Edge Weight Based Entropy of Different Topologies of Carbon Nanotubes

XUEWU ZUO¹, MUHAMMAD FAISAL NADEEM², MUHAMMAD KAMRAN SIDDIQUI², AND MUHAMMAD AZEEM³

¹Department of General Education, Anhui Xinhua University, Hefei 230088, China
²Department of Mathematics, COMSATS University Islamabad, Lahore Campus, Lahore 54000, Pakistan
³Department of Aerospace Engineering, Faculty of Engineering, Universiti Putra Malaysia, Seri Kembangan 43400, Malaysia

Corresponding author: Muhammad Faisal Nadeem (mfaisalnadeem@ymail.com)

This work was supported in part by the Anhui Xinhua University School-Level Natural Science Foundation under Project 2019zr006, and in part by the Anhui Provincial Natural Science Foundation under Project KJ2020A0780.

ABSTRACT The measure or determination of uncertainty of a system is known as entropy. After the rich idea of entropy, it gains attraction and interest in graph theory, due to its applications in applied mathematical chemistry. First time the idea graph entropy was used in 1955, to know the structural information of chemical networks or graphs. In mathematical chemistry, structures are the build-up of atoms/vertices and bonds/edges. Carbon nanotubes are also very famous since they have been used for memory devices and tissue engineering. This productive chemical structure is studied in this paper by inserting a cap on one and both ends. We measure the entropy of these three topologies of carbon nanotube. Some comparative work is also given, along with the analytical study of entropy measures of armchair carbon nanotubes.

INDEX TERMS Edge weight based entropy, topological indices, armchair carbon nanotube, capped and semi-capped nanotubes.

I. INTRODUCTION

The entropy of a probability distribution known as a measure of the unpredictability of information content or a measure of the uncertainty of a system. This definition was based on the concept of entropy and put forward by [1]. After the statistics approach of this concept, it becomes famous for graphs and chemical structures as well. Numerous information of the structures or graphs and chemical topologies are known by this parameter. In 1955, the very first time this concept of entropy was used on graphs. Entropy or graph-based entropy is very applicable in sociology, ecology, biology, chemistry, and many other disciplines of engineering [2], [3]. The extrinsic and intrinsic measures are the classifications of graph-based entropy measures computed by different elements (of graphs) and associated with probability distributions. To explore networks as an information functionals, the degree-powers is a parameter from the network science and application from the mathematics of graph theory [4], [5]. The entropy of a physically sound for a network is proposed by [6].

The entropy formulas brought up by [1], with the idea that it is helpful to know about the network’s content and structural information [7]. In developing this concept, this idea was used on graphs and extensively helped to know more and explore living systems. For example, by making graphs of biological and chemical systems, it has been used to explore living systems. These biological and chemical applicable works can found in [8], [9]. For more information on the applications of entropy in structural chemistry, computer science, and even in the biological, we refer to see [10]. In network heterogeneity work, this entropy can be found in [7], [11].

The electron transfer property of nanotechnology and its low-cost implementations in various modern technology make the study of nano-structure a current trend. In 1990, nano-structures were discovered. In this decade, a lot of varieties of carbon nanotubes have been evolved. In 1991, carbon nanotube was discovered [12], after the discovery of nanotube in 1985 [13]. More developed and high-performance electrochemical sensors are expected in near future, because of the material property and electron transfer property of carbon nanotubes [14]. The electrochemical sensors, which are most assorted, are already made by carbon nanotubes [15]. Not only electrochemical, biochemical sensors are also in the
advance stage due to the blessings of carbon nanotubes [16]. These biological sensors are used to know the DNA and proteins from the body [17]. These biochemical sensors also determine pyrophosphate, lactate, glucose, cholesterol, alcohols, and numerous analytes [16]. Nanotubes delivers the development and optimized functionality of biosensors. Biological recognition in biosensors architecture is also worked by nanotube. Immobilization of respective molecule is also from carbon nanotubes [18].

Carbon nanotubes (CNTs) comprise of carbon atoms organized in a series of benzene rings rolled up into a tubular structure. A significant aspect that controls the properties arises from a disparity of tube structures that are produced by the rolling up of the graphene sheet into a tube. There are three different ways for rolling the sheet, which produce three types of nanotubes, armchair, zigzag, and chiral. Detail construction of carbon nanotubes can be found in [19], [20]. By looking at the structure of nanotubes in a topological perspective, there are three main shapes of carbon nanotubes. Both sides are closed, known as capped nanotube, and one-side closed, or one-side open is known as semi-capped carbon nanotube. All these and many other topological behaviors of armchair carbon nanotube, we refer to see [21].

