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# On R, S and Van entropies of beta graphene

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## Abstract

Topological indices are graph-theoretically based characteristics that allow for the characterization of a molecular structure's underlying connectivity. Degree-based topological indices have been the subject of substantial research and have been connected to numerous chemical characteristics. Gaining relevance is the study of graph entropy indices as a tool for characterizing structural features and as a gauge of the complexity of the connectivity underneath them. The focus of current research is on substructures like beta graphene (β-GN), that are generated from hexagonal honeycomb graphite lattices. In this study, we investigate R, S and Van topological indices of beta graphene structures by using Shannon's entropy model, we generated the graph-based entropies of these structures.

Keywords: Beta graphene, Shannon's entropy, Topological descriptors, Van index, S index, R index

## 1. Introduction

Topological indices, which are structural invariants generated from molecular graphs and determine the fundamental connectivity of the molecular network, have drawn a lot of attention in recent years due to their applications in quantitative structure-activity and quantitative structure-property relationships (QSPR) relations [1-4]. The physicochemical properties of molecular structures have been predicted using degree-based topological indices, which have been the subject of substantial research [1–5]. Through information entropy measurements, the information complexity of complicated chemical structures like GN, GY, and GDY can be identified. The idea of information entropy was initially developed by Shannon to study and measure the complexity of data and information transmission, but it has since been widely used in a range of scientific domains. Studying the complexity of molecular structures and their quantum chemical electron densities [6] is one of the most significant uses of information entropy.

In QSAR and QSPR research, topological indices combined with entropy metrics may be a more effective tool. Information entropy has been discovered to directly correlate with the physical characteristics of fullerenes, including their formal carbon atom oxidation states and rotational symmetry numbers in several types of natural substances [7].

Due to its promising characteristics, including variable band gaps, charge-carrier mobilities, and energy level alignment, two-dimensional (2D) derivatives of graphite structures like GN, GY, and GDY are becoming more and more significant. GN is a 2D sheet made up of hexagons and carbon atoms that have undergone $sp^2$ hybridization. It has attracted significant interest due to its remarkable physical, thermal, mechanical, chemical, and electrical properties [8,9]. Since 2010 when "groundbreaking experiments relating to the 2D substance graphene" won the Nobel Prize in Physics, GN-based materials have drawn a lot of interest [10]. The states of $sp^2$ atoms remain comparable when the bonds connecting three coordinated atoms in a GN layer are replaced by carbyne chains, and GY layers are created [11]. GYs are 2D materials created by adding acetylenic linkages to honeycomb structures made of C atoms that have undergone *sp* hybridization.

Because acetylenic groups are present, these structures exhibit a wide variety of electrical, optical, and mechanical properties [12]. The first synthetic carbon-based nanomaterial, GDY, contains carbon atoms that are $sp^2$ hybridized with benzene rings and *sp* hybridized with acetenyl groups. This brand-new substance, which contains both $sp^2$ and sp hybridized carbon atoms, has been created [13]. The most popular GN and its variant configurations are the α,β,γ-type architectures [14]. Topological indices related to α-type structures have been examined among them [15-17]. Due to their significant applications, topological descriptors for the and structures of the GNs have not yet been explored; however, this calls for further research into the topological indices of these various networks in order to compare and contrast the complexity of these structures [18]. Additionally, fluctuations in the relative entropies of the various types of structures would accompany phase transitions between them, and these variations might be well recorded by the topologically based entropy measurements that we propose here.

For use in a variety of fields, including energy, the environment, future materials, bio-medicine, biosensor, and heat-sink applications, GN has a number of distinctive properties. GN is used in a variety of products, including lithium-ion batteries, flexible or micro-supercapacitors, lithium-air batteries, lithium-sulfur batteries, electrodes for fuel cells, and solar cells [18]. Because of GN's exceptional thermal conductivity, high opacity, and high chemical reactivity, scientists are considering employing it in the biomedical sector[18]. Because of its great conductivity, GN is a fantastic material for use in high-speed electronics. GN could be utilized as an energy storage device in the construction of supercapacitors and nonvolatile memory due to its huge inner surface area [9]. The loading and release of the medication is challenging to control since GN derivatives clump in salt or biological solutions and have some cytotoxicity, despite the fact that they might be employed for drug delivery [19]. Due to the presence of acetylenic groups, GYs are thought to have potential uses in optoelectronic devices [20].

Small GY flakes can be dispersed throughout a polymer matrix in composite materials to increase stiffness and strength. The band gap of GY can be mechanically changed, according to computational research, making it possible to produce transistors with a variety of characteristics that depend on the band gap with relative ease. Due of GY's enormous elastic strain range, it is possible to repeatedly stretch it without permanently changing its shape. As a result, it has reliable electromechanical coupling for a variety of uses, including temperature monitoring [21,22]. Field-Effect Transistors (FETs), solar cells, and a range of other applications [24,25] are just a few examples where GDY's exceptional electrical properties are used.

Degree based and neighboring sum degree based entropies of the β-GN, β-GY, and β-GDY and structures have been calculted in the references [26,27].

In this work, we investigate the R, S, and Van topological indices and related entropy measures for the β-GN structures.

## 2. Topological indices and entropies

Let *G* be a chemical graph and *v* a vertex(atom) of *G*. The degree of vertex *v*, denoted as deg*(v)*, is the total number of edges which is incident to *v*. $N(v)$ is the set of all neighbouring vertices of *v*. The sum degree of the vertex *v*, denoted as $S_v$, is the total number of all the degrees of neighbouring vertices of *v*. The multiplication degree of the vertex *v*, denoted as $M_v$, is the multiplication of total number of all the degrees of neighbouring vertices of *v*. Van degree of the vertex *v*, defined as; $van(v) = \frac{S_v}{M_v}$ [28]. Also, reverse Van degree of the vertex *v*, defined as; $rvan(v) = \frac{M_v}{S_v}$. Van topological indices defined as [28];

The first Van index of a simple connected graph *G* defined as; $Van^1(G) = \sum_{v\in V(G)} van(v)^2$ .

The second Van index of a simple connected graph *G* defined as; $Van^2(G) = \sum_{uv\in E(G)} van(u)van(v)$.

The third Van index of a simple connected graph *G* defined as; $Van^3(G) = \sum_{uv\in E(G)}[van(u) + van(v)]$.

The first reverse Van index of a simple connected graph *G* defined as; $Van^{1r}(G) = \sum_{v\in V(G)} rvan(v)^2$ .

The second reverse Van index of a simple connected graph *G* defined as; $Van^{2r}(G) = \sum_{uv\in E(G)} rvan(u)rvan(v)$.

The third reverse Van index of a simple connected graph *G* defined as; $Van^{3r}(G) = \sum_{uv\in E(G)}[rvan(u) + rvan(v)]$.

R degree of the vertex *v*, defined as; $r(v) = M_v + S_v$ [29]. Also, reverse R degree of the vertex *v*, defined as; $rr(v) = \frac{1}{M_v+S_v}$. R topological indices defined as [29]:

The first R index of a simple connected graph *G* defined as; $R^1(G) = \sum_{v\in V(G)} r(v)^2$ .

The second R index of a simple connected graph *G* defined as; $R^2(G) = \sum_{uv\in E(G)} r(u)r(v)$.

The third R index of a simple connected graph *G* defined as; $R^3(G) = \sum_{uv\in E(G)}[r(u) + r(v)]$.

