

Degree-based entropies of graphene, graphyne and graphdiyne using Shannon's approach

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Abstract

Topological indices are numerical indicators that are used to study the physical and chemical properties of a molecule. Many chemical properties have been linked to degree-based topological indices, which have been extensively studied. The study of entropy measures of graphs as a measure of complexity and as a tool for the characterization of structural properties has also been gaining importance recently. Current work deals with certain carbon allotropes, a prominent sector of research and development due to their unique bonding properties. Carbon atoms are closely bonded in a hexagonal honeycomb lattice to form graphene. Graphyne and graphdiyne are two-dimensional graphene derivatives that have potential applications in various fields. This paper investigates numerous degree-based topological indices of these carbon allotropes by using the edge partition method. Furthermore, by expressing the topological indices as probability functions, the probabilistic entropies of these structures are determined using Shannon's entropy model.

Keywords: Topological descriptors; edge partition method; Shannon's entropy; graphene derivatives.

1 Introduction

Chemical graph theory is a branch of mathematics that employs graph theory to model molecular atomic structures. Topological indices are structural invariants based on molecular graph modelling of these atomic structures that have piqued the interest of mathematical chemists due to statistical

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correlations between their structures and their physicochemical properties. A topological index is a numerical parameter of a graph that describes the molecular shape numerically and is applied in the advancement of quantitative structure-activity relationships (QSAR) and quantitative structure property relationships (QSPR) [1]. Wiener discovered the concept of a topological index in 1947 while investigating the boiling temperature of paraffin, and various mathematical analyses have been carried out to connect the physical features of a molecule using this index, which has been predicted as a good approach to avoid expensive and time-consuming laboratory tests. Degree-based topological indices were studied extensively and correlated with many of the residues of the understudy molecular compounds [2]. When it comes to the structural analysis of complex molecules, the measure of information entropy also plays a major role. Despite the fact that Shannon introduced the concept of information entropy to analyse and quantify the complexity of data and information transmission, it has since been applied in a variety of scientific fields. One of the most important is the chemical application of information entropy. It is used in chemistry to study the complexity of molecular structures as well as the electron density [3].

Topological indices merged with entropy can be a stronger tool in QSAR and QSPR studies. It has been found that information entropy has a direct correlation with physicochemical properties of fullerene like rotational symmetry number and formal carbon atom oxidation states in different class of natural compounds [4]. Their application of various carbon allotropes such as graphene, graphyne and graphdiyne in a variety of industries is growing as a result of their promising features, such as band-gap, charge carrier mobility, and energy level alignment. Graphene is a hexagonal structure made up of sp^2 hybridized carbon atoms. Because of its exceptional physical, thermal, mechanical, chemical, and electrical properties, it has sparked a lot of curiosity [5]. Graphene is known as the mother of all graphitic carbon compounds since it is the fundamental component of carbon nanotubes and graphite [6]. Since the Nobel Prize in Physics was awarded in 2010 for “ground breaking experiments relating to the two-dimensional (2D) substance graphene,” the scientific world has been paying more attention to graphene [7]. When the bonds between three coordinated atoms in a layer are replaced by carbyne chains, the states of sp^2 atoms remain equivalent and graphyne layers are formed [8]. Graphynes are two-dimensional carbon allotropes made from graphene by introducing acetylenic links into a honeycomb structure with C atoms that are either sp^2 or sp hybridized. These structures have a wide range of electrical, optical, and mechanical characteristics due to the presence of acetylenic groups [9]. Among the most known configurations of graphyne are α , β , and γ graphynes [10] and the study of topological indices pertaining to α -type structures has already been done in a few papers [11]. Graphdiyne is the first synthetic carbon-based nanomaterial with sp^2 hybridized carbon atoms from benzene rings and sp hybridised carbon atoms from acetyl groups. This novel carbon allotrope with

both sp^2 and sp -hybridized carbon atoms has been created since it was initially synthesized [11].

Graphene has a number of unique features that make it ideal for use in a variety of disciplines, including energy, the environment, future materials, bio-medicine, bio-sensor, and heat-sink applications. Lithium-ion batteries, flexible or micro-super capacitors, lithium air batteries, lithium-sulfur batteries, electrodes for fuel cells, and solar cells all use graphene. Scientists are looking into the possibility of using graphene in the biomedical industry because of its high opacity, high chemical reaction and unparalleled thermal conductivity [12]. Graphene has a high conductivity, making it excellent for use in high-speed electronics. Because graphene has a large interior surface area, it could be used as an energy storage device in super-capacitor technology. If research is focused on increasing storage capacity, graphene could eventually replace present solid-state technology. According to storing properties of graphene oxides, indium tin oxide electrodes modified with polymers and graphene oxide show the write-read-erase-rewrite cycle for a non-volatile memory system [6].

Although graphene derivatives could be used for drug administration, the loading and release of the medication is difficult to manage since it clumps in salt or biological solutions and has some cytotoxicity [13]. Graphynes are believed to have potential applications in optoelectronic devices due to the presence of acetylenic groups [14]. In composite materials, small flakes of graphyne can be distributed in a polymer matrix to boost stiffness and strength. Computational studies show that the band gap of graphyne may be adjusted mechanically, allowing for the simple production of transistors with a variety of features that depend on the band gap. Graphyne has a huge elastic strain range, allowing it to be strained, relaxed to its original shape, and strained again without permanent deformation. This allows it to have durable electromechanical coupling in a range of applications, including temperature monitoring [15, 32].

