

## Research Article

# Computing the Entropy Measures for the Line Graphs of Some Chemical Networks

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Chemical Graph entropy plays a significant role to measure the complexity of chemical structures. It has explicit chemical uses in chemistry, biology, and information sciences. A molecular structure of a compound consists of many atoms. Especially, the hydrocarbons is a chemical compound that consists of carbon and hydrogen atoms. In this article, we discussed the concept of subdivision of chemical graphs and their corresponding line chemical graphs. More precisely, we discuss the properties of chemical graph entropies and then constructed the chemical structures namely triangular benzenoid, hexagonal parallelogram, and zigzag edge coronoid fused with starphene. Also, we estimated the degree-based entropies with the help of line graphs of the subdivision of above mentioned chemical graphs.

## 1. Introduction

Mathematical chemistry is a field of theoretical chemistry that uses mathematical approaches to discuss molecular structure without necessarily referring to quantum mechanics [1]. Chemical Graph Theory is a branch of mathematical chemistry where a chemical phenomenon is theoretically described using graph theory [2, 3]. The growth of organic disciplines has been aided by Chemical Graph Theory [4, 5]. In mathematical chemistry, graph invariants or topological indices are numeric quantities that describe various essential features of organic components and are produced from an analogous molecular graph [6, 7]. Degree-based indices are among the topological indices used to predict bioactivity, boiling point, draining energy, stability, and physico-chemical properties of certain chemical compounds [8, 9]. Due to their chemical applications, these indices have significant role in theoretical chemistry. Zhang et al. [10–12] discuss the

topological indices of generalized bridge molecular graphs, Carbon Nanotubes and product of chemical graphs. Zhang et al. [13–15] provided the physical analysis of heat for formation and entropy of Ceria Oxide. For further study about indices, see [16, 17]. Shannon [18] originated the conception of information entropy in communication theory. However, it was later discovered as a quantity that applied to all things with a set nature [19, 20], including molecular graphs [21–23]. In chemistry, information entropy is now used in two modes. Firstly, it is a structural descriptor for assessing the complexity of chemical structures [24]. Information entropy is useful in this regard for connecting structural and physico-chemical features [25], numerically distinguishing isomers of organic molecules [26], and classifying natural products and synthetic chemicals [27, 28]. The physico-chemical sounding of information entropy is a different mode of application. As a result, Terenteva and Kobozev demonstrated its utility in analyzing physico-chemical processes that simulate

information transmission [29]. Zhdanov [30] used entropy values to study organic compound chemical processes. The information entropy is defined as:

$$\begin{aligned} ENT_{\psi}(\mathcal{F}) &= -\sum_{i=1}^q N_i \frac{\Lambda(l_i m_i)}{In} \log \frac{\Lambda(l_i m_i)}{In}, \\ &= \log(In) - \frac{1}{In} \sum_{i=1}^q N_i \Lambda(l_i m_i) \log \Lambda(l_i m_i). \end{aligned} \quad (1)$$

Here, the logarithm is considered to be with base  $e$  while  $\mathcal{F}_V$ ,  $\mathcal{F}_E$  and  $\Lambda(lm)$  represent the vertex set, the edge set and the edge weight of the edge  $(lm)$  in  $\Lambda$ . Many graph entropies have been calculated in the literature utilising characteristic polynomials, vertices degree, and graph order [31–34]. Graph entropies, which are based on independent sets, matchings, and the degree of vertices [35], have been estimated in recent years. Dehmer and Mowshowits proposed several graph complexity and Hosoya entropy relationships [23, 32, 36, 37]. For further study, see [19, 21, 38–42, 59, 60]. The graph  $\mathcal{F}$  is structured into ordered pairs, with one object being referred to as a vertex set ( $\mathcal{F}_V$ ) and the other as an edge set ( $\mathcal{F}_E$ ), and these vertices and edges being connected. When two vertices of  $\mathcal{F}$  share an edge, they are said to be neighboring. The sum of the degrees of all neighboring vertices of  $l$  is denoted by  $A_l$ , and the degree of a vertex  $l$  is represented by  $\hat{N}(l)$ . By replacing each of  $S(\mathcal{F})$ 's edges with a path of length two, the subdivision graph  $S(\mathcal{F})$  is formed. The line graph is denoted by the symbol  $L(\mathcal{F})$  in which  $|V(L(\mathcal{F}))| = |E(\mathcal{F})|$  and two vertices of  $L(\mathcal{F})$  are adjacent iff their corresponding edges share a common end points in  $\mathcal{F}$ .

*1.1. Randić Entropy* [43, 44]. If  $\Lambda(lm) = (\hat{N}(l) \times \hat{N}(m))^\alpha$ , with  $\alpha = 1, -1, 1/2, -1/2$ , then

$$\sum_{lm \in \mathcal{F}_E} \Lambda(lm) = \sum_{lm \in \mathcal{F}_E} (\hat{N}(l) \times \hat{N}(m))^\alpha = R_\alpha. \quad (2)$$

Now (1) represent the Randic Entropy.

$$\begin{aligned} ENT_{R_\alpha}(\mathcal{F}) &= \log(R_\alpha) - \frac{1}{(R_\alpha)} \sum_{i=1}^q \sum_{lm \in \mathcal{F}_E} [(\hat{N}(l) \times \hat{N}(m))^\alpha] \\ &\quad \cdot \log [(\hat{N}(l) \times \hat{N}(m))^\alpha]. \end{aligned} \quad (3)$$

*1.2. Atom Bond Connectivity Entropy* [45]. If  $\Lambda(lm) = \sqrt{\hat{N}(l) \times \hat{N}(m) - 2/\hat{N}(l) \times \hat{N}(m)}$ , then

$$\sum_{lm \in \mathcal{F}_E} \Lambda(lm) = \sum_{lm \in \mathcal{F}_E} \sqrt{\frac{\hat{N}(l) + \hat{N}(m) - 2}{\hat{N}(l) \times \hat{N}(m)}} = ABC(\mathcal{F}). \quad (4)$$

Thus (1) is converted in the following form:

$$\begin{aligned} ENT_{ABC}(\mathcal{F}) &= \log(ABC) \\ &\quad - \frac{1}{(ABC)} \sum_{i=1}^q \sum_{lm \in \mathcal{F}_E} \left[ \sqrt{\frac{\hat{N}(l) + \hat{N}(m) - 2}{\hat{N}(l) \times \hat{N}(m)}} \right] \\ &\quad \cdot \log \left[ \sqrt{\frac{\hat{N}(l) + \hat{N}(m) - 2}{\hat{N}(l) \times \hat{N}(m)}} \right]. \end{aligned} \quad (5)$$

*1.3. The Geometric Arithmetic Entropy* [43, 44]. If  $\Lambda(lm) = 2\sqrt{\hat{N}(l) \times \hat{N}(m)}/\hat{N}(l) + \hat{N}(m)$ , then

$$\sum_{lm \in \mathcal{F}_E} \Lambda(lm) = \sum_{lm \in \mathcal{F}_E} \frac{2\sqrt{\hat{N}(l) \times \hat{N}(m)}}{\hat{N}(l) + \hat{N}(m)} = GA(\mathcal{F}). \quad (6)$$

Now (1) takes the form as given below.

$$\begin{aligned} ENT_{GA}(\mathcal{F}) &= \log(GA) \\ &\quad - \frac{1}{(GA)} \sum_{i=1}^q \sum_{lm \in \mathcal{F}_E} \left[ \frac{2\sqrt{\hat{N}(l) \times \hat{N}(m)}}{\hat{N}(l) + \hat{N}(m)} \right] \\ &\quad \cdot \log \left[ \frac{2\sqrt{\hat{N}(l) \times \hat{N}(m)}}{\hat{N}(l) + \hat{N}(m)} \right]. \end{aligned} \quad (7)$$

*1.4. The Fourth Atom Bond Connectivity Entropy* [35]. If  $\Lambda(lm) = \sqrt{A_l + A_m - 2/A_l A_m}$ , then

$$\sum_{lm \in E(\mathcal{F})} \Lambda(lm) = \sum_{lm \in E(\mathcal{F})} \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} = ABC_4(\mathcal{F}). \quad (8)$$

Now (1) converted in the following form as:

$$\begin{aligned} ENT_{ABC_4}(\mathcal{F}) &= \log(ABC_4(\mathcal{F})) - \frac{1}{(ABC_4(\mathcal{F}))} \sum_{i=1}^q \sum_{lm \in E_i(\mathcal{F})} \\ &\quad \cdot \log \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right]^{\left[ \sqrt{A_l + A_m - 2/A_l A_m} \right]}. \end{aligned} \quad (9)$$

*1.5. The Fifth Geometric Arithmetic Entropy* [35]. If  $\Lambda(lm) = 2\sqrt{A_l A_m}/A_l + A_m$ , then

$$\sum_{lm \in E(\mathcal{F})} \Lambda(lm) = \sum_{lm \in E(\mathcal{F})} \frac{2\sqrt{A_l A_m}}{A_l + A_m} = GA_5(\mathcal{F}). \quad (10)$$

Equation (1) is now changed to the following form, which is known as fifth geometric arithmetic entropy.

$$ENT_{GA_5}(\mathcal{F}) = \log(GA_5(\mathcal{F})) - \frac{1}{(GA_5(\mathcal{F}))} \sum_{i=1}^q \sum_{lm \in E_i(\mathcal{F})} \left[ \log \left[ \frac{2\sqrt{A_l A_m}}{A_l + A_m} \right] \left[ \frac{2\sqrt{A_l A_m}}{A_l + A_m} \right] \right]. \quad (11)$$

See [35, 44] for further information on these entropy measures.

## 2. Formation of Triangular Benzenoid $T_x \forall x \in \mathbb{N}$

Triangular benzenoids are a group of benzenoid molecular graphs and are denoted by  $T_x$ , where  $x$  characterizes the number of hexagons at the bottom of the graph and  $1/2x(x+1)$  represents the total number of hexagons in  $T_x$ . Triangular benzenoids are a generalization of the benzene molecule  $C_6H_6$ , with benzene rings forming a triangular shape. In physics, chemistry, and nanosciences, the benzene molecule is a common molecule. Synthesizing aromatic chemicals is quite fruitful [46]. Raut [47] calculated some topological indices for the triangular benzenoid system. Hussain et al. [48] discussed the irregularity determinants of some benzenoid systems.

Kwun [49] calculated degree-based indices by using  $M$  polynomials. For further details, see [50, 51]. The hexagons are placed in rows, with each row increasing by one hexagon. For  $T_1$ , there are only one type of edges  $e_1 = (2, 2)$  and  $|e_1| = 6$ . Therefore,  $V(T_1) = 6$  and  $E(T_1) = 6$  while three kinds of edges are there in  $T_2$  e.g.  $e_1 = (2, 2)$ ,  $e_2 = (2, 3)$ ,  $e_3 = (3, 3)$  and  $|e_1| = 6$ ,  $|e_2| = 6$ ,  $|e_3| = 3$ . Therefore,  $V(T_2) = 13$  and  $E(T_2) = 15$ . Continuing in this way,  $|V(T_x)| = x^2 + 4x + 1$  and  $|E(T_x)| = 3/2x(x+3)$ . The subdivision graph of  $T_x$  and its line graph are demonstrated in Figure 1. It is to be noted that  $|V(L(S(T_x)))| = 3x(x+3)$  and  $|E(L(S(T_x)))| = 3/2(3x^2 + 7x - 2)$ .

Let  $\mathcal{F} = L(S(T_x))$ . i.e.  $\mathcal{F}$  is the line graph of the subdivision graph of triangular benzenoid  $T_x$ . We will use the edge partition and vertices counting technique to compute our abstracted indices and entropies. The degree of each edge's terminal vertices is used in the edge partitioning of  $\mathcal{F}$ . It is easy to see that there are only three types of edges shown in Table 1.

**2.1. Entropy Measure for  $L(S(T_x))$ .** We'll calculate the entropies of  $\mathcal{F} = L(S(T_x))$  in this section.

