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Research Article

VDB Entropy Measures and Irregularity-Based Indices for the Rectangular Kekulene System

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Theoretical chemists are fascinated by polycyclic aromatic hydrocarbons (PAHs) because of their unique electromagnetic and other significant properties, such as superaromaticity. The study of PAHs has been steadily increasing because of their wide-ranging applications in several fields, like steel manufacturing, shale oil extraction, coal gasification, production of coke, tar distillation, and nanosciences. Topological indices (TIs) are numerical quantities that give a mathematical expression for the chemical structures. They are useful and cost-effective tools for predicting the properties of chemical compounds theoretically. Entropic network measures are a type of TIs with a broad array of applications, involving quantitative characterization of molecular structures and the investigation of some specific chemical properties of molecular graphs. Irregularity indices are numerical parameters that quantify the irregularity of a molecular graph and are used to predict some of the chemical properties, including boiling points, resistance, enthalpy of vaporization, entropy, melting points, and toxicity. This study aims to determine analytical expressions for the VDB entropy and irregularity-based indices in the rectangular Kekulene system.

1. Introduction

Chemical graph theory is one of the important branches of mathematics, which helps researchers to explore chemical compounds by reconstructing their underlying molecular structures as graphs. A *molecular graph* is a simple graph that represents the skeleton of an organic chemical compound in which the vertices of the molecular graph represent carbon atoms, and its edges represent the links between those carbon atoms [1]. According to IUPAC, the molecular structural descriptor is described as "A *molecular structural descriptor* is a numerical quantity associated with the chemical constitution that can be used to correlate chemical structure with several physical characteristics, biological activity, or chemical reactivity" [2].

Cycloarenes are conjugated macrocyclic chemical compounds composed of circularly fused benzene rings that enclose a cavity with inward-facing C-H bonds. Thus, cycloarenes are a subdivision of the Kekulene system. The magnetic susceptibility, aromaticity, and vibrational frequencies of cycloarenes have all been the subject of theoretical research [3, 4].

The rectangular Kekulene system $RK(m, n)$ is a type of polycyclic aromatic compound that has a broad range of applications, from everyday materials to cutting-edge industries like nanotechnology. As a result, theoretical chemists have long been attracted to the study of their fundamental features, including carcinogenicity, toxicity, observed bioactivities, and other relevant features. The fascinating potential of increased stability with interesting magnetic and magnetocaloric effects is offered by the structure of the Kekulene molecule, which has 12 annulated benzene rings and a central cavity.

Numerous theoretical and experimental studies on coronoids have been sparked by the synthesis of Kekulene and septulene [5–7]. Due to their intriguing property of superaromaticity, the study of Kekulene systems is also gaining momentum. Extra thermodynamic stability owing to macrocyclic conjugation in super-ring compounds like Kekulene is referred to as superaromaticity or macrocyclic aromaticity, and it accounts for a minor portion of global aromaticity. All of the coronoids that have been investigated so far are superaromatic in some way, with positive superaromatic stabilisation energies (SSEs). This gives rise to a more in-depth investigation of the features of Kekulene systems and their linkages to the underlying molecular structures. This research can be used in a variety of nanotechnology fields.

The cavities, which are an intrinsic element of the Kekulene system, serve as prototypes for developing and synthesizing novel nanomaterials with applications in nanotechnology and biotechnology, as well as the burgeoning field of nanomedicine. They have also been used in the design and synthesis of porous and mesoporous materials based on calixarenes and mesoporous silica for the storage and complex formation of hazardous nuclear waste and other contaminants [8–10]. It has been demonstrated that by utilizing Kekulene system knowledge, one can accurately compute total pi-electron energy, resonance energy, and coronoid hydrocarbon enumeration [11].

Graph-theoretical techniques are more efficient in acquiring the properties of the Kekulene system than computationally intensive quantum chemical calculations. Aihara [12] pointed out in a recent study that graph theory is beneficial not only for predicting topological resonance energies but also for exposing severe flaws in prior aromaticity theories. Recently, Julietraja and Venugopal computed the degree-based indices for coronoid structures [13]. Julietraja et al. analyzed the degree-based molecular descriptors using M-polynomial for certain classes of benzenoid systems [14, 15]. Julietraja et al. used entropy measures to investigate three prominent classes of PAHs [16].

However, despite the several promising applications of the rectangular kekulene systems, there have been no attempts till now to study these systems from a structural perspective. Our research, detailed in this article, is an effort towards bridging this research gap. The objective of this article is to compute the VDB entropy measures and irregularity-based indices for the rectangular Kekulene system. Since we tackle two open problems in this article, the number of known TIs for these systems will be doubled. This increased number of known molecular descriptors will contribute to the current body of knowledge on these systems. The TIs will also form the basis on which new Kekulene structures can be designed and synthesised.

The subsequent sections cover a literature survey on graph-theoretical concepts, degree-based entropy measures, and irregularity-based indices. There is a brief summary of the methods used for research, followed by the computation of the analytical expressions of both entropy measures and irregularity indices for rectangular Kekulene systems. The analytical expressions of the descriptors are used to compute the numerical values and observe their behaviour using graphical plots.

2. Graph-Theoretical Concepts

In this article, $\Gamma_1 (V, E)$ denotes a connected graph, where V and E denote the vertex and edge sets, respectively. The degree of a vertex m_1 in a graph Γ_1 is the number of edges that are adjacent to that vertex m_1 and is denoted by $\deg_{\Gamma_1}(m_1)$ [17]. There is a large body of knowledge about degree-based topological descriptors, which have a strong co-relation with numerous physicochemical properties of PAHs such as Zagreb and its co-indices, ABC index, GA index, Randić index, sum-connectivity index, and SDD index. These indices are also used to generate degree-based entropy measures.

2.1. Edge Weight- and Degree-Based Entropy. Let n be the order of a graph of size m and φ be some meaningful information function. The Shannon's entropy [18, 19] of a graph Γ_1 is defined as

$$\mathrm{ENT}_{\varphi}(\Gamma_1) = -\sum_{l=1}^{n} \frac{\varphi\left(\deg_{\Gamma_1}(v_l)\right)}{\sum_{m=1}^{n} \varphi\left(\deg_{\Gamma_1}(v_m)\right)} \log\left[\frac{\varphi\left(\deg_{\Gamma_1}(v_l)\right)}{\sum_{m=1}^{n} \varphi\left(\deg_{\Gamma_1}(v_m)\right)}\right]. \quad (1)$$

Let $v_l \in V(\Gamma_1)$ and the degree of v_l be represented by the information function $\varphi(v_l)$, that is, $\varphi(v_l) = \deg_{\Gamma_1}(v_l)$. Then, equation (1) can be rewritten as

$$\mathrm{ENT}_{\varphi}(\Gamma_1) = -\sum_{l=1}^{n} \frac{\deg_{\Gamma_1}(v_l)}{\sum_{m=1}^{n} \deg_{\Gamma_1}(v_m)} \log\left[\frac{\deg_{\Gamma_1}(v_l)}{\sum_{m=1}^{n} \deg_{\Gamma_1}(v_m)}\right]. \quad (2)$$

According to the fundamental theorem of graph theory, $\sum_{m=1}^{n} \deg_{\Gamma_1}(v_m) = 2E$. Hence, equation (2) reduces to

$$\mathrm{ENT}_{\varphi}(\Gamma_1) = \log(2E) - \frac{1}{2E}\log\left[\sum_{l=1}^{n}\left(\deg_{\Gamma_1}(v_l)\right)^{\deg_{\Gamma}(v_l)}\right]. \quad (3)$$

The entropy measure of an edge-weighted graph was first proposed by Chen et al. [20]. If $\Gamma_1 = (V(\Gamma_1); E(\Gamma_1); \varphi(l_1 m_1)$ is an edge-weighted graph, where $V(\Gamma_1)$, $E(\Gamma_1)$, and $\varphi(l_1 m_1)$ represents vertex set, edge set, and edge weight of the edge $(l_1 m_1)$ of Γ_1, then we have

$$\mathrm{ENT}_{\varphi}(\Gamma_1) = -\sum_{l_1'm_1' \in E(\Gamma)} \frac{\varphi(l_1'm_1')}{\sum_{l_1m_1 \in E(\Gamma_1)} \varphi(l_1m_1)} \log\left[\frac{\varphi(l_1'm_1')}{\sum_{l_1m_1 \in E(\Gamma_1)} \varphi(l_1m_1)}\right]. \tag{4}$$

By using the equations of (1), (3), and (4), we get the VDB entropy measures listed in Table 1.

