Bol. Soc. Paran. Mat.
©SPM – E-ISSN-2175-1188
SPM: www.spm.uem.br/bspm

(3s.) **v. 2025 (43)** : 1–22.
ISSN-0037-8712
doi:10.5269/bspm.77385

Computation of Degree Based Molecular Descriptors and Entropies Coronene Fractal Structures

Muhammad Asif Javed, A. Q. Baig, Mukhtar Ahmad*, Suzila Binti Mohd Kasim, Ibrahim K. Alsulami and Ather Qayyum

ABSTRACT: This study focuses on computing entropy and degree-based molecular descriptors for two-dimensional coronene fractal structures at three iterative levels. Key topological indices—including Randic, atom-bond connectivity (ABC_4), geometric-arithmetic (GA), Zagreb, and Sanskurti entropy—are calculated. These indices support the analysis of structure–property and structure–activity relationships, aiding in applications such as drug development and QSAR/QSPR modeling.

Key Words:: Topological indices, randic index, atom-bond connectivity (ABC_4), geometric-arithmetic (GA) index, Sanskurti entropy, Entropy descriptors, Coronene fractal structures.

Contents

1. Introduction

Chemical graph theory provides a powerful mathematical framework for analyzing molecular structures. By representing molecules as graphs, researchers can explore their properties through well-defined mathematical tools. This approach enhances the understanding of molecular behavior and structural characteristics in chemistry [4].

A central concept in chemical graph theory is the use of topological indices—numerical descriptors that capture structural features of chemical graphs. These indices are used to predict various chemical, physical, and biological properties of molecules [25]. They serve as a bridge between molecular structure and observable behavior, making them essential tools in cheminformatics and computational chemistry.

This theory has proven particularly useful for modeling and predicting the physicochemical properties and biological activity of compounds. Techniques like quantitative structure–property relationships (QSPR) and quantitative structure–activity relationships (QSAR) rely heavily on topological indices for predictive modeling [7,8].

In this study, we represent a chemical structure as a simple, connected graph G, where $V(G)$ denotes the set of vertices (atoms) and $E(G)$ the set of edges (bonds). The degree of a vertex u is denoted by $\vartheta(u)$. Bonds are represented by edges between vertices, and the total number of atoms associated with a vertex v_j is expressed as ξ_{v_j}.

* Corresponding author.

Submitted June 19, 2025. Published August 24, 2025
2010 *Mathematics Subject Classification:* 05C90, 05C92, 05C12.

A graph with m atoms and n bonds is characterized by an order $|G|$ and a size $S(G)$, both represented by n. A path in G is an alternating sequence of atoms and bonds. If every pair of atoms is connected by such a path, the graph is considered connected. In this context, the geodesic between two vertices u_i and v_j is the shortest path connecting them, with the number of bonds representing the distance, denoted as $\xi(u_i, v_j)$ [2].

This research focuses on the zigzag and armchair hexagonal coronene fractals, denoted by $ZHCF_{(n)}$. We compute the first through fourth redefined Zagreb entropies, as well as the Sanskurti entropy, atom-bond connectivity entropy, and fifth geometric-arithmetic entropy. The entropy framework is based on the work of Shazia Manzoor [17].

These coronene fractal structures, particularly in zigzag and armchair configurations, have not been extensively studied. Our analysis offers valuable insights for chemists interested in the physicochemical characteristics of these complex molecular systems.

2. Literature Review

Redefined versions of the Zagreb indices $ReZG_1$, $ReZG_2$, and $ReZG_3$ were introduced in 2013 by Ranjini et al. [20]. These have been created as

$$ReZG_1 = \sum_{\upsilon_i \nu_j \in E_(G)} \frac{\xi_{\upsilon_i} + \xi_{\nu_j}}{\xi_{\upsilon_i} \times \xi_{\nu_j}} \tag{2.1}$$

$$ReZG_2 = \sum_{\upsilon_i \nu_j \in E_(G)} \frac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j}} \tag{2.2}$$

$$ReZG_3 = \sum_{u_i v_j \in E_(G)} \left(\xi_{\upsilon_i} + \xi_{\nu_j}\right)\left(\xi_{\upsilon_i} \times \xi_{\nu_j}\right) \tag{2.3}$$

2.1. Atom-bond connectivity index

The degree-based molecular descriptor known as the atom-bond connectivity (ABC) index has garnered significant attention recently and has a wide range of applications in chemistry. Ghorbani and Hosseinzadeh introduced the $ABC4$ index in 2010, representing the fourth iteration of the ABC index. This concept was first introduced by Estrada et al. in 1998, using a similar formulation. Below is the numerical formula for the $ABC4$ [10].

$$ABC_4(G) = \sum_{ts \in E(G)} \sqrt{\frac{\varsigma_t + \varsigma_s - 2}{\varsigma_t \times \varsigma_s}} \tag{2.4}$$

2.2. Geometric-Arithmetic index

The geometric arithmetic index GA5 of a graph G was introduced in its fifth iteration by Graovac et al. [9] in 2011.

$$GA(G) = \sum_{ts \in E(G)} \frac{2\sqrt{\varsigma_t \times \varsigma_s}}{(\varsigma_t + \varsigma_s)} \tag{2.5}$$

2.3. Sanskruti index

The Sanskruti index, abbreviated as S_G and indicated by $S(G)$, was first introduced by Hosamani in 2017 [11] for a molecular graph G as follows.

$$S(G) = \sum_{ts \in E_(G)} \left\{\frac{\varsigma_t \times \varsigma_s}{\varsigma_t + \varsigma_s - 2}\right\}^3 \tag{2.6}$$

Shannon first introduced the concept of entropy in his renowned 1948 paper [23]. The entropy of a probability distribution serves as a measure of uncertainty or unpredictability within a system. Later, the concept of entropy was further developed to better understand structural information in chemical networks and graphs.

Recently, the application of graph entropies has expanded across various fields, including ecology, biology, chemistry, and sociology. The degree of each atom is particularly significant, and extensive research has been conducted in both graph theory and network theory on invariants, which have long been utilized as information functionals in scientific studies.

In this context, we will discuss the graph entropy measures that have been employed to analyze chemical and biological networks, presented in the order of their application.

In the present article, we establish zigzag and armchair hexagonal coronene fractals $ZHCF_{(n)}$, Rectangular coronene fractals $RCF_{(n)}$. calculate its first, second, and third redefined Zagreb entropies. Sanskurti entropy, fifth geometry arithmetic entropy, and fourth atom-bond connectivity entropy using their indices. We made use of the entropy concept found in Shazia Manzoor's article [12,18].

3. Applications of Entropy

In information theory, graph entropy is a significant measure that analyzes chemical graphs and complex networks to uncover structural details. Distance-based entropy is particularly impactful in various contexts, including biology, mathematics, chemical graph theory, and organic chemistry. Shannon's concept of entropy introduces a topological index to graphs, and since topological indices serve as molecular descriptors, they are essential tools in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) research.

Modern information theory began in 1948 with the publication of Shannon's groundbreaking work [22]. After its initial applications in electrical engineering and linguistics, information theory found extensive use in biology and chemistry, notably around 1953 [16]. In 2004, Shannon's entropy formulas were employed to assess the structural information content of networks [24], closely aligning with the work of Trucco (1956) and Rashevsky (1955).

The following sections will cover various graph entropy measures that have been utilized to explore biological and chemical networks sequentially. Entropy measures for graphs have been widely applied in the natural sciences, computer science, and structural chemistry (see, for example, 2011; [6]). The applications of entropies network measures are diverse, encompassing quantitative structure characterization in structural chemistry as well as investigations into the general chemical and biological properties of molecular graphs.

It is important to note that these applications aim to address fundamental problems in data analysis, such as clustering and classification. In this paper, we propose a new assessment method for zigzag and armchair hexagonal coronene fractals $ZHCF_{(n)}$ and Rectangular coronene fractals $RCF_{(n)}$.

4. Degree-Based Entropy

The definition of entropy of an edge-weighted graph G was put forth by Chen et al. in 2014 [5]. The represents an edge-weighted graph, where V_G, E_G, and $\Im(u_iv_j)$ represent, respectively, the set of vertices, the edge set, and the edge-weight of edge. The definition of an edge-weighted graph's entropy is

$$ENT_{\Im(G)} = \sum_{\upsilon_i\nu_j\in E_{(G)}} \frac{\Im(u_iv_j)}{\sum_{\upsilon_i\nu_j\in E_{(G)}}\Im(u_iv_j)} - \log\left\{\frac{\Im(u_iv_j)}{\sum_{\upsilon_i\nu_j\in E_{(G)}}\Im(u_iv_j)}\right\} \tag{4.1}$$

Additional entropies were discovered with the aid of equation 7 and were represented mathematically as follows:

(i) First redefined Zagreb entropy

Let $\Im(u_iv_j) = \dfrac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}$ afterward, the initial, redefined Zagreb index (1) is provided by

$$ReZG_1 = \sum_{\upsilon_i\nu_j\in E_{(G)}} \left\{\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right\} = \sum_{\upsilon_i\nu_j\in E_{(G)}} \Im(u_iv_j) \tag{4.2}$$

Now, by using these values in (7), the first redefined Zagreb entropy is

$$ENT_{(ReZG_1)} = \log(ReZG_1) - \frac{1}{ReZG_1} \log \left\{ \prod_{\upsilon_i \nu_j \in E_{(G)}} \left[\frac{\xi_{\upsilon_i} + \xi_{\nu_j}}{\xi_{\upsilon_i} \times \xi_{\nu_j}} \right]^{\left[\frac{\xi_{\upsilon_i} + \xi_{\nu_j}}{\xi_{\upsilon_i} \times \xi_{\nu_j}} \right]} \right\} \tag{4.3}$$