**2.1.1. Randic Entropy of  $L(S(T_x))$ .** The Randic index and entropy for  $\alpha = 1, -1, 1/2, -1/2$ , with the help of Table 1, and equation (3) is:

$$ENT_{R_\alpha}(\mathcal{F}) = \log(R_\alpha) - \frac{1}{(R_\alpha)} \sum_{i=1}^3 \sum_{lm \in E_i(\mathcal{F})} [(\hat{N}(l) \times \hat{N}(m))^\alpha] \log [(\hat{N}(l) \times \hat{N}(m))^\alpha] \quad (12)$$

$$= \log(R_\alpha) - \frac{1}{(R_\alpha)} \left[ [4^\alpha(3x+9) \times \log(4^\alpha)] + [6^\alpha(6x-6) \times \log(6^\alpha)] + \left[ \frac{3^{(2\alpha+1)}}{2} (3x^2+x-4) \times \log(9^\alpha) \right] \right].$$

By putting  $\alpha = 1, -1, 1/2, -1/2$ , in (3), we get the Randic entropies as given below:

$$ENT_{R_1}(\mathcal{F}) = \log\left(\frac{3}{2}(27x^2 + 41x - 52)\right) - \frac{12(x+3) \times \log[4]}{(3/2)(27x^2 + 41x - 52)} - \frac{36(x-1) \times \log[6]}{(3/2)(27x^2 + 41x - 52)} - \frac{27/2(3x^2+x-4) \times \log[9]}{(3/2)(27x^2 + 41x - 52)}$$

$$ENT_{R_{-1}}(\mathcal{F}) = \log\left(\frac{1}{12}(6x^2 + 23x + 7)\right) + \frac{3/4(x+3) \times \log[4]}{(1/12)(6x^2 + 23x + 7)} + \frac{(x-1) \times \log[6]}{(1/12)(6x^2 + 23x + 7)} + \frac{1/6(3x^2+x-4) \times \log[9]}{(1/12)(6x^2 + 23x + 7)},$$

$$ENT_{R_{1/2}}(\mathcal{F}) = \log\left(\frac{3}{2}(9x^2 + (7+4\sqrt{6})x - 4\sqrt{6})\right) - \frac{6(x+3) \times \log[2]}{(3/2)(9x^2 + (7+4\sqrt{6})x - 4\sqrt{6})} - \frac{6\sqrt{6}(x-1) \times \log[\sqrt{6}]}{(3/2)(9x^2 + (7+4\sqrt{6})x - 4\sqrt{6})}$$

$$- \frac{9/2(3x^2+x-4) \times \log[3]}{(3/2)(9x^2 + (7+4\sqrt{6})x - 4\sqrt{6})},$$

$$ENT_{R_{-1/2}}(\mathcal{F}) = \log\left(\frac{1}{2}(3x^2 + 2(2+\sqrt{6})x + 5)\right) + \frac{3/2(x+3) \times \log[2]}{(1/2)(3x^2 + 2(2+\sqrt{6})x + 5)} + \frac{\sqrt{6}(x-1) \times \log[\sqrt{6}]}{(1/2)(3x^2 + 2(2+\sqrt{6})x + 5)}$$

$$+ \frac{1/2(3x^2+x-4) \times \log[3]}{(1/2)(3x^2 + 2(2+\sqrt{6})x + 5)}.$$

(13)

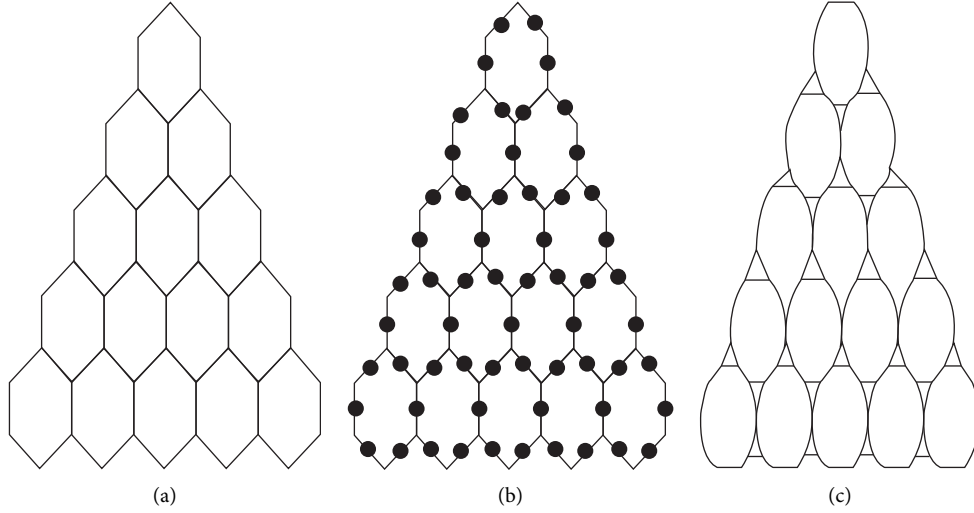


FIGURE 1: (a) Triangular benzenoid  $T_5$ , (b) Subdivision of  $T_5$ , (c) The line graph of subdivision graph of  $T_5$ .

TABLE 1: Edge partition of  $L(S(T_x))$ .

$(\widehat{N}(l), \widehat{N}(m))$	$N_i$	Set of Edges
(2, 2)	$2(x + 3)$	$E_1$
(2, 3)	$6(x - 1)$	$E_2$
(3, 3)	$3/2(3x^2 + x - 4)$	$E_3$

2.1.2. *The ABC Entropy of  $L(S(T_x))$ .* The ABC index and entropy measure with the help of Table 1 and equation (5) is:

$$\begin{aligned}
 \text{ABC}(\mathcal{F}) &= 3x^2 + \left(\frac{9}{\sqrt{2}} + 1\right)x + \frac{3}{\sqrt{2}} - 4, \\
 \text{ENT}_{\text{ABC}}(\mathcal{F}) &= \log(\text{ABC}) - \frac{1}{(\text{ABC})} \sum_{i=1}^3 \sum_{lm \in E_i(\mathcal{F})} \left[ \sqrt{\frac{\widehat{N}(l) + \widehat{N}(m) - 2}{\widehat{N}(l) \times \widehat{N}(m)}}} \right] \log \left[ \sqrt{\frac{\widehat{N}(l) + \widehat{N}(m) - 2}{\widehat{N}(l) \times \widehat{N}(m)}}} \right] \\
 &= \log \left( 3x^2 + \left(\frac{9}{\sqrt{2}} + 1\right)x + \frac{3}{\sqrt{2}} - 4 \right) + \frac{1/\sqrt{2}(9x + 3) \times \log[\sqrt{2}]}{(3x^2 + (9/\sqrt{2} + 1)x + 3/\sqrt{2} - 4)} - \frac{(3x^2 + x - 4) \times \log[2/3]}{(3x^2 + (9/\sqrt{2} + 1)x + 3/\sqrt{2} - 4)}.
 \end{aligned} \tag{14}$$

2.1.3. *The Geometric Arithmetic Entropy of  $L(S(T_x))$ .*

The GA index and entropy measure with the help of Table 1 and equation (7) is:

$$\begin{aligned}
 \text{GA}(\mathcal{F}) &= \frac{9}{2}x^2 + \frac{3x}{10}(8\sqrt{6} + 15) - \frac{3}{5}(4\sqrt{6} - 5), \\
 \text{ENT}_{\text{GA}}(\mathcal{F}) &= \log(\text{GA}) - \frac{1}{(\text{GA})} \sum_{i=1}^3 \sum_{lm \in E_i(\mathcal{F})} \left[ \frac{2\sqrt{\widehat{N}(l) \times \widehat{N}(m)}}{\widehat{N}(l) + \widehat{N}(m)} \right] \log \left[ \frac{2\sqrt{\widehat{N}(l) \times \widehat{N}(m)}}{\widehat{N}(l) + \widehat{N}(m)} \right] \\
 &= \log \left( \frac{9}{2}x^2 + \left(\frac{24\sqrt{6} + 45}{10}\right)x + \frac{15 - 12\sqrt{6}}{5} \right) - \frac{12\sqrt{6}/5(x - 1) \times \log[2\sqrt{6}/5]}{(9/2x^2 + (24\sqrt{6} + 45/10)x + 15 - 12\sqrt{6}/5)}.
 \end{aligned} \tag{15}$$

TABLE 2: Edge partition of  $L(S(T_x))$ .

$(A_l, A_m)$	$N_i$	Set of Edges
(4, 4)	9	$\mathcal{F}_{E_1}$
(4, 5)	6	$\mathcal{F}_{E_2}$
(5, 5)	$3(x-2)$	$\mathcal{F}_{E_3}$
(5, 8)	$6(y-1)$	$\mathcal{F}_{E_4}$
(8, 8)	$3(x-1)$	$\mathcal{F}_{E_5}$
(8, 9)	$6(x-1)$	$\mathcal{F}_{E_6}$
(9, 9)	$3/2(3x^2 + 2 - 5x)$	$\mathcal{F}_{E_7}$

2.1.4. *The  $ABC_4$  Entropy of  $L(S(T_x))$ .* The edge partition of the graph  $L(S(T_x))$  is grounded on the degree addition of terminal vertices of every edge, as shown in Table 2.

$$\begin{aligned}
 ENT_{ABC_4}(\mathcal{F}) &= \log(ABC_4) - \frac{1}{(ABC_4)} \sum_{i=1}^7 \sum_{lm \in E_i(\mathcal{F})} \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right] \log \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right], \\
 ENT_{ABC_4}(\mathcal{F}) &= \log(ABC_4) - \frac{[3\sqrt{6}/2] \log [\sqrt{6}/4]}{(ABC_4)} - \frac{[3\sqrt{7}/\sqrt{5}] \log [\sqrt{7}/2\sqrt{5}]}{(ABC_4)} \\
 &\quad - \frac{[6\sqrt{2}/5](x-1) \log [2\sqrt{2}/5]}{(ABC_4)} - \frac{[3\sqrt{11}/\sqrt{10}](x-1) \log [\sqrt{11}/2\sqrt{10}]}{(ABC_4)} \\
 &\quad - \frac{[3\sqrt{14}/8](x-1) \log [\sqrt{14}/8]}{(ABC_4)} - \frac{[\sqrt{15}/\sqrt{2}](x-1) \log [\sqrt{15}/6\sqrt{2}]}{(ABC_4)} - \frac{2/3(3x^2 - 5x + 2) \log [4/9]}{(ABC_4)}.
 \end{aligned} \tag{17}$$

If we consider  $x = 1$ , Then  $ABC_4(\mathcal{F}) = 9\sqrt{6}/4$ , and  $ENT_{ABC_4}(\mathcal{F}) = 2.1972$ .

