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 formulation was the foundation as described in [1] as a proposal for the idea of entropy. Following the statistical methodology of this concept, it became well-known for graphs and chemical structures. This parameter imparts a lot of information about structures, graphs, and chemical topologies. It was in 1955 that this term was used for graphs. Entropy, also known as graph-based entropy, has applications in chemistry, biology, ecology, sociology and a variety of other technical fields [2], [3]. Intrinsic and extrinsic measures are two types of entropy measurements based on graphs, that are computed by distinct elements (of graphs) and linked to probability distributions. From the network theory, there is a parameter known as degree-powers which is an application from graph theory mathematics to investigate networks as information functionals (reference [4], [5]). The authors in [6], put forward the idea of entropy for wide variety of networks. The entropy formulae put forward by [1], with the notion that knowing about the contents of a network and also for the structural information [7]. This notion was developed by using graphs, which greatly aided in learning more about and exploring biological systems. It has been used to investigate
alcohols, and a variety of other analytes, according to [16]. Biosensors can be developed and brought into function better than nanotubes. Nanotubes also help in biological identification in biosensor design. Carbon nanotubes are also utilized to immobilize the relevant chemical, according to [18].

There are three major forms of carbon nanotubes while looking at their structure from a topological perspective. Capped carbon nanotubes have both sides closed, while semi-capped carbon nanotubes have one side closed or open. See [19] for all these and many more topological characteristics of armchair carbon nanotubes.

In literature, there are several studies and applications of carbon nanotubes. Following are some of the studies and applications of this structure. In [20], the quantum scale analysis of this new topology is described. Many technologies are used to identify nanotubes, but the detection of surface defects is investigated in [21]. It was utilized in photovoltaic [22] and saturable absorbers. In [23], the benefits of carbon nanotubes for this film are described, whereas in [24], the benefits of carbon nanotubes for fuel cells are highlighted. CVD development by palm oil pioneer is described in [25]. Nanotubes have also been used to enhance pharmaceutical applications, such as regenerative medications [26], [27]. It’s also utilized to record dates and for the memory device [28] functionality. See [29], [30] for data on carbon nanotubes in biomedical engineering, particularly in tissue function. Solar cell coating nanotubes are also employed as a key element in anti-reflection, according to [31]. The definitions of topological indices that we used to discover our major conclusions and create formulæ for edge weight based entropy are listed below.

**Definition 1:** The first and second Zagreb index is introduced in 1972 by Gutman [32], [33] as:

\[
M_1(G) = \sum_{ab \in E(G)} (\xi_a + \xi_b) \quad (1)
\]

\[
M_2(G) = \sum_{ab \in E(G)} (\xi_a \times \xi_b) \quad (2)
\]

**Definition 2:** Shirdel et al. [34] introduced Hyper-Zagreb index as:

\[
HM(G) = \sum_{ab \in E(G)} [\xi_a + \xi_b]^2 \quad (3)
\]

**Definition 3:** Furtula et al. [35] defined Augmented Zagreb index as:

\[
AZI(G) = \sum_{ab \in E(G)} \left( \frac{\xi_a \times \xi_b}{\xi_a + \xi_b - 2} \right)^3 \quad (4)
\]

**Definition 4:** Ranjini et al. [36], defined, the redefined first, second and third Zagreb indices for a graph G as:

\[
ReZG_1(G) = \sum_{ab \in E(G)} \frac{\xi_a + \xi_b}{\xi_a \times \xi_b} \quad (5)
\]

\[
ReZG_2(G) = \sum_{ab \in E(G)} \frac{\xi_a \times \xi_b}{\xi_a + \xi_b} \quad (6)
\]

\[
ReZG_3(G) = \sum_{ab \in E(G)} \frac{\xi_a \times \xi_b (\xi_a + \xi_b)}{\xi_a \times \xi_b} \quad (7)
\]

**Definition 5:** In 2014, the entropy for an edge-weighted graph was introduced [37]. Let a graph \(G = (V(G), E(G), \psi(ab))\), with \(V(G)\) denotes the vertex set, \(E(G)\) stand for edge set and the important or new factor is \(\psi(ab)\) is a weight for an edge \(ab\). Now following is the main formula of this research work is the entropy for an edge weighted graph;

\[
\Omega_\psi (G) = - \sum_{a'b' \in E(G)} \sum_{ab \in E(G)} \psi (a'b') \log \left( \frac{\psi (a'b')}{\sum_{ab \in E(G)} \psi (ab)} \right) . \quad (8)
\]

The researchers in [38], [39] established the following entropy for an edge weighted based graph by making the edge of a weight equal to the major portion of the topological index. The following are some key formulæ for this study, all of which are based on the Equation (8).

**Definition 6:** The first and second Zagreb entropies are defined as following [38], [40];

\[
\Omega_{M_1} (G) = - \frac{1}{M_1(G)} \log \left( \prod_{ab \in E(G)} [\xi_a + \xi_b]^{\xi_a + \xi_b} \right) + \log (M_1 (G)) . \quad (9)
\]

\[
\Omega_{M_2} (G) = - \frac{1}{M_2(G)} \log \left( \prod_{ab \in E(G)} [\xi_a \xi_b]^{\xi_a \xi_b} \right) + \log (M_2 (G)) . \quad (10)
\]

**Definition 7:** The hyper and augmented Zagreb entropies are defined as following [38];

\[
\Omega_{HM} (G) = - \frac{1}{HM(G)} \log \left( \prod_{ab \in E(G)} [(\xi_a + \xi_b)^2]^{(\xi_a + \xi_b)^2} \right) + \log (HM (G)) . \quad (11)
\]

\[
\Omega_{AZI} (G) = - \frac{1}{AZI(G)} \log \left( \prod_{ab \in E(G)} \left[ \left( \frac{\xi_a \xi_b}{\xi_a + \xi_b - 2} \right)^3 \right] \right) + \log (AZI (G)) . \quad (12)
\]
Definition 8: The first, second and third redefined Zagreb entropies are defined as following [39]:

\[
\Omega_{ReZG_1}(G) = -\frac{1}{ReZG_1(G)} \log \left[ \prod_{ab \in E(G)} \left( \frac{\xi_a + \xi_b}{\xi_a \xi_b} \right)^{\frac{\xi_a + \xi_b}{\xi_a \xi_b}} \right] + \log (ReZG_1(G)).
\]

