. Soc.* **69**(1), 17–20 (1947).
3. Gutman, I., &Trinajstić, N. Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **17**(4), 535–538 (1972).
4. Furtula, B. & Gutman, I. A forgotten topological index. *J. Math. Chem.* **53**(4), 1184–1190 (2015).
5. Estrada, E., Torres, L., Rodriguez, L. & Gutman, I. An atom-bond connectivity index modelling the enthalpy of formation of alkanes. *Indian J. Chem.* **37A**, 849–855 (1998).
6. Vukicevic, B. & Furtula, B. Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. *J. Math. Chem.* **46**, 1369–1376 (2009).
7. Shegehall, V. S. & Kanabur, R. Arithmetic-geometric indices of path graph. *J. Math. Comput. Sci.* **16**, 19–24 (2015).
8. Hui, Z.-H., Yousaf, S., Aslam, A., Binyamin, M. A. & Kanwal, S. On expected values of some degree based topological descriptors of random phenylene chains. *Mol. Phys.* **121**, 16. https://doi.org/10.1080/00268976.2023.2225648 (2023).
9. Huang, R.-R., Aftab, S., Noureen, S. & Aslam, A. Analysis of porphyrin, PETIM and zinc porphyrin dendrimers by atom-bond sum-connectivity index for drug delivery. *Mol. Phys.* **121**, 15. https://doi.org/10.1080/00268976.2023.2214073 (2023).
10. Yun, Z., Aslam, A., Kanwal, S., Saeed, S. & Razzaque, A. Physio-chemical properties of $HCP(U)$ and $HEX(U)$ crystal structure lattice via eccentricity dependent chemical invariants. *Mol. Phys.* **121**, 13. https://doi.org/10.1080/00268976.2023.2202267 (2023).
11. Hui, Z.-H., Naeem, M., Rauf, A. & Aslam, A. Estimating the physicochemical properties of antiemetics using degree-based topological descriptors. *Mol. Phys.* **121**, 5. https://doi.org/10.1080/00268976.2023.2189491 (2023).
12. Wei, S., Ke, X. & Wang, Y. Wiener indices in random cyclooctane chains. *Wuhan Univ. J. Nat. Sci.* **23**(6), 498–502 (2018).

13. Hechao, L. I. U., Rangwei, W. U., &Lihua, Y. O. U. Three types of Kirchhoff indices in the random cyclooctane chains. 华南师范大学学报 *(自然科学版)* **53**(2), 96–103 (2021).
14. Liu, J. B., Gu, J. J. & Wang, K. The expected values for the Gutman index, Schultz index, and some Sombor indices of a random cyclooctane chain. *Int. J. Quantum Chem.* **123**(3), e27022 (2023).
15. Raza, Z. Zagreb connection indices for some benzenoid systems. *Polycycl. Aromat. Compds.* **42**(4), 1814–1827 (2022).
16. Raza, Z. & Imran, M. Expected values of some molecular descriptors in random cyclooctane chains. *Symmetry* **13**(11), 2197 (2021).
17. Huang, G., Kuang, M. & Deng, H. The expected values of Kirchhoff indices in the random polyphenyl and spiro chains. *ARS Math. Contemp.* **9**(2), 197–207 (2015).
18. Fang, X., You, L. & Liu, H. The expected values of Sombor indices in random hexagonal chains, phenylene chains and Sombor indices of some chemical graphs. *Int. J. Quantum Chem.* **121**(17), e26740 (2021).
19. Huang, G., Kuang, M. & Deng, H. The expected values of Hosoya index and Merrifield–Simmons index in a random polyphenylene chain. *J. Comb. Optim.* **32**(2), 550–562 (2016).
20. Liu, H., Zeng, M., Deng, H. & Tang, Z. Some indices in the random spiro chains. *Iran. J. Math. Chem.* **11**(4), 255–270 (2020).
21. Liu, J. B., Gu, J. J., & Wang, K. The expected values and limiting behaviours for the Gutman index, Schultz index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random cyclooctane chain. *arXiv preprint* arXiv:2203.12923 *(2022).*
22. Qi, J., Fang, M. & Geng, X. The expected value for the wiener index in the random spiro chains. *Polycycl. Aromat. Compd.* **43**(2), 1788–1798 (2023).
23. Qi, J., Ni, J. & Geng, X. The expected values for the Kirchhoff indices in the random cyclooctatetraene and spiro chains. *Discrete Appl. Math.* **321**, 240–249 (2022).
24. Raza, Z., Arockiaraj, M., Bataineh, M. S., &Maaran, A. Cyclooctane chains: mathematical expected values based on atom degree and sum-degree of Zagreb, harmonic, sum-connectivity, and Sombor descriptors. *Eur. Phys. J. Spec. Top.* **4**, 1–10 (2023).
25. Sigarreta, S., Sigarreta, S., & Cruz-Suárez, H. On bond incident degree indices of random spiro chains. *Polycycl. Aromat. Compds.* **8**, 1–13 (2022).
26. Sigarreta, S. C., & Cruz-Suarez, H. Degree based topological indices of a general random chain. *arXiv preprint* arXiv:2205.06385 (2022).
27. Wei, S., Ke, X. & Hao, G. Comparing the excepted values of atom-bond connectivity and geometric–arithmetic indices in random spiro chains. *J. Inequal. Appl.* **2018**(1), 45 (2018).
28. Mansoor, S. *et al.* Recent advancements in Se- and Te-enriched cocatalysts for boosting photocatalytic splitting of water to produce hydrogen. *Res. Chem. Intermed.* **49**, 3723–3745. https://doi.org/10.1007/s11164-023-05077-5 (2023).
29. Tayyab, M., Liu, Y., Liu, Z., Xu, Z., Yue, W., Zhou, L., Lei, J. & Zhang, J. A new breakthrough in photocatalytic hydrogen evolution by amorphous and chalcogenide enriched cocatalysts. *Chem. Eng. J. 5*, 140601 (2022).
30. Liu, Y. *et al.* Single-atom Pt loaded zinc vacancies ZnO–ZnS induced type-V electron transport for efficiency photocatalytic H_2 evolution. *Sol. RRL* **5**, 2100536. https://doi.org/10.1002/solr.202100536 (2021).

Acknowledgements
This work was supported by the China Henan International Joint Laboratory for Multidimensional Topology and Carcinogenic Characteristics Analysis of Atmospheric Particulate Matter PM 2.5; the Key Research Project in Universities of Henan Province (grant no. 21B110004) and Researchers Supporting Project Number (RSP2024R401), King Saud University, Riyadh, Saudi Arabia.

Author contributions
All the author contributed equally.

Competing interests
The authors declare no competing interests.

Additional information
Correspondence and requests for materials should be addressed to A.I.

Reprints and permissions information is available at www.nature.com/reprints.

Publisher's note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.