2.2. Irregularity-Based Indices for QSPR Analysis. Irregularity indices are numerical parameters that quantify the irregularity of a molecular graph. The study of irregular graphs was brought to the limelight by Paul Erdös in [21]. Erdös raised an open question on irregular graphs [22], at the Second Krakow Conference on Graph Theory.

If a topological descriptor becomes zero for a normal graph and nonzero for a nonregular graph, it is known as an irregularity index. Bell proposed the first irregularity index in [23]. Irregularity indices have proved to be particularly useful in quantifying the topology of nonregular graphs. In QSPR and QSAR studies, irregularity of graphs is used to predict a range of physical and chemical properties, including melting and boiling points, enthalpy of vaporization, resistance, entropy, and toxicity. It has been proved that using regression analysis in [24], 4-octane isomer properties such as enthalpy of vaporization (HVAP), entropy, acentric factor (AcenFac), and standard enthalpy of vaporization (DHVAP) can be determined using irregularity indices with a correlation coefficient of magnitude higher than 0.9. Some commonly used irregularity indices and their analytical expressions are listed in Table 2.

The recent work and development of irregularity indices can be seen more elaborately in [25–29].

3. Methods

In this paper, the computations are performed using graph-theoretical methods, the edge partition method, and analytical techniques. Maple is utilized in obtaining the analytical expressions for the degree-based entropy measures. Maple is used to calculate the numerical values of the VDB entropy measures and irregularity indices based on analytical expressions. The numerical results are represented visually using Origin, and Chem Draw Ultra is used for describing the molecular structures of the three PAHs.

3.1. Degree-Based Entropy for the Rectangular Kekulene System. Let Γ be a rectangular Kekulene system $\mathrm{RK}(r,s)$. The number of vertices and edges of $\mathrm{RK}(r,s)$ is $V(\Gamma_1) = 36rs + 14s - 2r$ and $E(\Gamma_1) = 48rs + 16s - 4r$. $\mathrm{RK}(r,s)$ consists of $12rs + 10s + 2r$ vertices of degree 2 and $24rs + 4s - 4r$ vertices of degree 3. It is picturised in Figure 1. The edge partition table of rectangular Kekulene system $\mathrm{RK}(r,s)$ is represented in Table 3.

3.2. First Zagreb Entropy. By using the edge partition in Table 3,

$$M_1(\Gamma_1) = (264s - 28)r + 76s. \tag{5}$$

Then, using the equation of first Zagreb entropy, the result is obtained as

$$\begin{aligned}
\mathrm{ENT}_{M_1}(\Gamma_1) &= \log(M_1(\Gamma_1)) - \frac{1}{M_1(\Gamma_1)} \log\left[\prod_{l_1m_1 \in E(\Gamma_1)} \left[\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)\right]^{\left[\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)\right]}\right] \\
&= \log(M_1(\Gamma)) - \frac{1}{M_1(\Gamma)} \log\left[\begin{array}{l}
\prod_{l_1m_1 \in E_{\{2,2\}}} \left[\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)\right]^{\left[\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)\right]} \\
\times \prod_{l_1m_1 \in E_{\{2,3\}}} \left[\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)\right]^{\left[\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)\right]} \\
\times \prod_{l_1m_1 \in E_{\{3,3\}}} \left[\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)\right]^{\left[\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)\right]}
\end{array}\right] \\
&= \log((264s - 28)r + 76s) - \frac{1}{[(264s - 28)r + 76s]} \\
&\quad \log\left[\left[[4s + 2r] \times [4]^{[4]}\right] \times \left[[24rs + 12s] \times [5]^{[5]}\right] \times \left[[24rs - 6r] \times [6]^{[6]}\right]\right].
\end{aligned} \tag{6}$$

Table 1: Edge weight- and degree-based entropy.

