

## Research Article

# The Edge-Weighted Graph Entropy Using Redefined Zagreb Indices

Jing Lu <sup>1</sup>, Hafiz Mutee-ur-Rehman <sup>2</sup>, Saima Nazeer,<sup>3</sup> and Xuemei An<sup>4</sup>

<sup>1</sup>Foundation Department, Changchun Sci-Tech University, Changchun 130600, China

<sup>2</sup>Department of Mathematics, Division of Science and Technology, University of Education, Lahore, Pakistan

<sup>3</sup>Department of Mathematics, Lahore College for Woman University, Lahore, Pakistan

<sup>4</sup>Hebei Institute of Mechanical and Electronic Technology, Xintai 054000, China

Correspondence should be addressed to Jing Lu; [jing1lu@outlook.com](mailto:jing1lu@outlook.com)

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Measurements of graphs and retrieving structural information of complex networks using degree-based network entropy have become an informational theoretical concept. This terminology is extended by the concept of Shannon entropy. In this paper, we introduce entropy with graphs having edge weights which are basically redefined Zagreb indices. Some bounds are calculated to idealize the performance in limiting different kinds of graph entropy. In addition, we discuss the structural complexity of connected graphs representing chemical structures. In this article, we have discussed the edge-weighted graph entropy with fixed number of vertices, with minimum and maximum degree of a vertex, regular graphs, complete graphs, complete bipartite graphs, and graphs associated with chemical structures.

## 1. Introduction

In network theory, entropy measure has become an interesting field during last 5 decades due to Shannon [1]. Rashevsky [2] defined partitions of vertex orbits to study structural information. Later on, Mowshowitz [3] used the same concept to prove certain properties for some operations of graphs (see [4]). Graph entropy measurement was used by Rashevsky to study structural complexity of graphs based on Shannon's entropy. Mowshowitz [3] introduced applications of graph entropy in information technology. The other applications of graph entropy include characterizing graph patterns in chemistry, biology, and computer sciences [5]. In the literature, the graph entropy was defined in different ways. An important example is Körner's entropy [6] introduced with an information theory-specific point of view.

The basic properties of graph entropy were discussed in [7]. The graph entropy satisfies *subadditive* property in union of graphs which can be extended in graph covering problem and the problem of perfect hashing.

Graph entropy used for minimum number of perfect hash functions over a given range of hash for all  $k$ -subsets of a set of given size is discussed in [8]. Another application of graph entropy is due to Kahn and Kim [9], who proposed an algorithm based on graph entropy of an appropriate comparability graph. Csiszar et al. [10] in 1990 characterized minimal pairs of convex corners which generate the probability density  $p = (p_1, p_2, \dots, p_k) \in$  in a  $k$ -dimensional space. Due to this fact, another definition of graph entropy in terms of vertex packing polytope of a graph was introduced. They also gave characterization of a perfect graph using the subadditivity property of graph entropy (see [6]). Their examinations prompted the thought of a class of graphs called *normal graphs*, a generalization of perfect graphs given in [11]. Alon and Orlitsky [12] examined the connection between the base entropy shading of a graph and the graph entropy. Distinctive graph invariants are utilized to create graph entropy estimates, for example, eigenvalue and network data [13], weighted graph entropy with distance-based TIs as edge weights [14], and weighted graph entropy with degree-

based TIs as edge weights [15]. There are various uses of graph entropy in interchanges and financial matters.

Different graph invariants such as connectivity information, distance-based topological indices (Wiener related index), degree-based topological indices, the no. of vertices, the vertex degree sequences, the second neighbor degree sequences, the third neighbor degree sequences, eigenvalues, and so on were used to define graph entropy in the literature (see[16]). The properties of graph entropies based on information functionals by using degree powers of graphs have been explored in [17, 18]. The most important graph invariants are the Zagreb index [19] and the zeroth-order Randić index [20]. Chen et al. [21] proposed the idea of graph entropy for unique weighted graphs by utilizing Randić edge weights and demonstrated extremal properties of graph entropy for some basic groups. Kwun et al. [22] established the weighted entropy with atomic bond connectivity edge weights.

In this paper, the idea presented in [23] is used to study the weighted graph entropy by using redefined Zagreb indices as edge weights. Some degree-based indices are portrayed by researching the boundaries of the entropy of certain class of graphs [22]. Our aim is also to address the issue proposed by Chen et al. in [21] and Kwun et al. in [24]. The paper is organized into different sections to discuss the proposed problems.