(13)

\[
\Omega_{ReZG_2}(G) = -\frac{1}{ReZG_2(G)} \log \left[ \prod_{ab \in E(G)} \left( \frac{\xi_a \xi_b}{\xi_a + \xi_b} \right)^{\frac{\xi_a \xi_b}{\xi_a + \xi_b}} \right] + \log (ReZG_2(G)).
\]

(14)

\[
\Omega_{ReZG_3}(G) = -\frac{1}{ReZG_3(G)} \log \left[ \prod_{ab \in E(G)} \left[ (\xi_a \xi_b + \xi_a + \xi_b) \right]^{\frac{\xi_a \xi_b (\xi_a + \xi_b)}{\xi_a \xi_b + \xi_a + \xi_b}} \right] + \log (ReZG_3(G)).
\]

(15)

The major contribution of this paper is to broaden the range of uses for armchair carbon nanotubes by investigating various edge weight-based entropies. The notions ACNT (β, γ), ACSCNT (β, γ) and ACCNT (β, γ), are armchair carbon semi-capped nanotubes and armchair carbon capped nanotubes, respectively. Furthermore, we analyzed these entropies and compared the three stated structures using instances from Table 9 to Table 15 in the next section, and presented the findings in Figure 5 to Figure 11. The article [41] has additional information on this structure of armchair carbon nanotube and its variants.

II. RESULTS FOR THE UNCAPPED CARBON NANOTUBE ACNT (β, γ)

The notion ACNT (β, γ), is for an armchair carbon nanotube, it has two types of vertices according to degree defined in Table 1 and edge types defined in Table 2, and \( p_1 \) is the order and \( q_1 \), size of ACNT (β, γ).

Authors of [42], determined the topological indices based on the degree of armchair carbon nanotube ACNT (β, γ). We defined the main results in Table 3, we will use these results in our main prove of theorems.

Furthermore, a three-dimensional image of an armchair carbon nanotube ACNT (β, γ) is shown in Figure 1.

![Figure 1: Three-dimensional sight of armchair carbon nanotube ACNT (β, γ)](image-url)
in
\[\Omega_{M_1}(G) = - \frac{1}{9\gamma - 10\beta} \log \left[ (2 + 2)^\beta (2 + 3)^{2\beta (2 + 3)} \times (3 + 3)^{3\beta - 8\beta (3 + 3)} \right] + \log (9\beta - 10\beta),\]
\[\Omega_{M_2}(G) = - \frac{2\log [256^\beta \times 176787236^\beta \times 19683^\beta - 8\beta]}{27\beta - 40\beta}
+ \log \left( \frac{27\beta - 40\beta}{2} \right).\]

\[\text{Proof. By using the Table 2 given for the edge varieties of }\]
\[ACNT (\beta, \gamma)\text{ graph, second Zagreb index is determined in the Table 3. Now for the entropy of second Zagreb, we will use the the value of second Zagreb index in the Equation 10, and resulted in}\]
\[\Omega_{M_2}(G) = - \frac{1}{27\beta - 40\beta} \log \left[ (2 + 2)^\beta (2 + 3)^{2\beta (2 + 3)} \times (3 + 3)^{3\beta - 8\beta (3 + 3)} \right] + \log \left( \frac{27\beta - 40\beta}{2} \right),\]
\[\Omega_{M_2}(G) = - \frac{2\log [256^\beta \times 176787236^\beta \times 19683^\beta - 8\beta]}{27\beta - 40\beta}
+ \log \left( \frac{27\beta - 40\beta}{2} \right).\]

\[\text{Theorem 10: Let }\Omega_{M_2}\text{ is the edge weight based second Zagreb entropy for the graph } G \cong ACNT (\beta, \gamma), \text{ then }\]
\[\Omega_{M_2}(G) = - \frac{1}{27\beta - 40\beta} \log \left[ (2 + 2)^\beta (2 + 3)^{2\beta (2 + 3)} \times (3 + 3)^{3\beta - 8\beta (3 + 3)} \right] + \log \left( \frac{27\beta - 40\beta}{2} \right).\]

\[\text{Theorem 11: Let }\Omega_{HM}\text{ is the edge weight based hyper Zagreb entropy for the graph } G \cong ACNT (\beta, \gamma), \text{ then }\]
\[\Omega_{HM}(G) = \log (54\beta - 78\beta) - \frac{\log [4^{2\beta} \times 5^{100\beta} \times 6^{54\beta} - 144\beta]}{54\beta - 78\beta}.\]

\[\text{Proof. By using the Table 2 given for the edge varieties of }\]
\[ACNT (\beta, \gamma)\text{ graph, hyper Zagreb index is determined in the Table 3. Now for the entropy of hyper Zagreb, we will use the the value of hyper Zagreb index in the Equation 11, and resulted in}\]
\[\Omega_{HM}(G) = \log (54\beta - 78\beta) - \frac{\log [4^{2\beta} \times 5^{100\beta} \times 6^{54\beta} - 144\beta]}{54\beta - 78\beta}.\]

\[\text{Theorem 12: Let }\Omega_{AZI}\text{ is the edge weight based augmented Zagreb entropy for the graph } G \cong ACNT (\beta, \gamma), \text{ then }\]
\[\Omega_{AZI}(G) = - \frac{1}{2187\beta - 345\beta} \log \left[ \left( \frac{2 + 2}{3 + 3} \right)^{2\beta (2 + 2)} \times \left( \frac{2 + 3}{3 + 3} \right)^{2\beta (2 + 3)} \times \left( \frac{3 + 3}{3 + 3} \right)^{2\beta (3 + 3)} \right] + \log \left( \frac{2187\beta - 345\beta}{128} \right),\]
\[\Omega_{AZI}(G) = - \frac{1}{2187\beta - 345\beta} \log \left[ \left( \frac{2 + 2}{3 + 3} \right)^{2\beta (2 + 2)} \times \left( \frac{2 + 3}{3 + 3} \right)^{2\beta (2 + 3)} \times \left( \frac{3 + 3}{3 + 3} \right)^{2\beta (3 + 3)} \right] + \log \left( \frac{2187\beta - 345\beta}{128} \right).\]

