

Research Article

Degree-Based Entropy for a Non-Kekulean Benzenoid Graph

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Tessellations of kekulenes and cycloarenes have a lot of potential as nanomolecular belts for trapping and transporting heavy metal ions and chloride ions because they have the best electronic properties and pore sizes. The aromaticity, superaromaticity, chirality, and novel electrical and magnetic properties of a class of cycloarenes known as kekulenes have been the subject of several experimental and theoretical studies. Through topological computations of superaromatic structures with pores, we investigate the entropies and topological characterization of different tessellations of kekulenes. Using topological indices, the biological activity of the underlying structure is linked to its physical properties in (QSPR/QSAR) research. There is a wide range of topological indices accessible, including degree-based indices, which are used in this work. With the total π -electron energy, these indices have a lot of iteration. In addition, we use graph entropies to determine the structural information of a non-Kekulean benzenoid graph. In this article, we study the crystal structure of non-Kekulean benzenoid graph \mathcal{K}_n and then calculate some entropies by using the degree-based topological indices. We also investigate the relationship between degree-based topological indices and degree-based entropies. This relationship is very helpful for chemist to study the physicochemical characterization of non-Kekulean benzenoid chemical. These numerical values correlate with structural facts and chemical reactivity, biological activities, and physical properties.

1. Introduction

Chemical graph theory is used to mathematically model molecules in order to review their physical properties. It is also a good idea to characterize chemical structures. Chemical graph theory could be a mathematical branch that combines graph theory and chemistry.

Topological indices are molecular descriptors that can be used to describe these characteristics and specific chemical graphs [1]. The topological index of a chemical composition is a numerical value or continuation of a given structure under consideration that indicates chemical, physical, and biological properties of a chemical molecule structure [2].

It also belongs to a category of nontrivial chemical graph theory applications for exact molecular problem solutions.

This theory is essential in the field of chemical sciences and chemical graph theory. More information is on quantity structure activity relationship (QSAR) and quantity structure property relationship (QSPR), which are used to predict biobiota and physicochemical properties in chemical compounds [3, 4].

In this article, G is the connected simple chemical structure, with $V(G)$ vertices set and $E(G)$ edges set. Degree of any vertex u is denoted by $\mathfrak{R}(u)$. The edge between vertices u and v is denoted by uv . The total number of atoms linked to v_j of G is denoted by d_{v_j} , and it is the atom-bond of every atom of G . If G is a graph which contains m atoms and n atom-bonds, then order of G , denoted by $|G|$, is m and the size of G denoted by $S(G)$ is n . An alternating sequence of atoms and atom-bonds in a graph G is known as a path in G .

If there exists a path between every two atoms in G , then G is said to be a connected graph. A $u_i \sim v_j$ geodesic is the shortest path between two atoms u_i and v_j in a connected graph G . The number of atom-bonds (length) in a $u_i \sim v_j$ geodesic is called the distance between u_i and v_j , denoted by $d(u_i, v_j)$ for $u_i, v_j \in V_G$, in a connected graph [5]. In this article, we construct the non-Kekulean benzenoid graph \mathcal{K}_n and computed the 1st redefined Zagreb entropy, 2nd redefined Zagreb entropy, 3rd redefined Zagreb entropy, 4th atom-bond connectivity entropy, 5th geometry arithmetic entropy, and Sanskurti entropy by using their indices. We used the concept of entropy from Shazia Manzoor' article [6]. The huge amount of infirmations were missing for non-Kekulean benzenoid structure that we find in this paper. This information is much helpful for the chemists to study the physio-chemical properties of the non-Kekulean benzenoid structure.

2. Literature Review

In 2013, Ranjini et al. [7] introduced redefined version of Zagreb indices $ReZG_1$, $ReZG_2$, and $ReZG_3$. These are formulated as

$$ReZG_1 = \sum_{u_i, v_j \in E_G} \frac{d_{u_i} + d_{v_j}}{d_{u_i} \times d_{v_j}}, \quad (1)$$

$$ReZG_2 = \sum_{u_i, v_j \in E_G} \frac{d_{u_i} \times d_{v_j}}{d_{u_i} + d_{v_j}}, \quad (2)$$

$$ReZG_3 = \sum_{u_i, v_j \in E_G} (d_{u_i} \times d_{v_j})(d_{u_i} + d_{v_j}). \quad (3)$$

In 2010, Ghorbani and Hosseinzadeh [8] introduced the fourth version of the atom-bond connectivity index ABC_4 of a graph G and formulated as

$$ABC_4 = \sum_{u_i, v_j \in E_G} \sqrt{\frac{S_{u_i} + S_{v_j} - 2}{S_{u_i} \times S_{v_j}}}. \quad (4)$$

In 2011, Graovac et al. [9] introduced the fifth version of the geometric arithmetic index GA_5 of a graph G as

$$GA_5(G) = \sum_{u_i, v_j \in E_G} \frac{2\sqrt{S_{u_i} \times S_{v_j}}}{S_{u_i} + S_{v_j}}. \quad (5)$$

In 2017, Hosamani introduced the Sanskurti index [10] S_G for a molecular graph G as follows and have worked on it till now in 2021 [11], denoted by $S(G)$,

$$S(G) = \sum_{u_i, v_j \in E_G} \left\{ \frac{S_{u_i} \times S_{v_j}}{S_{u_i} + S_{v_j} - 2} \right\}^3, \quad (6)$$

Shannon first introduced the idea of entropy in his famous article [12] in 1948. The unpredictability of information content or the uncertainty of a system is measured by

the entropy of a probability distribution. Later on, entropy was applied to graphs and chemical networks and it was developed to better understand the structural information in these networks. Graph entropies have recently gained popularity in fields such as biology, chemistry, ecology, and sociology to name a few. Degree of every atom is extremely important; graph theory and network theory have both conducted extensive research on invariants, which are used as information functionals in science and have been around for a long time. In the following paragraphs, we will go over graph entropy measures that have been used to investigate biological and chemical networks in chronological order [13–15].