The first reverse R index of a simple connected graph *G* defined as; $R^{1r}(G) = \sum_{v\in V(G)} rr(v)^2$ .

The second reverse R index of a simple connected graph *G* defined as; $R^{2r}(G) = \sum_{uv\in E(G)} rr(u)rr(v)$.

The third reverse R index of a simple connected graph *G* defined as; $R^{3r}(G) = \sum_{uv\in E(G)}[rr(u) + rr(v)]$.

S degree of the vertex *v*, defined as; $s(v) = |M_v - S_v|$ [30]. Also, reverse S degree of the vertex *v*, defined as; $rs(v) = \frac{1}{|M_v-S_v|+1}$ . R topological indices defined as [30]:

The first S index of a simple connected graph *G* defined as; $S^1(G) = \sum_{v\in V(G)} s(v)^2$ .

The second S index of a simple connected graph *G* defined as; $S^2(G) = \sum_{uv\in E(G)} s(u)s(v)$.

The third S index of a simple connected graph *G* defined as; $S^3(G) = \sum_{uv\in E(G)}[s(u) + s(v)]$.

The first reverse S index of a simple connected graph *G* defined as; $S^{1r}(G) = \sum_{v\in V(G)} rs(v)^2$ .

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The second reverse S index of a simple connected graph $G$ defined as; $S^{2r}(G)=\sum_{uv\in E(G)} rs(u)rs(v)$.

The third reverse S index of a simple connected graph $G$ defined as; $S^{3r}(G)=\sum_{uv\in E(G)}[rs(u)+rs(v)]$.

Entropy is a measure of the unpredictable nature of pertinent information or a technique to gauge the uncertainty of a system, according to Shannon's fundamental work. The modern information theory was founded on the findings of this research. The structural informativeness of a network has been measured using entropy formulas [31]. Though information theory was first only employed in linguistics and electrical engineering, its adaptability led to its usage in fields like biology and chemistry [32] as well as graph theory for chemical networks. In order to measure the topological information of chemical networks and graphs, the concept of graph entropy was proposed. Based on the orbits of the vertex points, Rashevsky [33] created the idea of graph entropy.

Mathematicians can associate graph elements like edges and vertices with probability distributions using the graph entropy measures, which are divided into intrinsic and extrinsic measures. Numerous disciplines, such as chemistry, ecology, sociology, and biology, use graph entropies extensively [34,35]. Dehmer developed graph entropies based on information functionals, analyzed their characteristics, and introduced them [36,37]. In addition to analyzing the walk-based graph entropies, Estrada et al. [38] presented a physically sound measure of graph entropy. Applications for entropy network measurements include investigating the biological and chemical properties of molecular graphs as well as quantitatively defining a molecular structure [39]. There are numerous uses for entropy metrics in the study of chemical graphs. They are used to examine chemical characteristics of complicated networks. According to the definition of topological index $T$ based Shannon's entropy [40] for 2D networks, calculated as,

$$\boldsymbol{Entropy_T(G)=Ent_T(G)}$$

$$=\boldsymbol{log(T(G))-\frac{1}{T(G)}\sum_{uv\in E(G)} f(uv)log\big(f(uv)\big)} \qquad (1)$$

where $f$ is the topological index's structural-functional identifier. In the case of the second Van index, for instance

$\boldsymbol{f(uv)=van(u)van(v)}$ and in the case of the third Van index, for instance $\boldsymbol{f(uv)=van(u)+van(v)}$.

**3. Main results**

In this section we firstly calculate Van, R, S topological indcies and after that corresponding entropies of these indices for beta graphene families. According to its structural similarities to graphite, fullerene, carbon nanotubes, graphyne, and other closely related materials including amorphous carbon, carbon fiber, and charcoal, as well as aromatic compounds like polycyclic aromatic hydrocarbons, graphene can be seen as the fundamental building block of these materials. Despite having extremely various sizes and shapes, they all have some characteristics because they have the same structural makeup. As a result, understanding the above-mentioned materials is aided by the structural research of graphene. Figure 1 shows that the (2,1) beta graphene (β-GN(2,1)). It follows that the vertex set V(β-GN(m,n)) = 12mn + 2m + 10n and the edge set E(β-GN(m,n)) = 18mn + m + 11n make up the β-GN(m, n).

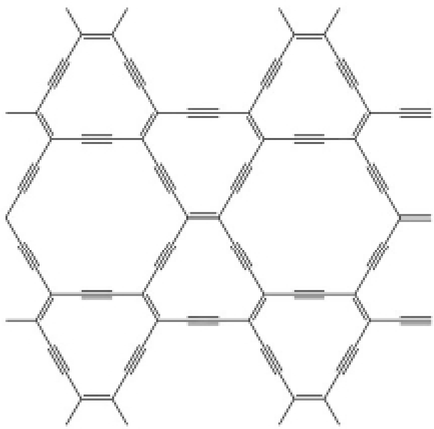

*Figure 1 2D model for beta graphene $\beta$-GN(2,1)*

β-GN(m,n) beta graphene has the following sum and multiplication edge end vertex degree partitions which are shown in Table 1.

**Table 1** Edge end vertex sum and multiplication degree partition of β-GN(m,n).

| Cardinality | $(S_u,S_v)$ | $(M_u,M_v)$ |
|---|---|---|
| $4m+2n$ | (5,5) | (6,6) |
| $4m+8$ | (5,7) | (6,12) |
| $4m+4n-8$ | (5,8) | (6,18) |
| $2m+4$ | (7,9) | (12,27) |
| $4m-8$ | (8,8) | (18,18) |

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| | | |
|---|---|---|
| $8m+4n-12$ | (8,9) | (18,27) |
| $18mn-21m-n+10$ | (9,9) | (27,27) |

With the help of Table 1, the Van, R and S edge end vertex degree partitions of β-GN(m,n) are calculated and given in Tables 2-4.

**Table 2** Van edge end vertex degree partition of β-GN(m,n)

| Cardinality | $(van(u), van(v))$ | $(rvan(u), rvan(v))$ |
|---|---|---|
| $4m+2n$ | (5/6,5/6) | (6/5,6/5) |
| $4m+8$ | (5/6,7/12) | (6/5,12/7) |
| $4m+4n-8$ | (5/6,4/9) | (6/5,9/4) |
| $2m+4$ | (7/12,1/3) | (12/7,3) |
| $4m-8$ | (4/9,4/9) | (9/4,9/4) |
| $8m+4n-12$ | (4/9,1/3) | (9/4,3) |
| $18mn-21m-n+10$ | (1/3,1/3) | (3,3) |

**Table 3** S edge end vertex degree partition of β-GN(m,n)

| Cardinality | $(s(u), s(v))$ | $(rs(u), rs(v))$ |
|---|---|---|
| $4m+2n$ | (1,1) | (1/2,1/2) |
| $4m+8$ | (1,5) | (1/2,1/6) |
| $4m+4n-8$ | (1,10) | (1/2,1/11) |
| $2m+4$ | (5,18) | (1/6,1/19) |
| $4m-8$ | (10,10) | (1/11,1/11) |
| $8m+4n-12$ | (10,18) | (1/11,1/19) |
| $18mn-21m-n+10$ | (18,18) | (1/19,1/19) |

**Table 4** R edge end vertex degree partition of of β-GN(m,n)

| Cardinality | $(r(u), r(v))$ | $(rr(u), rr(v))$ |
|---|---|---|
| $4m+2n$ | (11,11) | (1/11,1/11) |
| $4m+8$ | (11,19) | (1/11,1/19) |
| $4m+4n-8$ | (11,26) | (1/11,1/26) |
| $2m+4$ | (19,36) | (1/19,1/36) |
| $4m-8$ | (26,26) | (1/26,1/26) |
| $8m+4n-12$ | (26,36) | (1/27,1/36) |
| $18mn-21m-n+10$ | (36,36) | (1/36,1/36) |

### 3.1 Topological indices beta graphene

The following theorems give the overall Van, R, and S indices representation of β-GN(m,n).