\[\text{Theorem 13: Let }\Omega_{RZG_1}\text{ is the edge weight based redefined first Zagreb entropy for the graph } G \cong ACNT (\beta, \gamma), \text{ then }\]
\[\Omega_{RZG_1}(G) = - \frac{1}{2187\beta - 345\beta} \log \left[ \left( \frac{2 + 2}{3 + 3} \right)^{2\beta (2 + 2)} \times \left( \frac{2 + 3}{3 + 3} \right)^{2\beta (2 + 3)} \times \left( \frac{3 + 3}{3 + 3} \right)^{2\beta (3 + 3)} \right] + \log \left( \frac{2187\beta - 345\beta}{128} \right).\]
**Theorem 14:** Let $\Omega_{ReZG_2}$ is the edge weight based redefined second Zagreb entropy for the graph $G \cong ACNT(\beta, \gamma)$, then $\Omega_{ReZG_2}(G) = \log\left[\frac{1.548941^\beta \times 1.355403^{3\beta\gamma-8\beta}}{9.5^4 - 13\beta^4} + \log\left(\frac{9\beta\gamma}{4} - \frac{13\beta}{5}\right)\right]$. 

Proof. By using the Table 2 given for the edge varieties of $ACNT(\beta, \gamma)$ graph, redefined second Zagreb index is determined in the Table 3. Now for the entropy of redefined second Zagreb, we will use the the value of redefined second Zagreb index in the Equation 14, and resulted in $\Omega_{ReZG_2}(G) = \log\left[\frac{1.548941^\beta \times 1.355403^{3\beta\gamma-8\beta}}{9.5^4 - 13\beta^4} + \log\left(\frac{9\beta\gamma}{4} - \frac{13\beta}{5}\right)\right] = 2\beta\gamma - 140\beta \quad (26)$

**Theorem 15:** Let $\Omega_{ReZG_3}$ is the edge weight based redefined third Zagreb entropy for the graph $G \cong ACNT(\beta, \gamma)$, then $\Omega_{ReZG_3}(G) = \log\left[\frac{16^{2\beta} \times 30^{6\beta} \times 5^4 \gamma(3\beta\gamma-8\beta)}{81\beta\gamma - 140\beta}\right]$. 

Proof. By using the Table 2 given for the edge varieties of $ACNT(\beta, \gamma)$ graph, redefined third Zagreb index is determined in the Table 3. Now for the entropy of redefined third Zagreb, we will use the the value of redefined third Zagreb index in the Equation 15, and resulted in $\Omega_{ReZG_3}(G) = \log\left[\frac{16^{2\beta} \times 30^{6\beta} \times 5^4 \gamma(3\beta\gamma-8\beta)}{81\beta\gamma - 140\beta}\right] = 2\beta\gamma - 140\beta \quad (27)$

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

The notion $ACSCNT(\beta, \gamma)$ is for the armchair carbon semi-capped nanotube, which has two different types of vertices, according to the fact established in Table 4, while edge distribution is defined in Table 5, given $p_2$, $q_2$, are the order and size of $ACSCNT(\beta, \gamma)$, respectively.

The data of the topological indices for the structure of $ACSCNT(\beta, \gamma)$, namely armchair semi-capped nanotube, given in [43]. The main results of this research work is useful here and we summarized in the Table 6, and we will use these results in our main prove of theorems.

Moreover, the 3D view of armchair semi-capped nanotube $ACSCNT(\beta, \gamma)$ is shown in Figure 2.

**Theorem 16:** Let $\Omega_{M_1}$ is the edge weight based first Zagreb entropy for the graph $G = \cong ACSCNT(\beta, \gamma)$, then $\Omega_{M_1}(G) = \log\left[\frac{16^{2\beta} \times 30^{6\beta} \times 5^4 \gamma(3\beta\gamma-8\beta)}{81\beta\gamma - 140\beta}\right] = 2\beta\gamma - 140\beta \quad (28)$

**III. RESULTS FOR THE UNCAPPED CARBON NANOTUBE $ACSCNT(\beta, \gamma)$**

| Table 4: $ACSCNT(\beta, \gamma)$ graph’s Vertex partition |
|---------------------------------------------------------|
| $\xi_a$ | Frequency | Set of Vertices |
| 2       | $\beta$  | $V_1$         |
| 3       | $\beta(\gamma-1)$ | $V_2$ |
| $p_2$   | $\beta\gamma$ |               |

| Table 5: $ACSCNT(\beta, \gamma)$ graph’s Edge partition |
|---------------------------------------------------------|
| $(\xi_a, \xi_b)$ | Frequency | Set of Edges |
| (2, 2)   | $\frac{\beta}{2}$ | $E_1$ |
| (2, 3)   | $\beta$        | $E_2$ |
| (3, 3)   | $\frac{3\beta\gamma-4\beta}{2}$ | $E_3$ |
| $q_2$    | $\frac{3\beta\gamma-\beta}{2}$ | |

| Table 6: $ACSCNT(\beta, \gamma)$ graph’s Topological Indices |
|---------------------------------------------------------------|
| $I$ | $I(ACSCNT(\beta, \gamma))$ |
| $M_1$ | $9\beta\gamma - 2\beta$ |
| $M_2$ | $\frac{27\beta\gamma - 11\beta}{2}$ |
| $HM$ | $54\beta\gamma - 21\beta$ |
| $AZI$ | $12\beta + \frac{729(3\beta\gamma - 3\beta)}{128}$ |
| $ReZG_1$ | $\beta\gamma + \frac{3}{2}$ |
| $ReZG_2$ | $\frac{9\beta\gamma - 9\beta}{4} + \frac{17\beta}{10}$ |
| $ReZG_3$ | $81\beta\gamma - 43\beta$ |
Theorem 18: Let $\Omega_{HM}$ is the edge weight based hyper Zagreb entropy for the graph $G = \cong ACSCNT (\beta, \gamma)$, then $\Omega_{HM} (G)$ is

$$
\Omega_{HM} (G) = \log (54\beta\gamma - 21\beta) - \log \left[ \frac{4^{16}\beta \times 5^{50}\beta \times 6^{54}\beta\gamma - 72\beta}{54\beta\gamma - 21\beta} \right].
$$