There is a lot of study and applications of carbon nanotubes are available in the literature. Few of the research and applications of this structure are given below. The quantum size study of this novel topology are discussed in [22]. The detection of nanotubes is made by any means of technology, but the surface defects detection is studied in [23]. It was used in/as saturable absorbers, and photo-voltaic [24]. The blessings made by carbon nanotube for this film are discussed in [25], for fuel cell [26]. By palm oil precursor, CVD growth are made advancements in pharmacy like regenerative medicines [28], [29]. It is also used to store data, and for the functionality of memory device [30]. The data of carbon nanotubes in biomedical engineering, especially in tissue functioning, are available at [31], [32]. In anti-reflection, solar cell coating nanotubes are also used as a vital factor [33].

Followings are some useful definitions of topological indices, which are helpful to find our main results and creating formulas for edge weight based entropy.

**Definition 1:** In 1988, Bollobás and Erdős [34] and Amic et al. [35] proposed the general Randić index independently. The general Randić index of a graph $G$ for the values of $\alpha = \pm 1, \pm \frac{1}{2}$ is defined as:

$$R_\alpha(G) = \sum_{a \in E(G)} (\xi_a \times \xi_b)'^\alpha,$$  \hspace{1cm} (1)

where $\xi_a$ and $\xi_b$ denote the degree of vertex $a$ and $b$.

**Definition 2:** Furtula and Gutman [36], presented forgotten topological index as:

$$F(G) = \sum_{a \in E(G)} \xi_a^2 + \xi_b^2.$$  \hspace{1cm} (2)

**Definition 3:** Balaban index for a graph $G$ of order $p$, and size $q$ is defined in [14] as follows:

$$J(G) = \frac{q}{q - p + 2} \sum_{a \in E(G)} \frac{1}{\sqrt{\xi_a \times \xi_b}}. \hspace{1cm} (3)$$

**Definition 4:** Estrada et al. [37] introduced the atom bond connectivity index as:

$$ABC(G) = \sum_{a \in E(G)} \sqrt{\xi_a + \xi_b - 2 \xi_a \times \xi_b}. \hspace{1cm} (4)$$

**Definition 5:** The geometric arithmetic index of a graph, is introduced by Vukičević and Furtula [38] as:

$$GA(G) = \sum_{a \in E(G)} 2 \sqrt{\xi_a \times \xi_b}. \hspace{1cm} (5)$$

**Definition 6:** In 2014 entropy for an edge weighted graph $G$ is introduced [39]:

$$\Omega_{\psi}(G) = -\sum_{a \in E(G)} \frac{\psi(a',b')}{\sum_{a \in E(G)} \psi(ab)} \times \log \left[ \frac{\psi(a',b')}{\sum_{a \in E(G)} \psi(ab)} \right]. \hspace{1cm} (6)$$

where $\psi(ab)$ is a weight for an edge $ab$.

By letting the edge of a weight equal to the main part of topological index, [40], [41] introduced the following entropies for an edge weighted based graph. Followings are some important formulae for this research work and all these are based on the Equation (6).

**Definition 7:** The Randić entropy is defined as following [40]:

$$\Omega_{R_\alpha}(G) = -\frac{1}{R_\alpha(G)} \log \left[ \prod_{a \in E(G)} (\xi_a \xi_b)^\alpha \right] + \log \left( R_\alpha(G) \right). \hspace{1cm} (7)$$

**Definition 8:** The forgotten and Balaban entropies are defined as following [40]:

$$\Omega_F(G) = -\frac{1}{F(G)} \log \left[ \prod_{a \in E(G)} ^{2} \left[ (\xi_a^2 + \xi_b^2)^2 \right] ^{\xi_a^2 + \xi_b^2} \right] + \log (F(G)). \hspace{1cm} (8)$$
TABLE 1. Vertex partition of ACNT ($\beta, \gamma$).

| $\xi_i$ | Frequency | Set of Vertices |
|--------|-----------|-----------------|
| 2      | $\beta$   | $V_1$           |
| 3      | $\beta(\gamma - 1)$ | $V_2$           |
| $p_1$  | $\beta \gamma$ | $p_2$           |

$\Omega_J (G) = -\frac{1}{J (G)} \log \prod_{ab \in E(G)} \left[ \frac{1}{q - p + 2} \times \frac{1}{\sqrt{\xi_a \xi_b}} \right]^{\frac{q}{\xi_a \xi_b}} + \log (J (G)).$  

(9)

Definition 9: The atom bond connectivity and geometric arithmetic entropies are defined as following [40];

$\Omega_{ABC} (G) = -\frac{1}{ABC (G)} \log \prod_{ab \in E(G)} \left[ \frac{1}{\xi_a + \xi_b - 2} \frac{1}{\xi_a \xi_b} \right]^{\frac{1}{\xi_a + \xi_b}} + \log (ABC (G)).$  

(10)

$\Omega_{GA} (G) = -\frac{1}{GA (G)} \log \prod_{ab \in E(G)} \left[ \frac{2}{\xi_a + \xi_b} \frac{2}{\xi_a \xi_b} \right]^{\frac{1}{\xi_a + \xi_b}} + \log (GA (G)).$  

(11)

For other kinds of entropy we suggested to see [42]–[44].