The extraordinary electrical properties of graphdiyne, according to the study in [16], can be immediately represented in its applications on Field-Effect Transistors (FETs). Graphdiyne can be employed in solar cells because of its high charge carrier mobility and intrinsic band gap [17]. Graphdiyne can be used to coat the surface of anode materials or current collectors, acting as an artificial solid electrolyte interphase (SEI) layer to prevent the anode and liquid electrolyte from reacting continuously. Graphdiyne's flexible shape and strong mechanical strength enable it to act as a seamless carbon protective and functional layer at the surface or interface, and its low-temperature synthesis allows it to grow on high-temperature sensitive materials [18].

In this work, we study the degree-based topological indices and their associated entropy measures for analyzing the physicochemical properties of different classes of compounds such as β -graphene, β -graphyne, β -graphydine, γ -graphene, γ -graphyne, and γ -graphydine. Section 2 of this paper contains the preliminaries of the topological indices and entropies, while the third section involves

main results that are further divided into two. In the first part, we calculate various degree based topological indices for the structures under consideration and the second part discusses the numerical values of corresponding entropies.

2 Degree-based topological indices and corresponding entropies

We define some fundamental concepts and notations that will be applied throughout the paper. Consider graphene and its derivatives' carbon atoms and bonds to be the vertex set $V(G)$ and edge set $E(G)$ of a simple graph respectively. The number of atoms to which a carbon atom is connected can be defined as $d(u)$, the degree of vertex u .

Three types of measurements are defined for each edge based on the degrees of end vertices and they are given below [1]. For an $e = uv \in E(G)$,

- $m^+(e) = d(u) + d(v)$
- $m^-(e) = d(u) - d(v)$
- $m^*(e) = d(u)d(v)$

Using these measurements, we now present various degree-based topological descriptors [1, 21–29] in Table 1.

Table 1: Degree-based topological indices

Topological index	Notation	Mathematical expression
First Zagreb	M_1	$\sum_{e \in E(G)} m^+(e)$
Second Zagreb	M_2	$\sum_{e \in E(G)} m^*(e)$
Randić	R	$\sum_{e \in E(G)} \frac{1}{\sqrt{m^*(e)}}$
Atom Bond Connectivity	ABC	$\sum_{e \in E(G)} \sqrt{\frac{m^+(e) - 2}{m^*(e)}}$
Harmonic	H	$\sum_{e \in E(G)} \frac{2}{m^+(e)}$
Sum Connectivity	SC	$\sum_{e \in E(G)} \frac{1}{\sqrt{m^+(e)}}$

Hyper Zagreb	$HM = \sum_{e \in E(G)} (m^+(e))^2$
Geometric Arithmetic	$GA = \sum_{e \in E(G)} 2 \frac{\sqrt{m^*(e)}}{m^+(e)}$
Irregularity Measure	$irr = \sum_{e \in E(G)} m^-(e) $
Sigma	$\sigma = \sum_{e \in E(G)} (m^-(e))^2$
Forgotten	$F = \sum_{e \in E(G)} ((m^+(e))^2 - 2m^*(e))$
Symmetric Division Degree	$SDD = \sum_{e \in E(G)} \left(\frac{(m^+(e))^2 - 2m^*(e)}{m^*(e)} \right)$
Augmented Zagreb	$AZ = \sum_{e \in E(G)} \left(\frac{m^*(e)}{m^+(e) - 2} \right)^3$

By considering X as the degree-based topological descriptors of G , it is defined in general as.

$$X(G) = \sum_{e \in E(G)} f(e)$$

where f is a structural functional that characterize the bond-additive topological index. For example, in the case of augmented Zagreb index,

$$f(e) = \left(\frac{m^*(e)}{m^+(e) - 2} \right)^3$$

The above-listed topological indices have potential applications in drug design, QSPR/QSAR analysis of molecules, thermodynamics, and so on. For example, it has been shown that there exists a good amount of correlation between the atom bond connectivity index, boiling points, and heats of formation of certain classes of isomeric octanes [4].

Graph entropy was introduced as an effort to characterize the complexity of graphs [30]. Even though it was introduced to express the complexity of communication and transmission of information, now it has major applications in different sciences like physical dissipative structures, biological systems, engineering sectors and so on [3]. There are two categories of graph entropies, deterministic and probabilistic. This work deals with the probabilistic category since it is widely applied in different fields like communication and characterization of chemical structures. Probabilistic methods are further classified into intrinsic and extrinsic categories. In intrinsic measures, a graph is partitioned into components sharing similar structures and a probability distribution is found over those

components. For extrinsic measures, a probability function is assigned to elements of the graph, i.e., vertices or edges. The numerical value of probabilistic measures of graph complexity is obtained by applying an entropy function to this probability distribution function [30]. Though many approaches to determining probabilistic entropy exist, Shannon's model is the leading one and we used the same for our computation.

In communication and transmission of information, the probability functions are assigned for each elements of the information in the form of symbols x_1, x_2, \dots, x_n and then the Shannon's original information entropy(h) measure is defined for it as,

$$h = - \sum_{i=1}^n p_i \log(p_i)$$

where $p_i = \frac{N_i}{N}$ and N_i denote the number of times x_i appear in the information and N is the total length of information [3]. In the case of chemical graphs, this is modified in order to characterize the structural property of the graphs. Edges of the chemical graph are considered as elements and probability value assigned to each edge using topological indices.

The entropy measured using that topological index X is defined as [3,31]

$$ENT_X(G) = - \sum_{e \in E(G)} p_e \log(p_e)$$

where the probability function p_e is given by

$$p_e = \frac{f(e)}{\sum_{e \in E(G)} f(e)} = \frac{f(e)}{X(G)}$$

Therefore,

$$\begin{aligned} ENT_X(G) &= - \sum_{e \in E(G)} p_e \log(p_e) \\ &= - \sum_{e \in E(G)} \frac{f(e)}{X(G)} \log \left(\frac{f(e)}{X(G)} \right) \\ &= - \sum_{e \in E(G)} \frac{f(e)}{X(G)} [\log(f(e)) - \log(X(G))] \\ &= - \frac{1}{X(G)} \sum_{e \in E(G)} f(e) [\log(f(e)) - \log(X(G))] \\ &= \log(X(G)) - \frac{1}{X(G)} \sum_{e \in E(G)} f(e) \log(f(e)) \end{aligned} \tag{1}$$

The formula above can be employed for the determination of graph entropies in the next section.