Proof. By using the Table 5 given for the edge varieties of $ACSCNT (\beta, \gamma)$ graph, hyper Zagreb index is determined in the Table 6. Now for the entropy of hyper Zagreb, we will use the value of hyper Zagreb index in the Equation 11, and resulted in

$$
\begin{align*}
\Omega_{HM} (G) &= - \frac{1}{54\beta\gamma - 21\beta} \log \left[ (2 + 2)^{\beta(2+2)} \times (2 + 3)^{\beta(2+3)} 
\times (3 + 3)^{\frac{3\beta - 4\beta}{2}(3+3)} \right] + \log (54\beta\gamma - 21\beta),
\end{align*}
$$

$$
= \log (54\beta\gamma - 21\beta) - \log \left[ \frac{4^{16}\beta \times 5^{50}\beta \times 6^{54}\beta\gamma - 72\beta}{54\beta\gamma - 21\beta} \right].
$$

Theorem 19: Let $\Omega_{AZI}$ is the edge weight based augmented Zagreb entropy for the graph $G = \cong ACSCNT (\beta, \gamma)$, then $\Omega_{AZI} (G)$ is

$$
\Omega_{AZI} (G) = - \log \left[ \frac{4096\beta \times 2^{24}\beta \times \left( \frac{27}{8} \right)^{\frac{3\beta - 4\beta}{2}}}{12\beta + \frac{729(3\beta - 3\beta)}{128}} \right] + \log \left( 12\beta + \frac{729(3\beta - 3\beta)}{128} \right).
$$

Proof. By using the Table 5 given for the edge varieties of $ACSCNT (\beta, \gamma)$ graph, augmented Zagreb index is determined in the Table 6. Now for the entropy of augmented Zagreb, we will use the value of augmented Zagreb index in the Equation 12, and resulted in

$$
\begin{align*}
\Omega_{AZI} (G) &= - \frac{1}{12\beta + \frac{729(3\beta - 3\beta)}{128}} \log \left[ \frac{2 \times 2^3 \times (\frac{27}{8})^{\frac{3\beta - 4\beta}{2}}}{2 + 2 - 2} \right] 
\times \left( \frac{2 \times 3}{2 + 3 - 2} \right)^{\frac{3\beta}{2}(\frac{3\beta - 4\beta}{2}) \times (3 + 3)} \times \left( \frac{3 \times 3}{3 + 3 - 2} \right)^{\frac{3\beta}{2}(\frac{3\beta - 4\beta}{2})} + \log \left( 12\beta + \frac{729(3\beta - 3\beta)}{128} \right),
\end{align*}
$$

$$
= - \log \left[ \frac{4096\beta \times 2^{24}\beta \times \left( \frac{27}{8} \right)^{\frac{3\beta - 4\beta}{2}}}{12\beta + \frac{729(3\beta - 3\beta)}{128}} \right] + \log \left( 12\beta + \frac{729(3\beta - 3\beta)}{128} \right).
$$
Theorem 20: Let $\Omega_{ReZG_1}$ is the edge weight based first redefined Zagreb entropy for the graph $G = \cong ACSCNT (\beta, \gamma)$, then $\Omega_{ReZG_1} (G)$ is

$$\Omega_{ReZG_1} (G) = -3 \log \left[ \frac{0.859044^3 \times 0.873580^{3\beta \gamma - 4\beta}}{3\beta \gamma + \beta} \right] + \log \left( \beta \gamma + \frac{\beta}{3} \right).$$

Proof. By using the Table 5 given for the edge varieties of $ACSCNT (\beta, \gamma)$ graph, redefined first Zagreb index is determined in the Table 6. Now for the entropy of redefined first Zagreb, we will use the the value of redefined first Zagreb index in the Equation 13, and resulted in

$$\Omega_{ReZG_1} (G) = -3 \log \left[ \frac{0.859044^3 \times 0.873580^{3\beta \gamma - 4\beta}}{3\beta \gamma + \beta} \right] + \log \left( \beta \gamma + \frac{\beta}{3} \right).$$

(38)

Theorem 21: Let $\Omega_{ReZG_2}$ is the edge weight based second redefined Zagreb entropy for the graph $G = \cong ACSCNT (\beta, \gamma)$, then $\Omega_{ReZG_2} (G)$ is

$$\Omega_{ReZG_2} (G) = -3 \log \left[ \frac{0.859044^3 \times 0.873580^{3\beta \gamma - 4\beta}}{3\beta \gamma + \beta} \right] + \log \left( \beta \gamma + \frac{\beta}{3} \right).$$

(39)

Proof. By using the Table 5 given for the edge varieties of $ACSCNT (\beta, \gamma)$ graph, redefined second Zagreb index is determined in the Table 6. Now for the entropy of redefined second Zagreb, we will use the the value of redefined second Zagreb index in the Equation 14, and resulted in

$$\Omega_{ReZG_2} (G) = -3 \log \left[ \frac{0.859044^3 \times 0.873580^{3\beta \gamma - 4\beta}}{3\beta \gamma + \beta} \right] + \log \left( \beta \gamma + \frac{\beta}{3} \right).$$

(40)

IV. RESULTS FOR THE UNCAPPED CARBON NANOTUBE $ACCN(T (\beta, \gamma)$

The notion $ACCN (\beta, \gamma)$, is for the armchair carbon capped nanotube, it has a solemn type of vertices and edge types defined in Table 7, along the fact $p_3$, $q_3$, are the order and size of $ACCN (\beta, \gamma)$, respectively.