In this article, we construct the non-Kekulean benzenoid graph \mathcal{K}_n and computed the 1st redefined Zagreb entropy, 2nd redefined Zagreb entropy, 3rd redefined Zagreb entropy, 4th atom-bond connectivity entropy, 5th geometry arithmetic entropy, and Sanskurti entropy by using their indices. We used the concept of entropy from Shazia Manzoor' article [15].

3. Applications of Entropy

In information theory, the graph entropy is a crucial quantity. It analyses chemical graphs and complex networks for structural information. Distance-based entropy is playing an important role in various forms including different problems in math, biology, chemical graph theory, organic chemistry. The graph is inserted with a topological index by Shannon's entropy concept and topological indices as molecular descriptors are important tools in (QSAR)/(QSPR) study. Shannon's seminal work [16] was published in 1948, marking the beginning of modern information theory. Information theory was widely used in biology and chemistry after its early applications in linguistics and electrical engineering (see, for example, in 1953, [17]). Shannon's entropy formulas [16] were used to figure out a network's structural information content in 2004 [18].

The work of Rashevsky in 1955 [19] and Trucco in 1956 [20] is closely related to these applications. The following sections go over graph entropy measures that have been used to study biological and chemical networks in chronological order. Entropy measures for graphs have also been widely used in biology, computer science, and structural chemistry (for example, in 2011, see [21]). Entopic network measures have a wide range of applications, ranging from quantitative structure characterization in structural chemistry to exploring biological or chemical properties of molecular graphs in general. We stress that the aforementioned applications are intended to solve a fundamental data analysis problem, such as clustering or classification. We hypothesise that the degree-based entropy introduced in this paper can be used to assess non-Kekulean benzenoid graph.

4. Degree-Based Entropy

In 2014, Chen et al. [22] proposed the definition of entropy of an edge-weighted graph G . The $G = (V_G, E_G, \Psi(u_i, v_j))$, for an edge-weighted graph, where V_G , E_G , and $\Psi(u_i, v_j)$

exemplify the set of vertices, the edge set, and the edge-weight of edge $(u_i v_j)$, respectively. The entropy of edge-weighted graph is defined as

$$ENT_{\Psi(G)} = \sum_{u_i, v_j \in E_G} \frac{\Psi(u_i v_j)}{\sum_{u_i, v_j \in E_G} \Psi(u_i v_j)} \log \left\{ \frac{\Psi(u_i v_j)}{\sum_{u_i, v_j \in E_G} \Psi(u_i v_j)} \right\}. \quad (7)$$

By the help of equation 7, other entropies were found [6] and mathematically denoted as follows:

$$ENT_{ReZG_1} = \log(ReZG_1) - \frac{1}{ReZG_1} \log \left\{ \prod_{u_i, v_j \in E_G} \left[\frac{d_{u_i} + d_{v_j}}{d_{u_i} d_{v_j}} \right]^{[d_{u_i} + d_{v_j} / d_{u_i} d_{v_j}]} \right\}. \quad (9)$$

(ii) Second redefined Zagreb entropy:

Let $\Psi(u_i v_j) = d_u + d_v / d_u d_v$. Then, the second redefined Zagreb index (2) is given by

$$ReZG_2 = \sum_{u_i, v_j \in E_G} \left\{ \frac{d_{u_i} d_{v_j}}{d_{u_i} + d_{v_j}} \right\} = \sum_{u_i, v_j \in E_G} \Psi(u_i v_j). \quad (10)$$

$$ENT_{ReZG_2} = \log(ReZG_2) - \frac{1}{ReZG_2} \log \left\{ \prod_{u_i, v_j \in E_G} \left[\frac{d_u d_v}{d_{u_i} + d_{v_j}} \right]^{[d_{u_i} d_{v_j} / d_{u_i} + d_{v_j}]} \right\}. \quad (11)$$

(iii) Third redefined Zagreb entropy:

Let $\Psi(u_i v_j) = \{(d_{u_i} d_{v_j})(d_{u_i} + d_{v_j})\}$. Then, the third redefined Zagreb index (3) is given by

$$ReZG_3 = \sum_{u_i, v_j \in E_G} \left\{ (d_{u_i} d_{v_j})(d_{u_i} + d_{v_j}) \right\} = \sum_{u_i, v_j \in E_G} \Psi(u_i v_j). \quad (12)$$

$$ENT_{ReZG_3} = \log(ReZG_3) - \frac{1}{ReZG_3} \log \left\{ \prod_{u_i, v_j \in E_G} \left[(d_{u_i} d_{v_j})(d_{u_i} + d_{v_j}) \right]^{[(d_{u_i} d_{v_j})(d_{u_i} + d_{v_j})]} \right\}. \quad (13)$$

(iv) Entropy of fourth atom-bond connectivity:

Let $\Psi(u_i v_j) = \left\{ \sqrt{S_{u_i} + S_{v_j} - 2 / S_{u_i} S_{v_j}} \right\}$. Then, the 4th atom-bond connectivity index (4) is

$$ABC_4(G) = \sum_{u_i, v_j \in E_G} \left\{ \sqrt{\frac{S_{u_i} + S_{v_j} - 2}{S_{u_i} S_{v_j}}} \right\} = \sum_{u_i, v_j \in E_G} \Psi(u_i v_j). \quad (14)$$