This article’s main contribution is to expand the number of applications and investigate various edge weight-based entropies of armchair carbon nanotubes, ACNT ($\beta, \gamma$), armchair carbon semi-capped nanotube, ACSCNT ($\beta, \gamma$), and armchair carbon capped nanotube, ACCNT ($\beta, \gamma$). Moreover, we analyze these entropies and compare all three described structures by taking examples which are shown in Table 9 to Table 12 in further next section, and depicted the results in Figure 5 to Figure 8. For more detail of this topology of armchair carbon nanotube and its variant are available in [45].

II. RESULTS FOR THE UNCAPPED CARBON NANOTUBE ACNT ($\beta, \gamma$)

Armchair carbon nanotube ACNT ($\beta, \gamma$), with two types of vertices according to degree defined in Table 1 and edge types defined in Table 2, and $p_1$, $q_1$, are the order and size of ACNT ($\beta, \gamma$), respectively.

Authors of [46], computed the degree based topological indices of armchair carbon nanotube ACNT ($\beta, \gamma$). We defined the main results in Table 3, we will used these results in our main proof of theorems.

Moreover, the 3D view of armchair carbon nanotube ACNT ($\beta, \gamma$) is shown in Figure 1.

Theorem 10: If $G$ be a graph of ACNT ($\beta, \gamma$) and $\Omega_{R_\alpha}$ is the edge weight based Randić entropy, then $\Omega_{R_\alpha} (G)$ is

$\Omega_{R_\alpha} (G) = \log \left[ \frac{4^{\alpha} \beta \times 36^{\alpha} \beta \times 3^{\alpha} \gamma (3 \beta \gamma - 8 \beta)}{\beta (4\alpha + 2 \times 6^\alpha - 4 \times 9^\alpha) + \frac{3}{2} \times 9^\alpha \beta \gamma} \right] \times \log \left[ \beta (4^\alpha + 2 \times 6^\alpha - 4 \times 9^\alpha) + \frac{3}{2} \times 9^\alpha \beta \gamma \right].$

(12)

Proof: As we know that Randić index is defined in the Table 3 by using the edge type of ACNT ($\beta, \gamma$) which is defined in the Table 2. Now using Randić index in the Equation (7), which gives

$\Omega_{R_\alpha} (G) = -\frac{1}{\beta (4^\alpha + 2 \times 6^\alpha - 4 \times 9^\alpha) + \frac{3}{2} \times 9^\alpha \beta \gamma} \times \log \left[ (2 \times 2)^{2\beta \times 2^\alpha} \times (2 \times 3)^{2\beta \times (2 \times 3)^\alpha} \times (3 \times 3)^{\alpha (3^{\beta \gamma - 8 \beta}) (3 \times 3)^\alpha} \right].$
+ \log \left[ \beta \left( 4^a + 2 \times 6^a - 4 \times 9^a \right) + \frac{3}{2} \times 9^a \beta \gamma \right],

= -\frac{1}{27 \beta \gamma - 38 \beta} \log \left[ 16777216^\beta \times 13^{26^\beta} \times 18^{9(3^\beta \gamma - 8^\beta)} \right]

\Omega_F (\mathbb{G}) = -log \left[ \frac{[16777216^\beta \times 13^{26^\beta} \times 18^{9(3^\beta \gamma - 8^\beta)}]}{27 \beta \gamma - 38 \beta} \right] + \log (27 \beta \gamma - 38 \beta).

(13)

\textbf{Theorem 11:} If \( \mathbb{G} \) be a graph of ACNT \((\beta, \gamma) \) and \( \Omega_F \) is the edge weight based forgotten entropy, then \( \Omega_F (\mathbb{G}) \) is

\Omega_F (\mathbb{G}) = -\log \left[ \frac{[16777216^\beta \times 13^{26^\beta} \times 18^{9(3^\beta \gamma - 8^\beta)}]}{27 \beta \gamma - 38 \beta} \right] + \log (27 \beta \gamma - 38 \beta).