The data on the topological indices based on the degree of graph $ACCN (\beta, \gamma)$ or armchair capped nanotube given in [43]. For the usage of that data we summarized in the Table 8, and we will take into account for the results of our main prove of theorems.

Furthermore, a three-dimensional image of an armchair carbon capped nanotube $ACCN (\beta, \gamma)$ is shown in Figure 3. While two-dimensional symmetry of this structure is shown in Figure 4.

Theorem 23: Let $\Omega_{M_1}$ is the edge weight based first Zagreb entropy for the graph $G = \cong ACCNT (\beta, \gamma)$, then $\Omega_{M_1} (G)$ is

$$\Omega_{M_1} (G) = - \log \left( \frac{216^{3\beta \gamma}}{9\beta \gamma} \right) + \log (9\beta \gamma).$$

(44)
TABLE 8: **ACCNT**(β, γ) graph’s Topological Indices

|   | \(I \text{(ACCNT}(\beta, \gamma))\) |
|---|---|
| \(M_1\) | 9\(\beta\gamma\) |
| \(M_2\) | \(\frac{27\beta\gamma}{2}\) |
| \(HM\) | 54\(\beta\gamma\) |
| \(AZI\) | \(\frac{2187\beta\gamma}{128}\) |
| \(ReZG_1\) | \(\beta\gamma\) |
| \(ReZG_2\) | \(\frac{9\beta\gamma}{4}\) |
| \(ReZG_3\) | 81\(\beta\gamma\) |

FIGURE 3: 3D view of armchair capped nanotube **ACCNT**(β, γ).

Proof. By using the Table 7 given for the edge varieties of **ACCNT** (β, γ) graph, first Zagreb index is determined in the Table 8. Now for the entropy of first Zagreb, we will use the the value of first Zagreb index in the Equation 9, and resulted in

\[
\Omega_{M_1}(G) = - \frac{1}{9\beta\gamma} \log \left( (3 + 3)^{\frac{3\beta\gamma}{2}} \right) + \log (9\beta\gamma),
\]

\[
= - \frac{\log (216^{3\beta\gamma})}{9\beta\gamma} + \log (9\beta\gamma). \tag{45}
\]

**Theorem 24:** Let \(\Omega_{M_2}\) is the edge weight based second Zagreb entropy for the graph \(G = \text{ACCNT} (\beta, \gamma)\), then \(\Omega_{M_2}(G)\) is

\[
\Omega_{M_2}(G) = - \frac{2\log (19683^{3\beta\gamma})}{27\beta\gamma} + \log \left( \frac{27\beta\gamma}{2} \right). \tag{46}
\]

Proof. By using the Table 7 given for the edge varieties of **ACCNT** (β, γ) graph, second Zagreb index is determined in the Table 8. Now for the entropy of second Zagreb, we will use the the value of second Zagreb index in the Equation 10, and resulted in

\[
\Omega_{M_2}(G) = - \frac{1}{27\beta\gamma} \log \left( (3 \times 3)^{\frac{3\beta\gamma}{2}} \right) + \log \left( \frac{27\beta\gamma}{2} \right),
\]

\[
= - \frac{2\log (19683^{3\beta\gamma})}{27\beta\gamma} + \log \left( \frac{27\beta\gamma}{2} \right). \tag{47}
\]

**Theorem 25:** Let \(\Omega_{HM}\) is the edge weight based hyper Zagreb entropy for the graph \(G = \text{ACCNT} (\beta, \gamma)\), then \(\Omega_{HM}(G)\) is

\[
\Omega_{HM}(G) = \log (54\beta\gamma) - \log \left( \frac{6^{54\beta\gamma}}{54\beta\gamma} \right). \tag{48}
\]

Proof. By using the Table 7 given for the edge varieties of **ACCNT** (β, γ) graph, hyper Zagreb index is determined in the Table 8. Now for the entropy of hyper Zagreb, we will use the the value of hyper Zagreb index in the Equation 11, and resulted in

\[
\Omega_{HM}(G) = - \frac{1}{54\beta\gamma} \log \left( (3 + 3)^{\frac{3\beta\gamma}{2}} \right) + \log (54\beta\gamma),
\]

\[
= \log (54\beta\gamma) - \frac{\log \left( \frac{6^{54\beta\gamma}}{54\beta\gamma} \right)}{54\beta\gamma}. \tag{49}
\]

**Theorem 26:** Let \(\Omega_{AZI}\) is the edge weight based augmented Zagreb entropy for the graph \(G = \text{ACCNT}(\beta, \gamma)\), then \(\Omega_{AZI}(G)\) is

\[
\Omega_{AZI}(G) = \log (54\beta\gamma) - \log \left( \frac{6^{54\beta\gamma}}{54\beta\gamma} \right). \tag{49}
\]
\[ \Omega_{AZ1}(G) = -\frac{1}{2187\beta\gamma} \log \left( \frac{3 	imes 3}{3 - 3 - 2} \right) + \log \left( \frac{2187\beta\gamma}{128} \right). \]  

Proof. By using the Table 7 given for the edge varieties of \( ACCNT(\beta, \gamma) \) graph, augmented Zagreb index is determined in the Table 8. Now for the entropy of augmented Zagreb, we will use the value of augmented Zagreb index in the Equation 12, and resulted in

\[ \Omega_{AZ1}(G) = \frac{1}{2187\beta\gamma} \log \left( \frac{3 	imes 3}{3 + 3} \right) + \log \left( \frac{2187\beta\gamma}{128} \right). \]  

Theorem 27: Let \( \Omega_{ReZG1} \) is the edge weight based first redefined Zagreb entropy for the graph \( G = \cong ACCNT(\beta, \gamma) \), then \( \Omega_{ReZG1}(G) \) is

\[ \Omega_{ReZG1}(G) = -\log \left( \frac{0.873580^{3\beta\gamma}}{\beta\gamma} \right) + \log (\beta\gamma). \]  