(i) First redefined Zagreb entropy:

Let $\Psi(u_i v_j) = d_u + d_v / d_u d_v$. Then, the first redefined Zagreb index (1) is given by

$$ReZG_1 = \sum_{u_i, v_j \in E_G} \left\{ \frac{d_{u_i} + d_{v_j}}{d_{u_i} d_{v_j}} \right\} = \sum_{u_i, v_j \in E_G} \Psi(u_i v_j). \quad (8)$$

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

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

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

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

$$ENT_{ABC_4(G)} = \log(ABC_4(G)) - \frac{1}{ABC_4(G)} \log \left\{ \prod_{u_i, v_j \in E_G} \left[\sqrt{\frac{S_{u_i} + S_{v_j} - 2}{S_{u_i} S_{v_j}}} \right]^{\left[\sqrt{S_{u_i} + S_{v_j} - 2 / S_{u_i} S_{v_j}} \right]} \right\}. \quad (15)$$

(v) Fifth geometry arithmetic entropy:

Let $\Psi(u_i v_j) = \left\{ 2 \sqrt{S_{u_i} S_{v_j} / S_{u_i} + S_{v_j}} \right\}$. Then, the fifth geometry arithmetic index (4) is given by

$$GA_5(G) = \sum_{u_i, v_j \in E_G} \left\{ \frac{2 \sqrt{S_{u_i} S_{v_j}}}{S_{u_i} + S_{v_j}} \right\} = \sum_{u_i, v_j \in E_G} \Psi(u_i v_j). \quad (16)$$

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

$$ENT_{GA_5(G)} = \log(GA_5(G)) - \frac{1}{GA_5(G)} \log \left\{ \prod_{u_i, v_j \in E_G} \left[\frac{2 \sqrt{S_{u_i} S_{v_j}}}{S_{u_i} + S_{v_j}} \right]^{\left[2 \sqrt{S_{u_i} S_{v_j} / S_{u_i} + S_{v_j}} \right]} \right\}. \quad (17)$$

(vi) Sanskruti entropy:

Let $\Psi(u_i v_j) = \left\{ S_{u_i} \times S_{v_j} / S_{u_i} + S_{v_j} - 2 \right\}^3$. Then, the Sanskruti index (6) is given by

$$S(G) = \sum_{u_i, v_j \in E_G} \left\{ \frac{S_{u_i} \times S_{v_j}}{S_{u_i} + S_{v_j} - 2} \right\}^3 = \sum_{u_i, v_j \in E_G} \Psi(u_i v_j). \quad (18)$$

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

$$ENT_{S(G)} = \log(S(G)) - \frac{1}{S(G)} \log \left\{ \prod_{u_i, v_j \in E_G} \left\{ \frac{S_{u_i} \times S_{v_j}}{S_{u_i} + S_{v_j} - 2} \right\}^3 \left\{ S_{u_i} \times S_{v_j} / S_{u_i} + S_{v_j} - 2 \right\}^3 \right\}. \quad (19)$$

The Kekulean and non-Kekulean structures of benzene are real and distinct due to the presence of rings in the benzenoid form. The specific arrangement of rings in the benzenoid system provides the transformation in series of benzenoid structures of the benzenoid graph that is the way the structures are changed. In the series of concealed non-Kekulean benzenoid graph \mathcal{K}_n , see [23], where n shows the number of bridges [24] in the center of \mathcal{K}_n , as shown in Figure 1. Similarly for $n = k$, there are k bridges. Here, in the non-

Kekulean benzenoid graph \mathcal{K}_n , we observed that there are three types of atom-bonds on the basis of valency of every atom. Therefore, by observing this concept of atom-bonds, there are two types of atoms v_i and v_j such that $d_{v_i} = 2$ and $d_{v_j} = 3$, where d_{v_i} and d_{v_j} mean the valency of atoms $\forall v_i, v_j \in \mathcal{K}_n$. The order and size of non-Kekulean benzenoid graphs \mathcal{K}_n are

$$\begin{aligned} |V(\mathcal{K}_n)| &= 2(6n + 7), \\ |E(\mathcal{K}_n)| &= 17n + 14. \end{aligned} \quad (20)$$

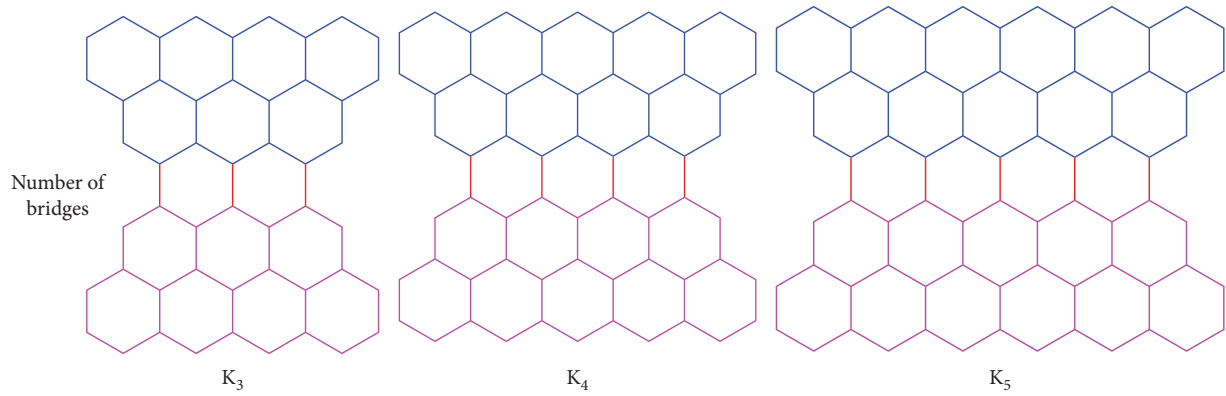


FIGURE 1: Non-Kekulean benzenoid graphs \mathcal{K}_n .