3 Main Results

In the first part of this section, the analytical expressions for various degree-based topological descriptors for β and γ types of graphene, graphyne and graphdiyne nanoribbons are derived. Then probabilistic entropy values for these nanoribbons are calculated and tabulated using computed topological indices. Entropy values are then plotted graphically and studied to find the regularities and irregularities of entropy values calculated using different topological descriptors. Crystal structures of various graphene derivatives under our consideration are shown in Figure 1. The red coloured carbon atoms are sp^2 hybridized and grey coloured carbon atoms are sp hybridized.

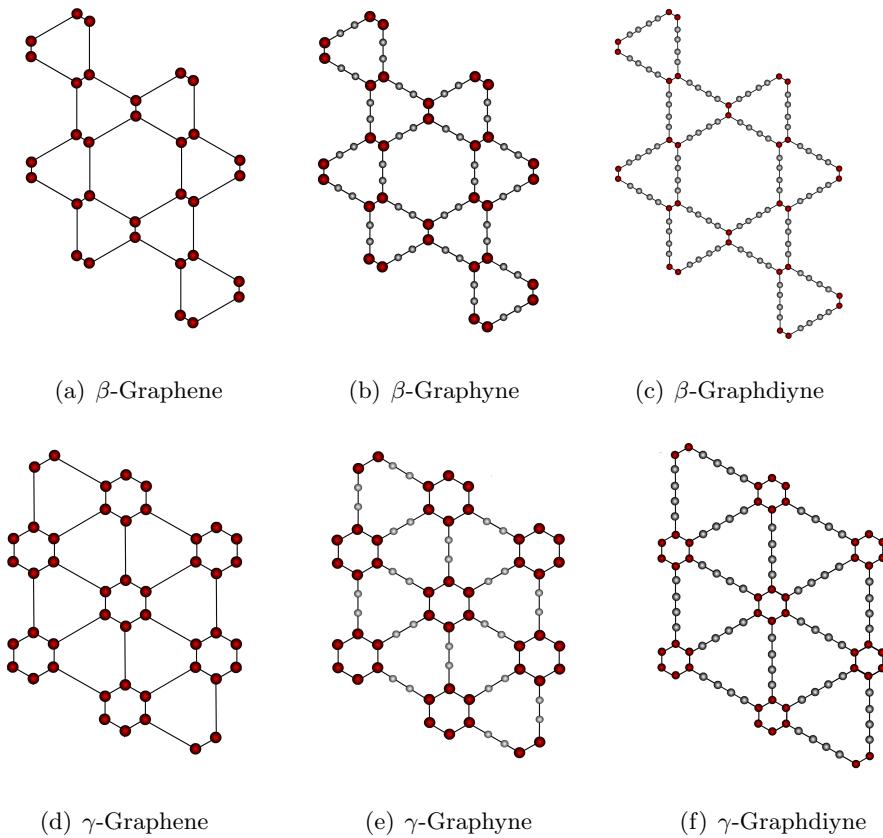


Figure 1: Crystal structures of β and γ graphene and their derivatives

We will use the notations $\beta\text{-}GN$ and $\gamma\text{-}GN$ to denote β and γ graphene, $\beta\text{-}GyN$ and $\gamma\text{-}GyN$ for β and γ graphyne and $\beta\text{-}GdN$ and $\gamma\text{-}GdN$ to denote β and γ graphdiyne structures. The structures of $\beta\text{-}GdN$ and $\gamma\text{-}GdN$ are given in Figures 2–3. Corresponding β and γ structures for graphyne can be obtained by removing two sp hybridized atoms between every pair of sp^2 hybridized carbon atoms. Deleting every sp hybridized atoms from Figures 2–3 and retaining only the sp^2 hybridized carbon atoms will yield respective structures of $\beta, \gamma\text{-}GN$. Throughout the paper, we will use m and n to denote the number of rows and columns of basic crystal structures of the compounds in the

nanoribbon. Then the total number of vertices and edges these nanoribbons are given in Table 2.