2.1.5. *The  $GA_5$  Entropy of  $L(S(T_x))$ .* After some simple calculations, the  $GA_5$  index may be calculated using Table 2 under the constraint that  $x \neq 1$ .

$$\begin{aligned}
 ENT_{GA_5}(\mathcal{F}) &= \log(GA_5) - \frac{1}{(GA_5)} \sum_{i=1}^7 \sum_{lm \in E_i(\mathcal{F})} \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right] \log \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right], \\
 ENT_{GA_5}(\mathcal{F}) &= \log(GA_5) - \frac{[8\sqrt{5}/3] \log [4\sqrt{5}/9]}{(GA_5)} - \frac{[24\sqrt{10}/13](x-1) \log [4\sqrt{10}/13]}{(GA_5)} - \frac{[72\sqrt{2}/17](x-1) \log [12\sqrt{2}/17]}{(GA_5)}.
 \end{aligned} \tag{19}$$

### 3. Formation of Hexagonal Parallelogram

**Nanotubes  $H(x, y)$ ,  $\forall x, y \in \mathbb{N}$**

Hexagonal parallelogram nanotubes are formed by arranging hexagons in a parallelogram fashion. Baig et al. [52] computed counting polynomials of benzoid carbon nanotubes. Also, see [53]. We will denote this structure by  $H(x, y) \forall x, y \in \mathbb{N}$ , in which  $x$  and  $y$  represent the quantity of hexagons in any row and column respectively. Also, the order and size of  $H(x, y)$  is  $2(x + y + xy)$  and  $3xy + 2x +$

After simple calculations, by using Table 2 subject to the condition that  $x \neq 1$ , we get

$$\begin{aligned}
 ABC_4(\mathcal{F}) &= \frac{3\sqrt{6}}{2} + \frac{3\sqrt{7}}{\sqrt{5}} + \frac{6\sqrt{2}}{5}(x-2) \\
 &\quad + \left( \frac{3\sqrt{11}}{\sqrt{10}} + \frac{3\sqrt{14}}{8} + \frac{\sqrt{15}}{\sqrt{2}} \right)(x-1) \\
 &\quad + \frac{2}{3}(3x^2 - 5x + 2).
 \end{aligned} \tag{16}$$

By using (9), the  $ABC_4$  entropy as follows:

$$\begin{aligned}
 GA_5(\mathcal{F}) &= 3 + \frac{8\sqrt{5}}{3} + 3x + \left( \frac{24\sqrt{10}}{13} + \frac{72\sqrt{2}}{17} + 3 \right)(x-1) \\
 &\quad + \frac{3}{2}(3x^2 - 5n + 2).
 \end{aligned} \tag{18}$$

Therefore, (11), with Table 2 converted in the form:

$2y - 1$  respectively. The subdivision graph of  $H(x, y)$  and its line graph is shown in Figure 2, see [46]. Let  $\mathcal{F} = L(S(H(x, y)))$ , then  $|\mathcal{F}_V| = 2(3xy + 2x + 2y - 1)$  and  $|\mathcal{F}_E| = 9xy + 4x + 4y - 5$ . To compute our results, we will use edge partition technique which is grounded on the degree of terminal vertices of every edge. It is to be noted that there are only three types of edges, see Figure 2. The edge partition of chemical graph  $L(S(H(x, y)))$  depending on the degree of terminal vertices is presented in Table 3.

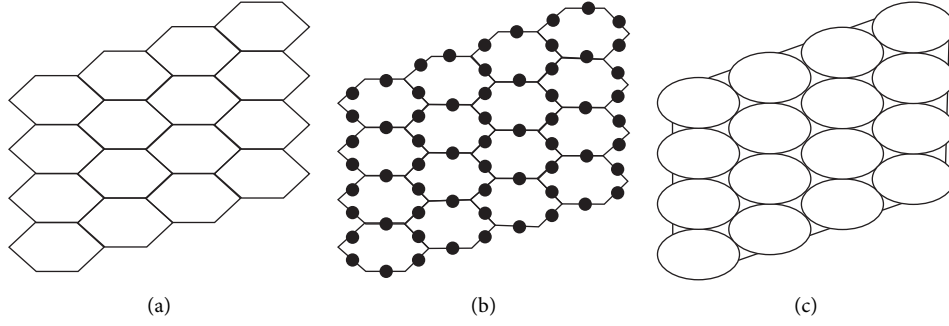


FIGURE 2: (a) Hexagonal parallelogram  $H(x, y)$ , (b) Subdivision of  $H(x, y)$ , (c) The line graph of subdivision graph of  $H(x, y)$ .

TABLE 3: Edge partition of  $L(S(H(x, y)))$ .

$(\widehat{\mathcal{N}}(l), \widehat{\mathcal{N}}(m))$	$N_i$	Kinds of Edges
(2, 2)	$2(4 + y + x)$	$\mathcal{F}_{E_1}$
(2, 3)	$4(-2 + y + x)$	$\mathcal{F}_{E_2}$
(3, 3)	$9xy - 2m - 2n - 5$	$\mathcal{F}_{E_3}$

3.1. Entropy Measure for  $L(S(H(x, y)))$ . We will enumerate the entropies of  $\mathcal{F} = L(S(H(x, y)))$  in this section.

3.1.1. Randić Entropy of  $\mathcal{F}$ . The Randić index for  $\alpha = 1, -1, 1/2, -1/2$ , by using Table 3 is:

$$R_\alpha(\mathcal{F}) = 2(x + y + 4) \times (4)^\alpha + 4(x + y - 2) \times (6)^\alpha + (9xy - 2x - 2y - 5) \times (9)^\alpha. \quad (20)$$

So the (3) with Table 3 gives the Randić entropy and is converted in the form:

$$\begin{aligned} ENT_{R_\alpha}(\mathcal{F}) &= \log(R_\alpha) - \frac{1}{(R_\alpha)} \sum_{i=1}^3 \sum_{lm \in E_i(\mathcal{F})} [(\widehat{\mathcal{N}}(l) \times \widehat{\mathcal{N}}(m))^\alpha] \log[(\widehat{\mathcal{N}}(l) \times \widehat{\mathcal{N}}(m))^\alpha] \\ &= \log(R_\alpha) - \frac{1}{(R_\alpha)} [[4^\alpha(2x + 2y + 8) \times \log(4^\alpha)] + t[6^\alpha(4x + 4y - 8) \times \log(6^\alpha)]n + q[9^\alpha(9xy - 2x - 2y - 5) \times \log(9^\alpha)]]. \end{aligned} \quad (21)$$

Now substitute  $\alpha = 1, -1, 1/2, -1/2$ , in (20), we get the Randić entropies as given below:

$$\begin{aligned} ENT_{R_1}(\mathcal{F}) &= \log(81xy + 14(x + y) - 61) - \frac{8(x + y + 4) \times [4]}{(81xy + 14(x + y) - 61)} - \frac{24(x + y - 2) \times \log[6]}{(81xy + 14(x + y) - 61)} - \frac{9(9xy - 2x - 2y - 5) \times \log[9]}{(81xy + 14(x + y) - 61)}. \\ ENT_{R_{-1}}(\mathcal{F}) &= \log\left(xy + \frac{17}{18}(x + y) + \frac{1}{9}\right) + \frac{1/2(x + y + 4) \times [4]}{(xy + 17/18(x + y) + 1/9)} + \frac{2/3(x + y - 2) \times \log[6]}{(xy + 17/18(x + y) + 1/9)} \\ &\quad + \frac{1/9(9xy - 2x - 2y - 5) \times \log[9]}{(xy + 17/18(x + y) + 1/9)}. \\ ENT_{R_{1/2}}(\mathcal{F}) &= \log(27xy + (4\sqrt{6} - 2)(x + y) + 1 - 8\sqrt{6}) - \frac{4(x + y + 4) \times [2]}{(27xy + (4\sqrt{6} - 2)(x + y) + 1 - 8\sqrt{6})} \\ &\quad - \frac{4\sqrt{6}(x + y - 2) \times \log[\sqrt{6}]}{(27xy + (4\sqrt{6} - 2)(x + y) + 1 - 8\sqrt{6})} - \frac{93(9xy - 2x - 2y - 5) \times \log[3]}{(27xy + (4\sqrt{6} - 2)(x + y) + 1 - 8\sqrt{6})}, \\ ENT_{R_{-1/2}}(\mathcal{F}) &= \log\left(3xy + \left(\frac{1}{3} + \frac{4}{\sqrt{6}}\right)(x + y) + \frac{7}{3} - \frac{8}{\sqrt{6}}\right) + \frac{(x + y + 4) \times \log[2]}{(3xy + (1/3 + 4/\sqrt{6})(x + y) + 7/3 - 8/\sqrt{6})} \\ &\quad + \frac{4/\sqrt{6}(x + y - 2) \times \log[\sqrt{6}]}{(3xy + (1/3 + 4/\sqrt{6})(x + y) + 7/3 - 8/\sqrt{6})} + \frac{1/3(9xy - 2x - 2y - 5) \times \log[9]}{(3xy + (1/3 + 4/\sqrt{6})(x + y) + 7/3 - 8/\sqrt{6})}. \end{aligned} \quad (22)$$

3.1.2. *The ABC Entropy of  $\mathcal{F}$* . With the use of Table 3 and equation (5), we can calculate the ABC index and entropy measure as follows:

$$ABC(\mathcal{F}) = 6xy + \left(\frac{9\sqrt{2} - 4}{3}\right)(x + y) - \frac{10}{3}. \quad (23)$$

Therefore, the equation (5), with Table 3 becomes as following and is called the atom bond connectivity entropy.

$$\begin{aligned} ENT_{ABC}(\mathcal{F}) &= \log(ABC) \\ &- \frac{1}{(ABC)} \sum_{i=1}^3 \sum_{lm \in E_i(\mathcal{F})} \left[ \sqrt{\frac{\hat{N}(l) + \hat{N}(m) - 2}{\hat{N}(l) \times \hat{N}(m)}}} \right] \\ &\cdot \log \left[ \sqrt{\frac{\hat{N}(l) + \hat{N}(m) - 2}{\hat{N}(l) \times \hat{N}(m)}}} \right], \\ &= \log \left( 6xy + \left(\frac{9\sqrt{2} - 4}{3}\right)(x + y) - \frac{10}{3} \right) \\ &+ \frac{\sqrt{2}(x + y + 4) \times [\sqrt{2}]}{(6xy + (9\sqrt{2} - 4/3)(x + y) - 10/3)} \\ &+ \frac{2\sqrt{2}(x + y - 2) \times \log[\sqrt{6}]}{(6xy + (9\sqrt{2} - 4/3)(x + y) - 10/3)} \\ &- \frac{2/3(9xy - 2x - 2y - 5) \times \log[2/3]}{(6xy + (9\sqrt{2} - 4/3)(x + y) - 10/3)}. \end{aligned} \quad (24)$$

3.1.3. *The Geometric Arithmetic Entropy of  $\mathcal{F}$* . We can calculate the GA index and entropy measure using Table 3 and equation (7) as follows:

$$GA(\mathcal{F}) = \frac{1}{5}(45xy + 8\sqrt{6}(x + y) + 15 - 16\sqrt{6}),$$

$$\begin{aligned} ENT_{GA}(\mathcal{F}) &= \log \left( \frac{1}{5}(45xy + 8\sqrt{6}(x + y) + 15 - 16\sqrt{6}) \right) \\ &- \frac{8\sqrt{6}/5(x + y - 2) \times \log[2\sqrt{6}/5]}{(1/5(45xy + 8\sqrt{6}(x + y) + 15 - 16\sqrt{6}))}. \end{aligned} \quad (25)$$

### 3.1.4. *The $ABC_4$ Entropy of $\mathcal{F}$*

Case 1. when  $x > 1, y \neq 1$

The edge partition of  $L(S(H(x, y)))$  is shown in Table 4.

Therefore, the  $ABC_4$  index and entropy measure with the help of Table 4 and equation (9) yield as:

TABLE 4: Edge partition of  $L(S(H(x, y)))$ .