(14)

\textbf{Proof:} As we know that forgotten index is defined in the Table 3 by using the edge type of ACNT \((\beta, \gamma) \) which is defined in the Table 2. Now using forgotten index in the Equation (8), which gives

\Omega_F (\mathbb{G}) = -\log \left[ \frac{1}{27 \beta \gamma - 38 \beta} \log \left[ \left( 2^2 + 2^2 \right)^{2(2^2 + 2^2)} \times \left( 2^2 + 3^2 \right)^{2(2^2 + 3^2)} \times \left( 3^2 + 2^2 \right)^{3(3^2 + 2^2)} \right] + \log (27 \beta \gamma - 38 \beta), \right]

\Omega_F (\mathbb{G}) = -\log \left[ \frac{1}{27 \beta \gamma - 38 \beta} \log \left[ \left( 2^2 + 2^2 \right)^{2(2^2 + 2^2)} \times \left( 2^2 + 3^2 \right)^{2(2^2 + 3^2)} \times \left( 3^2 + 2^2 \right)^{3(3^2 + 2^2)} \right] + \log (27 \beta \gamma - 38 \beta), \right]

\Omega_F (\mathbb{G}) = -\log \left[ \frac{1}{27 \beta \gamma - 38 \beta} \log \left[ \left( 2^2 + 2^2 \right)^{2(2^2 + 2^2)} \times \left( 2^2 + 3^2 \right)^{2(2^2 + 3^2)} \times \left( 3^2 + 2^2 \right)^{3(3^2 + 2^2)} \right] + \log (27 \beta \gamma - 38 \beta), \right]

(15)

\textbf{Theorem 12:} If \( \mathbb{G} \) be a graph of ACNT \((\beta, \gamma) \) and \( \Omega_J \) is the edge weight based Balaban entropy, then \( \Omega_J (\mathbb{G}) \) is

\Omega_J (\mathbb{G}) = \log \left[ \frac{[16777216^\beta \times 13^{26^\beta} \times 18^{9(3^\beta \gamma - 8^\beta)}]}{27 \beta \gamma - 38 \beta} \right] + \log (27 \beta \gamma - 38 \beta).

(16)

\textbf{Proof:} As we know that Balaban index is defined in the Table 3 by using the edge type of ACNT \((\beta, \gamma) \) which is defined in the Table 2. Now using Balaban index in the Equation (9), which gives

\Omega_J (\mathbb{G}) = \log \left[ \frac{[16777216^\beta \times 13^{26^\beta} \times 18^{9(3^\beta \gamma - 8^\beta)}]}{27 \beta \gamma - 38 \beta} \right] + \log (27 \beta \gamma - 38 \beta).

(17)

\textbf{Theorem 13:} If \( \mathbb{G} \) be a graph of ACNT \((\beta, \gamma) \) and \( \Omega_{ABC} \) is the edge weight based atom-bond connectivity entropy, then \( \Omega_{ABC} (\mathbb{G}) \) is

\Omega_{ABC} (\mathbb{G}) = -\log \left[ \frac{\left( \beta, \gamma \right)^{\beta \gamma}}{\left( \beta, \gamma \right)^{\beta \gamma}} \times \left( \gamma \right)^{\beta \gamma} \times \left( \frac{2}{3} \right)^{\beta \gamma} \right]

\Omega_{ABC} (\mathbb{G}) = -\log \left[ \frac{\left( \beta, \gamma \right)^{\beta \gamma}}{\left( \beta, \gamma \right)^{\beta \gamma}} \times \left( \gamma \right)^{\beta \gamma} \times \left( \frac{2}{3} \right)^{\beta \gamma} \right]

(18)

\textbf{Proof:} As we know that atom bond connectivity index is defined in the Table 3 by using the edge type of ACNT \((\beta, \gamma) \) which is defined in the Table 2. Now using atom bond connectivity index in the Equation (10), which gives

\Omega_{ABC} (\mathbb{G}) = -\log \left[ \frac{\left( \beta, \gamma \right)^{\beta \gamma}}{\left( \beta, \gamma \right)^{\beta \gamma}} \times \left( \gamma \right)^{\beta \gamma} \times \left( \frac{2}{3} \right)^{\beta \gamma} \right]

(19)

\textbf{Theorem 14:} If \( \mathbb{G} \) be a graph of ACNT \((\beta, \gamma) \) and \( \Omega_{GA} \) is the edge weight based geometric arithmetic entropy, then

\Omega_{GA} (\mathbb{G}) = -\log \left[ \frac{\left( \beta, \gamma \right)^{\beta \gamma}}{\left( \beta, \gamma \right)^{\beta \gamma}} \times \left( \gamma \right)^{\beta \gamma} \times \left( \frac{2}{3} \right)^{\beta \gamma} \right]

(20)
TABLE 4. Vertex partition of ACSCNT (β, γ).

| ξ_4 | Frequency | Set of Vertices |
|-----|-----------|-----------------|
| 2   | β         | V_1             |
| 3   | β(γ - 1)  | V_2             |

TABLE 5. Edge partition of ACSCNT (β, γ).

| (ξ_5, ξ_4) | Frequency | Set of Edges |
|------------|-----------|--------------|
| (2, 2)     | β         | E_1          |
| (2, 3)     | β         | E_2          |
| (3, 3)     | β(γ - 2)  | E_3          |
| p_2        | β(γ - 2)  |               |