(ii) Second redefined Zagreb entropy:

Let $\Im(u_i v_j) = \dfrac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j}}$ afterward, the second Zagreb index (2) is provided by

$$ReZG_2 = \sum_{\upsilon_i \nu_j \in E_{(G)}} \left\{ \frac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j}} \right\} = \sum_{\upsilon_i \nu_j \in E_{(G)}} \Im(u_i v_j) \tag{4.4}$$

Now, by using these values in (7), the second redefined Zagreb entropy is

$$ENT_{(ReZG_2)} = \log(ReZG_2) - \frac{1}{ReZG_2} \log \left\{ \prod_{\upsilon_i \nu_j \in E_{(G)}} \left[\frac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j}} \right]^{\left[\frac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j}} \right]} \right\} \tag{4.5}$$

(iii) Third redefined Zagreb entropy:

Let $\Im(u_i v_j) = \left(\xi_{\upsilon_i} + \xi_{\nu_j}\right)\left(\xi_{\upsilon_i} \times \xi_{\nu_j}\right)$ afterward, the third Zagreb index (2) is provided by

$$ReZG_3 = \sum_{\upsilon_i \nu_j \in E_{(G)}} \left\{ \frac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j}} \right\} = \sum_{\upsilon_i \nu_j \in E_{(G)}} \Im(u_i v_j) \tag{4.6}$$

Now, by using these values in (7), the third redefined Zagreb entropy

$$\begin{aligned} ENT_{ReZG_3} = \log(ReZG_3) - \frac{1}{ReZG_3} \\ \log \left\{ \prod_{\upsilon_i \nu_j \in E_{(G)}} \left[\left(\xi_{\upsilon_i} + \xi_{\nu_j}\right)\left(\xi_{\upsilon_i} \times \xi_{\nu_j}\right) \right]^{\left[\left(\xi_{\upsilon_i} + \xi_{\nu_j}\right)\left(\xi_{\upsilon_i} \times \xi_{\nu_j}\right) \right]} \right\} \end{aligned} \tag{4.7}$$

(iv) Entropy of fourth atom-bond connectivity:

Let $\Im(u_i v_j) = \frac{2\sqrt{\varsigma_t \times \varsigma_s}}{(\varsigma_t + \varsigma_s)}$ Consequently, the (4) atom-bond connectivity index is 4th

$$ABC_4(G) = \sum_{ts \in E(G)} = \left\{ \frac{2\sqrt{\varsigma_t \times \varsigma_s}}{(\varsigma_t + \varsigma_s)} \right\} = \sum_{\upsilon_i \nu_j \in E_{(G)}} \Im(u_i v_j) \tag{4.8}$$

Here, S_{u_j} is the neighborhood degree sum of vertex u_i. Now, by using these values in (7), the third redefined Zagreb entropy is

$$\begin{aligned} ENT_{ABC_4(G)} = \log(ABC_4(G)) - \frac{1}{(ABC_4(G))} \\ \log \left\{ \prod_{\upsilon_i \nu_j \in E_{(G)}} \left[\frac{2\sqrt{\varsigma_t \times \varsigma_s}}{(\varsigma_t + \varsigma_s)} \right]^{\left[\frac{2\sqrt{\varsigma_t \times \varsigma_s}}{(\varsigma_t + \varsigma_s)} \right]} \right\} \end{aligned} \tag{4.9}$$

(v) Fifth geometry arithmetic entropy:

Let $\Im(u_i v_j) = \frac{2\sqrt{\varsigma_t \times \varsigma_s}}{(\varsigma_t + \varsigma_s)}$ the fifth geometry arithmetic index is provided by

$$GA_5(G) = \sum_{\upsilon_i \nu_j \in E_{(G)}} \frac{2\sqrt{\varsigma_t \times \varsigma_s}}{(\varsigma_t + \xi_s)} = \sum_{\upsilon_i \nu_j \in E_{(G)}} \Im(u_i v_j) \tag{4.10}$$

Now, by using these values in (7), the fifth geometric arithmetic entropy is

$$ENT_{GA_5(G)} = \log(GA_5(G)) - \frac{1}{(GA_5(G))} \log\left\{ \prod_{\upsilon_i\nu_j \in E_{(G)}} \left[\frac{2\sqrt{\varsigma_t \times \varsigma_s}}{(\varsigma_t + \varsigma_s)}\right]^{\left[\frac{2\sqrt{\varsigma_t \times \varsigma_s}}{(\varsigma_t + \varsigma_s)}\right]} \right\} \tag{4.11}$$

(vi) Sanskruti entropy:

let $\Im(u_i v_j) = \left\{\frac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j} - 2}\right\}^3$ the Sanskruti index is provided by

$$S(G) = \sum_{\upsilon_i\nu_j \in E_{(G)}} \left\{\frac{\varsigma_{\upsilon_i} \times \varsigma_{\nu_j}}{\varsigma_{\upsilon_i} + \varsigma_{\nu_j} - 2}\right\}^3 = \sum_{\upsilon_i\nu_j \in E_{(G)}} \Im(u_i v_j) \tag{4.12}$$

Now, by using these values in equation (7), the Sanskruti entropy

$$ENT_S(G) = \log(S(G)) - \frac{1}{(S(G))} \log\left\{ \prod_{\upsilon_i\nu_j \in E_{(G)}} \left[\left\{\frac{\varsigma_{\upsilon_i} \times \varsigma_{\nu_j}}{\varsigma_{\upsilon_i} + \varsigma_{\nu_j} - 2}\right\}^3\right]^{\left[\left\{\frac{\varsigma_{\upsilon_i} \times \varsigma_{\nu_j}}{\varsigma_{\upsilon_i} + \varsigma_{\nu_j} - 2}\right\}^3\right]} \right\} \tag{4.13}$$

Klein et al. [15] conducted a systematic investigation of deterministic benzenoid fractals by methodically compounding benzene at various stages. The first stage involves benzene itself, while subsequent stages include benzenoid compounds such as kekulene, coronene, and singly connected benzene. Specifically, the coronoid family of benzenoid fractals is created by encircling benzene to form coronene, then fusing six copies of benzenoid perylenes through their bay regions. This process results in a hexabenzocoronene structure surrounded by six coronene-shaped frames, as illustrated in Figure 1. The nth stage fractal of the coronoid family is typically formed by combining six copies of the fractal structures from the $(n-1)$ stage, for $n \geq 1$. Synthetic organic chemists and materials scientists are interested in these materials as they serve as precursors to new nanomaterials in biotechnology and nanotechnology. El-Basil [3] has demonstrated that the characteristic scaling factor of molecular fractals corresponds to the golden ratio ($\tau = 1.618033989$), while Plavsic et al. [19] have explored the aromaticity of fractal benzenoids based on Clar structures. Although discussions about the potential synthesis of these fractal molecules began in the early 1990s [15], the process remains challenging to this day. This work aims to provide a theoretical characterization of these molecular fractals based on coronene, which will enhance our understanding of the behaviors of these fractal elements.

The zigzag and armchair hexagonal coronene fractals $ZHCF_{(n)}$, Rectangular coronene fractals $RCF_{(n)}$ structures because the benzenoid form contains rings. The specific arrangement of rings in the benzenoid system provides a series of benzenoid structures of the benzenoid graph, which is how the structures are changed. As seen in Figure 1, the number of [1] in the middle of the series of hidden zigzag and armchair hexagonal coronene fractals $ZHCF_{(n)}$, Rectangular coronene fractals $RCF_{(n)}$ benzenoid graph is shown in [13], where n show the number of level in the zigzag and armchair hexagonal and Rectangular coronene fractals as show in figurs. Similarly for n=$RCF_{(n)}$ and n=$RCF_{(n)}$. There are three different kinds of atom-bonds in the zigzag and armchair hexagonal coronene fractals $ZHCF_{(n)}$, Rectangular coronene fractals $RCF_{(n)}$ benzenoid graph , according to the valency of each atom. It is evident from this comprehension of atom-bonds that there are two types of atoms, v_i and v_j, such that $\xi = 2$ and $\xi = 3$, where ξ_i and ξ_j stand for the valency of atoms $\forall v_i, v_j \in ZHCF_{(n)}$. $ZHCF_{(n)}$ is the size and order of armchair hexagonal coronene fractals benzenoid graphs.