$(A_l, A_m)$	$N_i$	Kinds of edges
(4, 4)	8	$\mathcal{F}_{E_1}$
(4, 5)	8	$\mathcal{F}_{E_2}$
(5, 5)	$2(-4 + y + x)$	$\mathcal{F}_{E_3}$
(5, 8)	$4(-2 + y + x)$	$\mathcal{F}_{E_4}$
(8, 8)	$2(-2 + x + y)$	$\mathcal{F}_{E_5}$
(8, 9)	$2(-2 + x + y)$	$\mathcal{F}_{E_6}$
(9, 9)	$9xy - 8x - 8y + 7$	$\mathcal{F}_{E_7}$

$$\begin{aligned} ABC_4(\mathcal{F}) &= 4xy + \left(\frac{4\sqrt{2}}{5} + \frac{2\sqrt{11}}{\sqrt{10}} + \frac{\sqrt{14}}{4} + \frac{\sqrt{30}}{3} - \frac{32}{9}\right) \\ &\cdot (x + y) + 2\sqrt{6} + \frac{4\sqrt{7}}{\sqrt{5}} - \frac{16\sqrt{2}}{5} - \frac{4\sqrt{11}}{\sqrt{10}} \\ &- \frac{\sqrt{14}}{2} - \frac{2\sqrt{30}}{3} + \frac{28}{9}. \end{aligned} \quad (26)$$

Since  $\mathcal{F}$  has seven kinds of edges, So (9) by using Table 4 is converted in the form:

$$\begin{aligned} ENT_{ABC_4}(\mathcal{F}) &= \log(ABC_4) \\ &- \frac{1}{(ABC_4)} \sum_{i=1}^7 \sum_{lm \in E_i(\mathcal{F})} \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right] \\ &\cdot \log \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right], \\ ENT_{ABC_4}(\mathcal{F}) &= \log(ABC_4) - \frac{2\sqrt{6} \log[\sqrt{6}/4]}{(ABC_4)} \\ &- \frac{4\sqrt{7}/\sqrt{5} \log[\sqrt{7}/2\sqrt{5}]}{(ABC_4)} \\ &- \frac{4\sqrt{2}/5(x + y - 4) \log[2\sqrt{2}/5]}{(ABC_4)} \\ &- \frac{2\sqrt{11}/\sqrt{10}(x + y - 2) \log[\sqrt{11}/2\sqrt{10}]}{(ABC_4)} \\ &- \frac{\sqrt{14}/4(x + y - 2) \log[\sqrt{14}/8]}{(ABC_4)} \\ &- \frac{2\sqrt{15}/3\sqrt{2}(x + y - 2) \log[\sqrt{15}/6\sqrt{2}]}{(ABC_4)} \\ &- \frac{4/9(9xy - 8x - 8y + 7) \log[4/9]}{(ABC_4)}. \end{aligned} \quad (27)$$

Case 2. when  $x = 1, y \neq 1$

By using the same process, we get the closed expressions for the  $ABC_4$  index and  $ABC_4$  entropy as:

$$\begin{aligned}
BC_4(\mathcal{F}) &= \left( \frac{4\sqrt{2}}{5} + \frac{2\sqrt{11}}{\sqrt{10}} + \frac{\sqrt{14}}{4} + \frac{\sqrt{30}}{3} + \frac{4}{9} \right) y + \frac{5\sqrt{6}}{2} \\
&\quad + \frac{2\sqrt{7}}{\sqrt{5}} - \frac{8\sqrt{2}}{5} - \frac{2\sqrt{11}}{\sqrt{10}} - \frac{\sqrt{30}}{3} - \frac{\sqrt{14}}{4} - A \frac{9}{4}, \\
ENT_{ABC_4}(\mathcal{F}) &= \log(ABC_4) - \frac{5\sqrt{6}/2 \log[\sqrt{6}/4]}{(ABC_4)} \\
&\quad - \frac{2\sqrt{7}/\sqrt{5} \log[\sqrt{7}/2\sqrt{5}]}{(ABC_4)} \\
&\quad - \frac{4\sqrt{2}/5(y-2) \log[2\sqrt{2}/5]}{(ABC_4)} \\
&\quad - \frac{2\sqrt{11}/\sqrt{10}(y-1) \log[\sqrt{11}/2\sqrt{10}]}{(ABC_4)} \\
&\quad - \frac{\sqrt{14}/4(y-1) \log[\sqrt{14}/8]}{(ABC_4)} \\
&\quad - \frac{2\sqrt{15}/3\sqrt{2}(y-1) \log[\sqrt{15}/6\sqrt{2}]}{(ABC_4)} \\
&\quad - \frac{4/9(y-1) \log[4/9]}{(ABC_4)}. \tag{28}
\end{aligned}$$

### 3.1.5. The Fifth Geometric Arithmetic Entropy of $\mathcal{F}$

Case 3. when  $x > 1$ ,  $y \neq 1$  The fifth geometric arithmetic entropy can be estimated by using (11), and Table 4 in the following manner:

$$\begin{aligned}
GA_5(\mathcal{F}) &= 9xy + \left( \frac{16\sqrt{10}}{13} + \frac{48\sqrt{2}}{17} - 4 \right) (x+y) + 3 \\
&\quad + \frac{32\sqrt{5}}{9} - \frac{32\sqrt{10}}{13} - \frac{96\sqrt{2}}{17}. \tag{29}
\end{aligned}$$

So the (11), with Table 4 can be written as:

$$\begin{aligned}
ENT_{GA_5}(\mathcal{F}) &= \log(GA_5) - \frac{1}{(GA_5)} \sum_{i=1}^7 \sum_{lm \in E_i(\mathcal{F})} \\
&\quad \cdot \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right] \log \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right] \\
&= \log(GA_5) - \frac{32\sqrt{5}/9 \log[4\sqrt{5}/9]}{(GA_5)} \\
&\quad - \frac{16\sqrt{10}/13(x+y-2) \log[4\sqrt{10}/13]}{(GA_5)} \\
&\quad - \frac{48\sqrt{2}/17(x+y-2) \log[12\sqrt{2}/17]}{(GA_5)}. \tag{30}
\end{aligned}$$

TABLE 5: Edge partition of  $L(S(H(x, y)))$ , for  $x = 1$ .

$(A_l, A_m)$	$N_i$	Kinds of edges
(4, 4)	10	$\mathcal{F}_{E_1}$
(4, 5)	4	$\mathcal{F}_{E_2}$
(5, 5)	$2(y-2)$	$\mathcal{F}_{E_3}$
(5, 8)	$4(y-1)$	$\mathcal{F}_{E_4}$
(8, 8)	$2(y-1)$	$\mathcal{F}_{E_5}$
(8, 9)	$2(y-1)$	$\mathcal{F}_{E_6}$
(9, 9)	$y-1$	$\mathcal{F}_{E_7}$

Case 4. when  $x = 1$ ,  $y \neq 1$  By using Table 5 and using (11) we get the closed expressions for the  $GA_5$  index and  $GA_5$  entropy as:

$$\begin{aligned}
GA_5(\mathcal{F}) &= \left( 5 + \frac{16\sqrt{10}}{13} + \frac{48\sqrt{2}}{17} \right) y + 3 + \frac{16\sqrt{5}}{9} \\
&\quad - \frac{16\sqrt{10}}{13} - \frac{48\sqrt{2}}{17} - \frac{16\sqrt{10}}{13}, \\
ENT_{GA_5}(\mathcal{F}) &= \log(GA_5) - \frac{16\sqrt{5}/9 \log[4\sqrt{5}/9]}{(GA_5)} \\
&\quad - \frac{16\sqrt{10}/13(y-1) \log[4\sqrt{10}/13]}{(GA_5)} \\
&\quad - \frac{48\sqrt{2}/17(y-1) \log[12\sqrt{2}/17]}{(GA_5)}. \tag{31}
\end{aligned}$$

## 4. Formation from Fusion of Zigzag-Edge Coronoid with Starphene ZCS(x, y, z) Nanotubes

If a zigzag-edge coronoid  $ZC(x, y, z)$  is fused with a starphene  $St(x, y, z)$ , then we will obtain a composite benzenoid. It is to be noted that  $|V(ZCS(x, y, z))| = 36x - 54$  and  $|E(ZCS(x, y, z))| = -63 + 15(z + y + x)$ . The subdivision graph of  $ZCS(x, y, z)$  and its line graph are illustrated in Figure 3. We can see from figures that the order and the size in the line graph of the subdivision graph of  $ZCS(x, y, z)$  are  $-126 + 30(z + y + x)$  and  $-153 + 39(z + y + x)$  respectively [46]. Let  $\mathcal{F}$  represents the subdivision graph of  $ZCS(x, y, z)$ 's line graph. The edge division is determined by the degree of each edge's terminal vertices. Table 6 illustrates this.

4.1. Entropy Measure for  $L(S(ZCS(x, y, z)))$ . We'll calculate the entropies of  $\mathcal{F} = L(S(ZCS(x, y, z)))$  in this section.

4.1.1. Randić Entropy of  $\mathcal{F}$ . For  $\alpha = 1, -1, 1/2, -1/2$ , the Randić index with the help of Table 1 is

$$\begin{aligned}
R_\alpha(\mathcal{F}) &= 6(x + y + z - 5) \times (4)^\alpha + 12(x + y + z - 7) \\
&\quad \times (6)^\alpha + (21x + 21y + 21z - 39) \times (9)^\alpha. \tag{32}
\end{aligned}$$



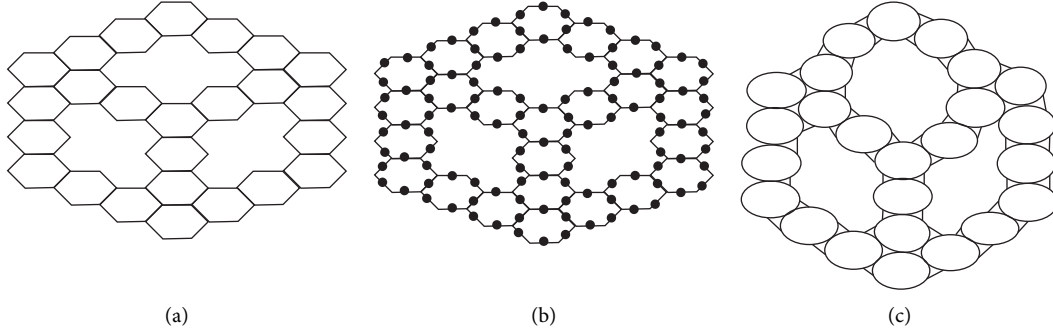

 FIGURE 3: (a)  $ZCS(4, 4, 4)$ , (b) subdivision of  $ZCS(4, 4, 4)$ , (c)  $L(S(ZCS(4, 4, 4)))$ .

 TABLE 6: Edge partition of  $L(S(ZCS))$ .

$(\hat{N}(l), \hat{N}(m))$	$N_i$	Kinds of Edges
(2, 2)	$6(-5 + z + y + x)$	$\mathcal{F}_{E_1}$
(2, 3)	$12(-7 + z + y + x)$	$\mathcal{F}_{E_2}$
(3, 3)	$-39 + 21(z + y + x)$	$\mathcal{F}_{E_3}$

Using (3) Randić entropy is:

$$\begin{aligned}
 ENT_{R_\alpha}(\mathcal{F}) &= \log(R_\alpha) - \frac{1}{(R_\alpha)} \sum_{i=1}^3 \sum_{lm \in E_i(\mathcal{F})} \left[ (\hat{N}(l) \times \hat{N}(m)^\alpha) \log [(\hat{N}(l) \times \hat{N}(m)^\alpha)] \right. \\
 &= \log(R_\alpha) - \frac{1}{(R_\alpha)} \left[ [4^\alpha (6(x + y + z - 5)) \times \log(4^\alpha)] + [6^\alpha (12(x + y + z - 7)) \times \log(6^\alpha)] \right. \\
 &\quad \left. \left. + [(21(x + y + z) - 39) \times \log(9^\alpha)] \right] \right].
 \end{aligned} \tag{33}$$

By putting  $\alpha = 1, -1, 1/2, -1/2$ , in (32), we get the Randić entropies as given below:

$$\begin{aligned}
 ENT_{R_1}(\mathcal{F}) &= \log(-975 + 285(z + y + x)) - \frac{24(-5 + z + y + x) \times \log[4]}{(-975 + 285(z + y + x))} - \frac{72(x + y + z - 7) \times \log[6]}{(-975 + 285(z + y + x))} \\
 &\quad - \frac{189(z + tyn + qx) - t351) \times \log[9]}{(-975 + 285(z + y + x))}, \\
 ENT_{R_{-1}}(\mathcal{F}) &= \log\left(-\frac{131}{6} + \frac{35}{6}(z + y + x)\right) + \frac{3/2(-5 + z + y + x) \times \log[4]}{(-131/6 + 35/6(z + y + x))} + \frac{2(-7 + z + y + x) \times \log[6]}{(-131/6 + 35/6(z + y + x))} \\
 &\quad + \frac{1/3(-13 + 7(z + y + x)) \times \log[9]}{(-131/6 + 35/6(z + y + x))}, \\
 ENT_{R_{1/2}}(\mathcal{F}) &= \log((3 + 12\sqrt{6})(x + y + z) - 177 - 84\sqrt{6}) - \frac{12(x + y + z - 5) \times \log[2]}{((3 + 12\sqrt{6})(x + y + z) - 177 - 84\sqrt{6})} \\
 &\quad - \frac{6\sqrt{6}(x + y + z - 7) \times \log[\sqrt{6}]}{((3 + 12\sqrt{6})(x + y + z) - 177 - 84\sqrt{6})} - \frac{9(7(x + y + z) - 13) \times \log[3]}{((3 + 12\sqrt{6})(x + y + z) - 177 - 84\sqrt{6})}, \\
 ENT_{R_{-1/2}}(\mathcal{F}) &= \log((10 + 2\sqrt{6})(x + y + z) - 28 - 14\sqrt{6}) + \frac{3(x + y + z - 5) \times \log[2]}{((10 + 2\sqrt{6})(x + y + z) - 28 - 14\sqrt{6})} \\
 &\quad + \frac{2\sqrt{6}(x + y + z - 7) \times \log[\sqrt{6}]}{((10 + 2\sqrt{6})(x + y + z) - 28 - 14\sqrt{6})} + \frac{(7(x + y + z) - 13) \times \log[3]}{((10 + 2\sqrt{6})(x + y + z) - 28 - 14\sqrt{6})}.
 \end{aligned} \tag{34}$$