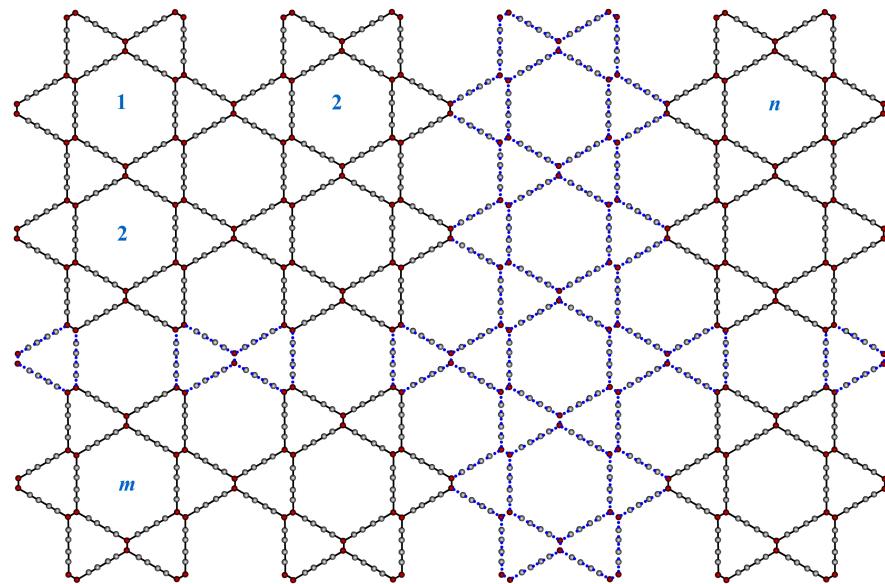


Figure 2: β -Graphdiyne nanoribbon $\beta\text{-GdN}(m, n)$

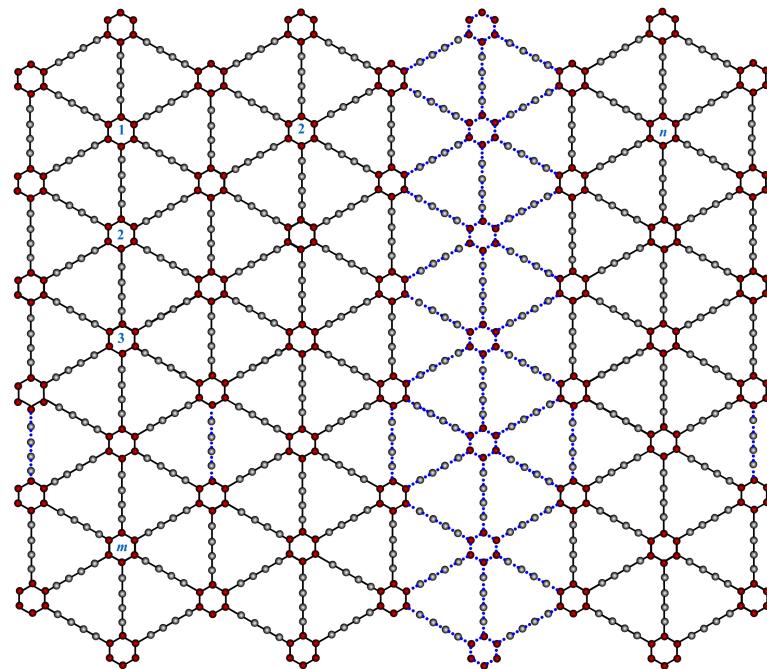


Figure 3: γ -Graphdiyne nanoribbon $\gamma\text{-GdN}(m, n)$

Table 2: Total number of vertices and edges of graphene and its derivatives

S.No.	G	Notation	$ V(G) $	$ E(G) $
1	β graphene	$\beta\text{-}GN$	$12mn + 2m + 10n$	$18mn + m + 11n$
2	γ graphene	$\gamma\text{-}GN$	$12mn + 6m + 18n + 6$	$18mn + 7m + 23n + 6$
3	β graphyne	$\beta\text{-}GyN$	$36mn + 2m + 24n$	$42mn + m + 23n$
4	γ graphyne	$\gamma\text{-}GyN$	$24mn + 8m + 28n + 6$	$30mn + 9m + 33n + 6$
5	β graphdiyne	$\beta\text{-}GdN$	$60mn + 2m + 34n$	$66nm + m + 35n$
6	γ graphdiyne	$\gamma\text{-}GdN$	$36mn + 10m + 38n + 6$	$42mn + 11m + 43n + 6$

3.1 Degree-based topological indices for graphene derivatives

An efficient edge partition method is presented to calculate various degree-based topological descriptors for different graphene derivative nanoribbons under consideration. To find the degree-based indices, first edge set is partitioned into different classes according to the degree of the end vertices of each edge in such a way that the ordered pairs of the degrees of the end vertices for the partitions are $(2, 2)$, $(2, 3)$ and $(3, 3)$. In the following, we use the notation d_{ij} , $i \leq j$ to denote the number of edges having i and j as the degrees of their end vertices. The values of d_{22} , d_{23} and d_{33} are given in Table 3.

 Table 3: The edge partition of graphene derivative nanoribbons G based on the degree of end vertices

S. No.	G	d_{22}	d_{23}	d_{33}
1	$\beta\text{-}GN$	$2m + 4n$	$4m + 8n$	$18mn - 5m - n$
2	$\gamma\text{-}GN$	$2m + 4n + 6$	$4m + 8n$	$18mn + m + 11n$
3	$\beta\text{-}GyN$	$12mn + 6m + 18n$	$24mn - 4m + 4n$	$6mn - m + n$
4	$\gamma\text{-}GyN$	$6mn + 3m + 9n + 6$	$12mn + 6m + 18n$	$12mn + 6n$
5	$\beta\text{-}GdN$	$36mn + 6m + 30n$	$24mn + 4m - 4n$	$6mn - m + n$
6	$\gamma\text{-}GdN$	$18mn + 5m + 19n + 6$	$12mn + 6m + 18n$	$12mn + 6n$

To compute each index, it is enough to calculate the values of $f(e)$ for one edge in each disjoint classes $\{e_{22}, e_{23}, e_{33}\}$ and then multiply them with total number of edges in respective classes. Finally, we add them up to get the exact analytical expression for each index.

$$X(G) = d_{22} \times f(e_{22}) + d_{23} \times f(e_{23}) + d_{33} \times f(e_{33}) \quad (2)$$