Following are the four figures of zigzag and armchair hexagonal and Rectangular coronene fractals graphs $Level_1$, $Level_2$, $Level_3$ and $Level_4$. According to the degree of the atoms, there are three types of atom-bonds in $ZHCF_{(n)}$: (2,2), (2,3)and (3,3). The atom-bonds partition of $ZHCF_{(n)}$ is shown as

$$
\begin{aligned}
E_{(2,2)} &= \{e = u, v; \forall u, v \in E(ZHCF_n) | \xi_u = 2; \xi_v = 3\} \\
E_{(2,3)} &= \{e = u, v; \forall u, v \in E(ZHCF_n) | \xi_u = 2; \xi_v = 3\} \qquad (4.14) \\
E_{(3,3)} &= \{e = u, v; \forall u, v \in E(ZHCF_n) | \xi_u = 2; \xi_v = 3\}
\end{aligned}
$$

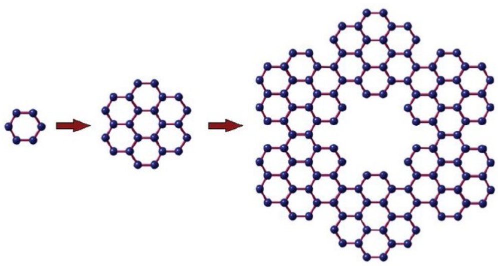


Figure 1: The Level one of zigzag and armchair hexagonal coronene fractals $ZHCF = 1$

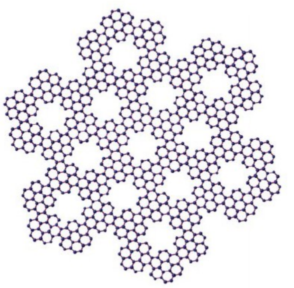


Figure 2: The Level two of zigzag and armchair hexagonal coronene fractals $ZHCF = 2$

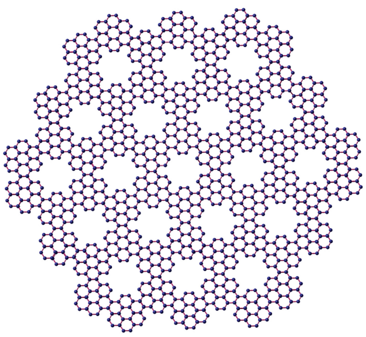


Figure 3: The Level three of zigzag and armchair hexagonal coronene fractals $ZHCF = 3$

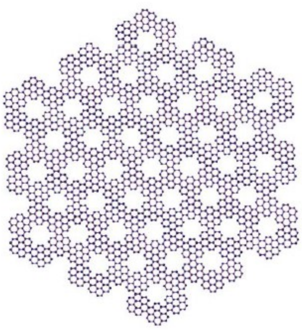


Figure 4: The Level four of zigzag and armchair hexagonal coronene fractals $ZHCF = 4$

The order and size of zigzag and armchair hexagonal coronene fractals $ZHCF_{(n)}$

$$|V| = 3(57n^2 + n)$$

$$|E| = 6(21n^2 + n)$$

Let $G = ZHCF(n)$ is the Coronene structures. Then 1st, 2nd and third Zagreb indices as:

Using Table 1 and (1) in (9), we are now computing the first redefined Zagrab entropy in the manner shown below:

$$ReZG_1(ZHCF_n) = 132\, n^2 + 8\, n$$

Types of atom-bonds	$E_{(2,2)}$	$E_{(2,3)}$	$E_{(3,3)}$
Frequency of atom-bonds	$3(9n^2+n)$	$6(9n^2+n)$	$6(15n^2+n)$

Table 1: Edge partition of zigzag and armchair hexagonal coronene fractals $ZHCF_{(n)}$

$$
\begin{aligned}
ENT_{ReZG_1} &= \log(ReZG_1) - \frac{1}{ReZG_1}\log\Bigg\{\prod_{\upsilon_i\nu_j\in E_{(2,2)}}\left[\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right]^{\left[\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right]} \\
&\times\prod_{\upsilon_i\nu_j\in E_{(2,3)}}\left[\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right]^{\left[\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right]}\times\prod_{\upsilon_i\nu_j\in E_{(3,3)}}\left[\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right]^{\left[\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right]}\Bigg\} \\
&= \log(132\,n^2+8\,n) - \frac{1}{\left(132\,n^2+8\,n\right)}\log\Bigg\{\left(3(9n^2+n)\right)\left(\frac{4}{4}\right)^{\left(\frac{4}{4}\right)} \\
&\times\left(6(9n^2+n)\right)\left(\frac{5}{6}\right)^{\left(\frac{5}{6}\right)}\times\left(6(15n^2+n)\right)\left(\frac{6}{9}\right)^{\left(\frac{6}{9}\right)}\Bigg\} \\
&= \log(132\,n^2+8\,n) - \frac{1}{132\,n^2+8\,n}\log\Bigg\{\left(3(9n^2+n)\right)\left(1\right) \\
&\times\left(6(9n^2+n)\right)\left(\frac{5}{6}\right)^{\left(\frac{5}{6}\right)}\times\left(6(15n^2+n)\right)\left(\frac{2}{3}\right)^{\left(\frac{2}{3}\right)}\Bigg\}
\end{aligned}
$$

$$
ENT_{ReZG_1} = log\,\left(132\,n^2+8\,n\right) - \frac{log\,\left\{15\,\left(9\,n^2+n\right)\left(9\,n^2+5\,n\right)5^{2/3}\sqrt[3]{6}\left(3\,n^2-n\right)\right\}}{132\,n^2+8\,n} \tag{4.15}
$$

Using Table 1 and (2) in (11), we are now computing the Sconed redefined Zagrab entropy in the manner shown below:

$$
ReZG_2(ZHCF_n) = \frac{1134\,n^2}{5} + \frac{51\,n}{5}
$$

$$ENT_{ReZG_2} = \log(ReZG_2) - \frac{1}{ReZG_2}\log\left\{\prod_{\upsilon_i\nu_j\in E(2,2)}\left[\frac{\xi_{\upsilon_i}\times\xi_{\nu_j}}{\xi_{\upsilon_i}+\xi_{\nu_j}}\right]^{\left[\frac{\xi_{\upsilon_i}\times\xi_{\nu_j}}{\xi_{\upsilon_i}+\xi_{\nu_j}}\right]}\right.$$

$$\left.\times\prod_{\upsilon_i\nu_j\in E(2,3)}\left[\frac{\xi_{\upsilon_i}\times\xi_{\nu_j}}{\xi_{\upsilon_i}+\xi_{\nu_j}}\right]^{\left[\frac{\xi_{\upsilon_i}\times\xi_{\nu_j}}{\xi_{\upsilon_i}+\xi_{\nu_j}}\right]}\times\prod_{\upsilon_i\nu_j\in E(3,3)}\left[\frac{\xi_{\upsilon_i}\times\xi_{\nu_j}}{\xi_{\upsilon_i}+\xi_{\nu_j}}\right]^{\left[\frac{\xi_{\upsilon_i}\times\xi_{\nu_j}}{\xi_{\upsilon_i}+\xi_{\nu_j}}\right]}\right\}$$

$$= \log\left(\frac{1134\,n^2}{5}+\frac{51\,n}{5}\right) - \frac{1}{\left(\frac{1134\,n^2}{5}+\frac{51\,n}{5}\right)}\log\left\{\left(3(9n^2+n)\right)\left(\frac{4}{4}\right)^{\left(\frac{4}{4}\right)}\right.$$

$$\left.\times\left(6(9n^2+n)\right)\left(\frac{6}{5}\right)^{\left(\frac{6}{5}\right)}\times\left(6(15n^2+n)\right)\left(\frac{9}{6}\right)^{\left(\frac{9}{6}\right)}\right\}$$

$$= \log\left(132\,n^2+8\,n\right) - \frac{1}{132\,n^2+8\,n}\log\left\{\left(3(9n^2+n)\right)\left(1\right)\right.$$

$$\left.\times\left(6(9n^2+n)\right)\left(\frac{6}{5}\right)^{\left(\frac{6}{5}\right)}\times\left(6(15n^2+n)\right)\left(\frac{3}{2}\right)^{\left(\frac{3}{2}\right)}\right\}$$

Using Table 1 and (3) in (13), we are now computing the third redefined Zagrab entropy in the manner shown below:

$$ReZG_3(ZHCF_n) = 6912\,n^2 + 228\,n$$

$$ENT_{ReZG_3} = \log(ReZG_3) - \frac{1}{ReZG_3}\log\left\{\prod_{\upsilon_i\nu_j\in E_{2,2}}\left(\xi_{\upsilon_i}+\xi_{\nu_j}\right)\left(\xi_{\upsilon_i}\times\xi_{\nu_j}\right)\right.$$

$$\left.\times\prod_{\upsilon_i\nu_j\in E_{2,3}}\left(\xi_{\upsilon_i}+\xi_{\nu_j}\right)\left(\xi_{\upsilon_i}\times\xi_{\nu_j}\right)\times\prod_{\upsilon_i\nu_j\in E_{3,3}}\left(\xi_{\upsilon_i}+\xi_{\nu_j}\right)\left(\xi_{\upsilon_i}\times\xi_{\nu_j}\right)\right\}$$

$$= \log(ReZG_3) - \frac{1}{ReZG_3}\log\left\{3(9n^2+n)\,(2+2)\,(2\times 2)^{(2+2)(2\times 2)}\right.$$

$$\left.+\,6(9n^2+n)\,(2+3)\,(2\times 3)^{(2+3)(2\times 3)} + 6(15n^2-n)\,(3+3)\,(3\times 3)^{(3+3)(3\times 3)}\right\}$$

$$ENT_{ReZG_3} = \log\left(6912\,n^2+228\,n\right) - \frac{1}{\left(6912\,n^2+228\,n\right)}$$

$$\log\left\{3(9n^2+n)(16)^{16}\times 6(9n^2+n)(30)^{30}\times 6(15n^2-n)(54)^{54}\right\}$$

Fourth atom-bond connectivity entropy of $ZHCF(n)$:

Based on the valency sum of the end atoms of each degree, Table 2 shows the atom-bond partition of the zigzag and armchair hexagonal coronene fractals $ZHCF_{(n)}$. Let $ZHCF_{(n)}$ represent the graph of armchair hexagonal coronene fractals. Next, Table 2 in (4) is used to obtain the fourth atom-bond connectivity index.