4.1.2. *The ABC Entropy of  $\mathcal{F}$* . The ABC index and entropy measure with the help of Table 6 and equation (5) are:

$$\begin{aligned}
 ABC(\mathcal{F}) &= (14 + 9\sqrt{2})(x + y + z) - 26 - 57\sqrt{2}, \\
 ENT_{ABC}(\mathcal{F}) &= \log((14 + 9\sqrt{2})(x + y + z) - 26 - 57\sqrt{2}) \\
 &\quad + \frac{3\sqrt{2}(3(x + y + z) - 19) \times \log[\sqrt{2}]}{((14 + 9\sqrt{2})(x + y + z) - 26 - 57\sqrt{2})} \\
 &\quad - \frac{(14(x + y + z) - 26)\log[2/3]}{((14 + 9\sqrt{2})(x + y + z) - 26 - 57\sqrt{2})}. \tag{35}
 \end{aligned}$$

TABLE 7: Edge partition of  $L(S(ZCS(x, y, z)))$  established on degree sum of terminal vertices, for every  $x = y = z \geq 4$

$(A_l, A_m)$	$N_i$	Kinds of Edges
(4, 4)	6	$\mathcal{F}_{E_1}$
(4, 5)	12	$\mathcal{F}_{E_2}$
(5, 5)	$6(x + y + z - 8)$	$\mathcal{F}_{E_3}$
(5, 8)	$12(x + y + z - 7)$	$\mathcal{F}_{E_4}$
(8, 8)	$6(x + y + z - 9)$	$\mathcal{F}_{E_5}$
(8, 9)	$12(x + y + z - 5)$	$\mathcal{F}_{E_6}$
(9, 9)	$3(x + y + z + 25)$	$\mathcal{F}_{E_7}$

4.1.3. *The Geometric Arithmetic Entropy of  $\mathcal{F}$* . The GA index and corresponding entropy with the help of Table 6 and equation (7) are:

$$GA(\mathcal{F}) = (x + y + z)(27 + 24\sqrt{6}/5) - 69 - 168\sqrt{6}/5,$$

$$ENT_{GA}(\mathcal{F}) = \log((x + y + z)(27 + 24\sqrt{6}/5) - 69 - 168\sqrt{6}/5) - \frac{24\sqrt{6}/5(x + y + z - 7) \times \log[2\sqrt{6}/5]}{(x + y + z)(27 + 24\sqrt{6}/5) - 69 - 168\sqrt{6}/5}. \tag{36}$$

4.1.4. *The  $ABC_4$  entropy of  $\mathcal{F}$* . Table 7 shows the graph  $L(S(ZCS(x, y, z)))$ 's edge partition, which is based on the degree addition of each edge's terminal vertices.

After simple calculations, the  $ABC_4$  index and entropy measure with the help of Table 7 and equation (9) subject to the condition that  $x = y = z \geq 41$

$$ABC_4(\mathcal{F}) = (x + y + z) \left( \sqrt{30} + \frac{4}{3} + \frac{12\sqrt{2}}{5} + \frac{3\sqrt{14}}{4} + \frac{6\sqrt{11}}{\sqrt{10}} \right) - 5\sqrt{30} + \frac{100}{3} - \frac{96\sqrt{2}}{5} + \frac{27\sqrt{14}}{4} - \frac{42\sqrt{11}}{\sqrt{10}} + \frac{3\sqrt{6}}{2} + \frac{6\sqrt{7}}{\sqrt{5}},$$

$$ENT_{ABC_4}(\mathcal{F}) = \log(ABC_4) - \frac{1}{(ABC_4)} \sum_{i=1}^7 \sum_{lm \in E_i(\mathcal{F})} \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right] \log \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right],$$

$$\begin{aligned}
 ENT_{ABC_4}(\mathcal{F}) &= \log(ABC_4) - \frac{[3\sqrt{6}/2]\log[\sqrt{6}/4]}{(ABC_4)} - \frac{[12\sqrt{2}/5](x + y + z - 8)\log[2\sqrt{2}/5]}{(ABC_4)} \\
 &\quad - \frac{[6\sqrt{11}/\sqrt{10}](x + y + z - 7)\log[\sqrt{11}/2\sqrt{10}]}{(ABC_4)} - \frac{3\sqrt{14}/4(x + y + z - 9)\log[\sqrt{14}/8]}{(ABC_4)} \\
 &\quad - \frac{\sqrt{30}(x + y + z - 5)\log[\sqrt{15}/6\sqrt{2}]}{(ABC_4)} - \frac{4/3(x + y + z + 25)\log[4/9]}{(ABC_4)} - \frac{[6\sqrt{7}/\sqrt{5}]\log[\sqrt{7}/2\sqrt{5}]}{(ABC_4)}. \tag{37}
 \end{aligned}$$

TABLE 8: Comparison of randic entropies for  $L(S(T_x))$ .

$[x]$	$ENT_{R_1}$	$ENT_{R_{-1}}$	$ENT_{R_{1/2}}$	$ENT_{R_{-1/2}}$
[46]	0.4055	2.5590	2.4849	2.6263
[52]	3.1863	3.0463	3.5667	3.5970
[25]	4.0316	3.6767	4.2203	4.2280
[26]	4.5797	4.2928	4.6981	4.6991
[24]	4.9945	4.8714	5.0779	5.0764
[23]	5.3312	5.4107	5.3942	5.3918
[27]	5.6159	5.9131	5.6658	5.6631
[2]	5.8632	6.3820	5.9041	5.9013
[56]	6.0820	6.8208	6.1164	6.1136
[31]	6.2785	7.2325	6.3080	6.3053

TABLE 9: Comparison of  $ENT_{ABC}$ ,  $ENT_{GA}$ ,  $ENT_{ABC_4}$ , and  $ENT_{GA_5}$  for  $L(S(T_x))$ .

$[x]$	$ENT_{ABC}$	$ENT_{GA}$	$ENT_{ABC_4}$	$ENT_{GA_5}$
[46]	2.3116	2.4849	2.1972	0
[52]	3.5239	3.5835	3.5749	3.5835
[25]	4.2025	4.2341	4.2263	4.2341
[26]	4.6897	4.7095	4.7028	4.7095
[24]	5.0739	5.0876	5.0817	5.0876
[23]	5.3926	5.4027	5.3975	5.4026
[27]	5.6655	5.6733	5.6687	5.6733
[2]	5.9046	5.91087	5.9066	5.9108
[56]	6.1174	6.1225	6.1187	6.1225
[31]	6.3093	6.3135	6.3100	6.3135

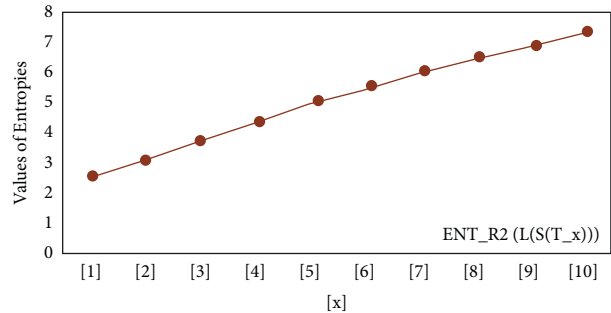
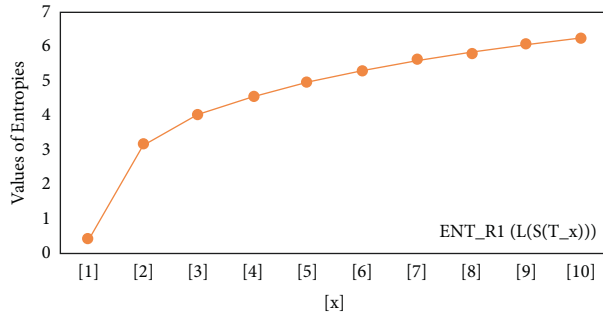


FIGURE 4: (a)  $R_1$  entropy, (b)  $R_{-1}$  entropy.

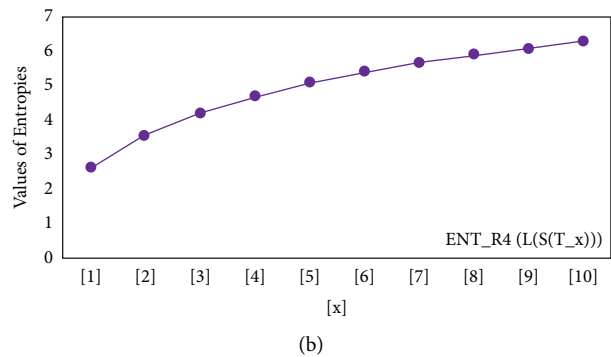
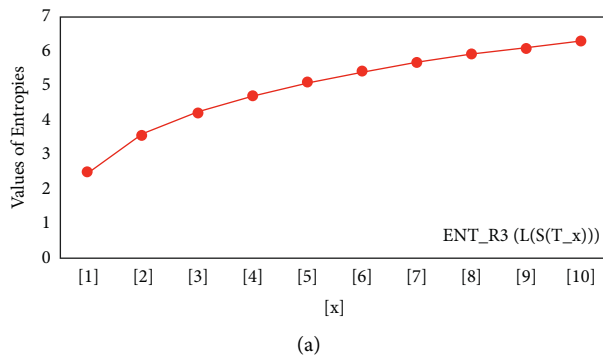


FIGURE 5: (a)  $R_{1/2}$  entropy, (b)  $R_{-1/2}$  entropy.

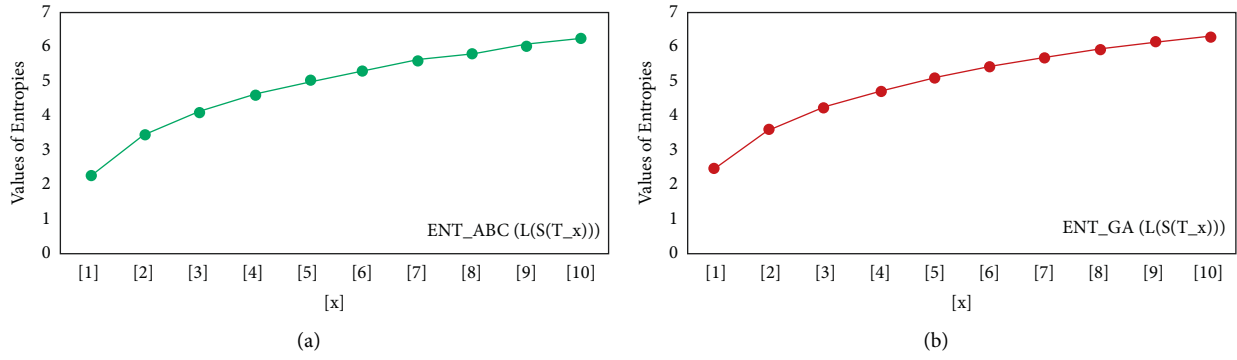


FIGURE 6: (a) The ABC entropy, (b) The GA entropy.