**Theorem 1.** Let β-GN(m,n) be a beta graphene network. Then, the second Van index of β-GN(m,n) is;

$$Van^2(\beta-\mathrm{GN(m,n)}) = 2mn+\frac{505}{81}m+\frac{181}{54}n-\frac{44}{81}$$

*Proof.* Considering that β-GN(m,n) is a beta graphene network. By definition;

$$Van^2(\beta-\mathrm{GN(m,n)}) = \sum\nolimits_{uv\in E(\beta-\mathrm{GN(m,n)})} van(u)van(v)$$

As a result by using Table 2;

$$\begin{aligned} Van^2(\beta-\mathrm{GN(m,n)}) &= (4m+2n)\times\frac{5}{6}\times\frac{5}{6}+(4m+8)\times\frac{5}{6}\times\frac{7}{12} + (4m+4n-8)\times\frac{5}{6}\times\frac{4}{9} \\ &+(2m+4)\times\frac{7}{12}\times\frac{1}{3}+(4m-8)\times\frac{4}{9}\times\frac{4}{9} + (8m+4n-12)\times\frac{4}{9}\times\frac{1}{3} \\ &+(18mn-21m-n+10)\times\frac{1}{3}\times\frac{1}{3}\end{aligned}$$

the conclusion follows.

3D plot of the second Van index of beta graphene network, β-GN(m,n), is shown in Figure 2.

**Theorem 2.** Let β-GN(m,n) be a graphene network. Then, the second reverse Van index of β-GN(m,n) is;

$$Van^{2r}(\beta-\mathrm{GN(m,n)}) = 162mn-\frac{55773}{700}m+\frac{792}{25}n-\frac{225}{14}$$

*Proof.* Considering that β-GN(m,n) is a beta graphene network. By definition;

$$Van^{2r}(G\beta - \mathrm{GN}(\mathrm{m,n})) = \sum_{uv\in E(\beta-\mathrm{GN}(\mathrm{m,n}))} rvan(u)rvan(v)$$

As a result by using Table 2;

$$Van^{2r}(\beta - \mathrm{GN}(\mathrm{m,n})) = (4m+2n)\times\frac{6}{5}\times\frac{6}{5}+(4m+8)\times\frac{6}{5}\times\frac{12}{7} + (4m+4n-8)\times\frac{6}{5}\times\frac{9}{4}$$
$$+(2m+4)\times\frac{12}{7}\times 3+(4m-8)\times\frac{9}{4}\times\frac{9}{4} + (8m+4n-12)\times\frac{9}{4}\times 3$$
$$+(18mn-21m-n+10)\times 3\times 3$$

the conclusion follows.

3D plot of the second reverse Van index of beta graphene network, β-GN(m,n), is shown in Figure 3.

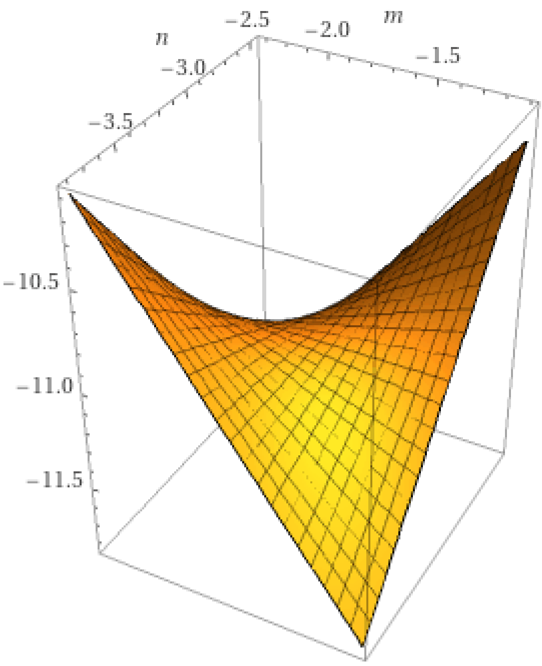

*Figure 2 3D plot of second Van index of β-GN(m,n)*

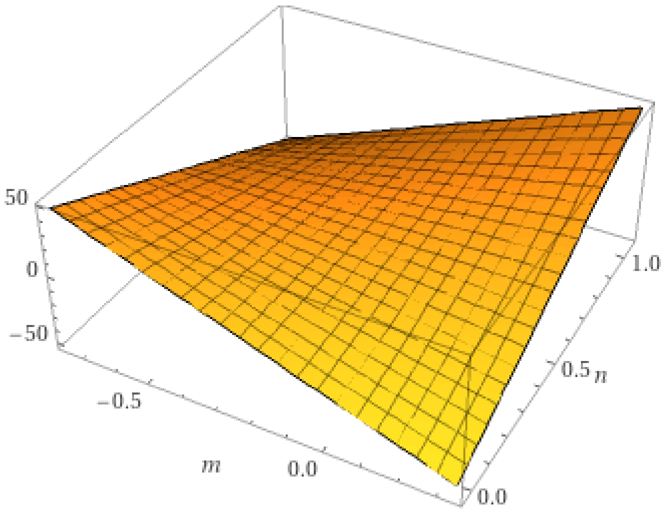

*Figure 3 3D plot of second reverse Van index of β-GN(m,n)*

**Theorem 3.** Let β-GN(m,n) be a graphene network. Then, the third Van index of β-GN(m,n) is;

$$Van^{3}(\beta - \mathrm{GN}(\mathrm{m,n})) = 12mn+\frac{271}{18}m-\frac{98}{9}n-5$$

*Proof.* Considering that β-GN(m,n) is a beta graphene network. By definition;

$$Van^{3}(\beta - \mathrm{GN}(\mathrm{m,n})) = \sum_{uv\in E(\beta-\mathrm{GN}(\mathrm{m,n}))} (van(u)+van(v))$$

As a result by using Table 2;

$$Van^{3}(G\beta - \mathrm{GN}(\mathrm{m,n})) = (4m+2n)\times\left(\frac{5}{6}+\frac{5}{6}\right) + (4m+8)\times\left(\frac{5}{6}+\frac{7}{12}\right)+(4m+4n-8)\times\left(\frac{5}{6}+\frac{4}{9}\right)$$
$$+(2m+4)\times\left(\frac{7}{12}+\frac{1}{3}\right)+(4m-8)\times\left(\frac{4}{9}+\frac{4}{9}\right) + (8m+4n-12)\times\left(\frac{4}{9}+\frac{1}{3}\right)$$
$$+(18mn-21m-n+10)\times\left(\frac{1}{3}+\frac{1}{3}\right)$$

the conclusion follows.

3D plot of the third Van index of β-GN(m,n) network is shown in Figure 4.