S. no.	Degree-based entropy	Mathematical expressions
1	First Zagreb entropy	$\mathrm{ENT}_{M_1}(\Gamma_1) = \log(M_1(\Gamma_1)) - (1/M_1(\Gamma_1))\log[\prod_{l_1m_1\in E(\Gamma_1)}[\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)]^{[\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)]}]$
2	Second Zagreb entropy	$\mathrm{ENT}_{M_2}(\Gamma_1) = \log(M_2(\Gamma_1)) - (1/M_2(\Gamma_1))\log[\prod_{l_1m_1\in E(\Gamma_1)}[\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)]^{[\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)]}]$
3	Second modified Zagreb entropy	$\mathrm{ENT}_{M_2^m}(\Gamma_1) = \log(M_2^m(\Gamma_1)) - (1/M_2^m(\Gamma_1))[\prod_{l_1m_1\in E(\Gamma_1)}[1/(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1))]^{[1/(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))]}]$
4	Reduced second Zagreb entropy	$\mathrm{ENT}_{RM_2}(\Gamma_1) = \log(RM_2(\Gamma_1)) - (1/RM_2(\Gamma_1))\log[\prod_{l_1m_1\in E(\Gamma_1)}[(\deg_{\Gamma_1}(l_1) - 1) \cdot (\deg_{\Gamma_1}(m_1) - 1)]^{[(\deg_{\Gamma_1}(l_1)-1)\cdot(\deg_{\Gamma_1}(m_1)-1)]}]$
5	Hyper Zagreb entropy	$\mathrm{ENT}_{\mathrm{HM}}(\Gamma_1) = \log(\mathrm{HM}(\Gamma_1)) - (1/\mathrm{HM}(\Gamma_1))\log[\prod_{l_1m_1\in E(\Gamma_1)}[\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)]^{2[\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)]^2}]$
6	Augmented Zagreb entropy	$\mathrm{ENT}_A(\Gamma_1) = \log(A(\Gamma_1)) - (1/A(\Gamma_1))\log[\prod_{l_1m_1\in E(\Gamma_1)}[(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1))/(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2)]^{3[(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))/(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)-2)]^3}]$
7	Atom bond connectivity entropy	$\mathrm{ENT}_{ABC}(\Gamma_1) = \log(ABC(\Gamma_1)) - (1/ABC(\Gamma_1))\log[\prod_{l_1m_1\in E(\Gamma_1)}[\sqrt{(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2)/(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1))}]^{\sqrt{(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)-2)/(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))}}]$
8	Geometric arithmetic entropy	$\mathrm{ENT}_{\mathrm{GA}}(\Gamma_1) = \log(\mathrm{GA}(\Gamma_1)) - (1/\mathrm{GA}(\Gamma_1))\log[\prod_{l_1m_1\in E(\Gamma_1)}[2\sqrt{(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1))/(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1))}]^{2\sqrt{(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))/(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1))}}]$
9	Symmetric division deg (SDD) entropy	$\mathrm{ENT}_{\mathrm{SDD}}(\Gamma_1) = \log(\mathrm{SDD}(\Gamma_1)) - (1/\mathrm{SDD}(\Gamma))\log[\prod_{l_1m_1\in E(\Gamma_1)}[(\deg_{\Gamma_1}(l_1)/\deg_{\Gamma_1}(m_1)) + (\deg_{\Gamma_1}(m_1)/\deg_{\Gamma_1}(l_1))]^{[(\deg_{\Gamma_1}(l_1)/\deg_{\Gamma_1}(m_1))+(\deg_{\Gamma_1}(m_1)/\deg_{\Gamma_1}(l_1))]}]$
10	Randić entropy	$\mathrm{ENT}_R(\Gamma_1) = \log(R(\Gamma_1)) - (1/R(\Gamma_1))\log[\prod_{l_1m_1\in E(\Gamma_1)}[1/\sqrt{(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1))}]^{[1/\sqrt{(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))}]}]$
11	Forgotten entropy	$\mathrm{ENT}_F(\Gamma_1) = \log(F(\Gamma_1)) - (1/F(\Gamma_1))\log[\prod_{l_1m_1\in E(\Gamma_1)}[\deg_{\Gamma_1}(l_1)^2 + \deg_{\Gamma_1}(m_1)^2]^{[\deg_{\Gamma_1}(l_1)^2+\deg_{\Gamma_1}(m_1)^2]}]$
12	Sum-connectivity entropy	$\mathrm{ENT}_\chi(\Gamma_1) = \log(\chi(\Gamma_1)) - (1/\chi(\Gamma_1))\log[\prod_{l_1m_1\in E(\Gamma_1)}[1/\sqrt{(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1))}]^{[1/\sqrt{(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1))}]}]$
13	First redefined Zagreb entropy	$\mathrm{ENT}_{\mathrm{ReZG}_1}(\Gamma_1) = \log(\mathrm{ReZG}_1(\Gamma_1)) - (1/\mathrm{ReZG}_1(\Gamma_1))\log[\prod_{l_1m_1\in E(\Gamma_1)}[(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1))/(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1))]^{[(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1))/(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))]}]$
14	Second redefined Zagreb entropy	$\mathrm{ENT}_{\mathrm{ReZG}_2}(\Gamma_1) = \log(\mathrm{ReZG}_2(\Gamma_1)) - (1/\mathrm{ReZG}_2(\Gamma_1))\log[\prod_{l_1m_1\in E(\Gamma_1)}[(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1))/(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1))]^{[(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))/(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1))]}]$

Table 2: Irregularity-based indices for QSPR analysis.

S. no.	Irregularity-based indices
1	$VAR(\Gamma_1) = \sum_{l_1 \in V(\Gamma_1)} (\deg_{\Gamma_1}(l_1) - (2m/n))^2 = (M_1(\Gamma)/n) - (2m/n)^2$
2	$IR1(\Gamma_1) = \sum_{l_1 \in V(\Gamma_1)} \deg_{\Gamma_1}(l_1)^3 - (2m/n) \sum_{l_1 \in V(\Gamma_1)} \deg_{\Gamma_1}(l_1)^2 = F(\Gamma) - (2m/n) M_1(\Gamma)$
3	$IR2(\Gamma_1) = \sqrt{\sum_{l_1 m_1 \in E(\Gamma_1)} [\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)]/m} - (2m/n) = \sqrt{M_2(\Gamma)/m} - (2m/n)$
4	$IRDIF(\Gamma_1) = \sum_{l_1 m_1 \in E(\Gamma_1)} \lvert (\deg_{\Gamma_1}(l_1)/\deg_{\Gamma_1}(m_1)) - (\deg_{\Gamma_1}(m_1)/\deg_{\Gamma_1}(m_1)) \rvert$
5	$AL(\Gamma_1) = \sum_{l_1 m_1 \in E(\Gamma_1)} \lvert \deg_{\Gamma_1}(l_1) - \deg_{\Gamma_1}(m_1) \rvert$
6	$IRL(\Gamma_1) = \sum_{l_1 m_1 \in E(\Gamma_1)} \lvert \ln \deg_{\Gamma_1}(l_1) - \ln \deg_{\Gamma_1}(m_1) \rvert$
7	$IRLU(\Gamma_1) = \sum_{l_1 m_1 \in E(\Gamma_1)} (\lvert \deg_{\Gamma_1}(l_1) - \deg_{\Gamma_1}(m_1) \rvert / \min(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)))$
8	$IRLF(\Gamma_1) = \sum_{l_1 m_1 \in E(\Gamma_1)} (\lvert \deg_{\Gamma_1}(l_1) - \deg_{\Gamma_1}(m_1) \rvert / \sqrt{(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1))})$
9	$IRF(\Gamma_1) = \sum_{l_1 m_1 \in E(\Gamma_1)} (d_u - d_v)^2 = F(\Gamma_1) - 2M_2(\Gamma_1)$
10	$IRLA(\Gamma_1) = \sum_{l_1 m_1 \in E(\Gamma_1)} (\lvert \deg_{\Gamma_1}(l_1) - \deg_{\Gamma_1}(m_1) \rvert / (\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)))$
11	$IRD_1(\Gamma_1) = \sum_{l_1 m_1 \in E(\Gamma_1)} \ln\left\{1 + \lvert \deg_{\Gamma_1}(l_1) - \deg_{\Gamma_1}(m_1) \rvert\right\}$
12	$IRA(\Gamma_1) = \sum_{l_1 m_1 \in E(\Gamma_1)} (\deg_{\Gamma_1}(l_1)^{-1/2} - \deg_{\Gamma_1}(m_1)^{-1/2})^2$
13	$IRB(\Gamma_1) = \sum_{l_1 m_1 \in E(\Gamma_1)} (\deg_{\Gamma_1}(l_1)^{-1/2} - \deg_{\Gamma_1}(m_1)^{-1/2})^2$
14	$IRB(\Gamma_1) = (\sum_{l_1 m_1 \in E(\Gamma_1)} \sqrt{(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1))}/m) - (2m/n) = (RR(\Gamma_1)/m) - (2m/n)$
15	$IRGA(\Gamma_1) = \sum_{l_1 m_1 \in E(\Gamma_1)} \ln(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)/2\sqrt{(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1))})$
16	$IRR_t(\Gamma_1) = (1/2) \sum_{l_1 m_1 \in E(\Gamma_1)} \lvert \deg_{\Gamma_1}(l_1) - \deg_{\Gamma_1}(m_1) \rvert$