TABLE 1: Atom-bonds-based partition of each atom of \mathcal{K}_n .

Types of atom-bonds	$E_{(2\sim 2)}$	$E_{(2\sim 3)}$	$E_{(3\sim 3)}$
Frequency of atom-bonds	8	$4(n+3)$	$(13n-6)$

Following are the three figures of non-Kekulean benzenoid graphs $K_3, K_4,$ and K_5 .

According to the degree of the atoms, there are three types of atom-bonds in \mathcal{K}_n : $(2 \sim 2), (2 \sim 3),$ and $(3 \sim 3)$. The atom-bonds partition of \mathcal{K}_n is shown as

$$\begin{aligned}
 E_{2\sim 2} &= \{e = u \sim v, \quad \forall u, v \in V(\mathcal{K}_n) | d_u = 2, d_v = 2\}, \\
 E_{2\sim 3} &= \{e = u \sim v, \quad \forall u, v \in V(\mathcal{K}_n) | d_u = 2, d_v = 3\}, \\
 E_{3\sim 3} &= \{e = u \sim v, \quad \forall u, v \in V(\mathcal{K}_n) | d_u = 3, d_v = 3\}.
 \end{aligned}
 \tag{21}$$

(vii) First redefined Zagreb entropy of \mathcal{K}_n

Let G be the non-Kekulean benzenoid graph \mathcal{K}_n . Then, by using Table 1 in (1), the first redefined Zagreb index is

$$\text{ReZG}_1(\mathcal{K}_n) = 2(6n+7). \tag{22}$$

Now, we are computing the first redefined Zagreb entropy by using Table 1 and (22) in (9) in the following way:

$$\begin{aligned}
 ENT_{\text{ReZG}_1}(\mathcal{K}_n) &= \log 2(6n+7) - \frac{1}{2(6n+7)} \log \left\{ \prod_{E_{(2\sim 2)}} \left[\frac{d_{u_i} + d_{v_j}}{d_{u_i} d_{v_j}} \right]^{[d_{u_i} + d_{v_j} / d_{u_i} d_{v_j}]} \times \prod_{E_{(2\sim 3)}} \left[\frac{d_{u_i} + d_{v_j}}{d_{u_i} d_{v_j}} \right]^{[d_{u_i} + d_{v_j} / d_{u_i} d_{v_j}]} \right. \\
 &\quad \left. \times \prod_{E_{(3\sim 3)}} \left[\frac{d_{u_i} + d_{v_j}}{d_{u_i} d_{v_j}} \right]^{[d_{u_i} + d_{v_j} / d_{u_i} d_{v_j}]} \right\} \\
 &= \log 2(6n+7) - \frac{1}{2(6n+7)} \log \left\{ 8 \left(\frac{4}{4} \right)^{4/4} \times 4(n+3) \left(\frac{5}{6} \right)^{5/6} \times (13n-6) \left(\frac{6}{9} \right)^{6/9} \right\}.
 \end{aligned}
 \tag{23}$$

After simplification, in the following equation, we get the actual amount of the first redefined Zagreb entropy.

$$ENT_{\text{ReZG}_1}(\mathcal{K}_n) = \log 2(6n+7) - \frac{1}{2(6n+7)} \log \left\{ 8 \times 4(n+3) \left(\frac{5}{6} \right)^{5/6} \times (13n-6) \left(\frac{2}{3} \right)^{2/3} \right\}. \tag{24}$$

TABLE 2: Edge partition (sum of valency of the neighborhood atoms).

(S_{u_i}, S_{v_j})	Number of atom-bonds
$S_{(4,5)}$	8
$S_{(5,7)}$	8
$S_{(6,7)}$	$4n$
$S_{(6,8)}$	4
$S_{(7,9)}$	$2n + 4$
$S_{(8,8)}$	2
$S_{(8,9)}$	4
$S_{(9,9)}$	$11n - 16$

(viii) Second redefined Zagreb entropy of \mathcal{K}_n :

Let G be the non-Kekulean benzenoid graph \mathcal{K}_n . Then, by using Table 1 in (2), the second redefined Zagreb index is

$$ReZG_2(\mathcal{K}_n) = \frac{243}{10}n + \frac{67}{5}. \tag{25}$$

Now, we are computing the second redefined Zagreb entropy by using Table 1 and (25) in (11) in the following way:

$$\begin{aligned} ENT_{ReZG_2}(\mathcal{K}_n) &= \log(ReZG_2) - \frac{1}{ReZG_2} \log \left\{ \prod_{E(2 \sim 2)} \left[\frac{d_{u_i} d_{v_j}}{d_{u_i} + d_{v_j}} \right]^{[d_{u_i} d_{v_j} / d_{u_i} + d_{v_j}]} \times \prod_{E(2 \sim 3)} \left[\frac{d_{u_i} d_{v_j}}{d_{u_i} + d_{v_j}} \right]^{[d_{u_i} d_{v_j} / d_{u_i} + d_{v_j}]} \right. \\ &\quad \left. \times \prod_{E(3 \sim 3)} \left[\frac{d_{u_i} d_{v_j}}{d_{u_i} + d_{v_j}} \right]^{[d_{u_i} d_{v_j} / d_{u_i} + d_{v_j}]} \right\} \tag{26} \\ &= \log\left(\frac{243}{10}n + \frac{67}{5}\right) - \frac{1}{((243/10)n + (67/5))} \log \left\{ 8\left(\frac{4}{4}\right)^{4/4} \times 4(n+3)\left(\frac{6}{5}\right)^{6/5} \times (13n-6)\left(\frac{9}{6}\right)^{9/6} \right\}. \end{aligned}$$