## 2. Topological Index

In chemical structures, various graph notions used are molecular descriptors (or topological index). Few of them are first and second Zagreb indices  $M_1(G)$  and  $M_2(G)$ , respectively, exhibiting applicability for deriving multi-linear regression models. Details on the chemical applications of these indices can be seen in [25, 26]. More results on Zagreb indices can be seen in [27, 28]. Applications of Zagreb indices in QSPR were exposed by modeling the structure-boiling point associated with  $C_3 - C_8$  alkanes using the CROMRsel method [29, 30]. A large number of studies have been conducted on these two indices.

Ranjini et al. [31] introduced redefined first, second, and third Zagreb indices as

$$\begin{aligned} RZ_1(\Gamma) &= \sum_{e=xy \in E(\Gamma)} \frac{d_x + d_y}{d_x \cdot d_y}, \\ RZ_2(\Gamma) &= \sum_{e=xy \in E(\Gamma)} \frac{d_x \cdot d_y}{d_x + d_y}, \\ RZ_3(\Gamma) &= \sum_{e=xy \in E(\Gamma)} (d_x \cdot d_y)(d_x + d_y). \end{aligned} \quad (1)$$

## 3. Entropy

The entropy of a graph is a functional depending both on the graph itself and on a probability distribution on its vertex set.

This graph functional originated from the problem of source coding in information theory and was introduced by Körner in 1973.

Consider a graph  $\Gamma$  having order  $q$  with degree of a vertex  $x$  denoted by  $d_x$ . For any edge  $xy$ , the probability density function is defined as

$$p_{xy} = \frac{w(xy)}{\sum_{y=1}^{d_x} w(xy)}, \quad (2)$$

where  $w(xy)$  is the weight  $xy$  and  $w(xy) > 0$ .

The weighted graph entropy is defined as

$$H(v_x) = - \sum p_{xy} \cdot \log(p_{xy}). \quad (3)$$

Extending this method, we introduced *entropy of the edge-weighted graph*. For an edge-weighted graph,  $\Gamma = (x, E, w)$ , where  $x, E$ , and  $w$  denote vertex sets, edge sets, and edge weights of  $\Gamma$ , respectively, where the edge weight is positive.

Let  $\Gamma = (x, E, w)$  be an edge-weighted graph, and the entropy of  $\Gamma$  is

$$I(\Gamma, w) = - \sum_{xy \in E(\Gamma)} p_{xy} \cdot \log(p_{xy}), \quad (4)$$

where  $p_{xy} = w(xy) / \sum_{xy \in E(\Gamma)} w(xy)$ .

## 4. Main Results

In this section, we extend the idea of graph entropy as edge-weighted graphs explained in [23] that tackled the issue of weighted synthetic graph entropy. We also addressed the issue proposed by Chen et al. in [21] and Kwun et al. in [24]. Now we present bounds of the weighted entropy for the connected graphs, regular graphs, complete graphs, complete bipartite graphs, and graphs associated with chemical structures. In these results, the edge weights are redefined first, second, and third Zagreb indices.

**Theorem 1.** *Let  $\Gamma$  be a connected graph with  $q, q \geq 3$  vertices; then, we have*

- (1)  $\log(RZ_1) - \log(3/(q-1)^2) \leq I(\Gamma, \text{Re}Z_1) \leq \log(RZ_1) - \log(q-1)$ .
- (2)  $\log(RZ_2) - \log(1/(q-2)) \leq I(\Gamma, \text{Re}Z_2) \leq \log(RZ_2) - \log((q-1)^2/3)$ .
- (3)  $\log(RZ_3) - \log(4q-8) \leq I(\Gamma, \text{Re}Z_3) \leq \log(RZ_3) - \log(3(q-1)^2)$ .

*Proof*

(1) In simple connected graph  $\Gamma$ , of order  $q$ , the maximum and minimum degrees for a vertex are  $q-1$  and 1, respectively. Therefore, for any edge  $xy$ , the minimum and maximum possible degrees of  $x$  and  $y$  are 1, 2 and  $q-1, q-1$ , respectively. Therefore, we have