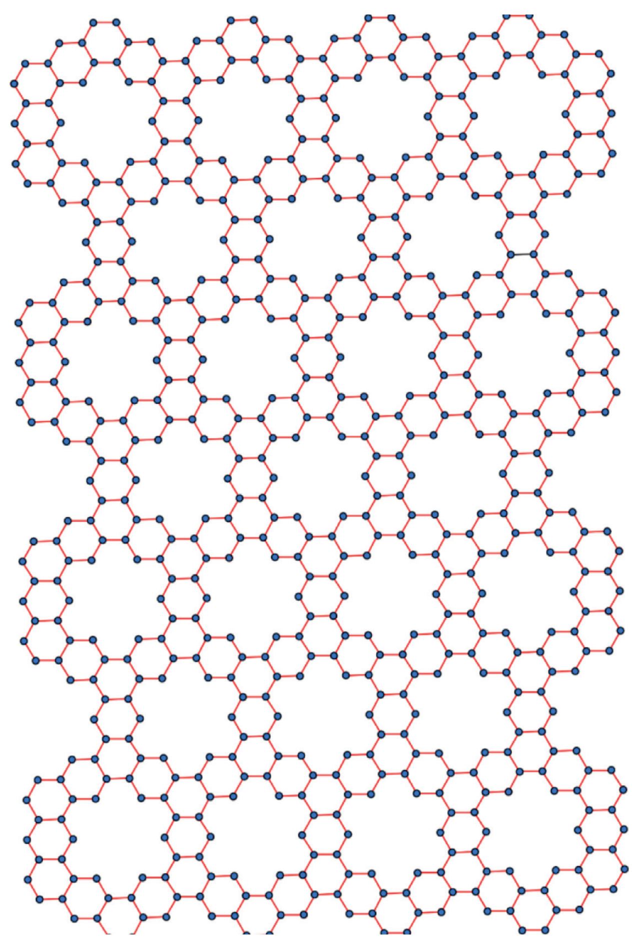

Figure 1: Rectangular Kekulene system.

Table 3: Edge partition table of $RK(r,s)$.

$(\deg_{\Gamma_1}(l_1), \deg_{\Gamma_1}(m_1))$	Total number of edges
$(2,2)$	$4s+2r$
$(2,3)$	$24rs+12s$
$(3,3)$	$24rs-6r$

3.3. Second Zagreb Entropy. By using the edge partition in Table 3,

$$M_2(\Gamma_1) = (360s-46)r+88s. \quad (7)$$

Then, using the equation of second Zagreb entropy, the result is obtained as

$$\begin{aligned}
\mathrm{ENT}_{M_2}(\Gamma_1) &= \log(M_2(\Gamma_1)) - \frac{1}{M_2(\Gamma_1)}\log\left[\prod_{l_1m_1\in E(\Gamma_1)}\left[\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right]^{\left[\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right]}\right] \\
&= \log(M_2(\Gamma_1)) - \frac{1}{M_2(\Gamma_1)}\log\begin{bmatrix}\prod_{l_1m_1\in E_{\{2,2\}}}\left[\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right]^{\left[\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right]} \\ \times\prod_{l_1m_1\in E_{\{2,3\}}}\left[\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right]^{\left[\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right]} \\ \times\prod_{l_1m_1\in E_{\{3,3\}}}\left[\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right]^{\left[\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right]}\end{bmatrix} \\
&= \log((360s-46)r+88s) - \frac{1}{[(360s-46)r+88s]} \\
&\quad \log\left[\left[[4s+2r]\times[4]^{[4]}\right]\times\left[[24rs+12s]\times[6]^{[6]}\right]\times\left[[24rs-6r]\times[9]^{[9]}\right]\right].
\end{aligned} \quad (8)$$

3.4. Second Modified Zagreb Entropy. By using the edge partition in Table 3,

$$M_2^m(\Gamma) = \frac{1}{6}(40s-1)r+3s. \quad (9)$$

Then, using the equation of the second modified Zagreb entropy, the result is obtained as

$$\begin{aligned}
\mathrm{ENT}_{M_2^m}(\Gamma_1) &= \log(M_2^m(\Gamma_1)) - \frac{1}{M_2^m(\Gamma_1)}\log\left[\prod_{l_1m_1\in E(\Gamma_1)}\left[\frac{1}{(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))}\right]^{\left[1/(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))\right]}\right] \\
&= \log(M_2^m(\Gamma_1)) - \frac{1}{M_2^m(\Gamma_1)}\log\begin{bmatrix}\prod_{l_1m_1\in E_{\{2,2\}}}\left[\frac{1}{(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))}\right]^{\left[1/(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))\right]} \\ \times\prod_{l_1m_1\in E_{\{2,3\}}}\left[\frac{1}{(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))}\right]^{\left[1/(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))\right]} \\ \times\prod_{l_1m_1\in E_{\{3,3\}}}\left[\frac{1}{(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))}\right]^{\left[1/(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1))\right]}\end{bmatrix} \\
&= \log\left(\frac{1}{6}(40s-1)r+3s\right) - \frac{1}{[(1/6)(40s-1)r+3s]}
\end{aligned}$$

$$\log\left[\left[[4s+2r]\times\left[\frac{1}{4}\right]^{[1/4]}\right]\times\left[[24rs+12s]\times\left[\frac{1}{6}\right]^{[1/6]}\right]\times\left[[24rs-6r]\times\left[\frac{1}{9}\right]^{[1/9]}\right]\right]. \tag{10}$$

3.5. Reduced Second Zagreb Entropy. By using the edge partition in Table 3,

$$RM_2(\Gamma)=((144s-22)r+28s. \tag{11}$$

Then, using the equation of reduced second Zagreb entropy, the result is obtained as

$$\begin{aligned}
\mathrm{ENT}_{RM_2}(\Gamma_1)&=\log(\mathrm{RM}_2(\Gamma_1))-\frac{1}{\mathrm{RM}_2(\Gamma_1)}\log\left[\prod_{l_1m_1\in E(\Gamma_1)}\left[\left(\deg_{\Gamma_1}(l_1)-1\right)\cdot\left(\deg_{\Gamma_1}(m_1)-1\right)\right]^{\left[\left(\deg_{\Gamma_1}(l_1)-1\right)\cdot\left(\deg_{\Gamma_1}(m_1)-1\right)\right]}\right]\\
&=\log(M_2^m(\Gamma_1))-\frac{1}{M_2^m(\Gamma_1)}\log\left[\begin{array}{l}\prod_{l_1m_1\in E_{\{2,2\}}}\left[\left(\deg_{\Gamma_1}(l_1)-1\right)\cdot\left(\deg_{\Gamma_1}(m_1)-1\right)\right]^{\left[\left(\deg_{\Gamma_1}(l_1)-1\right)\cdot\left(\deg_{\Gamma_1}(m_1)-1\right)\right]}\\ \times\prod_{l_1m_1\in E_{\{2,3\}}}\left[\left(\deg_{\Gamma_1}(l_1)-1\right)\cdot\left(\deg_{\Gamma_1}(m_1)-1\right)\right]^{\left[\left(\deg_{\Gamma_1}(l_1)-1\right)\cdot\left(\deg_{\Gamma_1}(m_1)-1\right)\right]}\\ \times\prod_{l_1m_1\in E_{\{3,3\}}}\left[\left(\deg_{\Gamma_1}(l_1)-1\right)\cdot\left(\deg_{\Gamma_1}(m_1)-1\right)\right]^{\left[\left(\deg_{\Gamma_1}(l_1)-1\right)\cdot\left(\deg_{\Gamma_1}(m_1)-1\right)\right]}\end{array}\right]\\
&=\log((144s-22)r+28)-\frac{1}{[(144s-22)r+28]}\\
&\quad\log\left[\left[[4s+2r]\times[1]^{[1]}\right]\times\left[[24rs+12s]\times[2]^{[2]}\right]\times\left[[24rs-6r]\times[4]^{[4]}\right]\right].
\end{aligned} \tag{12}$$