Proof. By using the Table 7 given for the edge varieties of \( ACCNT(\beta, \gamma) \) graph, first redefined Zagreb index is determined in the Table 8. Now for the entropy of first redefined Zagreb, we will use the value of first redefined Zagreb index in the Equation 13, and resulted in

\[ \Omega_{ReZG2}(G) = -\frac{1}{9\beta\gamma} \log \left( \frac{3 \times 3}{3 + 3} \right) + \log \left( \frac{9\beta\gamma}{4} \right). \]  

Theorem 28: Let \( \Omega_{ReZG2} \) is the edge weight based second redefined Zagreb entropy for the graph \( G = \cong ACCNT(\beta, \gamma) \), then \( \Omega_{ReZG2}(G) \) is

\[ \Omega_{ReZG2}(G) = -\frac{1}{9\beta\gamma} \log \left( \frac{3 \times 3}{3 + 3} \right) + \log \left( \frac{9\beta\gamma}{4} \right). \]  

V. CONCLUSION AND DISCUSSION

For three cases of armchair carbon nanotubes, we calculated entropy based on edge weight, namely armchair carbon nanotube, armchair carbon semi-capped nanotube, and armchair carbon capped nanotube, which are denoted by \( ACNT(\beta, \gamma) \), \( ACSCNT(\beta, \gamma) \), and \( ACCNT(\beta, \gamma) \), respectively. The edge weight based entropy is measured in this draft namely are first and second Zagreb, hyper Zagreb, augmented Zagreb, redefined first, second and third Zagreb entropy.

In the Equations 16, 18, 20, 22, 24, 26, and 28, the final findings are shown. Following the analytical results, we conducted a comparative analysis of the various operating parameters \((m, n)\) of each graph. Software MATLAB is used to generate numerical results which are shown in the Tables 9 to 15 and corresponding plots are constructed by Maple\textsuperscript{TM}, are shown in the Figures 5 to 11. Furthermore, all of the results are double-checked by authentic mathematical tool of Mathematica. In the Tables 9 to 15, graphs are renamed as \( G_1 = ACNT(m, n) \), \( G_2 = ACSCNT(m, n) \) and \( G_3 = ACCNT(m, n) \). The plots in the Figures 5 and 6 are extracted from the data in Tables 9 and 10. It shows that the edge weight based
first and second Zagreb entropy have different properties for different topologies of nanotubes. For example, the entropy of $G_2$ shape of nanotube which is $ACSCNT (m, n)$ or semi-capped nanotube is growing more rapidly in comparison to other shapes either $G_1$ and $G_3$. Similarly in the Figures 8 and 11 extracted from the Tables 12 and 15, plotting showing the same entropy measure and for semi-capped nanotube, the entropy is growing more rapidly than others. Just in the case shown in the Figures 7 and 10, the plot for entropies are overlapped for capped and semi-capped nanotubes. It shows that each entropy measure is different for different topologies of nanotubes. Either it is single-sided capped or both sided capped. The fact is shown by the exemplary analysis drawn below.

![Figure 5](image5.png)

**FIGURE 5:** For the first Zagreb entropy, plotting results of several topologies of nanotubes

![Figure 6](image6.png)

**FIGURE 6:** For the second Zagreb entropy, plotting results of several symmetries of nanotubes

| $(m, n)$ | $\Omega_{M_1} (G_1)$ | $\Omega_{M_1} (G_2)$ | $\Omega_{M_1} (G_3)$ |
|---------|------------------|------------------|------------------|
| (4, 3)  | 1.142368104      | 1.345150450      | 1.256272505      |
| (4, 4)  | 1.296427377      | 1.446050672      | 1.380211242      |
| (4, 5)  | 1.410724714      | 1.529064232      | 1.477121255      |
| (4, 6)  | 1.501365452      | 1.599191748      | 1.556302501      |
| (4, 7)  | 1.57614375       | 1.659772059      | 1.623249291      |
| (4, 8)  | 1.640432325      | 1.7130433102     | 1.681241238      |
| (4, 9)  | 1.696240012      | 1.760555358      | 1.732393760      |
| (4, 10) | 1.745700946      | 1.803420306      | 1.778151251      |
| (4, 11) | 1.790109730      | 1.842452964      | 1.819543936      |
| (4, 12) | 1.830401934      | 1.878295195      | 1.857332497      |

**TABLE 9:** Numerical results of several symmetries of nanotubes

| $(m, n)$ | $\Omega_{M_2} (G_1)$ | $\Omega_{M_2} (G_2)$ | $\Omega_{M_2} (G_3)$ |
|---------|------------------|------------------|------------------|
| (4, 3)  | 1.131367693      | 1.364856838      | 1.255272504      |
| (4, 4)  | 1.282879492      | 1.458404662      | 1.380211242      |
| (4, 5)  | 1.398654780      | 1.537870525      | 1.477121254      |
| (4, 6)  | 1.490882155      | 1.605963160      | 1.556302500      |
| (4, 7)  | 1.567246576      | 1.665242140      | 1.623249290      |
| (4, 8)  | 1.652320896      | 1.717641557      | 1.681241237      |
| (4, 9)  | 1.688981310      | 1.764473780      | 1.732393759      |
| (4, 10) | 1.739139888      | 1.806844037      | 1.778151250      |
| (4, 11) | 1.784127809      | 1.845496204      | 1.819543935      |
| (4, 12) | 1.824907412      | 1.881021944      | 1.857332496      |

**TABLE 10:** Numerical results of several symmetries of nanotubes
FIGURE 7: For the hyper Zagreb entropy, plotting results of several symmetries of nanotubes