$(\varsigma_t, \varsigma_s)$	Sum of valency of the neighborhood atoms	Frequency
$\varsigma_1(G)$	(5,5)	$3(9n^2+n)$
$\varsigma_2(G)$	(5,7)	$3(9n^2+5n)$
$\varsigma_3(G)$	(5,8)	$12(3n^2-n)$
$\varsigma_4(G)$	(7,9)	$12n$
$\varsigma_5(G)$	(8,9)	$12(3n^2-n)$
$\varsigma_6(G)$	(9,9)	$3(15n^2-n)$

Table 2: Edge partition sum of valency of the neighborhood atoms zigzag and armchair hexagonal coronene fractals $ZHCF_{(n)}$

$$ABC_4(G) = \Bigg\{\Big(\frac{54\sqrt{62}}{5} + \frac{27\sqrt{14630}}{35} + \frac{18\sqrt{1295}}{5} + 6\sqrt{611} + 20\sqrt{91}\Big)n^2 + \Big(\frac{6\sqrt{62}}{5} + \frac{3\sqrt{14630}}{7} - \frac{6\sqrt{1295}}{5} + \frac{4\sqrt{7042}}{7} - 2\sqrt{611} - \frac{4\sqrt{91}}{3}\Big)n\Bigg\} \tag{4.16}$$

Now let's calculate the fourth atom-bond connectivity entropy using Table 2 and Equation (4) in (15) as follows:

$$ENT_{ABC_4} = \log(ABC_4(G)) - \frac{1}{(ABC_4(G))}\log\Bigg\{3(9n^2+n)\left[\sqrt{\frac{5+5-2}{5\times5}}\right]^{\left[\sqrt{\frac{5+5-2}{5\times5}}\right]} + 3(9n^2+5n)\left[\sqrt{\frac{5+7-2}{5\times7}}\right]^{\left[\sqrt{\frac{5+7-2}{5\times5}}\right]} + 12(3n^2-n)\left[\sqrt{\frac{5+8-2}{5\times8}}\right]^{\left[\sqrt{\frac{5+8-2}{5\times8}}\right]} + 12n\left[\sqrt{\frac{7+9-2}{7\times9}}\right]^{\left[\sqrt{\frac{7+9-2}{7\times9}}\right]} + 12(3n^2-n)\left[\sqrt{\frac{8+9-2}{8\times9}}\right]^{\left[\sqrt{\frac{8+9-2}{8\times9}}\right]} + 3(15n^2-n)\left[\sqrt{\frac{9+9-2}{9\times9}}\right]^{\left[\sqrt{\frac{9+9-2}{9\times9}}\right]}\Bigg\}$$

$$ENT_{(ABC_4(G))} = \Bigg\{\Big(\frac{54\sqrt{62}}{5} + \frac{27\sqrt{14630}}{35} + \frac{18\sqrt{1295}}{5} + 6\sqrt{611} + 20\sqrt{91}\Big)n^2 + \Big(\frac{6\sqrt{62}}{5} + \frac{3\sqrt{14630}}{7} - \frac{6\sqrt{1295}}{5} + \frac{4\sqrt{7042}}{7} - 2\sqrt{611} - \frac{4\sqrt{91}}{3}\Big)n\Bigg\}$$

$$-\frac{1}{\left(\frac{54\sqrt{62}}{5}+\frac{27\sqrt{14630}}{35}+\frac{18\sqrt{1295}}{5}+6\sqrt{611}+20\sqrt{91}\right)n^2+\left(\frac{6\sqrt{62}}{5}+\frac{3\sqrt{14630}}{7}-\frac{6\sqrt{1295}}{5}+\frac{4\sqrt{7042}}{7}-2\sqrt{611}-\frac{4\sqrt{91}}{3}\right)n}$$

$$\begin{aligned}&\times\log\Bigg\{3(9n^2+n)\left[\frac{\sqrt{8}}{5}\right]^{\left[\frac{\sqrt{8}}{5}\right]}+3(9n^2+5n)\left[\sqrt{\frac{10}{35}}\right]^{\left[\sqrt{\frac{10}{35}}\right]}+12(3n^2-n)\left[\sqrt{\frac{11}{40}}\right]^{\left[\sqrt{\frac{11}{40}}\right]}\\&+12n\left[\sqrt{\frac{14}{63}}\right]^{\left[\sqrt{\frac{14}{63}}\right]}+12(3n^2-n)\left[\sqrt{\frac{15}{72}}\right]^{\left[\sqrt{\frac{15}{72}}\right]}+3(15n^2-n)\left[\frac{4}{9}\right]^{\left[\frac{4}{9}\right]}\Bigg\}\end{aligned} \tag{4.17}$$

Fifth geometry arithmetic entropy:

$$\begin{aligned}GA(G)=&\left(117+\frac{9\sqrt{35}}{2}+\frac{144\sqrt{10}}{13}+\frac{432\sqrt{2}}{17}\right)n^2-\left(3+\frac{5\sqrt{35}}{2}-\frac{48\sqrt{10}}{13}+\frac{9\sqrt{7}n}{2}-\right.\\&\left.\frac{144\sqrt{2}}{17}\right)n\end{aligned} \tag{4.18}$$

Now let's calculate the Fifth geometry arithmetic entropy using Table 2 and Equation (5) in (17) as follows:

$$\begin{aligned}ENT_{(GA)}=&\log(GA)-\frac{1}{(GA)}\log\Bigg\{3(9n^2+n))\left[\frac{2\sqrt{5\times5}}{(5+5)}\right]^{\left[\frac{2\sqrt{5\times5}}{(5+5)}\right]}\times3(9n^2+5n)\left[\frac{2\sqrt{5\times7}}{(5+7)}\right]^{\left[\frac{2\sqrt{5\times7}}{(5+7)}\right]}\\&\times12(3n^2-n)\left[\frac{2\sqrt{5\times8}}{(5+8)}\right]^{\left[\frac{2\sqrt{5\times8}}{(5+8)}\right]}\times12n\left[\frac{2\sqrt{7\times9}}{(7+9)}\right]^{\left[\frac{2\sqrt{7\times9}}{(7+9)}\right]}\\&\times12(3n^2-n)\left[\frac{2\sqrt{8\times9}}{(8+9)}\right]^{\left[\frac{2\sqrt{8\times9}}{(8+9)}\right]}\times3(15n^2-n)\left[\frac{2\sqrt{9\times9}}{(9+9)}\right]^{\left[\frac{2\sqrt{9\times9}}{(9+9)}\right]}\Bigg\}\end{aligned} \tag{4.19}$$

$$\begin{aligned}ENT_{(GA)}=&\left(117+\frac{9\sqrt{35}}{2}+\frac{144\sqrt{10}}{13}+\frac{432\sqrt{2}}{17}\right)n^2-\left(3+\frac{5\sqrt{35}}{2}-\frac{48\sqrt{10}}{13}+\frac{9\sqrt{7}n}{2}-\right.\\&\left.\frac{144\sqrt{2}}{17}\right)n\end{aligned}$$

$$-\frac{1}{\left(117+\frac{9\sqrt{35}}{2}+\frac{144\sqrt{10}}{13}+\frac{432\sqrt{2}}{17}\right)n^2-\left(3+\frac{5\sqrt{35}}{2}-\frac{48\sqrt{10}}{13}+\frac{9\sqrt{7}n}{2}-\frac{144\sqrt{2}}{17}\right)n}$$

$$\begin{aligned}&\times\log\Bigg\{3(9n^2+n)(1)\times3(9n^2+5n)\left[\frac{\sqrt{35}}{6}\right]^{\left[\frac{\sqrt{35}}{6}\right]}\times12(3n^2-n)\left[\frac{2\sqrt{40}}{13}\right]^{\left[\frac{2\sqrt{40}}{13}\right]}\times12n\left[\frac{\sqrt{63}}{8}\right]^{\left[\frac{\sqrt{63}}{8}\right]}\\&\times12(3n^2-n)\left[\frac{2\sqrt{72}}{17}\right]^{\left[\frac{2\sqrt{72}}{17}\right]}\times3(15n^2-n)(1)\Bigg\}\end{aligned}$$

Sanskruti entropy:

$$\begin{aligned}S(G)=&\left(27\left\{\frac{10}{23}\right\}^3+27\{4/11\}^3+36\left\{\frac{13}{38}\right\}^3+36\left\{\frac{17}{70}\right\}^3+45\left\{\frac{18}{79}\right\}^3\right)n^2\\&+\left(3\left\{\frac{10}{23}\right\}^3+15\{4/11\}^3-12\left\{\frac{13}{38}\right\}^3n+12\left\{\frac{16}{61}\right\}^3-12\left\{\frac{17}{70}\right\}^3-3\left\{\frac{18}{79}\right\}^3\right)n\end{aligned} \tag{4.20}$$