By substituting the values of d_{22} , d_{23} and d_{33} corresponding to $\beta\text{-}GN$, $\gamma\text{-}GN$, $\beta\text{-}GyN$, $\gamma\text{-}GyN$, $\beta\text{-}GdN$ and $\gamma\text{-}GdN$ in Eq. (2), we have

$$(i) \quad X(\beta\text{-GN}) = (2m + 4n)f(e_{22}) + (4m + 8n)f(e_{23}) + (18mn - 5m - n)f(e_{33})$$

$$(ii) \quad X(\gamma\text{-GN}) = (2m + 4n + 6)f(e_{22}) + (4m + 8n)f(e_{23}) + (18mn + m + 11n)f(e_{33})$$

$$(iii) \quad X(\beta\text{-GyN}) = (12mn + 6m + 18n)f(e_{22}) + (24mn - 4m + 4n)f(e_{23}) + (6mn - m + n)f(e_{33})$$

$$(iv) \quad X(\gamma\text{-GyN}) = (6mn + 3m + 9n + 6)f(e_{22}) + (12mn + 6m + 18n)f(e_{23}) + (12mn + 6n)f(e_{33})$$

$$(v) \quad X(\beta\text{-GdN}) = (36mn + 6m + 30n)f(e_{22}) + (24mn + 4m - 4n)f(e_{23}) + (6mn - m + n)f(e_{33})$$

$$(vi) \quad X(\gamma\text{-GdN}) = (18mn + 5m + 19n + 6)f(e_{22}) + (12mn + 6m + 18n)f(e_{23}) + (12mn + 6n)f(e_{33})$$

After substituting the values of $f(e_{22}), f(e_{23})$ and $f(e_{33})$ in these results, we obtain the following Theorems 3.1 - 3.3.

Theorem 3.1. Let G_1, G_2 denote β -GN and γ -GN nanoribbons respectively, $m, n \geq 1$. Then

1. β -Graphene

$$M_1(G_1) = 108mn - 2m + 50n$$

$$M_2(G_1) = 162mn - 13m + 55n$$

$$R(G_1) = \frac{1}{3}(18mn + (2\sqrt{6} - 2)m + (4\sqrt{6} + 5)n)$$

$$ABC(G_1) = \frac{1}{3}(36mn + m(9\sqrt{2} - 10) + n(18\sqrt{2} - 2))$$

$$H(G_1) = \frac{1}{15}(90mn + 14m + 73n)$$

$$SC(G_1) = \frac{1}{30}(90\sqrt{6}mn + (24\sqrt{5} - 25\sqrt{6} + 30)m + (48\sqrt{5} - 5\sqrt{6} + 60)n)$$

$$HM(G_1) = 648mn + 228n - 48m$$

$$GA(G_1) = \frac{1}{5}(90mn + (8\sqrt{6} - 15)m + (16\sqrt{6} + 15)n)$$

$$irr(G_1) = \sigma(G) = 4m + 8n$$

$$F(G_1) = 324mn + 118n - 22m$$

$$SDD(G_1) = \frac{2}{3}(54mn + 4m + 35n)$$

$$AZ(G_1) = \frac{1}{16}(1458mn + 107m + 943n)$$

2. γ -Graphene

$$M_1(G_2) = 108mn + 34m + 122n + 24$$

$$M_2(G_2) = 162mn + 41m + 163n + 24$$

$$\begin{aligned}
R(G_2) &= \frac{1}{3}(18mn + (2\sqrt{6} + 4)m + (4\sqrt{6} + 17)n + 9) \\
ABC(G_2) &= \frac{1}{3}(36mn + (9\sqrt{2} + 2)m + (18\sqrt{2} + 22)n + 9\sqrt{2}) \\
H(G_2) &= \frac{1}{15}(90mn + 44m + 133n + 45) \\
SC(G_2) &= \frac{1}{30}(90\sqrt{6}mn + (24\sqrt{5} + 5\sqrt{6} + 30)m + (48\sqrt{5} + 55\sqrt{6} + 60)n + 90) \\
HM(G_2) &= 648mn + 660n + 168m + 96 \\
GA(G_2) &= \frac{1}{5}(90mn + m(8\sqrt{6} + 15) + n(16\sqrt{6} + 75) + 30) \\
irr(G_2) &= \sigma(G) = 4m + 8n \\
F(G_2) &= 324mn + 86m + 334n + 48 \\
SDD(G_2) &= \frac{2}{3}(54mn + 22m + 71n + 18) \\
AZ(G_2) &= \frac{1}{16}(1458mn + 593m + 1915n + 768)
\end{aligned}$$

Theorem 3.2. Let G_3, G_4 denote β -GyN and γ -GyN nanoribbons respectively, $m, n \geq 1$. Then

1. β -Graphyne

$$\begin{aligned}
M_1(G_3) &= 204mn - 2m + 98n \\
M_2(G_3) &= 246mn - 9m + 105n \\
R(G_3) &= \frac{2}{3}((6\sqrt{6} + 12)mn - (\sqrt{6} - 4)m + (\sqrt{6} + 14)n) \\
ABC(G_3) &= \frac{1}{3}((54\sqrt{2} + 12)mn + (3\sqrt{2} - 2)m + (33\sqrt{2} + 2)n) \\
H(G_3) &= \frac{4}{15}(66mn + 4m + 41n) \\
SC(G_3) &= \frac{1}{30}((144\sqrt{5} + 30\sqrt{6} + 180)mn - (24\sqrt{5} + 5\sqrt{6} - 90)m + (24\sqrt{5} + 5\sqrt{6} + 270)n) \\
HM(G_3) &= 1008mn - 40m + 424n \\
GA(G_3) &= \frac{1}{5}((48\sqrt{6} + 90)mn - (8\sqrt{6} - 25)m + (8\sqrt{6} + 95)n) \\
irr(G_3) &= \sigma(G) = 24mn + 4m - 4n \\
F(G) &= 516mn - 22m + 214n \\
SDD(G_3) &= \frac{4}{3}(66mn + m + 35n) \\
AZ(G_3) &= \frac{1}{16}(3558mn + 431m + 2641n)
\end{aligned}$$