$$\begin{aligned}
I(\Gamma, RZ_1) &= - \sum_{xy \in E(\Gamma)} p_{xy} \log(p_{xy}) \\
&= - \sum_{xy \in E} (\Gamma) \frac{w(xy)}{\sum_{y=1}^{d_x} w(xy)} \cdot \log\left(\frac{w(xy)}{\sum_{y=1}^{d_x} w(xy)}\right) \\
&= - \sum_{xy \in E(\Gamma)} \frac{(d_x + d_y/d_x \cdot d_y)}{-\sum_{xy \in E(\Gamma)} (d_x + d_y/d_x \cdot d_y)} \\
&\quad \times \log\left(\frac{(d_x + d_y/d_x \cdot d_y)}{-\sum_{xy \in E(\Gamma)} (d_x + d_y/d_x \cdot d_y)}\right), \tag{5} \\
I(\Gamma, RZ_1) &= \frac{-1}{RZ_1} - \left( \sum_{xy \in E(\Gamma)} \left(\frac{d_x + d_y}{d_x \cdot d_y}\right) \cdot \log\left(\frac{d_x + d_y/d_x \cdot d_y}{RZ_1}\right) \right) \\
&= \frac{-1}{RZ_1} - \left( \sum_{xy \in E(\Gamma)} \left(\frac{d_x + d_y}{d_x \cdot d_y}\right) \cdot \log\left(\frac{d_x + d_y}{d_x \cdot d_y}\right) - \log(RZ_1) \right) \\
&\leq \log(RZ_1) - \frac{1}{RZ_1} \left( \sum_{xy \in E(\Gamma)} \left(\frac{d_x + d_y}{d_x \cdot d_y}\right) \times [\log(2q - 2) - \log(2)] \right) \\
&= \log(RZ_1) - \log(q - 1).
\end{aligned}$$

Also,

$$\begin{aligned}
I(\Gamma, RZ_1) &= - \sum_{xy \in E(\Gamma)} \frac{w(xy)}{\sum_{y=1}^{d_x} w(xy)} \cdot \log\left(\frac{w(xy)}{\sum_{y=1}^{d_x} w(xy)}\right) \\
&= - \sum_{xy \in E(\Gamma)} \frac{(d_x + d_y/d_x \cdot d_y)}{-\sum_{xy \in E(\Gamma)} (d_x + d_y/d_x \cdot d_y)} \\
&\quad \times \log\left(\frac{(d_x + d_y/d_x \cdot d_y)}{-\sum_{xy \in E(\Gamma)} (d_x + d_y/d_x \cdot d_y)}\right) \\
&= \frac{-1}{RZ_1} - \left( \sum_{xy \in E(\Gamma)} \left(\frac{d_x + d_y}{d_x \cdot d_y}\right) \cdot \log\left(\frac{d_x + d_y/d_x \cdot d_y}{RZ_1}\right) \right) \tag{6} \\
&= \frac{-1}{RZ_1} - \left( \sum_{xy \in E(\Gamma)} \left(\frac{d_x + d_y}{d_x \cdot d_y}\right) \cdot \log\left(\frac{d_x + d_y}{d_x \cdot d_y}\right) - \log(RZ_1) \right) \\
&\geq \log(RZ_1) - \frac{1}{RZ_1} \left( \sum_{xy \in E(\Gamma)} \left(\frac{d_x + d_y}{d_x \cdot d_y}\right) \times [\log(3) - \log(q - 1)^2] \right) \\
&= \log(RZ_1) - \log\left(\frac{3}{(q - 1)^2}\right).
\end{aligned}$$

Hence,

$$\begin{aligned} \log(\operatorname{Re}Z_1) - \log\left(\frac{3}{(q-1)^2}\right) &\leq I(\Gamma, \operatorname{Re}Z_1) \\ &\leq \log(\operatorname{Re}Z_1) - \log(q-1). \end{aligned} \tag{7}$$

The proofs of (2) and (3) follow the proof of (1).  $\square$

**Theorem 2.** Let  $\Gamma$  be a graph having  $q$  vertices with minimum and maximum degrees of  $\gamma$  being  $\delta$  and  $\Delta$ , respectively. Then, we have

$$(1) \log(RZ_1) - \log(2\delta/\Delta^2) \leq I(\Gamma, RZ_1) \leq \log(RZ_1) - \log(2\Delta/\delta^2).$$

$$(2) \log(RZ_2) - \log(\delta^2/2\Delta) \leq I(\Gamma, RZ_2) \leq \log(RZ_2) - \log(\Delta^2/2\delta).$$

$$(3) \log(RZ_3) - \log(2\Delta\delta^2) \leq I(\Gamma, RZ_3) \leq \log(RZ_3) - \log(2\delta\Delta^2).$$

*Proof*

(1) For a connected graph of order  $q$ , the minimum and maximum degrees for a vertex are 1 and  $q-1$ , respectively. For any edge  $xy$ , the minimum and maximum possible degrees of vertices  $x$  and  $y$  are 1, 2 and  $q-1$ ,  $q-1$ , respectively. Therefore, we have

$$\begin{aligned} I(\Gamma, RZ_1) &= \frac{-1}{RZ_1} - \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times \log\left(\frac{d_x + d_y}{d_x \cdot d_y}\right) - \log(RZ_1) \right) \\ &\leq \log(RZ_1) - \frac{1}{RZ_1} \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times [\log(2\Delta) - \log(\delta)^2] \right) \\ &= \log(RZ_1) - \log\left(\frac{2\Delta}{\delta^2}\right). \end{aligned} \tag{8}$$