Ω_{GA} (S) is

\[ Ω_{GA} (S) = - \frac{1}{4\sqrt{6} - 15\beta + 3\beta\gamma} + \log \left( \frac{4\sqrt{6} - 15\beta + 3\beta\gamma}{2} \right). \]

**Proof:** As we know that geometric arithmetic index is defined in the Table 3 by using the edge type of ACNT (β, γ) which is defined in the Table 2. Now using geometric arithmetic index in the Equation (11), which gives

\[ Ω_{GA} (S) = - \frac{1}{4\sqrt{6} - 15\beta + 3\beta\gamma} \log \left( \frac{4\sqrt{6} - 15\beta + 3\beta\gamma}{2} \right). \]

III. RESULTS FOR THE SEMI-CAPPED CARBON NANOTUBE ACSCNT (β, γ)

Armchair carbon semi-capped nanotube ACSCNT (β, γ), with two types of vertices according to degree defined in Table 4 and edge types defined in Table 5, and p_2, q_2, are the order and size of ACSCNT (β, γ), respectively.

Authors of [47], computed the degree based topological indices of armchair semi-capped nanotube ACSCNT (β, γ).

We defined the main results in Table 6, we will used these results in our main proof of theorems.

Moreover, the 3D view of armchair semi-capped nanotube ACSCNT (β, γ) is shown in Figure 2.

**Theorem 15:** If \( S \) be a graph of ACSCNT (β, γ) and \( Ω_{R_u} \) is the edge weight based Randić entropy, then \( Ω_{R_u} (S) \) is

\[ Ω_{R_u} (S) = - \frac{1}{\beta \left( \frac{4\alpha^2}{2} + 6\alpha^2 - 2 \times 9\alpha + \frac{3}{2} \times 9\alpha \beta \gamma \right)} + \log \left( \beta \left( \frac{4\alpha^2}{2} + 6\alpha^2 - 2 \times 9\alpha + \frac{3}{2} \times 9\alpha \beta \gamma \right) \right). \]

**Proof:** As we know that Randić index is defined in the Table 6 by using the edge type of ACSCNT (β, γ), which is defined in the Table 5. Now using Randić index in the Equation (7), which gives

\[ Ω_{R_u} (S) = - \frac{1}{\beta \left( \frac{4\alpha^2}{2} + 6\alpha^2 - 2 \times 9\alpha + \frac{3}{2} \times 9\alpha \beta \gamma \right)} \times \log \left( \beta \left( \frac{4\alpha^2}{2} + 6\alpha^2 - 2 \times 9\alpha + \frac{3}{2} \times 9\alpha \beta \gamma \right) \right), \]

\[ \ast \]

FIGURE 2. 3D view of armchair semi-capped nanotube ACSCNT (β, γ).
Theorem 16: If $\mathcal{G}$ be a graph of ACSCNT $(\beta, \gamma)$ and $\Omega_F$ is the edge weight based forgotten entropy, then $\Omega_F(\mathcal{G})$ is

$$\Omega_F(\mathcal{G}) = -\frac{1}{27\beta\gamma - 10\beta} \log \left[ \frac{4096^6 \times 1313 \times 18^{9(3\beta\gamma - 4\beta)}}{27\beta\gamma - 10\beta + \log (27\beta\gamma - 10\beta)} \right].$$

Proof: As we know that forgotten index is defined in the Table 6 by using the edge type of ACSCNT $(\beta, \gamma)$ which is defined in the Table 5. Now using forgotten index in the Equation (8), which gives

$$\Omega_F(\mathcal{G}) = -\frac{1}{27\beta\gamma - 10\beta} \log \left[ \frac{4096^6 \times 1313 \times 18^{9(3\beta\gamma - 4\beta)}}{27\beta\gamma - 10\beta + \log (27\beta\gamma - 10\beta)} \right].$$

(24)

Theorem 17: If $\mathcal{G}$ be a graph of ACSCNT $(\beta, \gamma)$ and $\Omega_J$ is the edge weight based Balaban entropy, then $\Omega_J(\mathcal{G})$ is

$$\Omega_J(\mathcal{G}) = -\frac{1}{j} \log \left[ \frac{0.840897^6 \times 0.693682^6}{0.832683^{3(3\beta\gamma - 4\beta)}} \right] + \log (j).$$

(26)

with $j = \beta^3(3\gamma - 2)(3 + 2\sqrt{6} + 6\gamma) - 48 + (12\gamma - 24\beta)^2$. 