Now let's calculate the Sanskruti entropy using Table 2 and Equation (6) in (19) as follows:

$$ENT_S(G) = \log(S(G)) - \frac{1}{(S(G))} \log \Bigg\{ 3(9n^2+n)\left[\left\{\frac{5\times 5}{(5+5)-2}\right\}^3\right]^{\left[\left\{\frac{5\times 5}{(5+5)-2}\right\}^3\right]}$$
$$+ 3(9n^2+5n)\left[\left\{\frac{5\times 7}{(5+7)-2}\right\}^3\right]^{\left[\left\{\frac{5\times 7}{(5+7)-2}\right\}^3\right]}$$
$$+ 12(3n^2-n)\left[\left\{\frac{5\times 8}{(5+8)-2}\right\}^3\right]^{\left[\left\{\frac{5\times 8}{(5+8)-2}\right\}^3\right]}$$
$$+ 12n\left[\left\{\frac{7\times 9}{(7+9)-2}\right\}^3\right]^{\left[\left\{\frac{7\times 9}{(7+9)-2}\right\}^3\right]}$$
$$+ 12(3n^2-n)\left[\left\{\frac{8\times 9}{(8+9)-2}\right\}^3\right]^{\left[\left\{\frac{8\times 9}{(8+9)-2}\right\}^3\right]}$$
$$+ 3(15n^2-n)\left[\left\{\frac{9\times 9}{(9+9)-2}\right\}^3\right]^{\left[\left\{\frac{9\times 9}{(9+9)-2}\right\}^3\right]} \Bigg\}$$

$$\begin{aligned} ENT_S(G) = \log(S(G)) - \frac{1}{(S(G))} \log \Bigg\{ & 3(9n^2+n)\left[\left\{\frac{25}{8}\right\}^3\right]^{\left[\left\{\frac{25}{8}\right\}^3\right]} \\ & + 3(9n^2+5n)\left[\left\{\frac{35}{10}\right\}^3\right]^{\left[\left\{\frac{35}{10}\right\}^3\right]} + 12(3n^2-n)\left[\left\{\frac{40}{11}\right\}^3\right]^{\left[\left\{\frac{40}{11}\right\}^3\right]} \\ & + 12n\left[\left\{\frac{9}{2}\right\}^3\right]^{\left[\left\{\frac{9}{2}\right\}^3\right]} + 12(3n^2-n)\left[\left\{\frac{24}{5}\right\}^3\right]^{\left[\left\{\frac{24}{5}\right\}^3\right]} \\ & + 3(15n^2-n)\left[\left\{\frac{81}{16}\right\}^3\right]^{\left[\left\{\frac{81}{16}\right\}^3\right]} \Bigg\} \end{aligned} \tag{4.21}$$

Comparison of (a) and (b)

The rectangular coronene fractals structures $RCF_{(n)}$ benzenoid graph have three different types of atom-bonds depending on the valency of each atom. It is evident from this understanding of atom-bonds that there are two different types of atoms: v_i and v_j. These atoms are such that $\xi = 2$ and $\xi = 3$, where the valencies of atoms $\forall v_i, v_j \in RCF_{(n)}$ are represented by the variables ξ_i and ξ_j. $RCF_{(n)}$ represents the size and order of Rectangular coronene fractals structures $RCF_{(n)}$.

Following are the figures of Rectangular coronene fractals structures graphs $Level_1$, $Level_2$, $Level_3$ and $Level_4$. According to the degree of the atoms, there are three types of atom-bonds in $RCF_{(n)}$: (2,2), (2,3) and (3,3). The atom-bonds partition of $RCF_{(n)}$ is shown as

$$\begin{aligned} E_{(2,2)} &= \{e = u, v; \forall u, v \in E(RCF_n) | \xi_u = 2; \xi_v = 3\} \\ E_{(2,3)} &= \{e = u, v; \forall u, v \in E(RCF_n) | \xi_u = 2; \xi_v = 3\} \\ E_{(3,3)} &= \{e = u, v; \forall u, v \in E(RCF_n) | \xi_u = 2; \xi_v = 3\} \end{aligned} \tag{4.22}$$

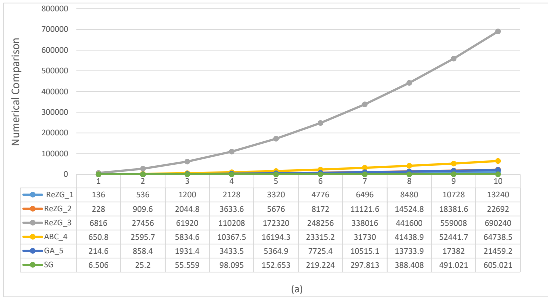


Figure 5: Comparison of $ReZG_1(ZHCF_n)$, $ReZG_2(ZHCF_n)$, $ReZG_3(ZHCF_n)$, $ABC_4(ZHCF_n)$, $GA_5(ZHCF_n)$, $SG(ZHCF_n)$.

The order and size of Rectangular coronene fractals structures $RCF_{(n)}$

$$|V| = 12(7n^2 + 4n)$$

$$|E| = 6(19n^2 + 10n)$$

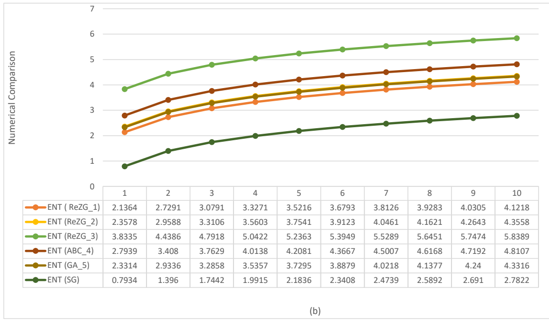
Types of atom-bonds	$E_{(2,2)}$	$E_{(2,3)}$	$E_{(3,3)}$
Frequency of atom-bonds	$6(3n^2 + 2n)$	$12(3n^2 + 2n)$	$12(5n^2 + 2n)$

Table 3: Edge partition of Rectangular coronene fractals structures $RCF_{(n)}$

Let $G = RCF(n)$ is the Coronene structures. Then 1st, 2nd and third Zagreb indices as:

Using Table 3 and (1) in (9), we are now computing the first redefined Zagrab entropy in the manner shown below:

$$ReZG_1(RCF_n) = 88\,n^2 + 48\,n$$



	1	2	3	4	5	6	7	8	9	10
ENT (ReZG_1)	2.1364	2.7291	3.0791	3.3271	3.5216	3.6793	3.8126	3.9283	4.0305	4.1218
ENT (ReZG_2)	2.3578	2.9588	3.3106	3.5603	3.7541	3.9123	4.0461	4.1621	4.2643	4.3558
ENT (ReZG_3)	3.8335	4.4386	4.7918	5.0422	5.2363	5.3949	5.5289	5.6451	5.7474	5.8389
ENT (ABC_4)	2.7939	3.408	3.7629	4.0138	4.2081	4.3667	4.5007	4.6168	4.7192	4.8107
ENT (GA_5)	2.3314	2.9336	3.2858	3.5357	3.7295	3.8879	4.0218	4.1377	4.24	4.3316
ENT (SG)	0.7934	1.396	1.7442	1.9915	2.1836	2.3408	2.4739	2.5892	2.691	2.7822

Figure 6: Comparison of $ENTReZG_1(ZHCF_n)$, $ENTReZG_2(ZHCF_n)$, $ENTReZG_3(ZHCF_n)$, $ENTABC_4(ZHCF_n)$, $ENTGA_5(ZHCF_n)$, $ENTSG(ZHCF_n)$.

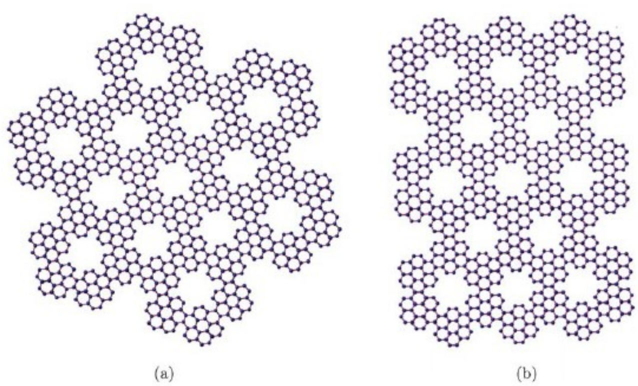


Figure 7: Coronene fractals structures (a) $ZHCF(2)$ and (b)$RCF(3,3)$

$$
\begin{aligned}
ENT_{ReZG_1} &= \log(ReZG_1) - \frac{1}{ReZG_1}\log\Bigg\{\prod_{\upsilon_i\nu_j\in E_{(2,2)}}\left[\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right]^{\left[\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right]} \\
&\times \prod_{\upsilon_i\nu_j\in E_{(2,3)}}\left[\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right]^{\left[\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right]} \times \prod_{\upsilon_i\nu_j\in E_{(3,3)}}\left[\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right]^{\left[\frac{\xi_{\upsilon_i}+\xi_{\nu_j}}{\xi_{\upsilon_i}\times\xi_{\nu_j}}\right]}\Bigg\} \\
&= \log(88\,n^2+48\,n) - \frac{1}{\left(88\,n^2+48\,n\right)}\log\Bigg\{\left(6(3n^2+2n)\right)\left(\frac{4}{4}\right)^{\left(\frac{4}{4}\right)} \\
&\times \left(12(3n^2+2n)\right)\left(\frac{5}{6}\right)^{\left(\frac{5}{6}\right)} \times \left(12(5n^2+2n)\right)\left(\frac{6}{9}\right)^{\left(\frac{6}{9}\right)}\Bigg\}
\end{aligned}
$$

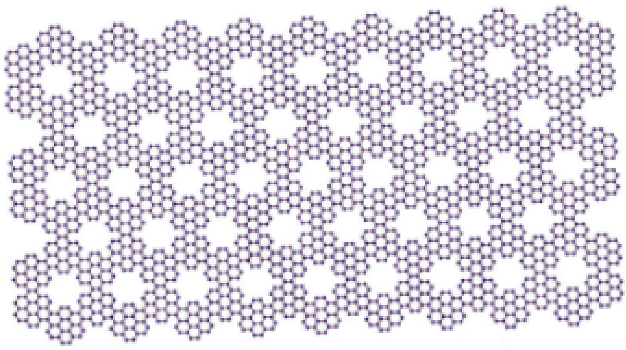


Figure 8: Rectangular coronene fractals $RCF_{(3,9)}$

$$ENT_{ReZG_1} = \log(132\,n^2 + 8\,n) - \frac{1}{132\,n^2 + 8\,n} \log\left\{ \Big(6(3n^2 + 2n)\Big)\Big(1\Big) \times \Big(12(3n^2 + 2n)\Big)\left(\frac{5}{6}\right)^{\left(\frac{5}{6}\right)} \times \Big(12(5n^2 + 2n)\Big)\left(\frac{2}{3}\right)^{\left(\frac{2}{3}\right)} \right\} \tag{4.23}$$