Also,

$$\begin{aligned} I(\Gamma, RZ_1) &= \frac{-1}{RZ_1} - \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times \log\left(\frac{d_x + d_y}{d_x \cdot d_y}\right) - \log(RZ_1) \right) \\ &\geq \log(RZ_1) - \frac{1}{RZ_1} \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times [\log(2\delta) - \log(\Delta^2)] \right) \\ &= \log(AZI) - \log\left(\frac{2\delta}{\Delta^2}\right). \end{aligned} \tag{9}$$

Hence,

$$\begin{aligned} \log(AZI) - \log\left(\frac{2\delta}{\Delta^2}\right) &\leq I(\Gamma, AZI) \\ &\leq \log(\operatorname{Re}Z_1) - \log\left(\frac{2\Delta}{\delta^2}\right). \end{aligned} \tag{10}$$

The proofs of (2) and (3) follow the proof of (1).  $\square$

**Theorem 3.** For a regular graph  $\Gamma = (V, E, w)$  of order  $q$ ,  $q \geq 3$ , we have

$$(1) \log(RZ_1) \leq I(\Gamma, RZ_1) \leq \log(RZ_1 (q-1)/2).$$

$$(2) \log(RZ_2) \leq I(\Gamma, RZ_2) \leq \log \log(2RZ_2/(q-1)).$$

$$(3) \log(RZ_3/16) \leq I(\Gamma, RZ_3) \leq \log(RZ_3/2 (q-1)^3).$$

Moreover,  $\log(RZ_1) = I(\Gamma, RZ_1)$  iff  $\Gamma$  is cyclic graph and  $\log(AZI) - \log(RZ_1 (q-1)/2)$  iff  $\Gamma$  is complete graph.

*Proof.* For a  $t$  regular graph  $t \geq 2$ , as  $\Gamma$  is connected with  $q \geq 3$ ,

$$\begin{aligned} I(\Gamma, RZ_1) &= \frac{-1}{RZ_1} - \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times \log\left(\frac{d_x + d_y}{d_x \cdot d_y}\right) - \log(RZ_1) \right) \\ &\leq \log(RZ_1) - \frac{1}{RZ_1} \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times [\log(2q-2) - \log(q-1)^2] \right) \\ &= \log\left(\frac{RZ_1 (q-1)}{2}\right). \end{aligned} \tag{11}$$

Also

$$\begin{aligned}
 I(\Gamma, RZ_1) &= \frac{-1}{RZ_1} - \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times \log \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) - \log(RZ_1) \right) \\
 &\geq \log(RZ_1) - \frac{1}{RZ_1} \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times [\log(2q - 2) - \log(q - 1)^2] \right) \\
 &= \log(RZ_1) - ([\log(4) - \log(4)]) \\
 &= \log(RZ_1).
 \end{aligned} \tag{12}$$

Hence,

$$\begin{aligned}
 \log(RZ_1) &\leq I(\Gamma, RZ_1) \\
 &\leq \log\left(\frac{RZ_1(q-1)}{2}\right).
 \end{aligned} \tag{13}$$

The proofs of (2) and (3) follow the proof of (1).  $\square$

**Theorem 4.** Let  $\Gamma = (V, E, w)$  be an arbitrary complete graph of order  $q$ ; then, we have

- (1)  $I(\Gamma, RZ_1) \leq q^2/2 - \log(q/2)$ .
- (2)  $I(\Gamma, RZ_2) \leq (q^2/2) - \log(q/2)$ .
- (3)  $I(\Gamma, RZ_3) \leq 2q^2 - \log(2q)$ .

*Proof.* For an arbitrary complete graph  $\Gamma$  of order  $q$ , we have  $RZ_1 \leq (q^2/2)$ ; therefore, the result is obvious.  $\square$

**Theorem 5.** For an arbitrary complete bipartite graph  $\Gamma = (V, E, w)$  with  $q$  vertices, we have

- (1)  $\log(RZ_1) - \log(q/q - 1) \leq I(\Gamma, RZ_1) \leq \log(RZ_1) - \log(2/(q/2))$ .
- (2)  $\log(RZ_2) - \log(q - 1/q) \leq I(\Gamma, RZ_2) \leq \log(\Gamma, RZ_2) - \log((q/2)^2/2(q/2))$ .
- (3)  $\log(RZ_3) - \log(q^2 - n) \leq I(\Gamma, RZ_3) \leq \log(RZ_3) - \log(2(q/2)^3)$ .