**Theorem 4.** Let β-GN(m,n) be a graphene network. Then, the third reverse Van index of β-GN(m,n) is;

$$Van^{3r}(\beta - \mathrm{GN}(\mathrm{m,n})) = 108mn-\frac{753}{35}m+\frac{168}{5}n-\frac{171}{7}$$

*Proof.* Considering that β-GN(m,n) is a beta graphene network. By definition;

$$Van^{3r}(G\beta - \mathrm{GN}(\mathrm{m,n})) = \sum_{uv\in E(\beta-\mathrm{GN}(\mathrm{m,n}))} (rvan(u) + rvan(v))$$

As a result by using Table 2;

$$Van^{3r}(\beta - \mathrm{GN}(\mathrm{m,n})) = (4m+2n)\times\left(\frac{6}{5}+\frac{6}{5}\right) + (4m+8)\times\left(\frac{6}{5}+\frac{12}{7}\right) + (4m+4n - 8)\times\left(\frac{6}{5}+\frac{9}{4}\right)$$

$$+(2m+4)\times\left(\frac{12}{7}+3\right) + (4m-8)\times\left(\frac{9}{4}+\frac{9}{4}\right) + (8m+4n-12)\times\left(\frac{9}{4}+3\right)$$

$$+(18mn - 21m - n + 10)\times(3+3)$$

the conclusion follows.

3D plot of the third reverse Van index of beta graphene network, β-GN(m,n), is shown in Figure 5.

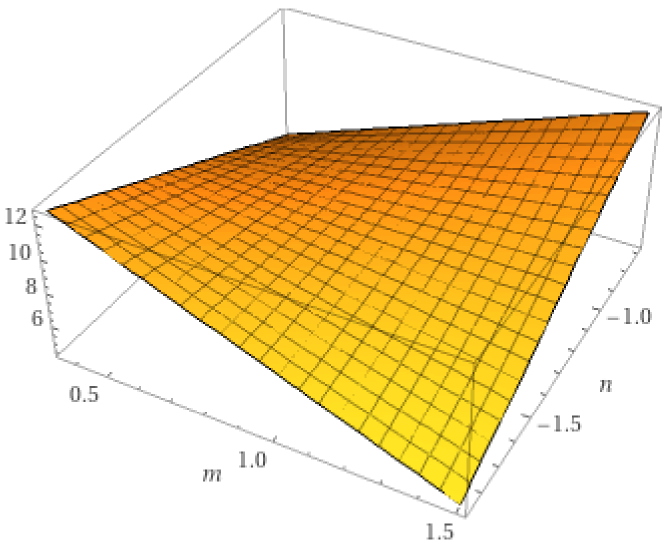


*Figure 4 3D plot of the third Van index of β-GN(m,n)*

**Theorem 5.** Let β-GN(m,n) be a beta graphene network. Then, the second S index of β-GN(m,n) is;

$$S^2(\beta - \mathrm{GN}(\mathrm{m,n})) = 5832mn - 4720m + 438n + 600$$

*Proof.* Considering that β-GN(m,n) is a beta graphene network. By definition;

$$S^2(\beta - \mathrm{GN}(\mathrm{m,n})) = \sum_{uv\in E(\beta-\mathrm{GN}(\mathrm{m,n}))} s(u)s(v)$$

As a result by using Table 3;

$$S^2(\beta - \mathrm{GN}(\mathrm{m,n})) = (4m+2n)\times 1\times 1 + (4m+8)\times 1\times 5 + (4m+4n-8)\times 1\times 10$$

$$+(2m+4)\times 5\times 18 + (4m-8)\times 10\times 10 + (8m+4n-12)\times 10\times 18$$

$$+(18mn - 21m - n + 10)\times 18\times 18$$

the conclusion follows.

3D plot of the second S index of beta graphene network, β-GN(m,n), is shown in Figure 6.

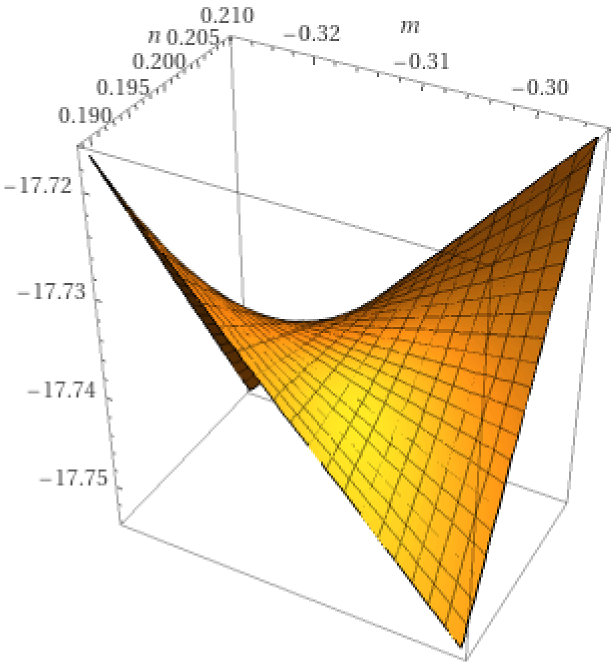


*Figure 5 3D plot of the third reverse Van index of β-GN(m,n)*

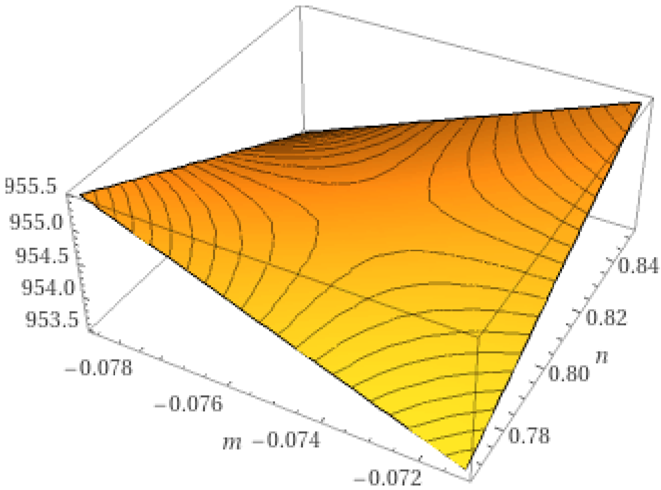


*Figure 6 3D plot of the second S index of β-GN(m,n)*

**Theorem 6.** Let β-GN(m,n) be a graphene network. Then, the second reverse S index of β-GN(m,n) is;

$$S^{2r}(\beta - \mathrm{GN}(\mathrm{m},\mathrm{n})) = \frac{18}{361}mn + \frac{202574}{131043}m + \frac{5545}{7942}n + \frac{31750}{131043}$$

*Proof.* Considering that β-GN(m,n) is a beta graphene network. By definition;

$$S^{2r}(G\beta - \mathrm{GN}(\mathrm{m},\mathrm{n})) = \sum_{uv\in E(\beta-\mathrm{GN}(\mathrm{m},\mathrm{n}))} rs(u)rs(v)$$

As a result by using Table 3;

$$S^{2r}(\beta - \mathrm{GN}(\mathrm{m},\mathrm{n})) = (4m+2n)\times\frac{1}{2}\times\frac{1}{2} + (4m+8)\times\frac{1}{2}\times\frac{1}{6} + (4m+4n-8)\times\frac{1}{2}\times\frac{1}{11}$$

$$+(2m+4)\times\frac{1}{6}\times\frac{1}{19} + (4m-8)\times\frac{1}{11}\times\frac{1}{11} + (8m+4n-12)\times\frac{1}{11}\times\frac{1}{19}$$

$$+(18mn-21m-n+10)\times\frac{1}{19}\times\frac{1}{19}$$

the conclusion follows.