Using Table 3 and (2) in (11), we are now computing the Sconed redefined Zagrab entropy in the manner shown below:

$$\begin{aligned} ENT_{ReZG_2} &= \log(ReZG_1) - \frac{1}{ReZG_1} \log\left\{ \prod_{\upsilon_i\nu_j \in E_{(2,2)}} \left[\frac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j}}\right]^{\left[\frac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j}}\right]} \right. \\ &\times \prod_{\upsilon_i\nu_j \in E_{(2,3)}} \left[\frac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j}}\right]^{\left[\frac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j}}\right]} \times \left. \prod_{\upsilon_i\nu_j \in E_{(3,3)}} \left[\frac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j}}\right]^{\left[\frac{\xi_{\upsilon_i} \times \xi_{\nu_j}}{\xi_{\upsilon_i} + \xi_{\nu_j}}\right]} \right\} \\ &= \log\left(\frac{1134\,n^2}{5} + \frac{51\,n}{5}\right) - \frac{1}{\left(\frac{1134\,n^2}{5} + \frac{51\,n}{5}\right)} \log\left\{ \Big(6(3n^2 + 2n)\Big)\left(\frac{4}{4}\right)^{\left(\frac{4}{4}\right)} \right. \\ &\times \left. \Big(12(3n^2 + 2n)\Big)\left(\frac{6}{5}\right)^{\left(\frac{6}{5}\right)} \times \Big(12(5n^2 + 2n)\Big)\left(\frac{9}{6}\right)^{\left(\frac{9}{6}\right)} \right\} \end{aligned}$$

$$ENT_{ReZG_2} = \log\left(\frac{756\,n^2}{5} + \frac{384\,n}{5}\right) - \frac{1}{\left(\frac{756\,n^2}{5} + \frac{384\,n}{5}\right)} \log\left\{ \Big(3(9n^2 + 2n)\Big)\Big(1\Big) \times \Big(6(9n^2 + 2n)\Big)\left(\frac{6}{5}\right)^{\left(\frac{6}{5}\right)} \times \Big(6(15n^2 + 2n)\Big)\left(\frac{3}{2}\right)^{\left(\frac{3}{2}\right)} \right\} \tag{4.24}$$

Using Table 3 and (3) in (13), we are now computing the third redefined Zagrab entropy in the manner shown below:

$$\begin{aligned}
ENT_{ReZG_3} &= \log(ReZG_3) - \frac{1}{ReZG_3}\log\Bigg\{\prod_{\upsilon_i\nu_j\in E_{2,2}}\left(\xi_{\upsilon_i}+\xi_{\nu_j}\right)\left(\xi_{\upsilon_i}\times\xi_{\nu_j}\right)\\
&\times\prod_{\upsilon_i\nu_j\in E_{2,3}}\left(\xi_{\upsilon_i}+\xi_{\nu_j}\right)\left(\xi_{\upsilon_i}\times\xi_{\nu_j}\right)\times\prod_{\upsilon_i\nu_j\in E_{3,3}}\left(\xi_{\upsilon_i}+\xi_{\nu_j}\right)\left(\xi_{\upsilon_i}\times\xi_{\nu_j}\right)\Bigg\}\\
&= \log(ReZG_3) - \frac{1}{ReZG_3}\log\Bigg\{6(3n^2+2n)\,(2+2)\,(2\times 2)^{(2+2)(2\times 2)}\\
&+ 12(3n^2+2n)\,(2+3)\,(2\times 3)^{(2+3)(2\times 3)} + 12(5n^2+2n)\,(3+3)\,(3\times 3)^{(3+3)(3\times 3)}\Bigg\}
\end{aligned} \tag{4.25}$$

$$\begin{aligned}
ENT_{ReZG_3} &= \log\left(6912\,n^2+228\,n\right) - \frac{1}{\left(6912\,n^2+228\,n\right)}\\
&\log\left\{6(3n^2+2n)(16)^{16}\times 12(3n^2+2n)(30)^{30}\times 12(5n^2+2n)(54)^{54}\right\}
\end{aligned}$$

$(\varsigma_t, \varsigma_s)$	Sum of valency of the neighborhood atoms	Frequency
$\varsigma_1(G)$	(5,5)	$6(3n^2+2n)$
$\varsigma_2(G)$	(5,7)	$6(3n^2+4n)$
$\varsigma_3(G)$	(5,8)	$24n^2$
$\varsigma_4(G)$	(7,9)	$12n$
$\varsigma_5(G)$	(8,9)	$24n^2$
$\varsigma_6(G)$	(9,9)	$6(5n^2+2n)$

Table 4: Edge partition (sum of valency of the neighborhood atoms Rectangular coronene Structures $RCF(n)$)

Entropy of fourth atom-bond connectivity:

$$\begin{aligned}
ABC_4(G) &= \Bigg\{\left(\frac{36\sqrt{62}}{5}+\frac{18\sqrt{14630}}{35}+\frac{12\sqrt{1295}}{5}+4\sqrt{611}+\frac{40\sqrt{91}}{3}\right)n^2\\
&+\left(\frac{24\sqrt{62}n}{5}+\frac{24\sqrt{14630}n}{35}+\frac{4\sqrt{7042}n}{7}+\frac{16\sqrt{91}n}{3}\right)n\Bigg\}
\end{aligned} \tag{4.26}$$

Using Table 4 and (4) in (15), we are now computing the third redefined Zagrab entropy in the manner shown below:

$$ENT_{(ABC_4(G))} = \log(ABC_4(G)) - \frac{1}{(ABC_4(G))}\log\Bigg\{3(9n^2+n)\left[\sqrt{\frac{5+5-2}{5\times5}}\right]^{\left[\sqrt{\frac{5+5-2}{5\times5}}\right]} +3(9n^2+5n)\left[\sqrt{\frac{5+7-2}{5\times7}}\right]^{\left[\sqrt{\frac{5+7-2}{5\times5}}\right]} + 12(3n^2-n)\left[\sqrt{\frac{5+8-2}{5\times8}}\right]^{\left[\sqrt{\frac{5+8-2}{5\times8}}\right]} +12n\left[\sqrt{\frac{7+9-2}{7\times9}}\right]^{\left[\sqrt{\frac{7+9-2}{7\times9}}\right]} + 12(3n^2-n)\left[\sqrt{\frac{8+9-2}{8\times9}}\right]^{\left[\sqrt{\frac{8+9-2}{8\times9}}\right]} +3(15n^2-n)\left[\sqrt{\frac{9+9-2}{9\times9}}\right]^{\left[\sqrt{\frac{9+9-2}{9\times9}}\right]}\Bigg\}$$

$$ENT_{(ABC_4(G))} = \Bigg\{\left(\frac{36\sqrt{62}}{5} + \frac{18\sqrt{14630}}{35} + \frac{12\sqrt{1295}}{5} + 4\sqrt{611} + \frac{40\sqrt{91}}{3}\right)n^2 + \left(\frac{24\sqrt{62}n}{5} + \frac{24\sqrt{14630}n}{35} + \frac{4\sqrt{7042}n}{7} + \frac{16\sqrt{91}n}{3}\right)n\Bigg\}$$

$$- \frac{1}{\left(\frac{36\sqrt{62}}{5} + \frac{18\sqrt{14630}}{35} + \frac{12\sqrt{1295}}{5} + 4\sqrt{611} + \frac{40\sqrt{91}}{3}\right)n^2 + \left(\frac{24\sqrt{62}n}{5} + \frac{24\sqrt{14630}n}{35} + \frac{4\sqrt{7042}n}{7} + \frac{16\sqrt{91}n}{3}\right)n}$$

$$\times \log\Bigg\{6(3n^2+2n)\left[\frac{\sqrt{8}}{5}\right]^{\left[\frac{\sqrt{8}}{5}\right]} + 6(3n^2+4n)\left[\sqrt{\frac{10}{35}}\right]^{\left[\sqrt{\frac{10}{35}}\right]} + 24n^2\left[\sqrt{\frac{11}{40}}\right]^{\left[\sqrt{\frac{11}{40}}\right]} + 12n\left[\sqrt{\frac{14}{63}}\right]^{\left[\sqrt{\frac{14}{63}}\right]} + 24n^2\left[\sqrt{\frac{15}{72}}\right]^{\left[\sqrt{\frac{15}{72}}\right]} + 6(5n^2+2n)\left[\frac{4}{9}\right]^{\left[\frac{4}{9}\right]}\Bigg\} \tag{4.27}$$

Fifth geometry arithmetic entropy:

$$GA(G) = \Bigg\{\left(78 + 3\sqrt{35} + \frac{96\sqrt{10}}{13} + \frac{288\sqrt{2}}{17}\right)n^2 + \left(36 + 4\sqrt{35} + \frac{9\sqrt{7}}{2}\right)n\Bigg\} \tag{4.28}$$