Moreover,  $\log(RZ_1) - \log(q/q - 1) = I(\Gamma, RZ_1)$  iff  $\Gamma$  is a star graph, and  $I(\Gamma, AZI) = \log(RZ_1) - \log(2/(q/2))$  iff  $\Gamma$  is complete bipartite graph (balanced).

*Proof*

(1) Assume that  $\Gamma$  is a complete bipartite graph with  $q$  vertices with two parts having  $s$  and  $t$  vertices, respectively. Therefore, we have  $s + t = q$ , and we have

$$\begin{aligned}
 I(\Gamma, RZ_1) &= \frac{-1}{RZ_1} - \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times \log \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) - \log(RZ_1) \right) \\
 &\leq \log(RZ_1) - \frac{1}{RZ_1} \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times [\log(s + t) - \log(st)] \right) \\
 &= \log(RZ_1) - \log\left(\frac{s+t}{st}\right).
 \end{aligned} \tag{14}$$

For minimum value, we take  $s = 1$  and  $a = q - 1$ , while for maximum value,  $s = a = (q/2)$ , and hence

$$\begin{aligned}
 \log(RZ_1) - \log\left(\frac{q}{q-1}\right) &\leq I(\Gamma, AZI) \\
 &\leq \log(RZ_1) - \log\left(\frac{2}{(q/2)}\right).
 \end{aligned} \tag{15}$$

The proofs of (2) and (3) follow the proof of (1).  $\square$

Chemical graphs are associated with structure of chemical compounds. Therefore, we consider atoms as vertices and chemical bonds as edges of that graph. The following theorem provides bounds for weighted graph entropy of chemical graph by assigning  $RZ_1$  as edge weights.

**Theorem 6.** Let  $\Gamma$  be a graph with  $q$  vertices associated with a chemical structure; then, we have

- (1)  $\log(16(RZ_1)/3) \leq I(\Gamma, RZ_1) \leq \log(RZ_1/4)$ .

$$(2) \log(4(RZ_2)) \leq I(\Gamma, RZ_2) \leq \log(3(RZ_2)/16).$$

$$(3) \log(RZ_3/16) \leq I(\Gamma, RZ_3) \leq \log((RZ_3)/48).$$

*Proof*

(1) For a chemical graph  $\Gamma'$ , for any edge  $xy$ , the maximum degrees of  $x$  and  $y$  are 4 and 4 and minimum possible degrees are 1 and 2. So, we have

$$\begin{aligned} I(G, RZ_1) &= \frac{-1}{RZ_1} - \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times \log \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) - \log(RZ_1) \right) \\ &\leq \log(RZ_1) - \frac{1}{RZ_1} \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times [\log(8) - \log(2)] \right) \\ &= \log \left( \frac{RZ_1}{4} \right). \end{aligned} \quad (16)$$

Similarly,

$$\begin{aligned} I(G, RZ_1) &= \frac{-1}{RZ_1} - \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times \log \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) - \log(RZ_1) \right) \\ &\geq \log(RZ_1) - \frac{1}{RZ_1} \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \times [\log(3) - \log(16)] \right) \\ &= \log \left( \frac{16(RZ_1)}{3} \right). \end{aligned} \quad (17)$$

Therefore,

$$\log \left( \frac{16(RZ_1)}{3} \right) \leq I(\Gamma, RZ_1) \leq \log \left( \frac{RZ_1}{4} \right). \quad (18)$$

The proofs of (2) and (3) follow the proof of (1).  $\square$

## 5. Numerical Examples

*Example 1.* The molecular graphs of carbon nanotubes  $VC_5C_7[p, q]$  are depicted in Figure 1. The structure of

$VC_5C_7[p, q]$  nanotubes consists of  $C_5$  loops and  $C_7$  net following the trivalent decoration. It can cover a cylinder or a ring. Two-dimensional lattice of  $VC_5C_7[p, q]$  is depicted in Figure 1. Now, we focus on calculating the entropy of a given structure.

It can be observed from Figure 1 that the edge set of  $VC_5C_7[p, q]$  has partition given in Table 1.

Therefore, the entropy of  $\Gamma$  is computed as

$$\begin{aligned} I(\Gamma, RZ_1) &= \log(RZ_1) - \frac{1}{RZ_1} \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \cdot \log \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \right) \\ &= \log(24pq + 2p) - \frac{1}{24pq + 2p} \left( |E_1| \left( \frac{4}{4} \right) \cdot \log \left( \frac{4}{4} \right) + |E_2| \left( \frac{2}{3} \right) \cdot \log \left( \frac{2}{3} \right) \right) \\ &= \log(24pq + 2p) - \frac{1}{24pq + 2p} \left( (24pq - 6p) \left( \frac{4}{4} \right) \cdot \log \left( \frac{4}{4} \right) + (12p) \left( \frac{2}{3} \right) \cdot \log \left( \frac{2}{3} \right) \right) \\ &= \log(24pq + 2p) + \frac{1.408738p}{24pq + 2p}. \end{aligned} \quad (19)$$

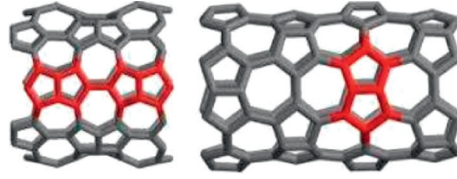


FIGURE 1:  $VC_5C_7[p, q]$ .