Proof: As we know that Balaban index is defined in the Table 6 by using the edge type of ACSCNT $(\beta, \gamma)$ which is defined in the Table 5. Now using Balaban index in the Equation (9), which gives

$$\Omega_J(\mathcal{G}) = -\frac{1}{j} \log \left[ \frac{\beta}{\sqrt[3]{2}} \times \frac{1}{\sqrt{2} \times 3} \times \left( \frac{1}{\sqrt{2} \times 3} \right)^{3\beta\gamma - 4\beta} \right] + \log (|j|) = -\frac{1}{j} \log \left[ \frac{0.840897^6 \times 0.693682^6}{0.832683^{3(3\beta\gamma - 4\beta)}} \right] + \log (j).$$

(27)

where $j = \beta^3(3\gamma - 2)(3 + 2\sqrt{6} + 6\gamma) - 48 + (12\gamma - 24\beta)^2$.

Theorem 18: If $\mathcal{G}$ be a graph of ACSCNT $(\beta, \gamma)$ and $\Omega_{ABC}$ is the edge weight based atom-bond connectivity entropy, then $\Omega_{ABC}(\mathcal{G})$ is

$$\Omega_{ABC}(\mathcal{G}) = -\frac{1}{(3\beta\gamma/4 + \beta\gamma - \beta)} \log \left[ \left( \frac{2 + 3 - 2}{2 \times 3} \right)^{3\beta\gamma - 4\beta/2} \times \left( \frac{3 + 3 - 2}{3 \times 3} \right)^{3\beta\gamma - 4\beta/2} \times \left( \frac{2}{3} \right)^{3\beta\gamma - 4\beta/3} \right] + \log \left( (3\sqrt{2}\beta/4 + \beta\gamma - \beta) \right).$$

(28)

Proof: As we know that atom bond connectivity index is defined in the Table 6 by using the edge type of ACSCNT $(\beta, \gamma)$ which is defined in the Table 5. Now using atom bond connectivity index in the Equation (10), which gives

$$\Omega_{ABC}(\mathcal{G}) = -\frac{1}{(3\sqrt{2}\beta/4 + \beta\gamma - \beta)} \log \left[ \left( \frac{2 + 3 - 2}{2 \times 3} \right)^{3\beta\gamma - 4\beta/2} \times \left( \frac{3 + 3 - 2}{3 \times 3} \right)^{3\beta\gamma - 4\beta/2} \times \left( \frac{2}{3} \right)^{3\beta\gamma - 4\beta/3} \right] + \log \left( (3\sqrt{2}\beta/4 + \beta\gamma - \beta) \right).$$

(29)

Theorem 19: If $\mathcal{G}$ be a graph of ACSCNT $(\beta, \gamma)$ and $\Omega_{GA}$ is the edge weight based geometric arithmetic entropy, then $\Omega_{GA}(\mathcal{G})$ is

$$\Omega_{GA}(\mathcal{G}) = -\frac{1}{\beta + 2\beta\sqrt{6} + 3\beta\gamma} \log \left[ \frac{\beta}{\sqrt{3}} \times \frac{\beta}{\sqrt{2}} \times \left( \frac{\beta}{\sqrt{2}} \right)^{\beta\gamma - \beta} \right] + \log \left( -\beta + 2\beta\sqrt{6} + 3\beta\gamma \right).$$

(30)

Proof: As we know that geometric arithmetic index is defined in the Table 6 by using the edge type of ACSCNT $(\beta, \gamma)$ which is defined in the Table 5. Now using geometric arithmetic index in the Equation (11), which
TABLE 7. Vertex and edge partition of ACCNT \((\beta, \gamma)\).

| \(\xi_i\) | Frequency | Order |
|-----------|-----------|-------|
| 3 \(\beta\gamma\) | \(|V_1| = p_3\) |
| \((\xi_0, \xi_3)\) | Frequency | Size |
| \((3, 3)\) | \(3\frac{\beta^2}{2}\) | \(|E_1| = q_3\) |
| \((\xi_1, \xi_3)\) | Frequency | Set of Edges |

TABLE 8. Topological indices of ACCNT \((\beta, \gamma)\) [47].

| \(I\) | \(I(\text{ACCNT} (\beta, \gamma))\) |
| \(R_a\) | \(\frac{4\beta^2\gamma^\alpha}{9}\) |
| \(F\) | \(2\beta\gamma\) |
| \(J\) | \(\beta^\alpha\gamma(3+3\alpha)(-2\sqrt{6}\beta\gamma+6\beta)\) |
| \(ABC\) | \(\beta\gamma\) |
| \(GA\) | \(\frac{3\beta^2\gamma}{2}\) |

gives
\[
\Omega_{GA} (\mathcal{E}) = -\frac{1}{-\beta + \frac{2\beta\sqrt{6}}{5} + \frac{3\beta\gamma}{2}} \times \log \left[ \frac{\beta^\alpha\gamma}{1 + \frac{3\beta\gamma}{2}} \right] + \log \left( -\beta + \frac{2\beta\sqrt{6}}{5} + \frac{3\beta\gamma}{2} \right)
\]
\[
= -\frac{1}{-\beta + \frac{2\beta\sqrt{6}}{5} + \frac{3\beta\gamma}{2}} + \log \left( -\beta + \frac{2\beta\sqrt{6}}{5} + \frac{3\beta\gamma}{2} \right).
\]
\[\text{(31)}\]