Using Table 4 and (5) in (17), we are now computing the third redefined Zagrab entropy in the manner shown below:

$$ENT_{GA} = \log(GA) - \frac{1}{GA}\log\Bigg\{6(3n^2+2n))\left[\frac{2\sqrt{5\times5}}{(5+5)}\right]^{\left[\frac{2\sqrt{5\times5}}{(5+5)}\right]} \times 6(3n^2+4n)\left[\frac{2\sqrt{5\times7}}{(5+7)}\right]^{\left[\frac{2\sqrt{5\times7}}{(5+7)}\right]} \times 24n^2\left[\frac{2\sqrt{5\times8}}{(5+8)}\right]^{\left[\frac{2\sqrt{5\times8}}{(5+8)}\right]} \times 12n\left[\frac{2\sqrt{7\times9}}{(7+9)}\right]^{\left[\frac{2\sqrt{7\times9}}{(7+9)}\right]} \times 24n^2\left[\frac{2\sqrt{8\times9}}{(8+9)}\right]^{\left[\frac{2\sqrt{8\times9}}{(8+9)}\right]} \times 6(5n^2+2n)\left[\frac{2\sqrt{9\times9}}{(9+9)}\right]^{\left[\frac{2\sqrt{9\times9}}{(9+9)}\right]}\Bigg\}$$

$$ENT_{(GA} = \Bigg\{\left(78 + 3\sqrt{35} + \frac{96\sqrt{10}}{13} + \frac{288\sqrt{2}}{17}\right)n^2 + \left(36 + 4\sqrt{35} + \frac{9\sqrt{7}}{2}\right)n\Bigg\}$$

$$-\frac{1}{\left(78+3\sqrt{35}+\frac{96\sqrt{10}}{13}+\frac{288\sqrt{2}}{17}\right)n^2+\left(36+4\sqrt{35}+\frac{9\sqrt{7}}{2}\right)n}$$
$$\times\log\left\{6(3n^2+2n)(1)\times 6(3n^2+4n)\left[\frac{\sqrt{35}}{6}\right]^{\left[\frac{\sqrt{35}}{6}\right]}\times 24n^2\left[\frac{2\sqrt{40}}{13}\right]^{\left[\frac{2\sqrt{40}}{13}\right]}\times 12n\left[\frac{\sqrt{63}}{8}\right]^{\left[\frac{\sqrt{63}}{8}\right]}\right.$$
$$\left.\times 24n^2\left[\frac{2\sqrt{72}}{17}\right]^{\left[\frac{2\sqrt{72}}{17}\right]}\times 6(5n^2+2n)(1)\right\} \tag{4.29}$$

Sanskruti entropy:

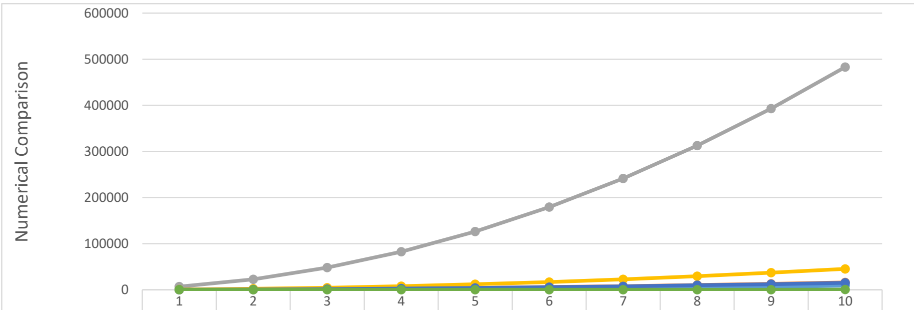
$$S(G)=\left\{\left(18\left\{\frac{10}{23}\right\}^3+18\{4/11\}^3+24\left\{\frac{13}{38}\right\}^3+24\left\{\frac{17}{70}\right\}^3+30\left\{\frac{18}{79}\right\}^3\right)n^2\right.$$
$$\left.+\left(12\left\{\frac{10}{23}\right\}^3+24\{4/11\}^3+12\left\{\frac{16}{61}\right\}^3+12\left\{\frac{18}{79}\right\}^3\right)n\right\} \tag{4.30}$$

Using Table 4 and (6) in (19), we are now computing the third redefined Zagrab entropy in the manner shown below:

$$ENT_S(G)=\log(S(G))-\frac{1}{(S(G))}\log\left\{6(3n^2+2n)\left[\left\{\frac{5\times 5}{(5+5)-2}\right\}^3\right]^{\left[\left\{\frac{5\times 5}{(5+5)-2}\right\}^3\right]}\right.$$
$$+6(3n^2+4n)\left[\left\{\frac{5\times 7}{(5+7)-2}\right\}^3\right]^{\left[\left\{\frac{5\times 7}{(5+7)-2}\right\}^3\right]}+24n^2\left[\left\{\frac{5\times 8}{(5+8)-2}\right\}^3\right]^{\left[\left\{\frac{5\times 8}{(5+8)-2}\right\}^3\right]}$$
$$+12n\left[\left\{\frac{7\times 9}{(7+9)-2}\right\}^3\right]^{\left[\left\{\frac{7\times 9}{(7+9)-2}\right\}^3\right]}+24n^2\left[\left\{\frac{8\times 9}{(8+9)-2}\right\}^3\right]^{\left[\left\{\frac{8\times 9}{(8+9)-2}\right\}^3\right]}$$
$$\left.+6(5n^2+2n)\left[\left\{\frac{9\times 9}{(9+9)-2}\right\}^3\right]^{\left[\left\{\frac{9\times 9}{(9+9)-2}\right\}^3\right]}\right\}$$

$$ENTS(G)=\log(S(G))-\frac{1}{(S(G))}\log\left\{6(3n^2+2n)\left[\left\{\frac{25}{8}\right\}^3\right]^{\left[\left\{\frac{25}{8}\right\}^3\right]}\right.$$
$$+6(3n^2+4n)\left[\left\{\frac{35}{10}\right\}^3\right]^{\left[\left\{\frac{35}{10}\right\}^3\right]}+24n^2\left[\left\{\frac{40}{11}\right\}^3\right]^{\left[\left\{\frac{40}{11}\right\}^3\right]}$$
$$+12n\left[\left\{\frac{9}{2}\right\}^3\right]^{\left[\left\{\frac{9}{2}\right\}^3\right]}+24n^2\left[\left\{\frac{24}{5}\right\}^3\right]^{\left[\left\{\frac{24}{5}\right\}^3\right]}$$
$$\left.+6(5n^2+2n)\left[\left\{\frac{81}{16}\right\}^3\right]^{\left[\left\{\frac{81}{16}\right\}^3\right]}\right\} \tag{4.31}$$

Comparison of (c) and (d)



	1	2	3	4	5	6	7	8	9	10
ReZG_1	136	448	936	1600	2440	3456	4648	6016	5760	9280
ReZG_2	228	758.4	1591.2	2726.4	4164	5904	7946.4	10291.2	12938.4	15888
ReZG_3	6816	22848	48096	82560	126240	179136	241248	312576	393120	482880
ABC_4	650.8	2164.4	4540.4	7779.5	11881	16845.2	22672.1	29361.6	36913.8	45328.6
GA_5	214.6	715.3	1502.2	2575.2	3934.3	5579.5	7510.8	9728.3	12231.9	15021.5
SG	6.503	21.0158	43.537	74.067	112.608	159.156	213.714	276.281	346.857	425.442

(c)

Figure 9: Comparison of $ReZG_1(RCF_n)$, $ReZG_2(RCF_n)$, $ReZG_3(RCF_n)$, $ABC_4(RCF_n)$, $GA_5(RCF_n)$, $SG(RCF_n)$.

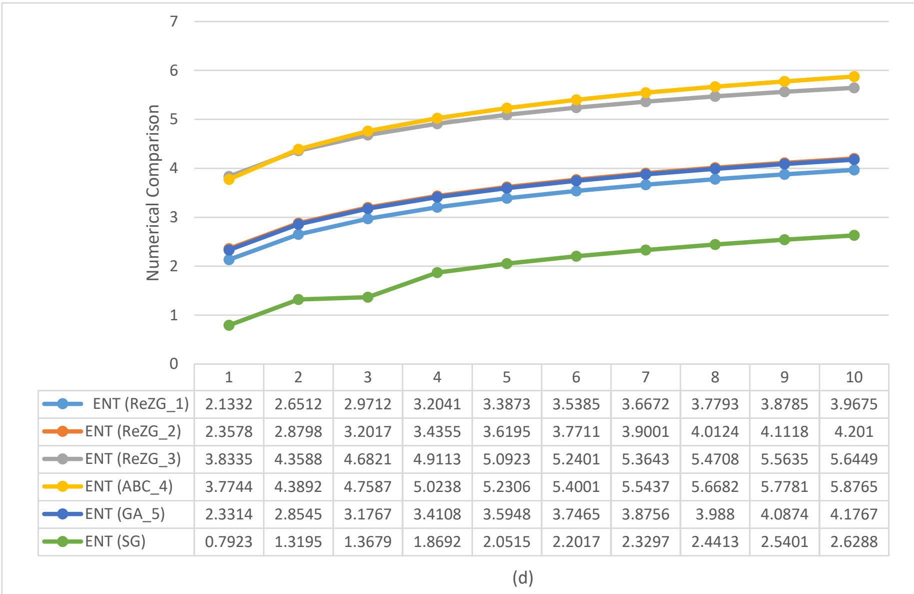
5. Discussions

The findings presented in this study offer significant insights into the structural and informational characteristics of chemical networks through the lens of entropy and degree-based molecular descriptors. The results indicate a strong correlation between certain descriptors and the centrality measures of chemical graph structures, suggesting their potential applicability in drug discovery, molecular characterization, and cheminformatics.

One key observation is the effectiveness of degree-based descriptors in capturing essential connectivity features, which directly relate to the network's robustness and information flow. Additionally, entropy measures provide a quantitative approach to assessing the disorder and complexity within molecular graphs, highlighting their utility in distinguishing between molecular topologies with varying degrees of regularity and randomness.

The analysis of specific chemical structures, such as hexagonal, tetragonal, and dendritic frameworks, further emphasizes how different graph models influence descriptor values. These structural variations suggest that selecting an appropriate descriptor depends not only on the graph type but also on the intended application — whether it be biological activity prediction or molecular similarity assessment.