TABLE 1: Edge partition based on end vertices' degree of  $VC_5C_7[p, q]$ .

$(d_a, d_b)$	(2, 2)	(3, 3)
Number of edges	$24pq - 6p$	$12p$

Also,

$$\begin{aligned}
 I(\Gamma, RZ_2) &= \log(RZ_2) - \frac{1}{RZ_2} \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x \cdot d_y}{d_x + d_y} \right) \cdot \log \left( \frac{d_x \cdot d_y}{d_x + d_y} \right) \right) \\
 &= \log(24pq + 12p) - \frac{1}{24pq + 12p} \left( |E_1| \left( \frac{4}{4} \right) \cdot \log \left( \frac{4}{4} \right) + |E_2| \left( \frac{3}{2} \right) \cdot \log \left( \frac{3}{2} \right) \right) \\
 &= \log(24pq + 12p) - \frac{1}{24pq + 12p} \left( (24pq - 6p) \left( \frac{4}{4} \right) \cdot \log \left( \frac{4}{4} \right) + (12p) \left( \frac{3}{2} \right) \cdot \log \left( \frac{3}{2} \right) \right) \\
 &= \log(24pq + 12p) - \frac{1.408738p}{24pq + 12p}.
 \end{aligned} \tag{20}$$

Moreover,

$$\begin{aligned}
 I(\Gamma, RZ_3) &= \log(RZ_3) - \frac{-1}{RZ_3} \\
 &\quad - \left( \sum_{xy \in E(\Gamma)} ((d_x + d_y)(d_x \cdot d_y) \cdot \log((d_x + d_y)(d_x \cdot d_y))) / ((d_x + d_y)) \right) \\
 &= \log(384pq - 552p) - \frac{1}{384pq - 552p} \left( |E_1|(16) \cdot \log(16) + |E_2|(54) \cdot \log(54) \right) \\
 &= \log(384pq - 552p) - \frac{1}{384pq - 552p} \left( (24pq - 6p)(16) \cdot \log(16) + (12p)(54) \cdot \log(54) \right) \\
 &= \log(384pq - 552p) - \left( \frac{462.3820pq - 115.5955p}{384pq - 552p} \right).
 \end{aligned} \tag{21}$$

*Example 2.* The molecular graphs of carbon nanotubes  $VC_5C_7[p, q]$  and  $HC_5C_7[p, q]$  are shown in Figures 2 and 3, respectively. The structure of these nanotubes consists of  $C_5$  loops and  $C_7$  net following the trivalent decoration. It can cover a cylinder or a ring. Two-dimensional lattice of  $VC_5C_7[p, q]$  is depicted in Figure 2 and that of  $HC_5C_7[p, q]$  is depicted in Figure 3. Now, we focus on calculating the

entropy of a given structure. From Figure 2, it can be observed that the edge set of  $VC_5C_7[p, q]$  has the following partitions.

It can be observed from Figure 3 that the edge set of  $HC_5C_7[p, q]$  can be divided into following three classes as given in Table 2.

Furthermore,

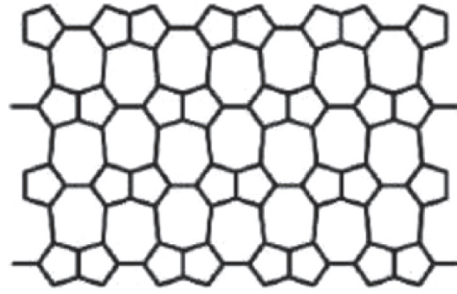
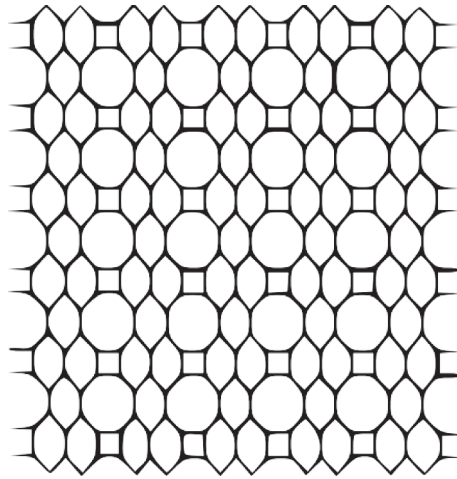
FIGURE 2:  $HC_5C_7[p, q]$ .