After simplification, we get the actual amount of second redefined Zagreb entropy in the following equation:

$$ENT_{ReZG_2}(\mathcal{K}_n) = \log \frac{1215n + 670}{50} - \frac{50}{1215n + 670} \log \left\{ 8 \times 4(n+3)\left(\frac{6}{5}\right)^{6/5} \times (13n-6)\left(\frac{3}{2}\right)^{3/2} \right\}. \tag{27}$$

(ix) Third redefined Zagreb entropy of \mathcal{K}_n :

Let G be the non-Kekulean benzenoid graph \mathcal{K}_n , then by using Table 1 in (3), the third redefined Zagreb index is

$$ReZG_3(\mathcal{K}_n) = 822n + 164. \tag{28}$$

Now, we are computing the third redefined Zagreb entropy by using Table 1 and (28) in (13) in the following way:

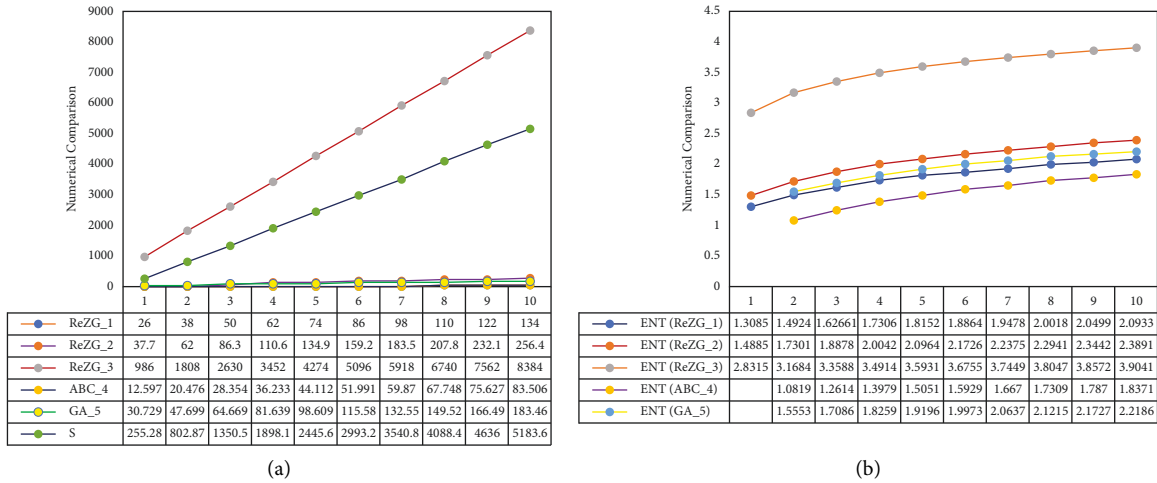


FIGURE 2: (a) Comparison of $ReZG_1(\mathcal{K}_n)$, $ReZG_2(\mathcal{K}_n)$, $ReZG_3(\mathcal{K}_n)$, $ABC_4(\mathcal{K}_n)$, $GA_5(\mathcal{K}_n)$, and $S(\mathcal{K}_n)$. (b) Comparison of $ENTReZG_1(\mathcal{K}_n)$, $ENTReZG_2(\mathcal{K}_n)$, $ENTReZG_3(\mathcal{K}_n)$, $ENTABC_4(\mathcal{K}_n)$, and $ENTGA_5(\mathcal{K}_n)$.

$$\begin{aligned}
 ENT_{ReZG_3}(\mathcal{K}_n) &= \log(ReZG_3) - \frac{1}{ReZG_3} \log \left\{ \prod_{E_{(2-2)}} [(d_{u_i}d_{v_j})(d_{u_i} + d_{v_j})] [(d_{u_i}d_{v_j})(d_{u_i} + d_{v_j})] \right. \\
 &\quad \times \prod_{E_{(2-3)}} [(d_{u_i}d_{v_j})(d_{u_i} + d_{v_j})] [(d_{u_i}d_{v_j})(d_{u_i} + d_{v_j})] \times \prod_{E_{(3-3)}} [(d_{u_i}d_{v_j})(d_{u_i} + d_{v_j})] [(d_{u_i}d_{v_j})(d_{u_i} + d_{v_j})] \left. \right\} \quad (29) \\
 &= \log(822n + 164) - \frac{1}{822n + 164} \log \{ 8(16)^{16} \times 4(n + 3)(30)^{30} \times (13n - 6)54^{54} \}.
 \end{aligned}$$

The above (29) is the actual amount of third redefined Zagreb entropy.

(x) Fourth atom-bond connectivity entropy of \mathcal{K}_n :

Table 2 shows the atom-bond-based partition of non-Kekulean graph \mathcal{K}_n , based on valency sum of end atoms of each degree.