3D plot of the second reverse S index of beta graphene network, β-GN(m,n), is shown in Figure 7.

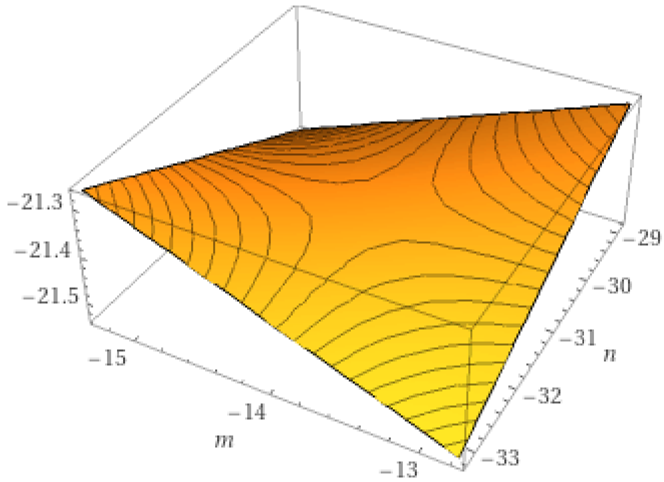


*Figure 7 3D plot of the second reverse S index of β-GN(m,n)*

**Theorem 7.** Let β-GN(m,n) be a beta graphene network. Then, the third S index of β-GN(m,n) is;

$$S^{3}(\beta - \mathrm{GN}(\mathrm{m},\mathrm{n})) = 648mn - 330m + 124n - 84$$

*Proof.* Considering that β-GN(m,n) is a beta graphene network. By definition;

$$S^{3}(\beta - \mathrm{GN}(\mathrm{m},\mathrm{n})) = \sum_{uv\in E(\beta-\mathrm{GN}(\mathrm{m},\mathrm{n}))} (s(u)+s(v))$$

As a result by using Table 3;

$$S^{3}(\beta - \mathrm{GN}(\mathrm{m},\mathrm{n})) = (4m+2n)\times(1+1) + (4m+8)\times(1+5) + (4m+4n-8)\times(1+10)$$

$$+(2m+4)\times(5+18) + (4m-8)\times(10+10) + (8m+4n-12)\times(10+18)$$

$$+(18mn-21m-n+10)\times(18+18)$$

the conclusion follows.

3D plot of the third S index of beta graphene network, β-GN(m,n), is shown in Figure 8.

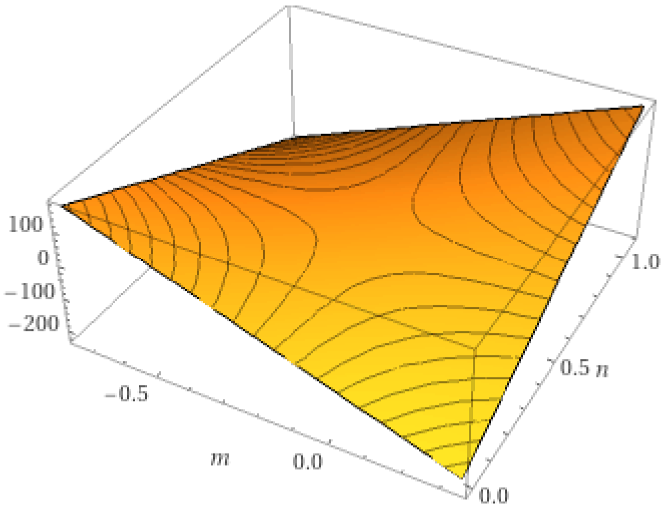


*Figure 8 3D plot of the third S index of β-GN(m,n)*

**Theorem 8.** Let β-GN(m,n) be a graphene network. Then, the third reverse S index of β-GN(m,n) is;

$$S^{3r}(\beta-\mathrm{GN(m,n)}\,)=\frac{36}{19}mn+\frac{1909}{209}m+\frac{1010}{209}n-\frac{134}{209}$$

*Proof.* Considering that β-GN(m,n) is a beta graphene network. By definition;

$$S^{3r}(G\beta-\mathrm{GN(m,n)}\,)=\sum\nolimits_{uv\in E(\beta-\mathrm{GN(m,n)}\,)}(rs(u)+rs(v))$$

As a result by using Table 3;

$$\begin{aligned}S^{3r}(\beta-\mathrm{GN(m,n)}\,)&\\&=(4m+2n)\times\left(\frac{1}{2}+\frac{1}{2}\right)\\&+(4m+8)\times\left(\frac{1}{2}+\frac{1}{6}\right)+(4m+4n\\&-8)\times\left(\frac{1}{2}+\frac{1}{11}\right)\end{aligned}$$

$$+(2m+4)\times\left(\frac{1}{6}+\frac{1}{19}\right)+(4m-8)\times\left(\frac{1}{11}+\frac{1}{11}\right)$$
$$+(8m+4n-12)\times\left(\frac{1}{11}+\frac{1}{19}\right)$$

$$+(18mn-21m-n+10)\times\left(\frac{1}{19}+\frac{1}{19}\right)$$

the conclusion follows.

3D plot of the third reverse S index of beta graphene network, β-GN(m,n), is shown in Figure 9.

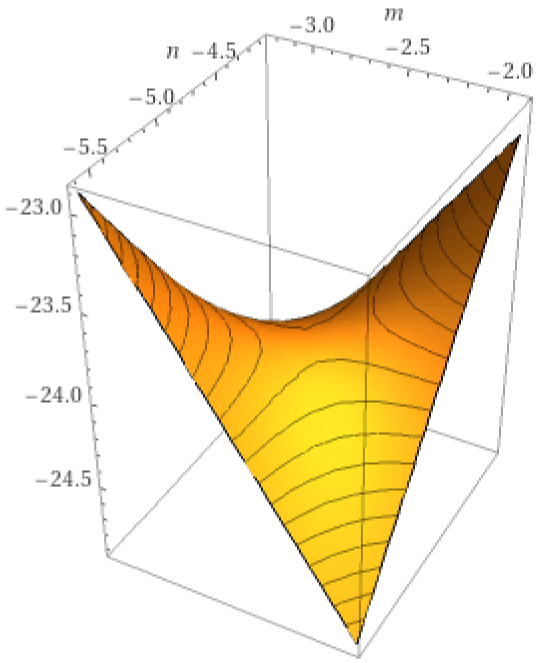


*Figure 9 3D plot of the third reverse S index of β-GN(m,n)*

**Theorem 9.** Let β-GN(m,n) be a beta graphene network. Then, the second R index of β-GN(m,n) is;

$$R^2(\beta-\mathrm{GN(m,n)}\,)=23328mn-13192m+3834n-1560$$

*Proof.* Considering that β-GN(m,n) is a beta graphene network. By definition;

$$R^2(\beta-\mathrm{GN(m,n)}\,)=\sum\nolimits_{uv\in E(\beta-\mathrm{GN(m,n)}\,)}r(u)r(v)$$

As a result by using Table 4;

$$\begin{aligned}R^2(\beta-\mathrm{GN(m,n)}\,)&\\&=(4m+2n)\times11\times11\\&+(4m+8)\times11\times19+(4m+4n\\&-8)\times11\times26\end{aligned}$$

$$+(2m+4)\times19\times36+(4m-8)\times26\times26$$
$$+(8m+4n-12)\times26\times36$$

$$+(18mn-21m-n+10)\times36\times36$$

the conclusion follows.