FIGURE 3: Naphthalenic nanotubes.

TABLE 2: Edge partition based on end vertices' degree of  $HC_5C_7[p, q]$ .

$(d_a, d_b)$	(2, 2)	(3, 3)	(2, 3)
Number of edges	$p$	$8p$	$24pq - 4p$

$$\begin{aligned}
 I(\Gamma, RZ_1) &= \log(RZ_1) - \frac{1}{RZ_1} \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \cdot \log \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \right) \\
 &= \log(20pq + 3p) - \frac{1}{20pq + 3p} \left( |E_1| \left( \frac{4}{4} \right) \cdot \log \left( \frac{4}{4} \right) + |E_2| \left( \frac{2}{3} \right) \cdot \log \left( \frac{3}{2} \right) \right) \\
 &\quad + \left( |E_3| \left( \frac{5}{6} \right) \cdot \log \left( \frac{5}{6} \right) \right) \\
 &= \log(20pq + 3p) - \frac{1}{20pq + 3p} \left( (p) \left( \frac{4}{4} \right) \cdot \log \left( \frac{4}{4} \right) + (8p) \left( \frac{2}{3} \right) \cdot \log \left( \frac{3}{2} \right) \right) \\
 &\quad + (24pq - 4p) \left( \frac{5}{6} \right) \cdot \log \left( \frac{5}{6} \right) \\
 &= \log(20pq + 3p) + \frac{1}{20pq + 3p},
 \end{aligned}$$



$$\begin{aligned}
I(\Gamma, RZ_2) &= \log(RZ_2) - \frac{1}{RZ_2} \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x \cdot d_y}{d_x + d_y} \right) \cdot \log \left( \frac{d_x \cdot d_y}{d_x + d_y} \right) \right) \\
&= \log \left( \frac{144pq}{5} + \frac{41p}{5} \right) - \frac{1}{(144pq/5) + (41p/5)} \left( |E_1| \left( \frac{4}{4} \right) \cdot \log \left( \frac{4}{4} \right) + |E_2| \left( \frac{3}{2} \right) + |E_3| \left( \frac{6}{5} \right) \right) \\
&= \log \left( \frac{144pq}{5} + \frac{41p}{5} \right) - \frac{1}{(144pq/5) + (41p/5)} \left( (p) \left( \frac{4}{4} \right) \cdot \log \left( \frac{4}{4} \right) \right. \\
&\quad \left. + (8p) \left( \left( \frac{3}{2} \right) \cdot \log \left( \frac{4}{4} \right) \right) + (24pq - 4p) \left( \left( \frac{5}{6} \right) \cdot \log \left( \frac{5}{6} \right) \right) \right) \\
&= \log(24pq + 12p) - \frac{1.408738p}{24pq + 12p}.
\end{aligned} \tag{22}$$

$$\begin{aligned}
I(\Gamma, RZ_3) &= \log(RZ_3) - \frac{-1}{RZ_3} \left( \sum_{xy \in E(\Gamma)} ((d_x + d_y)(d_x \cdot d_y)) \cdot \log((d_x + d_y)(d_x \cdot d_y)) \right) \\
&= \log(720pq - 80p) - \frac{1}{720pq - 80p} \left( |E_1|(16) \cdot \log(16) + |E_2|(6) \cdot \log(6) \right. \\
&\quad \left. + (|E_3|(30) \cdot \log(30)) \right) \\
&= \log(720pq - 80p) - \frac{1}{720pq - 80p} \left( (p)(16) \cdot \log(16) + (8p)(6) \cdot \log(6) \right. \\
&\quad \left. + (24pq - 4p)((30) \cdot \log(30)) \right) \\
&= \log(720pq - 80p) - \left( \frac{1}{720pq - 80p} \right).
\end{aligned} \tag{23}$$

*Example 3.* In nanosciences,  $SC_5C_7[p, q]$  (where  $p$  and  $q$  represent number of heptagons and number of cycles in each row separately in the entire lattice) nanotubes are a class  $C_5C_7$ , and this is generated by alternating  $C_5$  and  $C_7$ . The standard tiling of  $C_5$  and  $C_7$  can cover cylinders or rings, and each covers  $SC_5C_7[p, q]$ . Nanotubes  $NPHX[p, q]$  (where  $p$  and  $q$  are

expressed as the number of hexagon pairs in the first row and the other hexagons in the column) are trivalent modifications in the order of  $C_6, C_6, C_4, C_6, C_6, C_4, \dots$ . The first row of the sequence is  $C_6, C_8, C_6, C_8, \dots$  in the other rows. In other words, the nanolattice can be viewed as a tile of  $C_4, C_6$ , and  $C_8$ . Therefore, such tiles can cover cylinders or rings.