3.6. Hyper Zagreb Entropy. By using the edge partition in Table 3,

$$\mathrm{HM}(\Gamma_1)=(1464s-184)r+364s. \tag{13}$$

Then, using the equation of reduced second Zagreb entropy, the result is obtained as

$$\begin{aligned}
\mathrm{ENT}_{\mathrm{HM}}(\Gamma_1)&=\log(\mathrm{HM}(\Gamma_1))-\frac{1}{\mathrm{HM}(\Gamma_1)}\log\left[\prod_{l_1m_1\in E(\Gamma_1)}\left[\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right]^{2\left[\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right]^2}\right]\\
&=\log(\mathrm{HM}(\Gamma_1))-\frac{1}{\mathrm{HM}(\Gamma_1)}\log\left[\begin{array}{l}\prod_{l_1m_1\in E_{\{2,2\}}}\left[\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right]^{2\left[\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right]^2}\\ \times\prod_{l_1m_1\in E_{\{2,3\}}}\left[\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right]^{2\left[\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right]^2}\\ \times\prod_{l_1m_1\in E_{\{3,3\}}}\left[\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right]^{2\left[\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right]^2}\end{array}\right]
\end{aligned}$$

$$= \log((1464s - 184)r + 364s) - \frac{1}{[(1464s - 184)r + 364s]} \log\left[\left[[4s + 2r] \times [16]^{[16]}\right] \times \left[[24rs + 12s] \times [25]^{[25]}\right] \times \left[[24rs - 6r] \times [36]^{[36]}\right]\right]. \quad (14)$$

3.7. Augmented Zagreb Entropy. By using the edge partition in Table 3,

$$A(\Gamma_1) = \frac{1}{32}(14892s - 1675)r + 128s. \quad (15)$$

Then, using the equation of reduced second Zagreb entropy, the result is obtained as

$$\begin{aligned}
\mathrm{ENT}_A(\Gamma_1) &= \log(A(\Gamma_1)) - \frac{1}{A(\Gamma_1)} \log\left[\prod_{l_1 m_1 \in E(\Gamma_1)} \left[\frac{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2}\right]^{3\left[\left(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)\right)/\left(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2\right)\right]^3}\right] \\
&= \log(A(\Gamma_1)) - \frac{1}{A(\Gamma_1)} \log\left[\begin{array}{l}
\prod_{l_1 m_1 \in E_{\{2,2\}}} \left[\frac{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2}\right]^{3\left[\left(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)\right)/\left(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2\right)\right]^3} \\
\times \prod_{l_1 m_1 \in E_{\{2,3\}}} \left[\frac{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2}\right]^{3\left[\left(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)\right)/\left(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2\right)\right]^3} \\
\times \prod_{l_1 m_1 \in E_{\{3,3\}}} \left[\frac{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2}\right]^{3\left[\left(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)\right)/\left(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2\right)\right]^3}
\end{array}\right] \\
&= \log\left(\frac{1}{32}(14892s - 1675)r + 128s\right) - \frac{1}{[(1/32)(14892s - 1675)r + 128s]} \\
&\quad \log\left[\left[[4s + 2r] \times [8]^{[8]}\right] \times \left[[24rs + 12s] \times [8]^{[8]}\right] \times \left[[24rs - 6r] \times \left[\frac{729}{64}\right]^{[729/64]}\right]\right].
\end{aligned} \quad (16)$$

3.8. Atom Bond Connectivity Entropy. By using the edge partition in Table 3,

$$ABC(\Gamma_1) = ((12s + 1)r + 8s)\sqrt{2} + (16s - 4)r. \quad (17)$$

Then, using the equation of atom bond connectivity entropy, the result is obtained as

$$\mathrm{ENT}_{ABC}(\Gamma_1) = \log(ABC(\Gamma_1)) - \frac{1}{ABC(\Gamma_1)} \log\left[\prod_{l_1 m_1 \in E(\Gamma_1)} \left[\sqrt{\frac{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2}{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}}\right]^{\left[\sqrt{\left(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2\right)/\left(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)\right)}\right]}\right]$$

$$= \log\left(ABC\left(\Gamma_1\right)\right) - \frac{1}{ABC\left(\Gamma_1\right)} \log \left[\begin{array}{l} \prod_{l_1 m_1 \in E_{\{2,2\}}} \left[\sqrt{\frac{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2}{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}} \right]^{\left[\sqrt{\left(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2\right)/\left(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)\right)}\right]} \\ \times \prod_{l_1 m_1 \in E_{\{2,3\}}} \left[\sqrt{\frac{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2}{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}} \right]^{\left[\sqrt{\left(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2\right)/\left(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)\right)}\right]} \\ \times \prod_{l_1 m_1 \in E_{\{3,3\}}} \left[\sqrt{\frac{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2}{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}} \right]^{\left[\sqrt{\left(\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1) - 2\right)/\left(\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)\right)}\right]} \end{array} \right]$$

$$= \log\left(\left(\left(12s + 1\right)r + 8s\right)\sqrt{2} + \left(16s - 4\right)r\right) - \frac{1}{\left[\left(\left(12s + 1\right)r + 8s\right)\sqrt{2} + \left(16s - 4\right)r\right]} \log\left[\left[\left[4s + 2r\right] \times \left[\sqrt{\frac{1}{2}}\right]^{\left[\sqrt{1/2}\right]}\right] \times \left[\left[24rs + 12s\right] \times \left[\sqrt{\frac{1}{2}}\right]^{\left[\sqrt{1/2}\right]}\right] \times \left[\left[24rs - 6r\right] \times \left[\frac{2}{3}\right]^{[2/3]}\right]\right]. \quad (18)$$

3.9. Geometric Arithmetic Entropy. By using the edge partition in Table 3,

$$\mathrm{GA}\left(\Gamma_1\right) = 4s - 4r + \left(\frac{48}{5}\right)\sqrt{6}rs + \left(\frac{24}{5}\right)\sqrt{6}s + 24rs. \quad (19)$$

Then, using the equation of geometric arithmetic entropy, the result is obtained as

$$\mathrm{ENT}_{\mathrm{GA}}\left(\Gamma_1\right) = \log\left(\mathrm{GA}\left(\Gamma_1\right)\right) - \frac{1}{\mathrm{GA}\left(\Gamma_1\right)} \log\left[\prod_{l_1 m_1 \in E\left(\Gamma_1\right)} \left[\frac{2\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}}{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}\right]^{\left[2\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}/\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)\right]}\right]$$

$$= \log\left(\mathrm{GA}\left(\Gamma_1\right)\right) - \frac{1}{\mathrm{GA}\left(\Gamma_1\right)} \log \left[\begin{array}{l} \prod_{l_1 m_1 \in E_{\{2,2\}}} \left[\frac{2\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}}{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}\right]^{\left[2\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}/\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)\right]} \\ \times \prod_{l_1 m_1 \in E_{\{2,3\}}} \left[\frac{2\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}}{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}\right]^{\left[2\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}/\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)\right]} \\ \times \prod_{l_1 m_1 \in E_{\{3,3\}}} \left[\frac{2\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}}{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}\right]^{\left[2\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}/\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)\right]} \end{array} \right]$$

$$= \log\left(4s - 4r + \left(\frac{48}{5}\right)\sqrt{6}\,rs + \left(\frac{24}{5}\right)\sqrt{6}\,s + 24rs\right) - \frac{1}{\left[4s - 4r + (48/5)\sqrt{6}\,rs + (24/5)\sqrt{6}\,s + 24rs\right]} \log\left[\left[\left[4s + 2r\right] \times [1]^{[1]}\right] \times \left[\left[24rs + 12s\right] \times \left[\frac{2\sqrt{6}}{5}\right]^{\left[2\sqrt{6}/5\right]}\right] \times \left[\left[24rs - 6r\right] \times [1]^{[1]}\right]\right]. \quad (20)$$