3D plot of the second R index of beta graphene network, β-GN(m,n), is shown in Figure 10.

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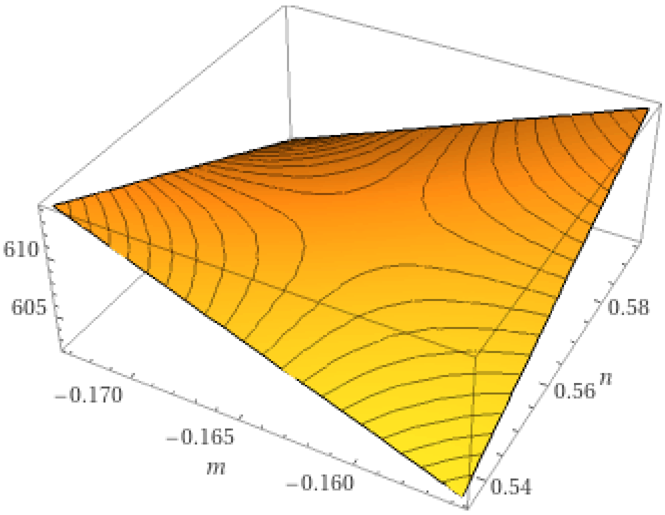


*Figure 10 3D plot of the second R index of β-GN(m,n)*

**Theorem 10.** Let β-GN(m,n) be a graphene network. Then, the second reverse R index of β-GN(m,n) is;

$$R^{2r}(\beta-\mathrm{GN(m,n)}\,) = \frac{1}{72}mn + \frac{101287067}{1510608528}m + \frac{207073}{6115824}n - \frac{2369}{7629336}$$

*Proof.* Considering that β-GN(m,n) is a beta graphene network. By definition;

$$R^{2r}(G\beta-\mathrm{GN(m,n)}\,) = \sum\nolimits_{uv\in E(\beta-\mathrm{GN(m,n)}\,)} rr(u)rr(v)$$

As a result by using Table 4;

$$R^{2r}(\beta-\mathrm{GN(m,n)}\,) = (4m+2n)\times\frac{1}{11}\times\frac{1}{11} + (4m+8)\times\frac{1}{11}\times\frac{1}{19} + (4m+4n-8)\times\frac{1}{11}\times\frac{1}{26}$$
$$+(2m+4)\times\frac{1}{19}\times\frac{1}{36} + (4m-8)\times\frac{1}{26}\times\frac{1}{26} + (8m+4n-12)\times\frac{1}{27}\times\frac{1}{36}$$
$$+(18mn-21m-n+10)\times\frac{1}{36}\times\frac{1}{36}$$

the conclusion follows.

3D plot of the second reverse R index of beta graphene network, β-GN(m,n), is shown in Figure 11.

**Theorem 11.** Let β-GN(m,n) be a beta graphene network. Then, the third R index of β-GN(m,n) is;

$$R^3(\beta-\mathrm{GN(m,n)}\,) = 1296mn - 342m + 368n - 276$$

*Proof.* Considering that β-GN(m,n) is a beta graphene network. By definition;

$$R^3(\beta-\mathrm{GN(m,n)}\,) = \sum\nolimits_{uv\in E(\beta-\mathrm{GN(m,n)}\,)} (r(u)+r(v))$$

As a result by using Table 4;

$$R^3(\beta-\mathrm{GN(m,n)}\,) = (4m+2n)\times(11+11) + (4m+8)\times(11+19) + (4m+4n-8)\times(11+26)$$
$$+(2m+4)\times(19+36) + (4m-8)\times(26+26) + (8m+4n-12)\times(26+36)$$
$$+(18mn-21m-n+10)\times(36+36)$$

the conclusion follows.

3D plot of the third R index of beta graphene network, β-GN(m,n), is shown in Figure 12.

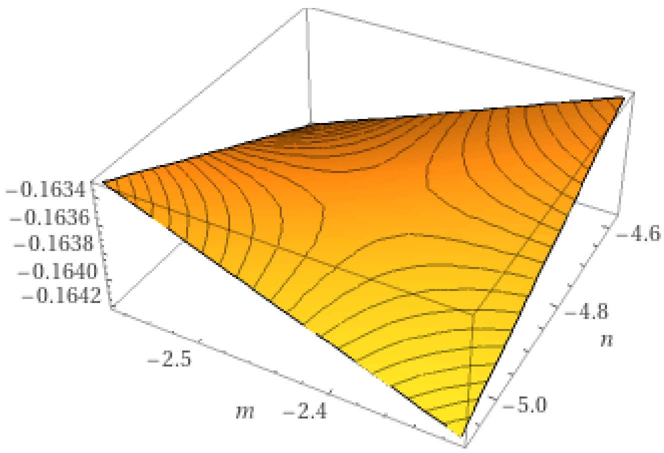


*Figure 11 3D plot of the second reverse R index of β-GN(m,n)*

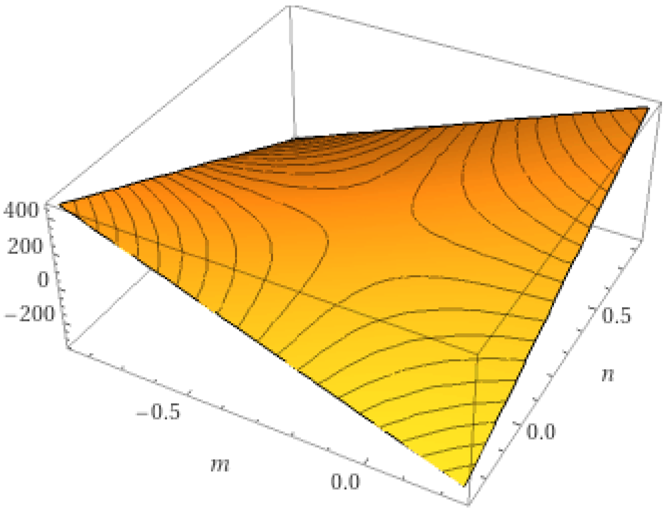


*Figure 12 3D plot of the third R index of β-GN(m,n)*

**Theorem 12.** Let β-GN(m,n) be a graphene network. Then, the third reverse R index of β-GN(m,n) is;

$$R^{3r}(\beta-\mathrm{GN(m,n)}\,)=mn+\frac{120256}{73359}m+\frac{8377}{7722}n-\frac{895}{2223}$$

*Proof.* Considering that β-GN(m,n) is a beta graphene network. By definition;

$$R^{3r}(G\beta-\mathrm{GN(m,n)}\,)=\sum\nolimits_{uv\in E(\beta-\mathrm{GN(m,n)}\,)}(rr(u)+rr(v))$$

As a result by using Table 4;

$$\begin{aligned}R^{3r}&(\beta-\mathrm{GN(m,n)}\,)\\&=(4m+2n)\times\left(\frac{1}{11}+\frac{1}{11}\right)\\&+(4m+8)\times\left(\frac{1}{11}+\frac{1}{19}\right)+(4m+4n\\&-8)\times\left(\frac{1}{11}+\frac{1}{26}\right)\\&+(2m+4)\times\left(\frac{1}{19}+\frac{1}{36}\right)+(4m-8)\times\left(\frac{1}{26}+\frac{1}{26}\right)\\&+(8m+4n-12)\times\left(\frac{1}{27}+\frac{1}{36}\right)\\&+(18mn-21m-n+10)\times\left(\frac{1}{36}+\frac{1}{36}\right)\end{aligned}$$

the conclusion follows.