FIGURE 8: For the augmented Zagreb entropy, plotting results of several symmetries of nanotubes

| $(m, n)$ | $\Omega_{HM} (G_1)$ | $\Omega_{HM} (G_2)$ | $\Omega_{HM} (G_3)$ |
|---------|---------------------|---------------------|---------------------|
| (4, 3)  | 1.298129246         | 1.998185255         | 2.03443756          |
| (4, 4)  | 1.689839004         | 2.132061781         | 2.158362493         |
| (4, 5)  | 1.910309252         | 2.234297720         | 2.255272505         |
| (4, 6)  | 2.061165240         | 2.317011745         | 2.33453751          |
| (4, 7)  | 2.175013537         | 2.386473577         | 2.40140541          |
| (4, 8)  | 2.266118393         | 2.443463897         | 2.459392488         |
| (4, 9)  | 2.341909744         | 2.49859744          | 2.510545011         |
| (4, 10) | 2.406721847         | 2.545883601         | 2.556302501         |
| (4, 11) | 2.463293060         | 2.588229320         | 2.597695186         |
| (4, 12) | 2.513459144         | 2.626811200         | 2.635483747         |

| $(m, n)$ | $\Omega_{AZI} (G_1)$ | $\Omega_{AZI} (G_2)$ | $\Omega_{AZI} (G_3)$ |
|---------|---------------------|---------------------|---------------------|
| (4, 3)  | 1.175901424         | 1.380098746         | 1.255272505         |
| (4, 4)  | 1.315688105         | 1.470862002         | 1.380211241         |
| (4, 5)  | 1.421414000         | 1.548279796         | 1.477121255         |
| (4, 6)  | 1.511594138         | 1.614865601         | 1.556325010         |
| (4, 7)  | 1.584678089         | 1.673004146         | 1.623429291         |
| (4, 8)  | 1.647394558         | 1.724490550         | 1.681241238         |
| (4, 9)  | 1.702209363         | 1.770641772         | 1.73293759          |
| (4, 10) | 1.750930075         | 1.812434610         | 1.778151250         |
| (4, 11) | 1.794766733         | 1.850607280         | 1.819543935         |
| (4, 12) | 1.834599229         | 1.885728708         | 1.857332497         |

TABLE 11: Numerical results of several symmetries of nanotubes

TABLE 12: Numerical results of several symmetries of nanotubes
FIGURE 9: For redefined first Zagreb entropy, plotting re-
sults of several symmetries of nanotubes

TABLE 13: Numerical results of several symmetries of nan-
otubes

| (m, n) | $\Omega_{ReZG_1}$ ($G_1$) | $\Omega_{ReZG_1}$ ($G_2$) | $\Omega_{ReZG_1}$ ($G_3$) |
|--------|-----------------|-----------------|-----------------|
| (4, 3) | 1.142736666 | 1.232780089 | 1.60745/103 |
| (4, 4) | 1.295809536 | 1.362473581 | 1.73295840 |
| (4, 5) | 1.409600029 | 1.462494047 | 1.829305853 |
| (4, 6) | 1.50034928 | 1.543862921 | 1.908487099 |
| (4, 7) | 1.575020041 | 1.612430371 | 1.975433888 |
| (4, 8) | 1.639040731 | 1.671670458 | 2.033425835 |
| (4, 9) | 1.694882276 | 1.72813506 | 2.084578358 |
| (4, 10) | 1.744390984 | 1.770376060 | 2.13035848 |
| (4, 11) | 1.788852848 | 1.812435901 | 2.171728534 |
| (4, 12) | 1.829199056 | 1.850786305 | 2.209517094 |

FIGURE 10: For the redefined second Zagreb entropy, plot-
ing results of several symmetries of nanotubes

TABLE 14: Numerical results of several symmetries of nan-
otubes

| (m, n) | $\Omega_{ReZG_2}$ ($G_1$) | $\Omega_{ReZG_2}$ ($G_2$) | $\Omega_{ReZG_2}$ ($G_3$) |
|--------|-----------------|-----------------|-----------------|
| (4, 3) | 1.142492831 | 1.272619456 | 1.259272508 |
| (4, 4) | 1.296004239 | 1.392636804 | 1.380211244 |
| (4, 5) | 1.410230553 | 1.486792325 | 1.477121257 |
| (4, 6) | 1.500888388 | 1.564215800 | 1.556302503 |
| (4, 7) | 1.575972146 | 1.629942966 | 1.623249292 |
| (4, 8) | 1.640026819 | 1.687042447 | 1.681241299 |
| (4, 9) | 1.695867858 | 1.737511408 | 1.732393763 |
| (4, 10) | 1.745358263 | 1.782792737 | 1.778151252 |
| (4, 11) | 1.789792822 | 1.823685174 | 1.819543938 |
| (4, 12) | 1.830107552 | 1.861112974 | 1.857332498 |
TABLE 15: Numerical results of several symmetries of nanotubes

| (m, n) | Ω_{ReZG_{3}} (G_{1}) | Ω_{ReZG_{3}} (G_{2}) | Ω_{ReZG_{3}} (G_{3}) |
|--------|----------------------|----------------------|----------------------|
| (4, 3) | 1.111267686 | 1.463898121 | 1.256272505 |
| (4, 4) | 1.263661939 | 1.527123430 | 1.390211241 |
| (4, 5) | 1.382605429 | 1.590416230 | 1.477121254 |
| (4, 6) | 1.477438084 | 1.648483043 | 1.556302501 |
| (4, 7) | 1.555758581 | 1.700942168 | 1.623249290 |
| (4, 8) | 1.623218784 | 1.748378626 | 1.681241254 |
| (4, 9) | 1.680135908 | 1.791499070 | 1.732397060 |
| (4, 10) | 1.731216752 | 1.830940078 | 1.778151250 |
| (4, 11) | 1.776955609 | 1.867235429 | 1.819543936 |
| (4, 12) | 1.813857774 | 1.900824030 | 1.857332496 |