3.10. Symmetric Division Deg (SDD) Entropy. By using the edge partition in Table 3,

$$\mathrm{SDD}(\Gamma_1) = 100rs - 8r + 34s. \tag{21}$$

Then, using the equation of Symmetric division deg entropy, the result is obtained as

$$\begin{aligned}
\mathrm{ENT}_{\mathrm{SDD}}(\Gamma_1) &= \log(\mathrm{SDD}(\Gamma_1)) - \frac{1}{\mathrm{SDD}(\Gamma_1)} \log\left[\prod_{l_1 m_1 \in E(\Gamma_1)} \left[\frac{\deg_{\Gamma_1}(l_1)}{\deg_{\Gamma_1}(m_1)} + \frac{\deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1)}\right]^{\left[\left(\deg_{\Gamma_1}(l_1)/\deg_{\Gamma_1}(m_1)\right) + \left(\deg_{\Gamma_1}(m_1)/\deg_{\Gamma_1}(l_1)\right)\right]}\right] \\
&= \log(\mathrm{SDD}(\Gamma_1)) - \frac{1}{\mathrm{SDD}(\Gamma_1)} \log\left[\begin{array}{l}
\prod_{l_1 m_1 \in E_{\{2,2\}}} \left[\frac{\deg_{\Gamma_1}(l_1)}{\deg_{\Gamma_1}(m_1)} + \frac{\deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1)}\right]^{\left[\left(\deg_{\Gamma_1}(l_1)/\deg_{\Gamma_1}(m_1)\right) + \left(\deg_{\Gamma_1}(m_1)/\deg_{\Gamma_1}(l_1)\right)\right]} \\
\times \prod_{l_1 m_1 \in E_{\{2,3\}}} \left[\frac{\deg_{\Gamma_1}(l_1)}{\deg_{\Gamma_1}(m_1)} + \frac{\deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1)}\right]^{\left[\left(\deg_{\Gamma_1}(l_1)/\deg_{\Gamma_1}(m_1)\right) + \left(\deg_{\Gamma_1}(m_1)/\deg_{\Gamma_1}(l_1)\right)\right]} \\
\times \prod_{l_1 m_1 \in E_{\{3,3\}}} \left[\frac{\deg_{\Gamma_1}(l_1)}{\deg_{\Gamma_1}(m_1)} + \frac{\deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1)}\right]^{\left[\left(\deg_{\Gamma_1}(l_1)/\deg_{\Gamma_1}(m_1)\right) + \left(\deg_{\Gamma_1}(m_1)/\deg_{\Gamma_1}(l_1)\right)\right]}
\end{array}\right] \\
&= \log(100rs - 8r + 34s) - \frac{1}{[100rs - 8r + 34s]} \\
&\quad \log\left[\left[[4s + 2r] \times [2]^{[2]}\right] \times \left[[24rs + 12s] \times \left[\frac{13}{6}\right]^{[13/6]}\right] \times \left[[24rs - 6r] \times [2]^{[2]}\right]\right].
\end{aligned} \tag{22}$$

3.11. Randić Entropy. By using the edge partition in Table 3,

$$R(\Gamma_1) = 4\sqrt{6}rs + 2\sqrt{6}s + 8rs - r + 2s. \tag{23}$$

Then, using the equation of Randić entropy, the result is obtained as

$$\begin{aligned}
\mathrm{ENT}_R(\Gamma_1) &= \log(R(\Gamma_1)) - \frac{1}{R(\Gamma_1)} \log\left[\prod_{l_1 m_1 \in E(\Gamma_1)} \left[\frac{1}{\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}}\right]^{\left[\left(1/\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}\right)\right]}\right] \\
&= \log(R(\Gamma_1)) - \frac{1}{R(\Gamma_1)} \log\left[\begin{array}{l}
\prod_{l_1 m_1 \in E_{\{2,2\}}} \left[\frac{1}{\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}}\right]^{\left[\left(1/\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}\right)\right]} \\
\times \prod_{l_1 m_1 \in E_{\{2,3\}}} \left[\frac{1}{\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}}\right]^{\left[\left(1/\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}\right)\right]} \\
\times \prod_{l_1 m_1 \in E_{\{3,3\}}} \left[\frac{1}{\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}}\right]^{\left[\left(1/\sqrt{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}\right)\right]}
\end{array}\right]
\end{aligned}$$

$$= \log(4\sqrt{6}rs + 2\sqrt{6}s + 8rs - r + 2s) - \frac{1}{[4\sqrt{6}rs + 2\sqrt{6}s + 8rs - r + 2s]} \log\left[\left[[4s + 2r] \times \left[\frac{1}{2}\right]^{[1/2]}\right] \times \left[[24rs + 12s] \times \left[\frac{1}{\sqrt{6}}\right]^{[1/\sqrt{6}]}\right] \times \left[[24rs - 6r] \times \left[\frac{1}{3}\right]^{[1/3]}\right]\right]. \tag{24}$$

3.12. Forgotten Entropy. By using the edge partition in Table 3,

$$F(\Gamma_1) = 744rs - 92r + 188s. \tag{25}$$

Then, using the equation of forgotten entropy, the result is obtained as

$$\begin{aligned} \mathrm{ENT}_F(\Gamma_1) &= \log(F(\Gamma_1)) - \frac{1}{F(\Gamma_1)} \log\left[\prod_{l_1m_1 \in E(\Gamma_1)} \left[\deg_{\Gamma_1}(l_1)^2 + \deg_{\Gamma_1}(m_1)^2\right]^{\left[\deg_{\Gamma_1}(l_1)^2 + \deg_{\Gamma_1}(m_1)^2\right]}\right] \\ &= \log(F(\Gamma_1)) - \frac{1}{F(\Gamma_1)} \log\left[\begin{array}{l} \prod_{l_1m_1 \in E_{\{2,2\}}} \left[\deg_{\Gamma_1}(l_1)^2 + \deg_{\Gamma_1}(m_1)^2\right]^{\left[\deg_{\Gamma_1}(l_1)^2 + \deg_{\Gamma_1}(m_1)^2\right]} \\ \times \prod_{l_1m_1 \in E_{\{2,3\}}} \left[\deg_{\Gamma_1}(l_1)^2 + \deg_{\Gamma_1}(m_1)^2\right]^{\left[\deg_{\Gamma_1}(l_1)^2 + \deg_{\Gamma_1}(m_1)^2\right]} \\ \times \prod_{l_1m_1 \in E_{\{3,3\}}} \left[\deg_{\Gamma_1}(l_1)^2 + \deg_{\Gamma_1}(m_1)^2\right]^{\left[\deg_{\Gamma_1}(l_1)^2 + \deg_{\Gamma_1}(m_1)^2\right]} \end{array}\right] \\ &= \log(744rs - 92r + 188s) - \frac{1}{[744rs - 92r + 188s]} \log\left[\left[[4s + 2r] \times [8]^{[8]}\right] \times \left[[24rs + 12s] \times [13]^{[13]}\right] \times \left[[24rs - 6r] \times [18]^{[18]}\right]\right]. \end{aligned} \tag{26}$$

3.13. Sum-Connectivity Entropy. By using the edge partition in Table 3,

$$\chi(\Gamma_1) = 2s + r + \left(\frac{24}{5}\right)\sqrt{5}rs + \left(\frac{12}{5}\right)\sqrt{5}s + 4\sqrt{6}rs - \sqrt{6}r. \tag{27}$$