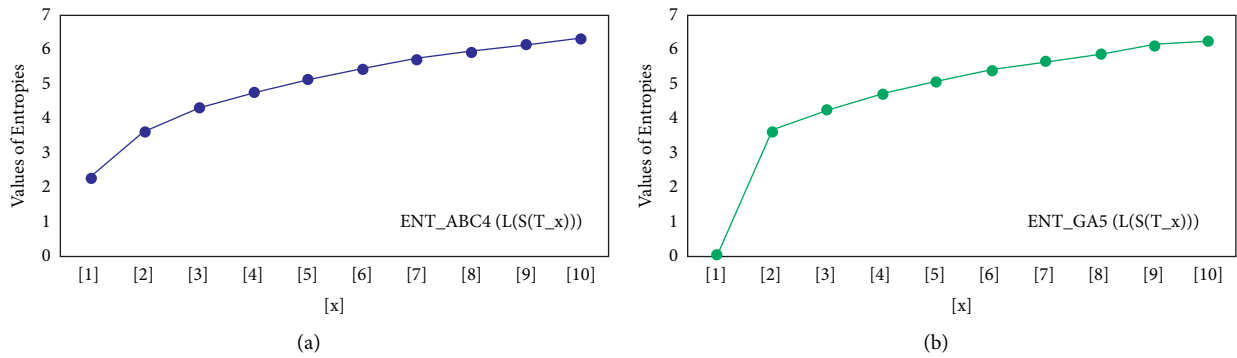


FIGURE 7: (a) The  $ABC_4$  entropy, (b) The  $GA_5$  entropy.

TABLE 10: Comparison of randic entropies for  $L(S(H(x, y)))$ .

$[x, y]$	$ENT_{R_1}$	$ENT_{R_{-1}}$	$ENT_{R_{1/2}}$	$ENT_{R_{-1/2}}$
[1, 1]	2.4849	2.4849	2.4849	2.4849
[2, 2]	3.7917	3.7830	3.8344	3.8332
[3, 3]	4.5635	4.5428	4.5933	4.5906
[4, 4]	5.1096	5.0872	5.1323	5.1294
[5, 5]	5.5345	5.5129	5.5530	5.5502
[6, 6]	5.8833	5.8630	5.8988	5.8962
[7, 7]	6.1794	6.1615	6.1928	6.1904
[8, 8]	6.4368	6.4194	6.4486	6.4464
[9, 9]	6.6646	6.6483	6.6751	6.6731
[10, 10]	6.8688	6.5370	6.8783	6.8822

TABLE 12: Comparison of  $ENT_{ABC_4}$  and  $ENT_{GA_5}$  Entropies for  $L(S(H(x, y)))$ ,  $x > 1$  and  $y \neq 1$ .

$[x, y]$	$ENT_{ABC_4}$	$ENT_{GA_5}$
[2, 2]	3.7879	3.4822
[3, 3]	4.5387	2.2596
[4, 4]	5.0783	4.8387
[5, 5]	5.5018	5.2952
[6, 6]	5.8509	5.6704
[7, 7]	6.1481	5.9882
[8, 8]	6.4068	6.2636
[9, 9]	6.6360	6.5064
[10, 10]	6.8417	6.7234

TABLE 11: Comparison of  $ENT_{ABC}$  and  $ENT_{GA}$  entropies for  $L(S(H(x, y)))$ .

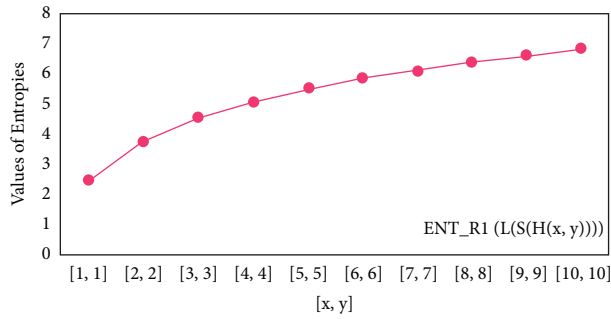
$[x, y]$	$ENT_{ABC}$	$ENT_{GA}$
[1, 1]	2.4849	2.4849
[2, 2]	3.8497	3.8501
[3, 3]	4.6048	4.6051
[4, 4]	5.1413	5.1416
[5, 5]	5.5604	5.5607
[6, 6]	5.9051	5.9053
[7, 7]	6.1982	6.1985
[8, 8]	6.4534	6.4536
[9, 9]	6.6794	6.6796
[10, 10]	6.8822	6.8824

TABLE 13: Comparison of  $ENT_{ABC_4}$  and  $ENT_{GA_5}$  entropies for  $L(S(H(x, y)))$ ,  $x = 1$  and  $y \neq 1$ .

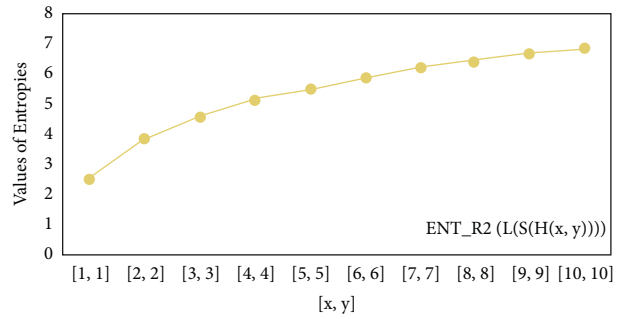
$[y]$	$ENT_{ABC_4}$	$ENT_{GA_5}$
[52]	3.1846	3.2958
[25]	3.5933	3.6888
[26]	3.8884	3.9702
[24]	4.1184	4.1896
[23]	4.3064	4.3694
[27]	4.4653	4.5217
[2]	4.6027	4.6539
[56]	4.7238	4.7706
[31]	4.8319	4.8751

TABLE 14: Comparison of randic entropies for  $L(S(ZCS(x, y, z)))$ .

$[x, y, z]$	$ENT_{R_1}$	$ENT_{R_{-1}}$	$ENT_{R_{1/2}}$	$ENT_{R_{-1/2}}$
[4, 4, 4]	5.7200	5.70060	5.7432	5.7407
[5, 5, 5]	6.0342	6.0165	6.0587	6.0565
[6, 6, 6]	6.2730	6.2564	6.2982	6.2961
[7, 7, 7]	6.4657	6.4497	6.4913	6.4893
[8, 8, 8]	6.6272	6.6117	6.6531	6.6511
[9, 9, 9]	6.7662	6.7511	6.7923	6.7904
[10, 10, 10]	6.8883	6.8734	6.9145	6.9126

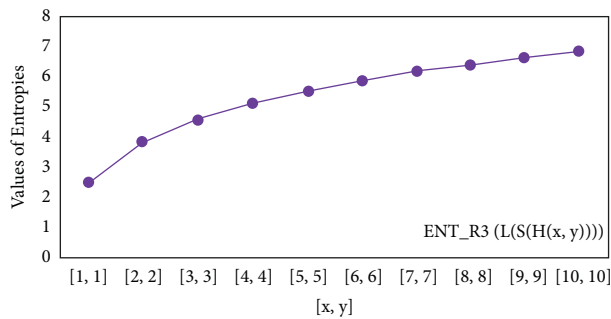


(a)

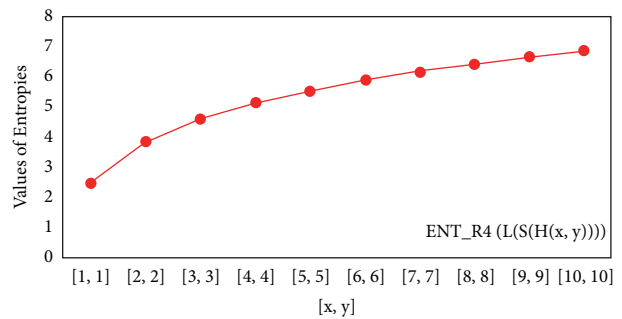


(b)

FIGURE 8: (a) $R_1$  entropy, (b) $R_{-1}$  entropy.

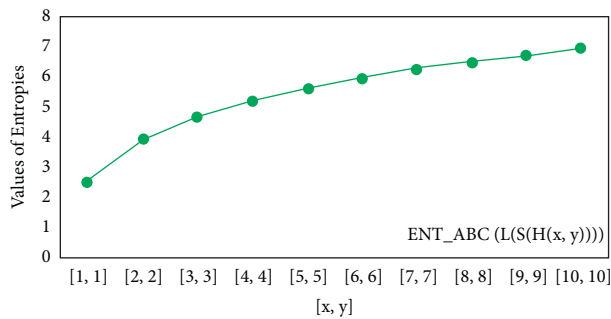


(a)

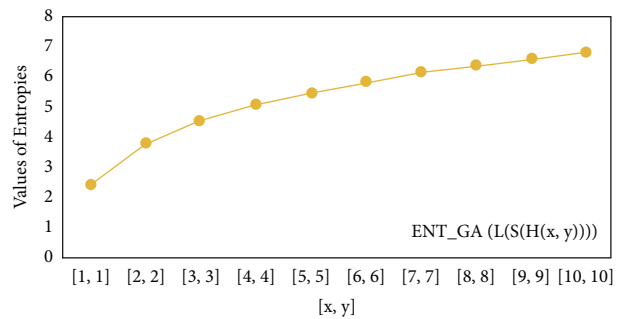


(b)

FIGURE 9: (a) $R_{1/2}$  entropy, (b) $R_{-1/2}$  entropy.



(a)



(b)

FIGURE 10: (a) The ABC entropy, (b) The GA, entropy.

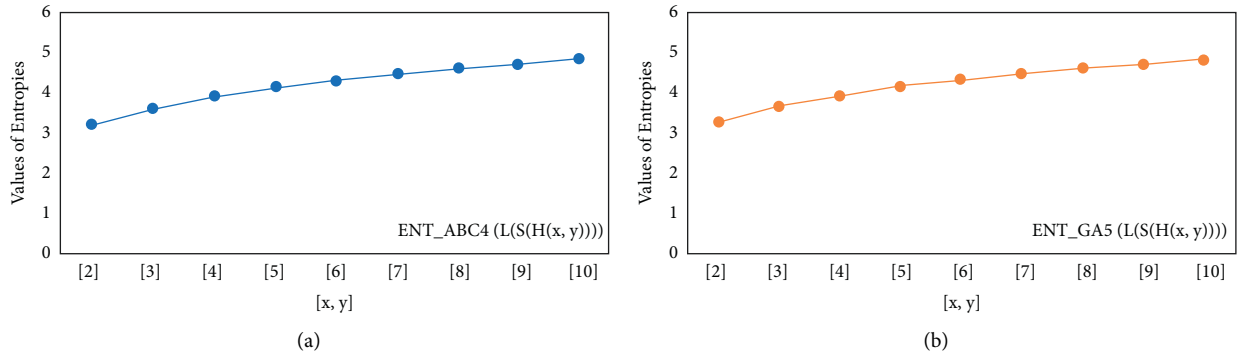


FIGURE 11: (a) The  $ABC_4$  entropy, (b) The  $GA_5$  entropy,  $x \geq 1, y \neq 1$ .

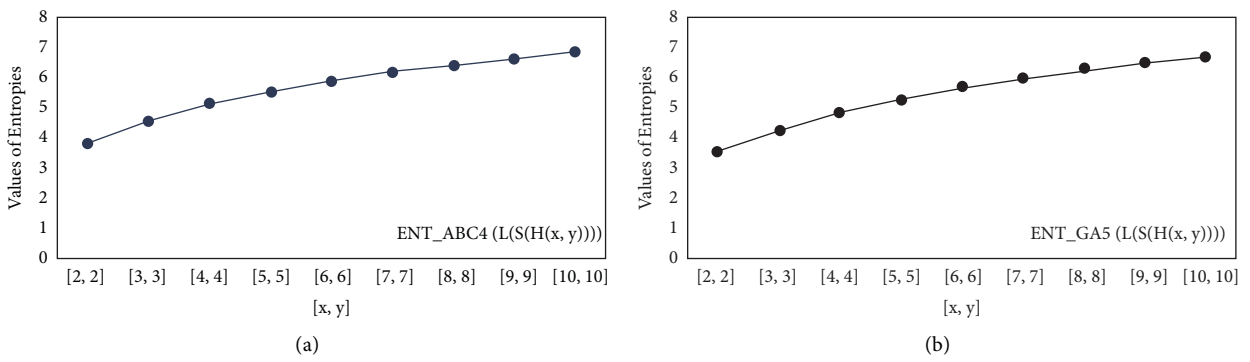


FIGURE 12: (a) The  $ABC_4$  entropy, (b) The  $GA_5$  entropy  $x = 1, y \neq 1$ .