Let \mathcal{K}_n be a non-Kekulean benzenoid graph. Then, by using Table 2 in (4), the fourth atom-bond connectivity index is

$$ABC_4(\mathcal{K}_n) = \left(\frac{44}{9} + \frac{2\sqrt{2}}{3} + 4\sqrt{\frac{11}{42}} \right) n + \left(2\sqrt{\frac{7}{5}} + 8\sqrt{\frac{2}{7}} + 2\sqrt{\frac{5}{6}} + \frac{4\sqrt{2}}{3} + \frac{\sqrt{14}}{4} - \frac{46}{7} \right). \quad (30)$$

Now, we are computing the fourth atom-bond connectivity entropy by using Table 2 and (30) in (15) in the following way:

$$\begin{aligned}
 ENT_{ABC_4}(\mathcal{K}_n) = \log(ABC_4(G)) - \frac{1}{ABC_4(G)} \log & \left\{ \prod_{S_{(4,5)}} \left(\sqrt{\frac{S_{u_i} + S_{v_j} - 2}{S_{u_i} S_{v_j}}} \right)^{\left(\sqrt{(S_{u_i} + S_{v_j} - 2)/S_{u_i} S_{v_j}} \right)} \right. \\
 & \times \prod_{S_{(5,7)}} \left(\sqrt{\frac{S_{u_i} + S_{v_j} - 2}{S_{u_i} S_{v_j}}} \right)^{\left(\sqrt{(S_{u_i} + S_{v_j} - 2)/S_{u_i} S_{v_j}} \right)} \times \prod_{S_{(6,7)}} \left(\sqrt{\frac{S_{u_i} + S_{v_j} - 2}{S_{u_i} S_{v_j}}} \right)^{\left(\sqrt{(S_{u_i} + S_{v_j} - 2)/S_{u_i} S_{v_j}} \right)} \\
 & \times \prod_{S_{(6,8)}} \left(\sqrt{\frac{S_{u_i} + S_{v_j} - 2}{S_{u_i} S_{v_j}}} \right)^{\left(\sqrt{(S_{u_i} + S_{v_j} - 2)/S_{u_i} S_{v_j}} \right)} \times \prod_{S_{(7,9)}} \left(\sqrt{\frac{S_{u_i} + S_{v_j} - 2}{S_{u_i} S_{v_j}}} \right)^{\left(\sqrt{(S_{u_i} + S_{v_j} - 2)/S_{u_i} S_{v_j}} \right)} \\
 & \times \prod_{S_{(8,8)}} \left(\sqrt{\frac{S_{u_i} + S_{v_j} - 2}{S_{u_i} S_{v_j}}} \right)^{\left(\sqrt{(S_{u_i} + S_{v_j} - 2)/S_{u_i} S_{v_j}} \right)} \times \prod_{S_{(8,9)}} \left(\sqrt{\frac{S_{u_i} + S_{v_j} - 2}{S_{u_i} S_{v_j}}} \right)^{\left(\sqrt{(S_{u_i} + S_{v_j} - 2)/S_{u_i} S_{v_j}} \right)} \\
 & \left. \times \prod_{S_{(9,9)}} \left(\sqrt{\frac{S_{u_i} + S_{v_j} - 2}{S_{u_i} S_{v_j}}} \right)^{\left(\sqrt{(S_{u_i} + S_{v_j} - 2)/S_{u_i} S_{v_j}} \right)} \right\}. \tag{31}
 \end{aligned}$$

After simplification, we get the exact value of fourth atom-bond connectivity entropy

$$\begin{aligned}
 ENT_{ABC_4}(\mathcal{K}_n) = \log & \left\{ \left(\frac{44}{9} + \frac{2\sqrt{2}}{3} + 4\sqrt{\frac{11}{42}} \right) n + \left(2\sqrt{\frac{7}{5}} + 8\sqrt{\frac{2}{7}} + 2\sqrt{\frac{5}{6}} + \frac{4\sqrt{2}}{3} + \frac{\sqrt{14}}{4} - \frac{46}{7} \right) \right\} \\
 & - \frac{1}{(44/9 + 2\sqrt{2}/3 + 4\sqrt{11/42})n + (2\sqrt{7/5} + 8\sqrt{2/7} + 2\sqrt{5/6} + 4\sqrt{2}/3 + \sqrt{14}/4 - 46/7)} \log \\
 & \cdot \left\{ 8 \left(\sqrt{\frac{7}{20}} \right)^{(\sqrt{7/20})} \times 8 \left(\sqrt{\frac{2}{7}} \right)^{(\sqrt{2/7})} \times (4n) \left(\sqrt{\frac{11}{42}} \right)^{\sqrt{11/42}} \times 4 \left(\frac{1}{2} \right)^{1/2} \times (2n+4) \left(\sqrt{\frac{14}{63}} \right)^{\sqrt{14/63}} \right. \\
 & \left. \times 2 \left(\sqrt{\frac{7}{32}} \right)^{\sqrt{7/32}} \times 4 \left(\sqrt{\frac{5}{24}} \right)^{\sqrt{5/24}} \times (11n-16) \left(\frac{4}{9} \right)^{4/9} \right\}. \tag{32}
 \end{aligned}$$

(xi) Fifth geometry arithmetic entropy of \mathcal{K}_n :

Let \mathcal{K}_n be a non-Kekulean benzenoid graph, then by using Table 2 in (4), the fifth geometry arithmetic index is

$$GA_A(\mathcal{K}_n) = 11n + \frac{8\sqrt{42}}{13}n + \frac{3\sqrt{7}}{4}n + \left(\frac{3\sqrt{7}}{2} + \frac{4\sqrt{35}}{3} + \frac{32\sqrt{5}}{9} + \frac{16\sqrt{3}}{7} + \frac{48\sqrt{2}}{17} - 14 \right). \quad (33)$$