Then, using the equation of sum-connectivity entropy, the result is obtained as

$$\mathrm{ENT}_\chi(\Gamma_1) = \log(\chi(\Gamma_1)) - \frac{1}{\chi(\Gamma_1)} \log\left[\prod_{l_1m_1 \in E(\Gamma_1)} \left[\frac{1}{\sqrt{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}}\right]^{\left[\left(1/\sqrt{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}\right)\right]}\right]$$

$$= \log\left(F\left(\Gamma_1\right)\right) - \frac{1}{F\left(\Gamma_1\right)} \log\left[\begin{array}{l} \prod_{l_1 m_1 \in E_{\{2,2\}}} \left[\frac{1}{\sqrt{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}}\right]^{\left[\left(1/\sqrt{\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)}\right)\right]} \\ \times \prod_{l_1 m_1 \in E_{\{2,3\}}} \left[\frac{1}{\sqrt{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}}\right]^{\left[\left(1/\sqrt{\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)}\right)\right]} \\ \times \prod_{l_1 m_1 \in E_{\{3,3\}}} \left[\frac{1}{\sqrt{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}}\right]^{\left[\left(1/\sqrt{\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)}\right)\right]} \end{array}\right]$$
$$= \log\left(2s + r + \left(\frac{24}{5}\right)\sqrt{5}\, rs + \left(\frac{12}{5}\right)\sqrt{5}\, s + 4\sqrt{6}\, rs - \sqrt{6}\, r\right) - \frac{1}{\left[2s + r + (24/5)\sqrt{5}\, rs + (12/5)\sqrt{5}\, s + 4\sqrt{6}\, rs - \sqrt{6}\, r\right]}$$
$$\log\left[\left[[4s + 2r] \times \left[\frac{1}{2}\right]^{[1/2]}\right] \times \left[[24rs + 12s] \times \left[\frac{1}{\sqrt{5}}\right]^{[1/\sqrt{5}\,]}\right] \times \left[[24rs - 6r] \times \left[\frac{1}{\sqrt{6}}\right]^{[1/\sqrt{6}\,]}\right]\right]. \tag{28}$$

3.14. First Redefined Zagreb Entropy. By using the edge partition in Table 3,

$$\mathrm{ReZG}_1\left(\Gamma_1\right) = 36rs - 2r + 14s. \tag{29}$$

Then, using the equation of first redefined Zagreb entropy, the result is obtained as

$$\mathrm{ENT}_{\mathrm{ReZG}_1}\left(\Gamma_1\right) = \log\left(\mathrm{ReZG}_1\left(\Gamma_1\right)\right) - \frac{1}{\mathrm{ReZG}_1\left(\Gamma_1\right)} \log\left[\prod_{l_1 m_1 \in E\left(\Gamma_1\right)} \left[\frac{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}\right]^{\left[\left(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right)/\left(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right)\right]}\right]$$
$$= \log\left(\mathrm{ReZG}_1\left(\Gamma_1\right)\right) - \frac{1}{\mathrm{ReZG}_1\left(\Gamma_1\right)} \log\left[\begin{array}{l} \prod_{l_1 m_1 \in E_{\{2,2\}}} \left[\frac{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}\right]^{\left[\left(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right)/\left(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right)\right]} \\ \times \prod_{l_1 m_1 \in E_{\{2,3\}}} \left[\frac{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}\right]^{\left[\left(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right)/\left(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right)\right]} \\ \times \prod_{l_1 m_1 \in E_{\{3,3\}}} \left[\frac{\deg_{\Gamma_1}(l_1) + \deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1) \cdot \deg_{\Gamma_1}(m_1)}\right]^{\left[\left(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right)/\left(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right)\right]} \end{array}\right]$$
$$= \log(36rs - 2r + 14s) - \frac{1}{[36rs - 2r + 14s]}$$
$$\log\left[\left[[4s + 2r] \times [1]^{[1]}\right] \times \left[[24rs + 12s] \times \left[\frac{5}{6}\right]^{[5/6]}\right] \times \left[[24rs - 6r] \times \left[\frac{2}{3}\right]^{[2/3]}\right]\right]. \tag{30}$$

3.15. Second Redefined Zagreb Entropy. By using the edge partition in Table 3,

$$\mathrm{ReZG}_1\left(\Gamma_1\right) = \left(\frac{92}{5}\right)s - 7r + \left(\frac{324}{5}\right)rs. \tag{31}$$

Then, using the equation of the second redefined Zagreb entropy, the result is obtained as

$$
\begin{aligned}
\mathrm{ENT}_{\mathrm{ReZG}_2}(\Gamma_1) &= \log\left(\mathrm{ReZG}_2(\Gamma_1)\right) - \frac{1}{\mathrm{ReZG}_2(\Gamma_1)}\log\left[\prod_{l_1m_1\in E(\Gamma_1)}\left[\frac{\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)}\right]^{\left[\left(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right)/\left(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right)\right]}\right]\\
&= \log\left(\mathrm{ReZG}_2(\Gamma_1)\right) - \frac{1}{\mathrm{ReZG}_2(\Gamma_1)}\log\left[\begin{array}{l}\prod_{l_1m_1\in E_{\{2,2\}}}\left[\frac{\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)}\right]^{\left[\left(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right)/\left(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right)\right]}\\
\times\prod_{l_1m_1\in E_{\{2,3\}}}\left[\frac{\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)}\right]^{\left[\left(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right)/\left(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right)\right]}\\
\times\prod_{l_1m_1\in E_{\{3,3\}}}\left[\frac{\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)}{\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)}\right]^{\left[\left(\deg_{\Gamma_1}(l_1)\cdot\deg_{\Gamma_1}(m_1)\right)/\left(\deg_{\Gamma_1}(l_1)+\deg_{\Gamma_1}(m_1)\right)\right]}\end{array}\right]\\
&= \log\left(\left(\frac{92}{5}\right)s - 7r + \left(\frac{324}{5}\right)rs\right) - \frac{1}{[(92/5)s - 7r + (324/5)rs]}\\
&\quad\log\left[\left[[4s+2r]\times[1]^{[1]}\right]\times\left[[24rs+12s]\times\left[\frac{6}{5}\right]^{[6/5]}\right]\times\left[[24rs-6r]\times\left[\frac{3}{2}\right]^{[3/2]}\right]\right].
\end{aligned}
\tag{32}
$$

Theorem 1. *If Γ_1 is the RK(r,s), then the irregularity-based descriptors are expressed as follows:*

(1) $VAR(\Gamma_1) = (2(36r^2s^2 + 36rs^2 - r^2 - 4rs + 5s^2)/(18rs - r + 7s)^2)$

(2) $IR1(\Gamma_1) = (4(180r^2s^2 + 1434rs^2 - 5r^2 - 115rs + 462s^2)/(18rs - r + 7s))$

(3) $IR2(\Gamma_1) = (1/2)(18\sqrt{2}\sqrt{(180rs - 23r + 44s)/(12rs - r + 4s)rs} - \sqrt{2}\sqrt{(180rs - 23r + 44s)/(12rs - r + 4s)r} + 7\sqrt{2}\sqrt{(180rs - 23r + 44s)/(12rs - r + 4s)s} - 96rs + 8r - 32s/(18rs - r + 7s))$