3D plot of the third reverse R index of beta graphene network, β-GN(m,n), is shown in Figure 13.

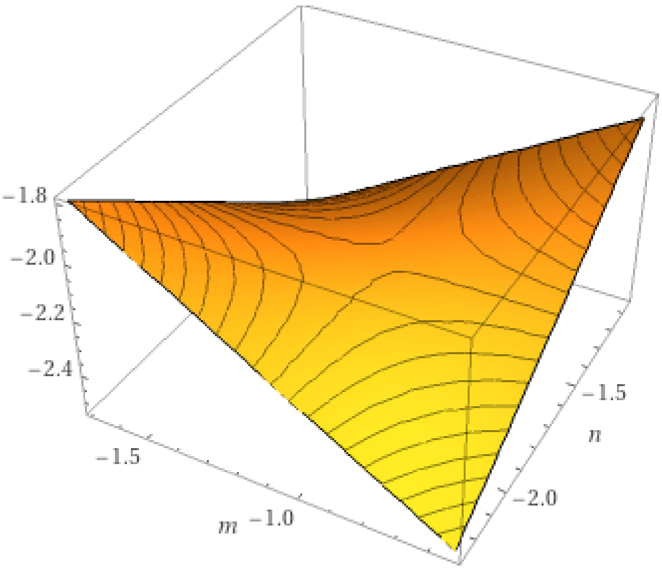


*Figure 13 3D plot of the third reverse R index of β-GN(m,n)*

### 3.2 Entropies of beta graphene

The following theorems give the overall entropies which are based on Van, R, and S indices representation of β-GN(m,n).

**Theorem 13.** Let G be a beta graphene network β-GN(m,n). Then, entropy of G which is based on the second Van index of β-GN(m,n) is;

$$\begin{aligned}Ent_{Van^2}(G)&=\log\left(2mn+\frac{505}{81}m+\frac{181}{54}n-\frac{44}{81}\right)\\&-\frac{1}{2mn+\frac{505}{81}m+\frac{181}{54}n-\frac{44}{81}}((4m+2n)\\&\times\frac{25}{36}\times\log\left(\frac{25}{36}\right)+(4m+8)\times\frac{35}{72}\times\log\left(\frac{35}{72}\right)\\&+(4m+4n-8)\times\frac{10}{27}\times\log\left(\frac{10}{27}\right)\\&+(2m+4)\times\frac{7}{36}\times\log\left(\frac{7}{36}\right)+(4m-8)\times\frac{16}{81}\times\log\left(\frac{16}{81}\right)\\&+(8m+4n-12)\times\frac{4}{27}\times\log\left(\frac{4}{27}\right)\\&+(18mn-21m-n+10)\times\frac{1}{9}\times\log\left(\frac{1}{9}\right))\end{aligned}$$

*Proof.* Considering that G is a beta graphene network. By definition;

$$\begin{aligned}Ent_{Van^2}(G)&=log(Van^2(G))\\&-\frac{1}{Van^2(G)}\sum\nolimits_{uv\in E(G)}f(uv)log\big(f(uv)\big)\end{aligned}$$

As a result by using Theorem 1, the conclusion follows.

**Theorem 14.** Let G be a beta graphene network β-GN(m,n). Then, entropy of G which is based on the second reverse Van index of β-GN(m,n) is;

$$Ent_{Van^{2r}}(G) = log\left(162mn - \frac{55773}{700}m + \frac{792}{25}n - \frac{225}{14}\right) - \frac{1}{162mn - \frac{55773}{700}m + \frac{792}{25}n - \frac{225}{14}G)}((4m+2n) \times \frac{36}{25} \times \log(\frac{36}{25}) + (4m+8) \times \frac{72}{35} \times \log(\frac{72}{35}) + (4m+4n-8) \times \frac{27}{10} \times \log(\frac{27}{10})$$
$$+(2m+4) \times \frac{36}{7} \times \log(\frac{36}{7}) + (4m-8) \times \frac{81}{16} \times \log(\frac{81}{16})$$
$$+ (8m+4n-12) \times \frac{27}{4} \times \log(\frac{27}{4})$$
$$+(18mn - 21m - n + 10) \times 9 \times \log(9))$$

*Proof.* Considering that G is a beta graphene network. By definition;

$$Ent_{Van^{2r}}(G) = log(Van^{2r}(G)) - \frac{1}{Van^{2r}(G)}\sum_{uv\in E(G)} f(uv)log\big(f(uv)\big)$$

As a result by using Theorem 2, the conclusion follows.

**Theorem 15.** Let G be a beta graphene network β-GN(m,n). Then, entropy of G which is based on the third Van index of β-GN(m,n) is;

$$Ent_{Van^{3}}(G) = log\left(12mn + \frac{271}{18}m - \frac{98}{9}n - 5\right) - \frac{1}{12mn + \frac{271}{18}m - \frac{98}{9}n - 5}((4m+2n) \times \frac{5}{3} \times \log(\frac{5}{3}) + (4m+8) \times \frac{17}{12} \times \log(\frac{17}{12}) + (4m+4n-8) \times \frac{23}{18} \times \log(\frac{23}{18})$$
$$+(2m+4) \times \frac{11}{12} \times \log(\frac{11}{12}) + (4m-8) \times \frac{8}{9} \times \log(\frac{8}{9})$$
$$+ (8m+4n-12) \times \frac{7}{9} \times \log(\frac{7}{9})$$
$$+(18mn - 21m - n + 10) \times \frac{2}{3} \times \log(\frac{2}{3}))$$

*Proof.* Considering that G is a beta graphene network. By definition;

$$Ent_{Van^{3}}(G) = log(Van^{3}(G)) - \frac{1}{Van^{3}(G)}\sum_{uv\in E(G)} f(uv)log\big(f(uv)\big)$$

As a result by using Theorem 3, the conclusion follows.

**Theorem 16.** Let G be a beta graphene network β-GN(m,n). Then, entropy of G which is based on the third reverse Van index of β-GN(m,n) is;

$$Ent_{Van^{3r}}(G) = log\left(108mn - \frac{753}{35}m + \frac{168}{5}n - \frac{171}{7}\right) - \frac{1}{108mn - \frac{753}{35}m + \frac{168}{5}n - \frac{171}{7}}((4m+2n) \times \frac{12}{5} \times \log(\frac{12}{5}) + (4m+8) \times \frac{102}{35} \times \log(\frac{102}{35}) + (4m+4n-8) \times \frac{69}{20} \times \log(\frac{69}{20})$$
$$+(2m+4) \times \frac{33}{7} \times \log(\frac{33}{7}) + (4m-8) \times \frac{9}{2} \times \log(\frac{9}{2})$$
$$+ (8m+4n-12) \times \frac{21}{4} \times \log(\frac{21}{4})$$
$$+(18mn - 21m - n + 10) \times 6 \times \log(6))$$

*Proof.* Considering that G is a beta graphene network. By definition;

$$Ent_{Van^{3r}}(G) = log(Van^{3r}(G)) - \frac{1}{Van^{3r}(G)}\sum_{uv\in E(G)} f(uv)log\big(f(uv)\big)$$

As a result by using Theorem 4, the conclusion follows.