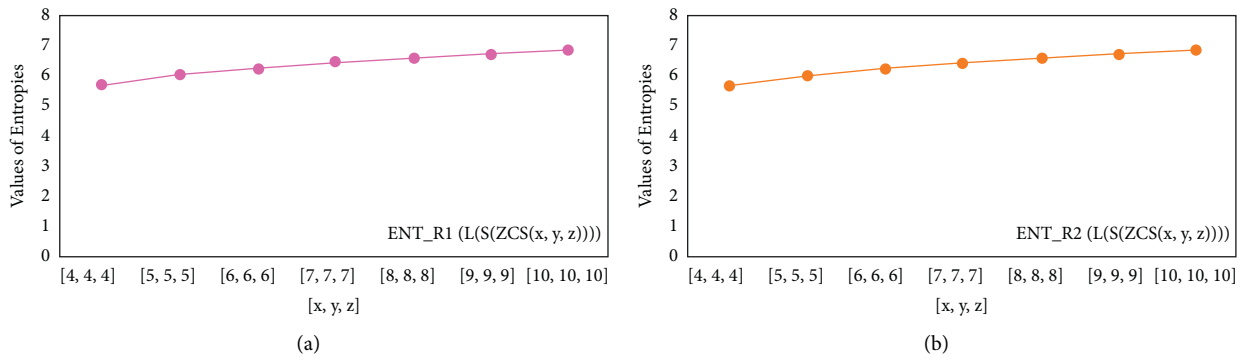


FIGURE 13: (a)  $R_1$  entropy, (b)  $R_{-1}$  entropy.

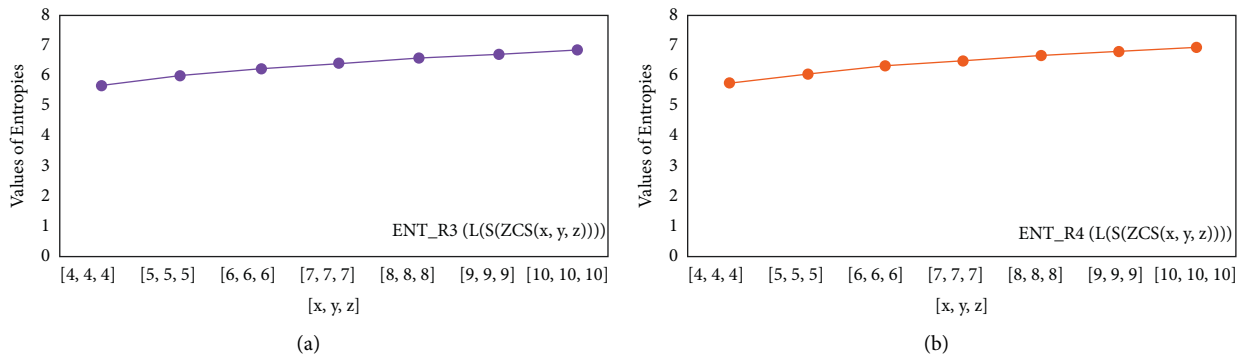


FIGURE 14: (a)  $R_{1/2}$  entropy, (b)  $R_{1/2}$  entropy.

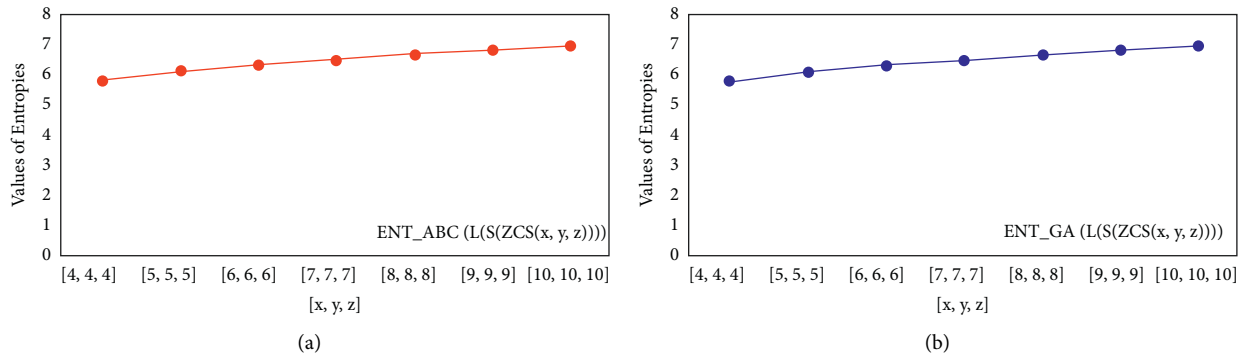
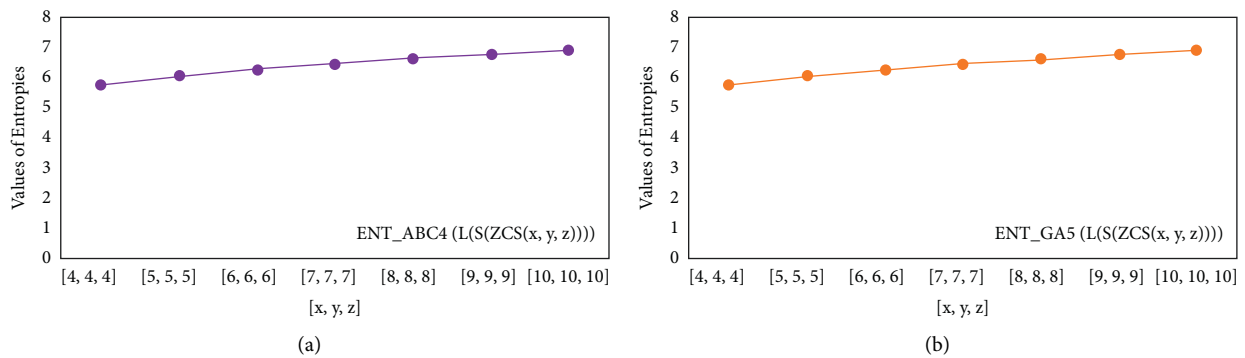


FIGURE 15: (a)ABC entropy, (b)The GA, entropy.


 FIGURE 16: (a)ABC<sub>4</sub> entropy, (b)GA<sub>5</sub> entropy.

4.1.5. *The GA<sub>5</sub> Entropy of  $\mathcal{F}$ .* After some simple calculations, the GA<sub>5</sub> index and corresponding entropy measure with the help of Table 7 and equation (11) subject to the condition that  $x = y = z \geq 4$ .

$$\begin{aligned}
 GA_5(\mathcal{F}) &= (x + y + z) \left( 15 + \frac{48\sqrt{10}}{13} + \frac{144\sqrt{2}}{17} \right) + 3 + \frac{16\sqrt{5}}{3} - \frac{336\sqrt{10}}{13} - \frac{720\sqrt{2}}{17}, \\
 ENT_{GA_5}(\mathcal{F}) &= \log(GA_5) - \frac{1}{(GA_5)} \sum_{i=1}^7 \sum_{lm \in E_i(\mathcal{F})} \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right] \log \left[ \sqrt{\frac{A_l + A_m - 2}{A_l A_m}} \right], \\
 ENT_{GA_5}(\mathcal{F}) &= \log(GA_5) - \frac{[16\sqrt{5}/3] \log [4\sqrt{5}/9]}{(GA_5)} - \frac{[48\sqrt{10}/13] (x + y + z - 7) \log [4\sqrt{10}/13]}{(GA_5)} \\
 &\quad - \frac{[144\sqrt{2}/17] (x + y + z - 5) \log [12\sqrt{2}/17]}{(GA_5)}.
 \end{aligned} \tag{38}$$

## 5. Concluding remarks for Computed Results

The applications of information-theoretic framework in many disciplines of study, such as biology, physics, engineering, and social sciences, have grown exponentially in the recent two decades. This phenomenal increase has been particularly impressive in the fields of soft computing, molecular biology, and information technology. As a result, the scientists may find our numerical and

graphical results useful [54, 55]. The entropy function is monotonic, which means that as the size of a chemical structure increases, so does the entropy measure, and as the entropy of a system increases, so does the uncertainty regarding its reaction.

For  $L(S(T_x))$ , the numerical and graphical results are shown in Tables 8 and 9 and Figures 4–7. In Table 9, the fifth arithmetic geometric entropy is zero which shows that the process is deterministic for  $x = 1$ . When the chemical

structure  $L(S(T_x))$  expands, the Randić entropy for  $\alpha = 1/2$  develops more quickly than other entropy measurements of  $L(S(T_x))$ , whereas the Randić entropy for  $\alpha = -1/2$  develops more slowly. This demonstrates that different topologies have varied entropy characteristics. For  $L(S(H(x, y)))$ , the numerical and graphical results are shown in Tables 10–13 and Figures 8–12. When the chemical structure  $L(S(H(x, y)))$  expands, the geometric arithmetic entropy develops more quickly than other entropy measurements of  $L(S(H(x, y)))$ , whereas the  $ABC_4$  entropy develops more slowly. Finally, for  $L(S(ZCS(x, y, z)))$ , the numerical and graphical results are shown in Table 14 and Figures 13–16. When the chemical structure  $L(S(ZCS(x, y, z)))$  expands, the geometric arithmetic entropy develops more quickly than other entropy measurements of  $L(S(ZCS(x, y, z)))$ , whereas the Randić entropy for  $\alpha = -1$  develops more slowly.

The novelty of this article is that entropies are computed for three types of benzenoid systems. These entropy measures are useful in estimating the heat of formation and many Physico-chemical properties. In statistical analysis of benzene structures, entropy measures showed more significant results as compared to topological indices. Therefore, we can say that the entropy measure is a newly introduced topological descriptor.

## 6. Conclusion

Using Shannon's entropy and Chen et al. [31] entropy definitions, we generated graph entropies associated to a new information function in this research. Between indices and information entropies, a relationship is created. Using the line graph of the subdivision of these graphs, we estimated the entropies for triangular benzenoids  $T_x$ , hexagonal parallelogram  $H(x, y)$  nanotubes, and  $ZCS(x, y, z)$ . Thermodynamic entropy of enzyme-substrate complexions [57, 58] and configuration entropy of glass-forming liquids [56] are two examples of thermodynamic entropy employed in molecular dynamics studies of complex chemical systems. Similarly, using information entropy as a crucial structural criterion could be a new step in this direction.

## Data Availability

The data used to support the findings of this study are cited at relevant places within the text as references.

## Conflicts of Interest

The authors declare that they have no conflicts of interest.

## Authors' Contributions

This work was equally contributed by all writers.