Limitations of the current work include the assumption of idealized topologies and the lack of experimental validation. Future research could explore real-world molecular data sets and consider integrating machine learning techniques to enhance the predictive capabilities of the descriptors.



	1	2	3	4	5	6	7	8	9	10
ENT (ReZG_1)	2.1332	2.6512	2.9712	3.2041	3.3873	3.5385	3.6672	3.7793	3.8785	3.9675
ENT (ReZG_2)	2.3578	2.8798	3.2017	3.4355	3.6195	3.7711	3.9001	4.0124	4.1118	4.201
ENT (ReZG_3)	3.8335	4.3588	4.6821	4.9113	5.0923	5.2401	5.3643	5.4708	5.5635	5.6449
ENT (ABC_4)	3.7744	4.3892	4.7587	5.0238	5.2306	5.4001	5.5437	5.6682	5.7781	5.8765
ENT (GA_5)	2.3314	2.8545	3.1767	3.4108	3.5948	3.7465	3.8756	3.988	4.0874	4.1767
ENT (SG)	0.7923	1.3195	1.3679	1.8692	2.0515	2.2017	2.3297	2.4413	2.5401	2.6288

Figure 10: Comparison of $ENTReZG_1(RCF_n)$, $ENTReZG_2(RCF_n)$, $ENTReZG_3(RCF_n)$, $ENTABC_4(RCF_n)$, $ENTGA_5(RCF_n)$, $ENTSG(RCF_n)$.

6. Conclusion

This study demonstrates the effectiveness of using entropy and degree-based molecular descriptors to analyze two-dimensional coronene fractal structures. By computing topological indices such as the Randic index, atom-bond connectivity (ABC_4), geometric-arithmetic (GA) index, Sanskurti entropy ($S(G)$), and the redefined Zagreb and atom-bond connectivity entropies, we provide a comprehensive topological characterization of zigzag and armchair coronene fractals. Our findings reveal that these indices capture essential structural features that are relevant to the physicochemical behavior and potential bioactivity of molecular compounds. These descriptors offer valuable tools for modeling structure–property and structure–activity relationships, which are critical in applications such as drug discovery, materials science, and nanotechnology. The significance of this work lies in extending the applicability of chemical graph theory to previously underexplored coronene-based fractal structures. The methodology presented serves as a foundation for future research involving more complex molecular systems.

References

1. A. Amrullah, A. Syahrul, M. Turmuzi, K. Baidowi, and K. Nani, "The bridge graphs partition dimension," Journal of Physics: Conference Series, vol. 1779, no. 1, Article ID 012086, 2021.

2. A. Ali, K. C. Das, D. Dimitrov, and B. Furtula, "Atombond connectivity index of graphs: a review over extremal results and bounds," Discrete Mathematics Letters, vol. 5, no. 1, pp. 68–93, 2021.

3. S.E. Basil, J. Chemical Society, Faraday Transactions. 90((15), 2201–2210 (1994).

4. P. C. S. Costa, J. S. Evangelista, I. Leal, and P. C. M. L. Miranda, "Chemical graph theory for property modeling in QSAR and QSPR-charming QSAR and QSPR," Mathematics, vol. 9, no. 1, p. 60, 2020.

5. Imran, M., Khan, A. R., Husin, M. N., Tchier, F., Ghani, M. U., and Hussain, S. (2023). Computation of Entropy Measures for Metal-Organic Frameworks. Molecules, 28(12), 4726.

6. M. Dehmer and A. Mowshowitz, "A history of graph entropy measures," Information Sciences, vol. 181, no. 1, pp. 57–78, 2011.

7. S. Ediza, I. iftia, Z. Tasb, M. Cancana, and M. Reza, "A Note on QSPR Analysis of Total Zagreb and Total Randic Indices of Octanes," Eurasian Chemical Communications, vol. 3, pp. 139–145, 2021.

8. Hakami, K. H., Khan, A. R., and Bhatti, S. A. (2025). Computation of Differential, Integral Operators and Quantitative Structure–Property Analysis of Boron α-Icosahedral Nanosheet. Journal of Mathematics, Volume 2025, Article ID 5607620, 17 pages. https://doi.org/10.1155/jom/5607620

9. Khan, A. R., Zia, A., Campeña, F. J. H., Siddiqui, M. K., Tchier, F., and Hussain, S. (2024). Investigations of Entropy Double & Strong Double Graph of Silicon Carbide.Silicon, 16, 4187–4197.

10. Ahmad, Mukhtar, et al. "Comprehensive Characterization and Metric Dimension Analysis of Circulant Subdivision Graphs", International Journal of Science, Mathematics and Technology Learning Volume 33 No. 1, (2025)

11. Hakami, K. H., Khan, A. R., and Zia, I. Bicubic Regression Analysis A Novel Approach for Estimation of Physicochemical Properties of Skin Cancer Drugs through Degree Based Entropy. Heliyon (2024).

12. W. Huang, Y. Zhang, Y. Yu et al. , "Historical data-driven risk assessment of railway dangerous goods transportation system: comparisons between Entropy Weight Method and Scatter Degree Method," Reliability Engineering and System Safety, vol. 205, Article ID 107236, 2021.

13. Khan, A. R., Bhatti, S. A., Imran, M., Tawfiq, F. M., Cancan, M., and Hussain, S. (2024). Computation of Differential and Integral Operators Using M-Polynomials of Gold Crystal. Heliyon, 10(14), 2024.

14. K. Julietraja, P. Venugopal, S. Prabhu, A. K. Arulmozhi, and M. K. Siddiqui, "Structural analysis of three types of PAH using entropy measures," Polycyclic Aromatic Compounds, pp. 1–31, 2021.

15. Khan A. R., Mutlib, A., Campeña, F. J. H., Tchier, F., Karim, M., and Hussain, S., (2024). Investigation of reduced reverse degree based polynomials & indices of gold crystals. Physica Scripta, 99, 075259.

16. Khan, A. R., Ullah, Z., Imran, M., Malik, S. A., Alamoudi, L. M., and Cancan, M. (2024). Molecular temperature descriptors as a novel approach for QSPR analysis of Borophene nanosheets. PLOS ONE, 19(6), e0302157.

17. S. Manzoor, M. K. Siddiqui, and S. Ahmad, "On entropy measures of molecular graphs using topological indices,"Arabian Journal of Chemistry, vol. 13, no. 8, pp. 6285–6298, 2020.

18. Khan, A. R., Zia, A., Campeña, F. J. H., Siddiqui, M. K., Tchier, F., and Hussain, S. (2024). Investigations of Entropy Double & Strong Double Graph of Silicon Carbide.Silicon, 16, 4187–4197.

19. R. M. Kashif, M. Ahmad, A. Qayyum, S. S. Supadi, M. J. Hussain, S. Raza, On Degree-Based Topological Indices of Toeplitz Graphs, Int.J.Anal. (2023). 21:111.

20. P. S. Ranjini, V. Lokesha, and A. Usha, “Relation between phenylene and hexagonal squeeze using harmonic index,” International Journal of Graph theory, vol. 1, no. 4, pp. 116–121, 2013.

21. M. Ahmad, S. Hussain, I. Zahid, U. parveen, M. Sultan and A. Qayyum, On degree based topological indices of petersen subdivision graph, European Journal of Mathematical Analysis 3 (2023)20.

22. C. E. Shannon, “A mathematical theory of communication,” ACM SIGMOBILE Mobile Computing and Communications Review, vol. 5, no. 1, pp. 3–55, 2001.

23. M. Ahmad, M. J. Hussain, G. Atta, S. Raza, I. Waheed, A. Qayyum, ”Topological Evaluation of Four Para-Line Graphs Absolute Pentacene Graphs Using Topological”, International Journal of Analysis and Applications (2023), 21:0.

24. M. Ahmad, Y. B. Yusof, A. Qayyum, L. Rathour, V. Singh, L. N. Mishra. “A New Development in Topological Analysis of Propane Para-Line Graphs with Application in Chemical Composition”, Discontinuity, Nonlinearity, and Complexity 14(4) (2025) 659-668.

25. M. Ahmad, A. Qayyum, G. Atta, S. S. Supadi, M. Saleem, U.Ali, ”A New Study on Degree Based Topological Indices of Harary Subdivision graphs With Application”, Int.J.Anal. (2024). 22:0.

26. E. Trucco, “A note on the information content of graphs,” Bulletinof Mathematical Biophysics, vol. 18, no. 2, pp. 129,135, 1956.

Muhammad Asif Javed,
Department of Mathematics and Statistics,
University Of Southern Punjab,
Pakistan.
E-mail address: asifaslam033333@gmail.com

and

A. Q. Baig,
Department of Mathematics and Statistics,
University Of Southern Punjab,
Pakistan.
E-mail address: aqbaig1@gmail.com

and

Mukhtar Ahmad,
Faculty of Computer Science and Mathematics, Universiti Malaysia Terengganu (UMT), Malaysia.
E-mail address: itxmemuktar@gmail.com

and

Suzila Binti Mohd Kasim ,
Centre of Foundation Studies Universiti Teknologi MARA,
Cawangan Selangor, Kampus Dengkil 43800 Dengkil, Selangor,
Malaysia.
E-mail address: suzilamk@uitm.edu.my

and

Ibrahim K. Alsulami,
Department of Science, King Abdulaziz Military Academy (KAMA), Riyadh 13959 Saudi Arabia.

E-mail address: dralsulami2@gmail.com

and

Ather Qayyum,
Department of Mathematics University of Southern Punjab Multan Pakistan.
E-mail address: atherqayyum@isp.edu.pk