(4) $IRDIF(\Gamma_1) = (1/3)(24rs + 12s)$

(5) $AL(\Gamma_1) = 24rs + 12s$

(6) $IRL(\Gamma_1) = 0.40545(24rs + 12s)$

(7) $IRLU(\Gamma_1) = (0.40545/2)(24rs + 12s)$

(8) $IRLF(\Gamma_1) = (1/\sqrt{6})(24rs + 12s)$

(9) $IRF(\Gamma_1) = 24rs + 12s$

(10) $IRLA(\Gamma_1) = (2/5)(24rs + 12s)$

(11) $IRD_1(\Gamma_1) = 0.69315(24rs + 12s)$

(12) $IRA(\Gamma_1) = 0.016832(24rs + 12s)$

(13) $IRB(\Gamma_1) = 0.10106(24rs + 12s)$

(14) $IRB(\Gamma_1) = (1/2)((216\sqrt{6}r^2s^2 - 12\sqrt{6}r^2s + 192\sqrt{6}rs^2 - 504r^2s^2 - 6\sqrt{6}rs + 42\sqrt{6}s^2 + 30r^2s - 444rs^2 - r^2 + 11rs - 100s^2)/(12rs - r + 4s))(18rs - r + 7s)$

(15) $IRGA(\Gamma_1) = 0.020391(24rs + 12s)$

(16) $IRR_t(\Gamma_1) = (1/2)(24rs + 12s)$

4. Numerical and Graphical Analysis of RK$(\mathbf{r}, \mathbf{s})$

In this section, by changing the values of the variables r and s from 1 to 9, the numerical values of VDB entropy measures are obtained using the analytical expressions of the rectangular Kekulene system. Tables 4 and 5 show the results of these calculations. By looking at their numerical values, the comparison can be done easily to see whether there are any similarities or differences between the individual topological indices. Figures 2 and 3 show this behaviour as three-dimensional graphical representations. The differences between each topological index for a specific structure can be seen in these 3D plots.

As it is evident from the above calculations, it is quite convenient to compute topological indices. Since topological indices correlate well with physiochemical properties, these can be directly used to predict the behaviour of compounds. Such a theoretical analysis based on topology significantly reduces the time and efforts required for analysis of compounds, when compared to intensive quantum chemical calculations or laborious experiments. But, not all properties of a compound can be mathematically associated to topological indices. Some features would still require practical experiments to be studied. The prediction accuracy of QSAR/QSPR methods which use TIs can also be comparatively less than that of

Table 4: Comparison table of $RK[r, s]$.

$RK[r, s]$	$ENT_{M_1}(\Gamma_1)$	$ENT_{M_2}(\Gamma_1)$	$ENT_{M_2^m}(\Gamma_1)$	$ENT_{RM_2}(\Gamma_1)$	$ENT_{HM}(\Gamma_1)$	$ENT_{A}(\Gamma_1)$	$ENT_{ABC}(\Gamma_1)$
[1, 1]	5.65	5.89	1.56	4.92	7.25	6.17	3.57
[2, 2]	7.02	7.30	3.17	6.30	8.69	7.57	4.94
[3, 3]	7.82	8.11	4.05	7.12	9.51	8.38	5.74
[4, 4]	8.38	8.68	4.66	7.71	10.08	8.95	6.31
[5, 5]	8.83	9.12	5.12	8.16	10.53	9.39	6.75

Table 5: Comparison table of $RK[r, s]$.

$RK[r, s]$	$ENT_{GA}(\Gamma_1)$	$ENT_{SDD}(\Gamma_1)$	$ENT_{R}(\Gamma_1)$	$ENT_{F}(\Gamma_1)$	$ENT_{\chi}(\Gamma_1)$	$ENT_{ReZG_1}(\Gamma_1)$	$ENT_{ReZG_2}(\Gamma_1)$
[1, 1]	3.96	4.84	2.89	6.60	3.03	3.72	4.24
[2, 2]	5.31	6.08	4.30	8.03	4.44	5.06	5.60
[3, 3]	6.11	6.87	5.11	8.84	5.25	5.85	6.40
[4, 4]	6.68	7.43	5.69	9.41	5.83	6.41	6.97
[5, 5]	7.12	7.87	6.13	9.85	6.27	6.85	7.42

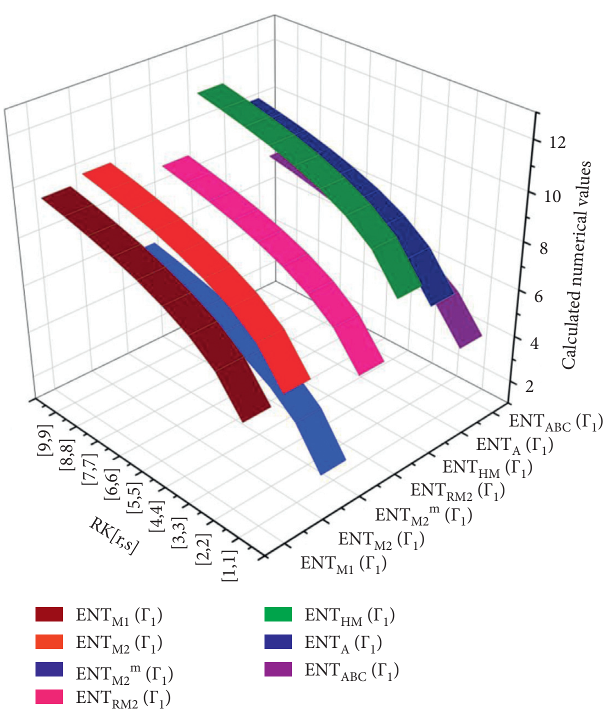

Figure 2: Graphical visualisation for Table 4.

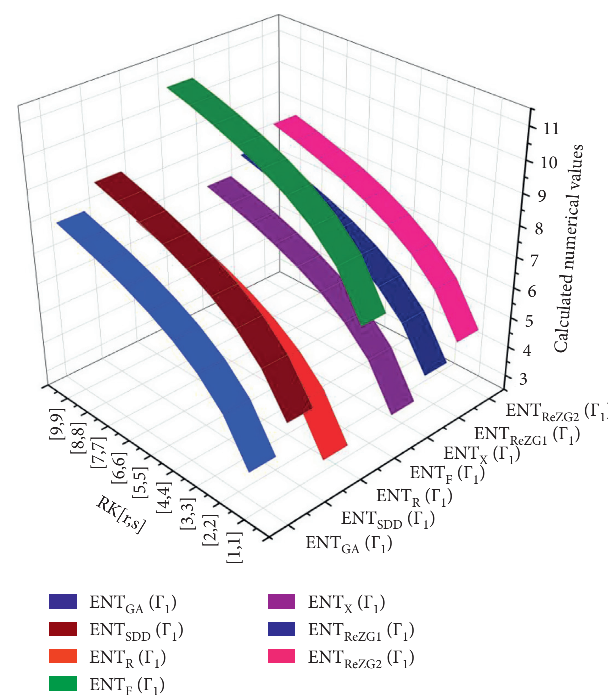

Figure 3: Graphical visualisation for Table 5.

experimental observations. However, TIs have been widely accepted by the scientific community as predictive methods for a subset of physiochemical properties due to their ease of use and universal applicability.

5. Conclusion

In this paper, the mathematical expressions of VDB entropy measures and irregularity-based indices have been computed for $RK(r, s)$. Furthermore, the numerical values for these expressions of VDB entropy measures and irregularity-based indices are calculated using the obtained analytical expressions. The 3D graphical comparisons of these analytical expressions of VDB entropy measures have been represented visually to find the behavioural pattern of the molecular compound. The study of Wiener polarity-based TIs, eccentricity-based TIs, and the recent development of VDB indices for this structure can also be explored as they have never been studied earlier. It is still an area where further research could be done in the future.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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