IV. RESULTS FOR THE CAPPED CARBON NANOTUBE

**ACCNT \((\beta, \gamma)\)**

Armchair carbon capped nanotube ACCNT \((\beta, \gamma)\), with single type of vertices according to degree and edge types defined in Table 7, and \(p_3, q_3\), are the order and size of ACCNT \((\beta, \gamma)\), respectively.

Authors of [47], computed the degree based topological indices of armchair capped nanotube ACCNT \((\beta, \gamma)\). We defined the main results in Table 8, we will used these results in our main proof of theorems.

Moreover, the 3D view of armchair capped nanotube ACCNT \((\beta, \gamma)\) is shown in Figure 3. While 2D view of this structure is shown in Figure 4.

**Theorem 20:** If \(\mathcal{G}\) be a graph of ACCNT \((\beta, \gamma)\) and \(\Omega_{R_a}\) is the edge weight based Randić entropy, then \(\Omega_{R_a} (\mathcal{E})\) is

\[
\Omega_{R_a} (\mathcal{E}) = -\frac{1}{\gamma^\alpha(3\times3)} \times \log \left( -\frac{2\beta\gamma^\alpha}{9} \right) + \log \left( \frac{9^\alpha \gamma}{2} \right). \tag{32}
\]

**Theorem 21:** If \(\mathcal{G}\) be a graph of ACCNT \((\beta, \gamma)\) and \(\Omega_F\) is the edge weight based forgotten entropy, then \(\Omega_F (\mathcal{E})\) is

\[
\Omega_F (\mathcal{E}) = -\frac{1}{27\beta\gamma} \times \log \left( \frac{9^\alpha \gamma}{2} \right) + \log \left( \frac{27\beta\gamma}{2} \right). \tag{33}
\]

**Proof:** As we know that forgotten index is defined in the Table 8 by using the edge type of ACCNT \((\beta, \gamma)\) which is defined in the Table 7. Now using forgotten index in the Equation (8), which gives

\[
\Omega_{R_a} (\mathcal{E}) = -\frac{1}{\gamma^\alpha(3\times3)} \times \log \left( -\frac{2\beta\gamma^\alpha}{9} \right) + \log \left( \frac{9^\alpha \gamma}{2} \right).
\]

**Proof:** As we know that forgotten index is defined in the Table 8 by using the edge type of ACCNT \((\beta, \gamma)\) which is defined in the Table 7. Now using forgotten index in the Equation (8), which gives

\[
\Omega_F (\mathcal{E}) = -\frac{1}{27\beta\gamma} \times \log \left( \frac{9^\alpha \gamma}{2} \right) + \log \left( \frac{27\beta\gamma}{2} \right).
\]

\[\text{(33)}\]
Theorem 22: If $G$ be a graph of $ACCNT(\beta, \gamma)$ and $\Omega_J$ is the edge weight based Balaban entropy, then $\Omega_J(G)$ is

$$\Omega_J(G) = -\frac{2 \log (0.832683^{3\beta\gamma})}{j\beta\gamma} + \log \left(\frac{j\beta\gamma}{2}\right),$$  

where $j = \left(\frac{3\beta\gamma - 2\beta}{\beta\gamma - 2\beta + 4}\right)$.

Proof: As we know that Balaban index is defined in the Table 8 by using the edge type of $ACCNT(\beta, \gamma)$ which is defined in the Table 7. Now using Balaban index in the Equation (9), which gives

$$\Omega_J(G) = -\frac{2 \log (0.832683^{3\beta\gamma})}{j\beta\gamma} + \log \left(\frac{j\beta\gamma}{2}\right).$$

where $j = \left(\frac{3\beta\gamma - 2\beta}{\beta\gamma - 2\beta + 4}\right)$. □

Theorem 23: If $G$ be a graph of $ACCNT(\beta, \gamma)$ and $\Omega_{ABC}$ is the edge weight based atom-bond connectivity entropy, then $\Omega_{ABC}(G)$ is

$$\Omega_{ABC}(G) = -\frac{1}{\beta\gamma} \log \left(\frac{3j^{\beta\gamma}}{\beta\gamma}\right) + \log (\beta\gamma).$$