Now, we are computing the fifth geometry arithmetic entropy of \mathcal{K}_n by using (33) and Table 2 in (17) in the following way:

$$\begin{aligned} ENT_{GA_5}(\mathcal{K}_n) &= \log(GA_5(G)) - \frac{1}{GA_5(G)} \log \left\{ \prod_{S_{(4,5)}} \left(\frac{2\sqrt{S_{u_i}S_{v_j}}}{S_{u_i} + S_{v_j}} \right)^{\binom{2\sqrt{S_{u_i}S_{v_j}}/S_{u_i}+S_{v_j}}}{\right.} \\ &\quad \times \prod_{S_{(5,7)}} \left(\frac{2\sqrt{S_{u_i}S_{v_j}}}{S_{u_i} + S_{v_j}} \right)^{\binom{2\sqrt{S_{u_i}S_{v_j}}/S_{u_i}+S_{v_j}}}{\times \prod_{S_{(6,7)}} \left(\frac{2\sqrt{S_{u_i}S_{v_j}}}{S_{u_i} + S_{v_j}} \right)^{\binom{2\sqrt{S_{u_i}S_{v_j}}/S_{u_i}+S_{v_j}}}{\right.} \\ &\quad \times \prod_{S_{(6,8)}} \left(\frac{2\sqrt{S_{u_i}S_{v_j}}}{S_{u_i} + S_{v_j}} \right)^{\binom{2\sqrt{S_{u_i}S_{v_j}}/S_{u_i}+S_{v_j}}}{\times \prod_{S_{(7,9)}} \left(\frac{2\sqrt{S_{u_i}S_{v_j}}}{S_{u_i} + S_{v_j}} \right)^{\binom{2\sqrt{S_{u_i}S_{v_j}}/S_{u_i}+S_{v_j}}}{\right.} \\ &\quad \times \prod_{S_{(8,8)}} \left(\frac{2\sqrt{S_{u_i}S_{v_j}}}{S_{u_i} + S_{v_j}} \right)^{\binom{2\sqrt{S_{u_i}S_{v_j}}/S_{u_i}+S_{v_j}}}{\times \prod_{S_{(8,9)}} \left(\frac{2\sqrt{S_{u_i}S_{v_j}}}{S_{u_i} + S_{v_j}} \right)^{\binom{2\sqrt{S_{u_i}S_{v_j}}/S_{u_i}+S_{v_j}}}{\right.} \\ &\quad \left. \times \prod_{S_{(9,9)}} \left(\frac{2\sqrt{S_{u_i}S_{v_j}}}{S_{u_i} + S_{v_j}} \right)^{\binom{2\sqrt{S_{u_i}S_{v_j}}/S_{u_i}+S_{v_j}}}{\right\} = \log(GA_5(G)) - \frac{1}{GA_5(G)} \log \left\{ 8 \left(\frac{2\sqrt{20}}{9} \right)^{\binom{(2\sqrt{20})}{9}} \times 8 \left(\frac{2\sqrt{35}}{12} \right)^{\binom{(2\sqrt{35})}{12}} \right. \\ &\quad \times 4n \left(\frac{2\sqrt{42}}{13} \right)^{\binom{(2\sqrt{42})}{13}} \times 4 \left(\frac{2\sqrt{48}}{14} \right)^{\binom{(2\sqrt{48})}{14}} \times 2(n+2) \left(\frac{2\sqrt{63}}{16} \right)^{\binom{(2\sqrt{63})}{16}} \times 2 \left(\frac{2\sqrt{64}}{16} \right)^{\binom{(2\sqrt{64})}{16}} \\ &\quad \left. \times 4 \left(\frac{2\sqrt{72}}{17} \right)^{\binom{(2\sqrt{72})}{17}} \times (11n-16) \left(\frac{2\sqrt{81}}{18} \right)^{\binom{(2\sqrt{81})}{18}} \right\}. \end{aligned} \quad (34)$$

By using the value of fifth geometry arithmetic index in the above expiration, we get the exact value of fifth geometry arithmetic entropy of \mathcal{K}_n :

$$\begin{aligned}
 ENT_{GA_5} = & \log \left[11n + \frac{8\sqrt{42}}{13}n + \frac{3\sqrt{7}}{4}n + \left(\frac{3\sqrt{7}}{2} + \frac{4\sqrt{35}}{3} + \frac{32\sqrt{5}}{9} + \frac{16\sqrt{3}}{7} + \frac{48\sqrt{2}}{17} - 14 \right) \right] / \\
 & - 11n + \frac{8\sqrt{42}}{13}n + \frac{3\sqrt{7}}{4}n + \left(\frac{3\sqrt{7}}{2} + \frac{4\sqrt{35}}{3} + \frac{32\sqrt{5}}{9} + \frac{16\sqrt{3}}{7} + \frac{48\sqrt{2}}{17} - 14 \right) \\
 & \times \log \left\{ 8 \left(\frac{4\sqrt{5}}{9} \right)^{(4\sqrt{5}/9)} \times 8 \left(\frac{\sqrt{35}}{6} \right)^{(\sqrt{35}/6)} \times 4n \left(\frac{2\sqrt{42}}{13} \right)^{(2\sqrt{42}/13)} \times 4 \left(\frac{4\sqrt{3}}{7} \right)^{(4\sqrt{3}/7)} \right. \\
 & \left. \times 2(n+2) \left(\frac{3\sqrt{7}}{8} \right)^{(3\sqrt{7}/8)} \times 2 \times 4 \left(\frac{12\sqrt{2}}{17} \right)^{(12\sqrt{2}/17)} \times (11n-16) \right\}.
 \end{aligned} \tag{35}$$