REFERENCES

[1] C. E. Shannon, “A mathematical theory of communication,” Bell System Technology Journal, vol. 27, pp. 379–423, 1948.
[2] M. Dehmer and M. Graber, “The discrimination power of molecular identification numbers revisited,” MATCH Community of Mathematics and Computational Chemistry, vol. 69, p. 785A–794, 2013.
[3] R. E. Ulanowicz, “Quantitative methods for ecological network analysis,” Computational Biology and Chemistry, vol. 28, pp. 321–339, 2004.
[4] S. Cao, M. Dehmer, and Y. Shi, “Extremality of degree-based graph entropies,” Information Science, vol. 278, pp. 22–33, 2014.
[5] E. Estrada and N. Hatano, “Statistical-mechanical approach to subgraph centrality in complex networks,” Chemical Physics Letters, vol. 439, pp. 247–251, 2007.
[6] R. V. Sol and S. I. Valverde, “Information theory of complex networks: on evolution and architectural constraints,” Complex Network Lectures Notes Physics, vol. 650, pp. 189–207, 2004.
[7] N. Rashevsky, “Life, information theory, and topology,” Bulletin of Mathematical Biophysics, vol. 17, pp. 229–235, 1955.
[8] E. Trucco, “A note on the information content of graphs,” Bulletin of Mathematical Biophysics, vol. 18, no. 2, pp. 129–135, 1956.
[9] M. Dehmer and A. Mowshowitz, “A history of graph entropy measures,” Information Science, vol. 181, pp. 57–78, 2011.
[10] Y. J. Tan and J. Wu, “Network structure entropy and its application to scale-free networks,” System Engineering-Theory & Practice, vol. 6, pp. 1–3, 2004.

FIGURE 11: For the redefined third Zagreb entropy, plotting results of several symmetries of nanotubes

VOLUME 4, 2020

This article has been accepted for publication in a future issue of this journal, but has not been fully edited. Content may change prior to final publication. Citation information: DOI 10.1109/ACCESS.2021.3119032, IEEE Access

This work is licensed under a Creative Commons Attribution 4.0 License. For more information, see https://creativecommons.org/licenses/by/4.0/
[36] P. S. Ranjini, V. Lokesh, and A. Usha, “Relation between phenylene and hexagonal squeeze using harmonic index,” International Journal of Graph Theory, vol. 1, pp. 116–121, 2013.

[37] Z. Chen, M. Dshner, and Y. Shi, “A note on distance based graph entropies,” Entropy, vol. 16, pp. 5416–5427, 2014.

[38] S. Manzoor, M. K. Siddiqui, and S. Ahmad, “On entropy measures of polyyclic hydroxychloroquine used for novel coronavirus (covid-19) treatment,” Polycyclic Aromatic Compounds, 2020.

[39] S. Manzoor, S. Ahmad, and M. K. Siddiqui, “On entropy measures of molecular graphs using topological indices,” Arabian Journal of Chemistry, vol. 13, no. 8, pp. 6285–6298, Aug 2020.

[40] X. Zuo, M. F. Nadeem, M. K. Siddiqui, and M. Azeem, “Edge weight based entropy of different topologies of carbon nanotubes,” IEEE Access, vol. 9, pp. 102,019–102,029, 2021.

[41] M. F. Nadeem, M. Azeem, and I. Farman, “Comparative study of topological indices for capped and uncapped carbon nanotubes,” Polycyclic Aromatic Compounds, 2020.

[42] M. Bača, J. Horváthová, M. Mokrišová, A. Semaničová, and A. Suhányiová, “On topological indices of carbon nanotube network,” Canadian Journal of Chemistry, vol. 90, pp. 1–5, 2015.

[43] M. F. Nadeem, M. Azeem, and H. M. K. Siddiqui, “Comparative study of zagreb indices for capped, semi-capped and uncapped carbon nanotubes,” Polycyclic Aromatic Compounds, 2020.

MUHAMMAD IMRAN: He received the Ph.D. degree in mathematics with a specialization in graph theory from the Abdus Salam School of Mathematical Sciences, Government College University, Lahore, Pakistan, in 2011, under the supervision of Prof. I. Tomescu of the Faculty of Mathematics and Informatics, University of Bucharest, Romania. He served as an Assistant Professor with the National University of Sciences and Technology (NUST), Islamabad, Pakistan, from May 2011 to July 2016. He is currently an Associate Professor with the Department of Mathematical Sciences, United Arab Emirates University, Al Ain, Abu Dhabi, United Arab Emirates. He successfully supervised one Ph.D. and six M.S. students of mathematics at NUST. He has published research articles in reputed international journals of mathematics and informatics. His research interests include metric graph theory, graph labeling, and spectral graph theory. He is a Referee for several international mathematical journals.

ALI AHMAD: He received M. Sc. Degree in Mathematics from Punjab University, Lahore, Pakistan in 2000, M. Phil degree in Mathematics from Bahauddin Zakariya University, Multan, Pakistan in 2005 and Ph.D. degree in Mathematics from Abdus Salam School of Mathematical Sciences, GC University, Lahore, Pakistan in 2010. He is currently an Assistant Professor with the College of Computer Science and Information Technology, Jazan University, Saudi Arabia. His research interest is graph labeling, metric dimension, minimal doubly resolving sets, distances in graphs and topological indices of graphs.

YASIR AHMAD: He received Bachelor in Computer Application (2003) from B.R Ambedkar Univ., India. He received M.S. in Information Technology (2005) from H.N.B Gharwal Univ. and M.Phil. (2009) in computer science from Madurai Kamaraj Univ., India. Currently, he is working as a lecturer in the College of Computer Science and Information Technology at Jazan University, Kingdom of Saudi Arabia. His research interests include networks security, software engineering, Intuitionistic fuzzy and Neutrosophic fuzzy sets.

MUHAMMAD AZEEM is a MS candidate in department of mathematics at COMSATS University Islamabad Lahore Campus and currently servicing at department of aerospace engineering, faculty of engineering, UPM, Malaysia. He received his BS degree from COMSATS University Islamabad Lahore Campus in 2018. He has published research articles in reputed international journals of mathematics and informatics. His research interests include control theory, metric graph theory, graph labeling, and spectral graph theory. He is a Referee for several international mathematical journals.

***