## References

- [1] Z. Q. Chu, M. K. Siddiqui, S. Manzoor, S. A. K. Kirmani, M. F. Hanif, and M. H. Muhammad, "On rational curve fitting between topological indices and entropy measures for graphite carbon nitride," *Polycyclic Aromatic Compounds*, vol. 5, pp. 1–18, 2022.
- [2] W. Gao and M. R. Farahani, "Degree-based indices computation for special chemical molecular structures using edge dividing method," *Applied Mathematics and Nonlinear Sciences*, vol. 1, no. 1, pp. 99–122, 2016.
- [3] E. Estrada, L. Torres, L. Rodríguez, and I. Gutman, "An atom-bond connectivity index. Modelling the enthalpy of formation of alkanes," *Indian Journal of Chemistry*, vol. 37A, pp. 849–855, 1998.
- [4] E. Estrada and N. Hatano, "Statistical-mechanical approach to subgraph centrality in complex networks," *Chemical Physics Letters*, vol. 439, no. 1-3, pp. 247–251, 2007.
- [5] E. Estrada, "Generalized walks-based centrality measures for complex biological networks," *Journal of Theoretical Biology*, vol. 263, no. 4, pp. 556–565, 2010.
- [6] W. Gao, M. K. Siddiqui, M. Naeem, and N. A. Rehman, "Topological characterization of carbon graphite and crystal cubic carbon structures," *Molecules*, vol. 22, no. 9, pp. 1496–1507, 2017.
- [7] M. Imran, M. K. Siddiqui, M. Naeem, and M. A. Iqbal, "On topological properties of symmetric chemical structures," *Symmetry*, vol. 10, no. 5, pp. 173–221, 2018.
- [8] M. Randić, "On characterization of molecular branching," *Journal of the American Chemical Society*, vol. 97, no. 23, pp. 6609–6615, 1975.
- [9] M. K. Siddiqui, M. Imran, and A. Ahmad, "On Zagreb indices, Zagreb polynomials of some nanostar dendrimers," *Applied Mathematics and Computation*, vol. 280, pp. 132–139, 2016.
- [10] X. Zhang, X. Wu, S. Akhter, M. K. Jamil, J. B. Liu, and M. R. Farahani, "Edge-version atom-bond connectivity and geometric arithmetic indices of generalized bridge molecular graphs," *Symmetry*, vol. 10, no. 12, pp. 751–786, 2018.
- [11] X. Zhang, H. M. Awais, M. Javaid, and M. K. Siddiqui, "Multiplicative Zagreb indices of molecular graphs," *Journal of Chemistry*, vol. 2019, Article ID 5294198, 19 pages, 2019.
- [12] X. Zhang, A. Rauf, M. Ishtiaq, M. K. Siddiqui, and M. H. Muhammad, "On degree based topological properties of two carbon nanotubes," *Polycyclic Aromatic Compounds*, vol. 42, no. 3, pp. 866–884, 2020.
- [13] X. Zhang, H. Jiang, J. B. Liu, and Z. Shao, "The cartesian product and join graphs on edge-version atom-bond connectivity and geometric arithmetic indices," *Molecules*, vol. 23, no. 7, pp. 1731–1817, 2018.
- [14] X. Zhang, M. Naeem, A. Q. Baig, and M. A. Zahid, "Study of hardness of superhard crystals by topological indices," *Journal of Chemistry*, vol. 2021, Article ID 9604106, 10 pages, 2021.
- [15] X. Zhang, M. K. Siddiqui, S. Javed, L. Sherin, F. Kausar, and M. H. Muhammad, "Physical analysis of heat for formation and entropy of Ceria Oxide using topological indices," *Combinatorial Chemistry & High Throughput Screening*, vol. 25, no. 3, pp. 441–450, 2022.
- [16] M. K. Siddiqui, M. Naeem, N. A. Rahman, and M. Imran, "Computing topological indices of certain networks," *Journal of Optoelectronics and Advanced Materials*, vol. 18, no. 9-10, pp. 884–892, 2016.
- [17] D. Vukicevic and B. Furtula, "Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges," *Journal of Mathematical Chemistry*, vol. 46, no. 4, pp. 1369–1376, 2009.
- [18] C. E. Shannon, "A mathematical theory of communication," *Bell System Technical Journal*, vol. 27, no. 3, pp. 379–423, 1948.



- [19] E. Trucco, "A note on the information content of graphs," *Bulletin of Mathematical Biophysics*, vol. 18, no. 2, pp. 129–135, 1956.
- [20] A. Mowshowitz, "Entropy and the complexity of graphs: I. An index of the relative complexity of a graph," *Bulletin of Mathematical Biophysics*, vol. 30, no. 1, pp. 175–204, 1968.
- [21] N. Rashevsky, "Life, information theory, and topology," *Bulletin of Mathematical Biophysics*, vol. 17, no. 3, pp. 229–235, 1955.
- [22] G. Karreman, "Topological information content and chemical reactions," *Bulletin of Mathematical Biophysics*, vol. 17, no. 4, pp. 279–285, 1955.
- [23] D. Bonchev, *Complexity in Chemistry, Introduction and Fundamentals*, vol. 2, pp. 1–100, Taylor & Francis, Boca Raton, FL, USA, 2003.
- [24] D. G. Bonchev, "Kolmogorov's information, shannon's entropy, and topological complexity of molecules," *Bulgarian Chemical Communications*, vol. 28, no. 3-4, pp. 567–582, 1995.
- [25] D. Bonchev and N. Trinajstić, "Information theory, distance matrix, and molecular branching," *The Journal of Chemical Physics*, vol. 67, no. 10, pp. 4517–4533, 1977.
- [26] D. Bonchev, O. V. Mekenyan, and N. Trinajstić, "Isomer discrimination by topological information approach," *Journal of Computational Chemistry*, vol. 2, no. 2, pp. 127–148, 1981.
- [27] G. Castellano and F. Torrens, "Information entropy-based classification of triterpenoids and steroids from Ganoderma," *Phytochemistry*, vol. 116, pp. 305–313, 2015.
- [28] M. Dehmer, K. Varmuza, S. Borgert, and F. Emmert-Streib, "On entropy-based molecular descriptors: statistical analysis of real and synthetic chemical structures," *Journal of Chemical Information and Modeling*, vol. 49, no. 7, pp. 1655–1663, 2009.
- [29] Z. Terenteva and N. I. Kobozev, "Possible relation between entropy of information-theory and thermodynamic entropy," *Zhurnal Fizicheskoi Khimii*, vol. 50, no. 4, pp. 877–881, 1976.
- [30] Y. A. Zhdanov, *Information Entropy in Organic Chemistry*, vol. 1, Rostov University, Rostov Oblast, Russia, 1979, in Russian.
- [31] Z. Chen, M. Dehmer, and Y. Shi, "A note on distance based graph entropies," *Entropy*, vol. 16, no. 10, pp. 5416–5427, 2014.
- [32] S. Cao, M. Dehmer, and Y. Shi, "Extremality of degree-based graph entropies," *Information Sciences*, vol. 278, pp. 22–33, 2014.
- [33] M. Dehmer, "Information processing in complex networks: graph entropy and information functionals," *Applied Mathematics and Computation*, vol. 201, no. 1-2, pp. 82–94, 2008.
- [34] M. Dehmer and A. Mowshowitz, "A history of graph entropy measures," *Information Sciences*, vol. 181, no. 1, pp. 57–78, 2011.
- [35] S. Manzoor, M. K. Siddiqui, and S. Ahmad, "On entropy measures of molecular graphs using topological indices," *Arabian Journal of Chemistry*, vol. 13, no. 8, pp. 6285–6298, 2020.
- [36] S. Cao and M. Dehmer, "Degree-based entropies of networks revisited," *Applied Mathematics and Computation*, vol. 261, pp. 141–147, 2015.
- [37] M. Dehmer, L. Sivakumar, and K. Varmuza, "Uniquely discriminating molecular structures using novel eigenvalue-based descriptors," *MATCH Communications in Mathematical*, vol. 67, pp. 147–172, 2012.
- [38] H. J. Morowitz, "Some order-disorder considerations in living systems," *Bulletin of Mathematical Biophysics*, vol. 17, no. 2, pp. 81–86, 1955.
- [39] N. Rashevsky, "Information theory in biology," *Bulletin of Mathematical Biophysics*, vol. 16, no. 2, pp. 183–185, 1954.
- [40] C. E. Shannon, "A mathematical theory of communication," *ACM SIGMOBILE - Mobile Computing and Communications Review*, vol. 5, no. 1, pp. 3–55, 2001.
- [41] R. V. Sol and S. I. Valverde, "Information theory of complex networks: on evolution and architectural constraints," *Complex Networks Lectures Notes in Physics*, vol. 650, pp. 189–207, 2004.
- [42] Y. J. Tan and J. Wu, "Network structure entropy and its application to scale-free networks," *Systems Engineering - Theory & Practice*, vol. 6, pp. 1–3, 2004.
- [43] S. Manzoor, M. K. Siddiqui, and S. Ahmad, "On physical analysis of degree-based entropy measures for metal-organic superlattices," *The European Physical Journal Plus*, vol. 136, no. 3, pp. 287–322, 2021.
- [44] S. Manzoor, M. K. Siddiqui, and S. Ahmad, "Degree-based entropy of molecular structure of hyaluronic acid-curcumin conjugates," *The European Physical Journal Plus*, vol. 136, no. 1, pp. 15–21, 2021.
- [45] M. A. Rashid, S. Ahmad, M. K. Siddiqui, S. Manzoor, and M. Dhlamini, "An Analysis of Eccentricity-Based Invariants for Biochemical Hypernetworks," *Complexity*, vol. 2021, Article ID 1974642, 14 pages, 2021.
- [46] S. Akhter and M. Imran, "On molecular topological properties of benzenoid structures," *Canadian Journal of Chemistry*, vol. 94, no. 8, pp. 687–698, 2016.
- [47] N. K. Raut, "Topological indices and topological polynomials of triangular benzenoid system," *International Journal of Mathematics Trends and Technology*, vol. 67, no. 6, pp. 90–96, 2021.
- [48] Z. Hussain, S. Rafique, M. Munir et al., "Irregularity molecular descriptors of hourglass, jagged-rectangle, and triangular benzenoid systems," *Processes*, vol. 7, no. 7, p. 413, 2019.
- [49] Y. C. Kwun, A. Ali, W. Nazeer, M. Ahmad Chaudhary, and S. M. Kang, "M-polynomials and degree-based topological indices of triangular, hourglass, and jagged-rectangle benzenoid systems," *Journal of Chemistry*, vol. 2018, Article ID 8213950, 8 pages, 2018.
- [50] V. R. Kulli, B. Chaluvaraju, and H. S. Boregowda, "Connectivity Bhatti indices for certain families of benzenoid systems," *Journal of Ultra Chemistry*, vol. 13, no. 04, pp. 81–87, 2017.
- [51] M. Ghorbani and M. Ghazi, "Computing some topological indices of Triangular Benzenoid," *Digest Journal of Nanomaterials and Biostructures*, vol. 5, no. 4, pp. 1107–1111, 2010.
- [52] A. Q. Baig, M. Imran, and H. Ali, "Computing Omega, Sadhana and PI polynomials of benzenoid carbon nanotubes," *Optoelectronics and advanced materials-rapid communications*, vol. 9, pp. 248–255, 2015.
- [53] K. G. Mirajkar and B. Pooja, "On Gourava indices of some chemical graphs," *International Journal of Applied Engineering Research*, vol. 14, no. 3, pp. 743–749, 2019.
- [54] A. Mehler, A. Lücking, and P. Weib, "A network model of interpersonal alignment in dialog," *Entropy*, vol. 12, no. 6, pp. 1440–1483, 2010.
- [55] A. Mowshowitz and M. Dehmer, "Entropy and the complexity of graphs revisited," *Entropy*, vol. 14, no. 3, pp. 559–570, 2012.
- [56] Y. Champion and N. Thurieau, "The sample size effect in metallic glass deformation," *Scientific Reports*, vol. 10, no. 1, Article ID 10801, 2020.
- [57] M. M. H. Graf, U. Bren, D. Haltrich, and C. Oostenbrink, "Molecular dynamics simulations give insight into d-glucose dioxidation at C2 and C3 by *Agaricus meleagris* pyranose

- dehydrogenase C-2 and C-3 by *Agaricus meleagris* pyranose dehydrogenase," *Journal of Computer-Aided Molecular Design*, vol. 27, no. 4, pp. 295–304, 2013.
- [58] M. V. Putz, A. M. Lacrama, and V. Ostafe, "Full analytic progress curves of enzymic reactions in vitro," *International Journal of Molecular Sciences*, vol. 7, no. 11, pp. 469–484, 2006.
- [59] M. Dehmer and M. Graber, "The discrimination power of molecular identification numbers revisited," *MATCH Communications in Mathematical*, vol. 69, pp. 785–794, 2013.
- [60] R. E. Ulanowicz, "Quantitative methods for ecological network analysis," *Computational Biology and Chemistry*, vol. 28, no. 5-6, pp. 321–339, 2004.