(xii) Sanskruti entropy of \mathcal{K}_n :

Let \mathcal{K}_n be a non-Kekulean benzenoid graph. Then, by using Table 2 in (6), Sanskruti index is

$$S(\mathcal{K}_n) = \frac{54759n - 29231}{100}. \tag{36}$$

Now, we are computing Sanskruti entropy by using (36) and Table 2 in (17) in the following way:

$$\begin{aligned}
 ENT_S(\mathcal{K}_n) = & \log S(\mathcal{K}_n) - \frac{1}{S(\mathcal{K}_n)} \log \left\{ \prod_{S_{(4,5)}} \left(\frac{S_{u_i} \times S_{v_j}}{S_{u_i} + S_{v_j} - 2} \right)^{3(S_{u_i} \times S_{v_j} / S_{u_i} + S_{v_j} - 2)^3} \right. \\
 & \times \prod_{S_{(5,7)}} \left(\frac{S_{u_i} \times S_{v_j}}{S_{u_i} + S_{v_j} - 2} \right)^{3(S_{u_i} \times S_{v_j} / S_{u_i} + S_{v_j} - 2)^3} \times \prod_{S_{(6,7)}} \left(\frac{S_{u_i} \times S_{v_j}}{S_{u_i} + S_{v_j} - 2} \right)^{3(S_{u_i} \times S_{v_j} / S_{u_i} + S_{v_j} - 2)^3} \\
 & \times \prod_{S_{(6,8)}} \left(\frac{S_{u_i} \times S_{v_j}}{S_{u_i} + S_{v_j} - 2} \right)^{3(S_{u_i} \times S_{v_j} / S_{u_i} + S_{v_j} - 2)^3} \times \prod_{S_{(7,9)}} \left(\frac{S_{u_i} \times S_{v_j}}{S_{u_i} + S_{v_j} - 2} \right)^{3(S_{u_i} \times S_{v_j} / S_{u_i} + S_{v_j} - 2)^3} \\
 & \times \prod_{S_{(8,8)}} \left(\frac{S_{u_i} \times S_{v_j}}{S_{u_i} + S_{v_j} - 2} \right)^{3(S_{u_i} \times S_{v_j} / S_{u_i} + S_{v_j} - 2)^3} \times \prod_{S_{(8,9)}} \left(\frac{S_{u_i} \times S_{v_j}}{S_{u_i} + S_{v_j} - 2} \right)^{3(S_{u_i} \times S_{v_j} / S_{u_i} + S_{v_j} - 2)^3} \\
 & \left. \times \prod_{S_{(9,9)}} \left(\frac{S_{u_i} \times S_{v_j}}{S_{u_i} + S_{v_j} - 2} \right)^{3(S_{u_i} \times S_{v_j} / S_{u_i} + S_{v_j} - 2)^3} \right\}.
 \end{aligned} \tag{37}$$

We get the actual amount of Sanskruti entropy of \mathcal{K}_n by using the value of Sanskruti index in the above expiration.

$$\begin{aligned}
ENT_S(\mathcal{K}_n) = & \log \frac{54759n - 29231}{100} \\
& - \frac{100}{54759n - 29231} \log \left\{ 8 \left(\frac{8000}{343} \right)^{8000/343} \times 8 \left(\frac{343}{8} \right)^{343/8} \times 4n \left(\frac{74088}{1331} \right)^{74088/1331} \times 4(64)^{64} \right. \\
& \left. \times 2(n+2) \left(\frac{729}{8} \right)^{729/8} \times 2 \left(\frac{32768}{343} \right)^{32768/343} \times 4 \left(\frac{13824}{125} \right)^{13824/125} \times (11n-16) \left(\frac{531441}{4096} \right)^{531441/4096} \right\}.
\end{aligned} \tag{38}$$

5. Numerical and Graphical Representation

The numerical representation and the graphical representation are dedicated in Figure 2. We can easily see, from Figure 2, that all indices are in increasing order as the value of n is increasing. Comparison of entropy for $ENTABC_4(\mathcal{K}_n)$ and $ENTGA_5(\mathcal{K}_n)$ is taken for $n > 1$.

6. Conclusion

For the construction of entropy-based measures to characterize the structure of complex networks, many graph invariants have been used. We study graph entropies based on vertex degrees using so-called information functionals, which are based on Shannon's entropy. There has been very little work done to find the extremal values of Shannon entropy-based graph measures. The main contribution of this paper is to prove some extreme values for the key focus area entropy of certain non-Kekulean benzenoid graph. In this research, we investigate the graph entropies associated with a new information function using Shannon's entropy and Chen et al's entropy definitions and evaluate a relationship between degree-based topological indices and degree-based entropies. The degree-based entropies for crystallographic structures of non-Kekulean benzenoid graph \mathcal{K}_n were calculated by their indices, which leads us to the physicochemical properties of the non-Kekulean benzenoid graph \mathcal{K}_n .

In the future, we hope to expand this concept to include various chemical structures with the help of chemists, allowing researchers to pursue new avenues in this field.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare no conflicts of interest.

Authors' Contributions

The authors contributed equally in the analysis and write up of the manuscript.

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