2. γ -Graphyne

$$\begin{aligned}
M_1(G_4) &= 156mn + 42m + 162n + 24 \\
M_2(G_4) &= 204mn + 48m + 198n + 24 \\
R(G_4) &= \frac{1}{2}((4\sqrt{6} + 14)mn + (2\sqrt{6} + 3)m + (6\sqrt{6} + 13)n + 6) \\
ABC(G_4) &= \frac{1}{2}((18\sqrt{2} + 16)mn + 9\sqrt{2}m + (27\sqrt{2} + 8)n + 6\sqrt{2}) \\
H(G_4) &= \frac{1}{10}(118mn + 39m + 137n + 30) \\
SC(G_4) &= \frac{1}{10}((24\sqrt{5} + 20\sqrt{6} + 30)mn + (12\sqrt{5} + 15)m + (36\sqrt{5} + 10\sqrt{6} + 45)n + 30) \\
HM(G_4) &= 828mn + 198m + 810n + 96
\end{aligned}$$

$$GA(G_4) = \frac{3}{5}((8\sqrt{6} + 30)mn + (4\sqrt{6} + 5)m + (12\sqrt{6} + 25)n + 10)$$

$$irr(G_4) = \sigma(G) = 12mn + 6m + 18n$$

$$F(G) = 420mn + 102m + 414n + 48$$

$$SDD(G_4) = 62mn + 19m + 69n + 12$$

$$AZ(G_4) = \frac{3}{8}(418mn + 128m + 465n + 128)$$

Theorem 3.3. Let G_5, G_6 denote β -GdN and γ -GdN nanoribbons respectively, $m, n \geq 1$. Then

1. β -Graphdiyne

$$M_1(G_5) = 300mn - 2m + 146n$$

$$M_2(G_5) = 342mn - 9m + 153n$$

$$R(G_5) = \frac{2}{3}((6\sqrt{6} + 30)mn - (\sqrt{6} - 4)m + (\sqrt{6} + 23)n)$$

$$ABC(G_5) = \frac{1}{3}((90\sqrt{2} + 12)mn + (3\sqrt{2} - 2)m + (51\sqrt{2} + 2)n)$$

$$H(G_5) = \frac{2}{15}(222mn + 8m + 127n)$$

$$SC(G_5) = \frac{1}{30}((144\sqrt{5} + 30\sqrt{6} + 540)mn - (24\sqrt{5} + 5\sqrt{6} - 90)m + (24\sqrt{5} + 5\sqrt{6} + 450)n)$$

$$HM(G_5) = 1392mn - 40m + 616n$$

$$GA(G_5) = \frac{1}{5}((48\sqrt{6} + 210)mn - (8\sqrt{6} - 25)m + (8\sqrt{6} + 155)n)$$

$$irr(G_5) = \sigma(G) = 24mn - 4m + 4n$$

$$F(G_5) = 708mn - 22m + 310n$$

$$SDD(G_5) = \frac{4}{3}(102mn + m + 53n)$$

$$AZ(G_5) = \frac{1}{16}(6630mn + 431m + 4177n)$$

2. γ -Graphdiyne

$$M_1(G_6) = 204mn + 50m + 202n + 24$$

$$M_2(G_6) = 252mn + 56m + 238n + 24$$

$$R(G_6) = \frac{1}{2}((4\sqrt{6} + 26)mn + (2\sqrt{6} + 5)m + (6\sqrt{6} + 23)n + 6)$$

$$ABC(G_6) = \frac{1}{2}((30\sqrt{2} + 16)mn + 11\sqrt{2}m + (37\sqrt{2} + 8)n + 6\sqrt{2})$$

$$H(G_6) = \frac{1}{10}(178mn + 49m + 187n + 30)$$

$$SC(G_6) = \frac{1}{10}((24\sqrt{5} + 20\sqrt{6} + 90)mn + (12\sqrt{5} + 25)m + (36\sqrt{5} + 10\sqrt{5} + 95)n + 30)$$

$$HM(G_6) = 1020mn + 230m + 970n + 96$$

$$GA(G_6) = \frac{1}{5}((24\sqrt{6} + 150)mn + (12\sqrt{6} + 25)m + (36\sqrt{6} + 125)n + 30)$$

$$irr(G_6) = \sigma(G) = 12mn + 6m + 18n$$

$$F(G_6) = 516mn + 118m + 494n + 48$$

$$SDD(G_6) = 86mn + 23m + 89n + 12$$

$$AZ(G_6) = \frac{1}{8}(2022mn + 512m + 2035n + 385)$$

3.2 Calculating topological index based entropy values

Calculation of entropy values following the Shannon's approach by defining probability function using degree-based topological indices is explained in this section. We will use Eq. (1) for calculating respective entropies. The method of calculation is demonstrated by finding out entropy value for β -GN nanoribbon using atom bond connectivity index.

Atom bond connectivity entropy for β -GN:

Let G denote β -GN, then using Eq. (1), atom bond connectivity entropy is derived as follows:

$$\begin{aligned} ENT_{ABC}(G) &= \log(ABC(G)) - \frac{1}{ABC(G)} \sum_{e \in E(G)} f(e) \log(f(e)) \\ &= \log(ABC(G)) - \frac{1}{ABC(G)} \sum_{uv \in E(G)} \sqrt{\frac{m^+(e) - 2}{m^*(e)}} \log \left(\sqrt{\frac{m^+(e) - 2}{m^*(e)}} \right) \end{aligned}$$

Upon substitution of various values from Table 3, we obtain the following

$$\begin{aligned} ENT_{ABC}(G) = \log(ABC(G)) - \frac{1}{ABC(G)} &\left[(2m + 4n) \sqrt{\frac{2+2-2}{2 \times 2}} \log \left(\sqrt{\frac{2+2-2}{2 \times 2}} \right) \right. \\ &+ (4m + 8n) \sqrt{\frac{2+3-2}{2 \times 3}} \log \left(\sqrt{\frac{2+3-2}{2 \times 3}} \right) \\ &\left. + (18mn - 5m - n) \sqrt{\frac{3+3-2}{3 \times 3}} \log \left(\sqrt{\frac{3+3-2}{3 \times 3}} \right) \right] \end{aligned}$$