Proof: As we know that atom bond connectivity index is defined in the Table 8 by using the edge type of $ACCNT(\beta, \gamma)$ which is defined in the Table 7. Now using atom bond connectivity index in the Equation (10), which gives

$$\Omega_{ABC}(G) = -\frac{1}{\beta\gamma} \log \left(\frac{3j^{\beta\gamma}}{\beta\gamma}\right) + \log (\beta\gamma).$$
Theorem 24: If $\mathcal{G}$ be a graph of $\text{ACCN}(\beta, \gamma)$ and $\Omega_{GA}$ is the edge weight based geometric arithmetic entropy, then $\Omega_{GA}(\mathcal{G})$ is

$$\Omega_{GA}(\mathcal{G}) = -\frac{1}{3\beta\gamma} \log(1) + \log \left(\frac{3\beta\gamma}{2}\right),$$

$$= \log \left(\frac{3\beta\gamma}{2}\right).$$

Proof: As we know that geometric arithmetic index is defined in the Table 8 by using the edge type of $\text{ACCN}(\beta, \gamma)$ which is defined in the Table 7. Now using geometric arithmetic index in the Equation (11), which gives

$$\Omega_{GA}(\mathcal{G}) = -\frac{1}{3\beta\gamma} \log \left[1 + \frac{3\beta\gamma}{2}\right],$$

$$= -\frac{1}{3\beta\gamma} \log (1) + \log \left(\frac{3\beta\gamma}{2}\right),$$

$$= \log \left(\frac{3\beta\gamma}{2}\right).$$

\(\square\)

V. CONCLUSION AND DISCUSSION

In this study we measure edge weight based entropy for three type of armchair carbon nanotubes, namely armchair carbon nanotube, armchair carbon semi-capped nanotube and armchair carbon capped nanotube which are symbolize by $\text{ACNT}(\beta, \gamma)$, $\text{ACSCNT}(\beta, \gamma)$ and $\text{ACCNT}(\beta, \gamma)$, respectively. The edge weight based entropy are measure in this draft namely are Randić, forgotten, atom bond connectivity and geometric arithmetic. The final results are shown in the Equations (12), (14), (18), and (20), respectively. After the analytical results we did some comparative study for the different running parameters ($m, n$) of each graph. The numerical results are made though MATLAB® are shown in the Tables 9 to 12 and associated plot are made by Maple™, are shown in the Figures 5 to 8. Moreover, all the results are verified by authentic mathematical tool of Mathematica®.

ACKNOWLEDGMENT

(Xuewu Zuo, Muhammad Faisal Nadeem, Muhammad Kamran Siddiqui, and Muhammad Azeem contributed equally to this work.)

COMPLIANCE WITH ETHICAL STANDARDS

CONFLICT OF INTEREST

The authors of this article declare that there is no conflict of interest

REFERENCES

[1] C. E. Shannon, “A mathematical theory of communication,” Bell Syst. Tech. J., vol. 27, no. 3, pp. 379–423, Jul./Oct. 1948.
[2] M. Dehmer and M. Graber, “The discrimination power of molecular identification numbers revisited,” MATCH Community Math. Comput. Chem., vol. 69, no. 3, pp. 785–794, 2013.
[3] R. E. Ulanowicz, “Quantitative methods for ecological network analysis,” Comput. Biol. Chem., vol. 28, nos. 5–6, pp. 521–539, Dec. 2004.
[4] S. Cao, M. Dehmer, and Y. Shi, “Extremality of degree-based graph entropies,” Inf. Sci., vol. 278, pp. 22–33, Sep. 2014.
[5] S. Cao and M. Dehmer, “Degree-based entropies of networks revisited,” Appl. Math. Comput., vol. 261, pp. 141–147, Jun. 2015.
MUHAMMAD FAISAL NADDEEM received the Ph.D. degree in mathematics from the Abdus Salam School of Mathematical Sciences, Government College University Lahore, in 2014. His current research interests include graph theory and its applications. He is currently an Assistant Professor with COMSATS University Islamabad, Lahore Campus. He is a Reviewer of Mathematical Reviews and Zentralblatt Math.

MUHAMMAD KAMRAN SIDDIQUI received the Ph.D. degree in discrete mathematics specialization in graph theory from the Abdus Salam School of Mathematical Sciences, Government College University Lahore, Pakistan, in 2014. Since 2014, he has been an Assistant Professor with the Department of Mathematics, COMSATS University Islamabad, Lahore Campus, Pakistan. Since 2018, he has been a Postdoctoral Fellow with the Department of Mathematical Sciences, United Arab Emirates University, United Arab Emirates. His current research interests include discrete mathematics, graph theory and its applications, chemical graph theory, and combinatorics.

MUHAMMAD AZEEM received the B.S. degree from COMSATS University Islamabad, Lahore Campus, in 2018, where he is currently pursuing the M.S. degree. He is currently working as a Research Assistant with the Department of Aerospace Engineering, Faculty of Engineering, UPM, Malaysia.

* * *