$$\begin{aligned}
I(\Gamma, RZ_1) &= \log(RZ_1) - \frac{1}{RZ_1} \left( \sum_{ij \in E(\Gamma)} \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \cdot \log \left( \frac{d_x + d_y}{d_x \cdot d_y} \right) \right) \\
&= \log(8pq) - \frac{1}{8pq} \left( |E_1| \left( \frac{4}{4} \right) \cdot \log \left( \frac{4}{4} \right) + |E_2| \left( \frac{3}{2} \right) \cdot \log \left( \frac{3}{2} \right) \right) \\
&\quad + |E_3| \left( \frac{5}{6} \right) \cdot \log \left( \frac{5}{6} \right) \\
&= \log(8pq) - \frac{1}{8pq} \left( (p) \left( \frac{4}{4} \right) \cdot \log \left( \frac{4}{4} \right) + (12pq - 9p) \left( \frac{3}{2} \right) \cdot \log \left( \frac{3}{2} \right) \right) \\
&\quad + (6p) \left( \left( \frac{5}{6} \right) \cdot \log \left( \frac{5}{6} \right) \right), \\
I(\Gamma, RZ_2) &= \log(RZ_2) - \frac{1}{RZ_2} \left( \sum_{xy \in E(\Gamma)} \left( \frac{d_x \cdot d_y}{d_x + d_y} \right) \cdot \log \left( \frac{d_x \cdot d_y}{d_x + d_y} \right) \right) \\
&= \log \left( 18pq - \frac{15p}{2} \right) - \frac{1}{18pq - (15p/2)} \left( |E_1| \left( \frac{4}{4} \right) \cdot \log \left( \frac{4}{4} \right) + |E_2| \left( \frac{2}{3} \right) \cdot \log \left( \frac{2}{3} \right) \right) \\
&\quad + |E_3| \left( \frac{6}{5} \right) \cdot \log \left( \frac{6}{5} \right) \\
&= \log \left( 18pq - \frac{15p}{2} \right) - \frac{1}{18pq - (15p/2)} \left( (p) \left( \frac{4}{4} \right) \cdot \log \left( \frac{4}{4} \right) + (12pq - 9p) \left( \frac{2}{3} \right) \cdot \log \left( \frac{2}{3} \right) \right) \\
&\quad + (6p) \left( \left( \frac{6}{5} \right) \cdot \log \left( \frac{6}{5} \right) \right), \\
I(\Gamma, RZ_3) &= \log(RZ_3) - \frac{-1}{RZ_3} \left( \sum_{xy \in E} (\Gamma) \left( (d_x + d_y)(d_x \cdot d_y) \right) \cdot \log \left( (d_x + d_y)(d_x \cdot d_y) \right) \right) \\
&= \log(72pq - 127p) - \frac{1}{72pq - 127p} \left( 16|E_1| \cdot \log(16) + 6|E_2| \cdot \log(6) \right) \\
&\quad + (30|E_3| \cdot \log(30)) \\
&= \log(720pq - 80p) - \frac{1}{720pq - 80p} \left( 16p \cdot \log(16) + 6(12pq - 9p) \cdot \log(6) \right) \\
&\quad + 6p(30 \cdot \log(30)) \\
&= \log(72pq - 127p) - \left( \frac{1}{72pq - 127p} \right).
\end{aligned} \tag{24}$$

## 6. Conclusions

In study of information theory, the graph entropy measures the information rate achievable by communicating symbols over a channel in which certain pairs of values may be confused [32–36]. This measure introduced by Körner in the 1970s has

proven itself useful in other settings, including combinatorics. In the present paper, we studied weighted graph entropy by using first, second, and third redefined Zagreb indices as edge weights. We also presented numerical examples to justify our results. Interesting work would be to study weighted graph entropy with other degree and distance-based topological

indices. The bounds achieved for degree-based network weighted graph entropy can be used for national security, social networks, Internet networks, structural chemistry, computational systems biology, and so on. These studies will play an important role in asymmetry in real networks and analyzing structural symmetry in future.

### Data Availability

The data used to support the findings of this study are included within this article.

### Conflicts of Interest

The authors declare that they have no conflicts of interest.

### Authors' Contributions

Jing Lu wrote the final version of the paper and used the software to prepare graphs and verify computational results. Hafiz Mutee-ur-Rehman computed the results. Saima Nazeer wrote the first version of the paper. Xuemei An analyzed and verified the results and arranged the funding for this study.

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