After simplifying this, we obtain

$$\begin{aligned} ENT_{ABC}(G) = \log\left(\frac{1}{3}(36mn + m(9\sqrt{2} - 10) + n(18\sqrt{2} - 2))\right) \\ + \frac{1}{\frac{1}{3}(36mn + m(9\sqrt{2} - 10) + n(18\sqrt{2} - 2))} \times \frac{1}{27021597764222976} \left[131475780704712042mn \right. \\ \left. + (28094916456744111\sqrt{2} - 36521050195753345)m \right. \\ \left. + (56189832913488222\sqrt{2} - 7304210039150669)n \right] \end{aligned}$$

The general entropy expression of each nanoribbons would be lengthy to present as theorems. With respect to each topological index, one can easily derive any degree-based entropies expression by following the above method. Numerical values and graphical representations of different entropies for all the variants of nanoribbons are discussed below in Tables 4 - 6 and Figure 4.

To compare entropy values of β and γ nanoribbons of these graphene and its derivatives corresponding to different topological indices, they can be plotted as graphs like shown in Figure 4. These graphs are plotted by using the values in Tables 4 - 6. While analysing the graph one can observe that

Table 4: Numerical values for degree-based entropies of β -GN and γ -GN nanoribbons when $m = n$

X	β -GN				γ -GN			
	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 2$	$m = 3$	$m = 4$	$m = 5$
M_1	4.5556	5.2813	5.8114	6.2296	4.9185	5.5462	6.0203	6.4022
M_2	4.5315	5.2626	5.7963	6.2169	4.8956	5.5286	6.0061	6.3902
R	4.5531	5.2786	5.8088	6.2272	4.9155	5.5433	6.0177	6.3998
ABC	4.5639	5.2879	5.8168	6.2342	4.9269	5.5526	6.0256	6.4066
H	4.5535	5.2790	5.8092	6.2276	4.9159	5.5437	6.0180	6.4001
SC	4.5618	5.2861	5.8153	6.2328	4.9246	5.5508	6.0241	6.4053
HM	4.5336	5.2643	5.7976	6.2181	4.8972	5.5299	6.0072	6.3912
GA	4.5643	5.2882	5.8171	6.2344	4.9272	5.5529	6.0258	6.4069
irr	3.1781	3.5835	3.8712	4.0943	3.1781	3.5835	3.8712	4.0943
σ	3.1781	3.5835	3.8712	4.0943	3.1781	3.5835	3.8712	4.0943
F	4.5354	5.2658	5.7989	6.2191	4.8985	5.5311	6.0082	6.3920
SDD	4.5637	5.2878	5.8167	6.2341	4.9268	5.5526	6.0255	6.4066
AZ	4.5507	5.2773	5.8080	6.2267	4.9153	5.5432	6.0177	6.3998

Table 5: Numerical values for degree-based entropies of β and γ -GyN nanoribbons when $m = n$

X	β -GyN				γ -GyN			
	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 2$	$m = 3$	$m = 4$	$m = 5$
M_1	5.3652	6.0994	6.6342	7.0553	5.3363	5.9857	6.4724	6.8625
M_2	5.3360	6.0710	6.6063	7.0278	5.3041	5.9537	6.4405	6.8307
R	5.3666	6.1005	6.6351	7.0561	5.3360	5.9852	6.4717	6.8617
ABC	5.3751	6.1091	6.6436	7.0646	5.3468	5.9961	6.4827	6.8728
H	5.3658	6.0998	6.6344	7.0554	5.3358	5.9850	6.4716	6.8617
SC	5.3729	6.1069	6.6414	7.0624	5.3443	5.9936	6.4803	6.8703
HM	5.3347	6.0700	6.6055	7.0271	5.3056	5.9555	6.4424	6.8327
GA	5.3752	6.1092	6.6437	7.0647	5.3471	5.9964	6.4831	6.8731
irr	4.5643	5.3753	5.9506	6.3969	4.5643	5.1930	5.6630	6.0403
σ	4.5643	5.3753	5.9506	6.3969	4.5643	5.1930	5.6630	6.0403
F	5.3330	6.0686	6.6043	7.0261	5.3067	5.9568	6.4439	6.8342
SDD	5.3745	6.1084	6.6430	7.0640	5.3463	5.9957	6.4823	6.8724
AZ	5.3679	6.1014	6.6357	7.0565	5.3332	5.9820	6.4684	6.8582

Table 6: Numerical values for degree-based entropies of β and γ -GdN nanoribbons when $m = n$

X	β -GdN				γ -GdN			
	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 2$	$m = 3$	$m = 4$	$m = 5$
M_1	5.8077	6.5442	7.0845	7.5022	5.6288	6.2892	6.7820	7.1761
M_2	5.7791	6.5151	7.0509	7.4727	5.5894	6.2488	6.7410	7.1347
R	5.8099	6.5464	7.0824	7.5043	5.6301	6.2904	6.7832	7.1772
ABC	5.8170	6.5538	7.0900	7.5119	5.6416	6.3023	6.7954	7.1896
H	5.8092	6.5457	7.0816	7.5035	5.6296	6.2899	6.7827	7.1768
SC	5.8150	6.5518	7.0879	7.5098	5.6388	6.2994	6.7924	7.1866
HM	5.7766	6.5127	7.0486	7.4704	5.5894	6.2489	6.7412	7.1350
GA	5.8171	6.5539	7.0900	7.5120	5.6419	6.3026	6.7957	7.1899
irr	4.5643	5.3753	5.9506	6.3969	4.5643	5.1930	5.6630	6.0403
σ	4.5643	5.3753	5.9506	6.3969	4.5643	5.1930	5.6630	6.0403
F	5.7739	6.5100	7.0460	7.4678	5.5889	6.2486	6.7411	7.1349
SDD	5.8164	6.5532	7.0894	7.5114	5.6412	6.3019	6.7950	7.1892
AZ	5.8121	6.5485	7.0845	7.5064	5.6301	6.2902	6.7829	7.1769

the lines joining entropy measures corresponding to various topological indices are almost straight lines that are parallel to the X -axis except sharp dip at irregularity index. So, it is clear that the entropies based on each degree-based indices are similar except $irr(G)$ and $\sigma(G)$. On the other hand the entropies calculated based on $irr(G)$ and $\sigma(G)$ are same in each graphene, graphyne and graphy-dine structures. From this an inference can be drawn that it is not ideal to use irregularity and sigma indices to calculate the entropies of β and γ versions of these graphene derivatives because even though the whole structure changes, these entropy measures are constant. While the size of the nanoribbon with m rows and n columns where $m = n$ increase, the distance between the lines keep on decreasing, which shows us a possibility of convergence of these lines.

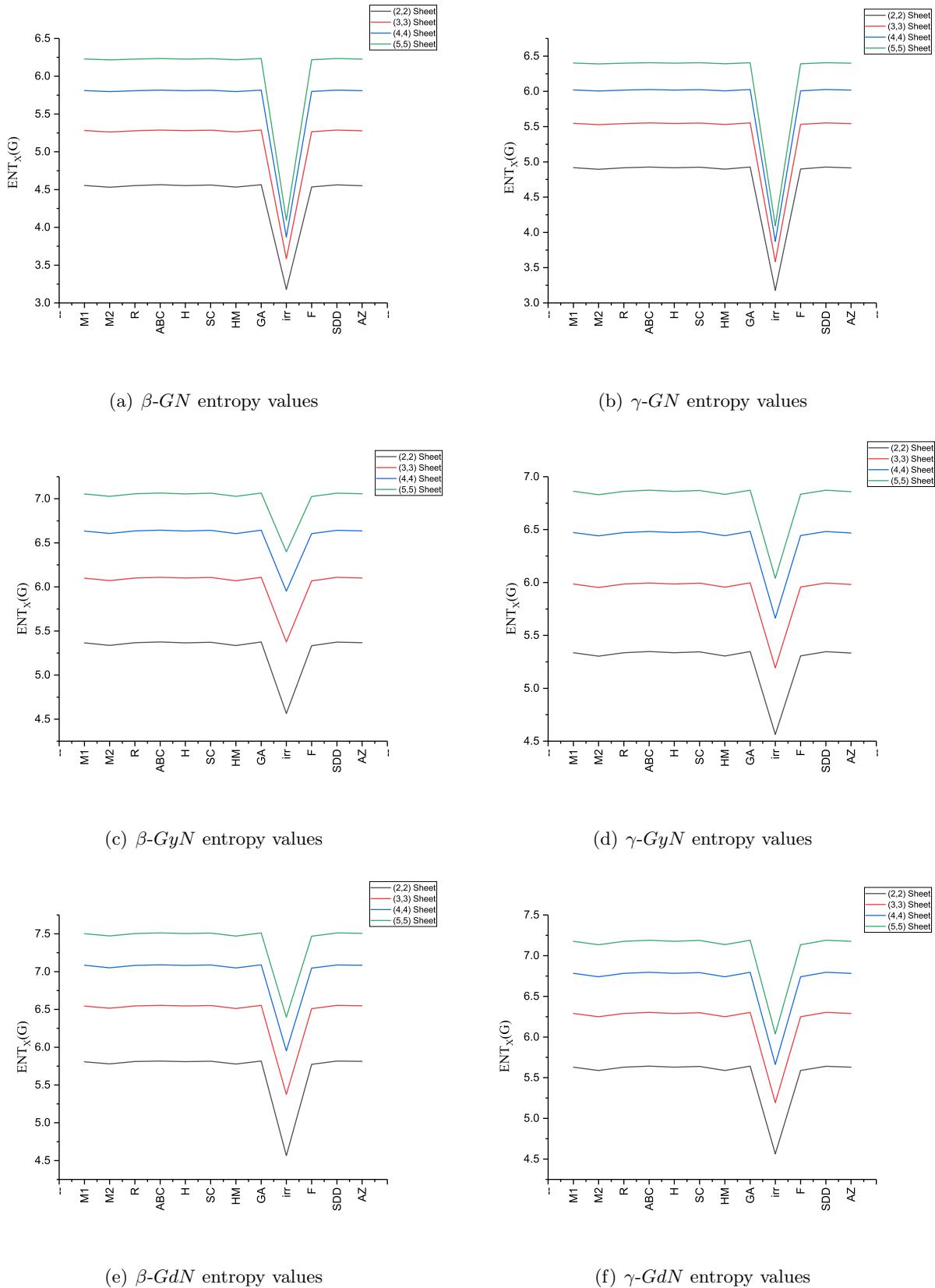


Figure 4: Plotted entropies of β , γ -GN, GyN and GdN nanoribbons

4 Concluding remarks

In this paper, we have presented the generalized analytical expression for degree-based topological indices of β and γ variants of graphene, graphyne and graphydine. These generalised analytical formulations have potential uses because of the relevance of these structures in thermochemistry due to their electrical, optical, and mechanical properties. The indices used to define the probability function in Shannon's formula are also used to generate various probabilistic entropy metrics. Using their respective degree-based topological indices, we establish a relationship between the degree-based entropies of β and γ variants. The findings of this study provide a substantial contribution to QSAR and QSPR by correlating the variants of β and γ nanoribbons with a large quantity of data on physicochemical qualities.

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