**Theorem 17.** Let G be a beta graphene network β-GN(m,n). Then, entropy of G which is based on the second S index of β-GN(m,n) is;

$$Ent_{S^2}(G) = log(5832mn - 4720m + 438n + 600) - \frac{1}{5832mn - 4720m + 438n + 600}((4m+2n) \times 2 \times \log(2) + (4m+8) \times 5 \times \log(5) + (4m+4n-8) \times 10 \times \log(10)$$
$$+(2m+4) \times 90 \times \log(90) + (4m-8) \times 100 \times 2\log(10)$$
$$+ (8m+4n-12) \times 180 \times \log(180)$$
$$+(18mn - 21m - n + 10) \times 324 \times 2\log(18))$$

*Proof.* Considering that G is a beta graphene network. By definition;

$$Ent_{S^2}(G) = log(S^2(G)) - \frac{1}{S^2(G)}\sum_{uv\in E(G)} f(uv)log\big(f(uv)\big)$$

As a result by using Theorem 5, the conclusion follows.

**Theorem 18.** Let G be a beta graphene network β-GN(m,n). Then, entropy of G which is based on the second reverse S index of β-GN(m,n) is;

$$Ent_{S^{2r}}(G) = log\left(\frac{18}{361}mn + \frac{202574}{131043}m + \frac{5545}{7942}n + \frac{31750}{131043}\right) - \frac{1}{\frac{18}{361}mn + \frac{202574}{131043}m + \frac{5545}{7942}n + \frac{31750}{131043}}((4m+2n) \times \frac{1}{4} \times \log(\frac{1}{4}) + (4m+8) \times \frac{1}{12} \times \log(\frac{1}{12}) + (4m+4n-8) \times \frac{1}{22} \times \log(\frac{1}{22})$$

$$+(2m+4) \times \frac{1}{114} \times \log(\frac{1}{114}) + (4m-8) \times \frac{1}{121} \times \log(\frac{1}{121}) + (8m+4n-12) \times \frac{1}{209} \times \log(\frac{1}{209})$$

$$+(18mn-21m-n+10) \times \frac{1}{361} \times \log(\frac{1}{361}))$$

*Proof.* Considering that G is a beta graphene network. By definition;

$$Ent_{S^{2r}}(G) = log(S^{2r}(G)) - \frac{1}{S^{2r}(G)} \sum_{uv \in E(G)} f(uv) log(f(uv))$$

As a result by using Theorem 6, the conclusion follows.

**Theorem 19.** Let G be a beta graphene network β-GN(m,n). Then, entropy of G which is based on the third S index of β-GN(m,n) is;

$$Ent_{S^3}(G) = log(648mn - 330m + 124n - 84) - \frac{1}{648mn-330m+124n-84}((4m+2n) \times 2 \times \log(2) + (4m+8) \times 6 \times \log(6) + (4m+4n-8) \times 11 \times \log(11)$$

$$+(2m+4) \times 23 \times \log(23) + (4m-8) \times 20 \times \log(20) + (8m+4n-12) \times 28 \times \log(28)$$

$$+(18mn-21m-n+10) \times 36 \times \log(36))$$

*Proof.* Considering that G is a beta graphene network. By definition;

$$Ent_{S^3}(G) = log(S^3(G)) - \frac{1}{S^3(G)} \sum_{uv \in E(G)} f(uv) log(f(uv))$$

As a result by using Theorem 7, the conclusion follows.

**Theorem 20.** Let G be a beta graphene network β-GN(m,n). Then, entropy of G which is based on the third reverse S index of β-GN(m,n) is;

$$Ent_{S^{3r}}(G) = log\left(\frac{36}{19}mn + \frac{1909}{209}m + \frac{1010}{209}n - \frac{134}{209}\right) - \frac{1}{\frac{36}{19}mn + \frac{1909}{209}m + \frac{1010}{209}n - \frac{134}{209}}((4m+8) \times \frac{2}{3} \times \log(\frac{2}{3}) + (4m+4n-8) \times \frac{13}{22} \times \log(\frac{13}{22})$$

$$+(2m+4) \times \frac{25}{114} \times \log(\frac{25}{114}) + (4m-8) \times \frac{2}{11} \times \log(\frac{2}{11}) + (8m+4n-12) \times \frac{30}{209} \times \log(\frac{30}{209})$$

$$+(18mn-21m-n+10) \times \frac{2}{19} \times \log(\frac{2}{19}))$$

*Proof.* Considering that G is a beta graphene network. By definition;

$$Ent_{S^3}r(G) = log(S^{3r}(G)) - \frac{1}{S^{3r}(G)} \sum_{uv \in E(G)} f(uv) log(f(uv))$$

As a result by using Theorem 8, the conclusion follows.

**Theorem 21.** Let G be a beta graphene network β-GN(m,n). Then, entropy of G which is based on the second R index of β-GN(m,n) is;

$$Ent_{R^2}(G) = log(23328mn - 13192m + 3834n - 1560) - \frac{1}{23328mn-13192m+3834n-1560}((4m+2n) \times 121 \times 2\log(11) + (4m+8) \times 209 \times \log(209) + (4m+4n-8) \times 286 \times \log(286)$$

$$+(2m+4) \times 684 \times \log(684) + (4m-8) \times 676 \times 2\log(26) + (8m+4n-12) \times 180 \times \log(180)$$

$$+(18mn-21m-n+10) \times 1296 \times 4\log(6))$$

*Proof.* Considering that G is a beta graphene network. By definition;

$$Ent_{R^2}(G) = log(R^2(G)) - \frac{1}{R^2(G)} \sum_{uv \in E(G)} f(uv) log(f(uv))$$

As a result by using Theorem 9, the conclusion follows.

**Theorem 22.** Let G be a beta graphene network β-GN(m,n). Then, entropy of G which is based on the second reverse R index of β-GN(m,n) is;

$$Ent_{R^{2r}}(G) = log\left(\frac{1}{72}mn + \frac{101287067}{1510608528}m + \frac{207073}{6115824}n - \frac{2369}{7629336}\right) - \frac{1}{\frac{1}{72}mn + \frac{101287067}{1510608528}m + \frac{207073}{6115824}n - \frac{2369}{7629336}}((4m+2n) \times \frac{1}{121} \times \log(\frac{1}{121}) + (4m+8) \times \frac{1}{209} \times \log(\frac{1}{209}) + (4m+4n-8) \times \frac{1}{286} \times \log(\frac{1}{286})$$

$$+(2m+4) \times \frac{1}{684} \times \log(\frac{1}{684}) + (4m-8) \times \frac{1}{676} \times \log(\frac{1}{676}) + (8m+4n-12) \times \frac{1}{180} \times \log(\frac{1}{180})$$

$$+(18mn-21m-n+10) \times \frac{1}{1296} \times \log(\frac{1}{1296}))$$

*Proof.* Considering that G is a beta graphene network. By definition;

$$Ent_{R^{2r}}(G) = log(R^{2r}(G)) - \frac{1}{R^{2r}(G)}\sum_{uv\in E(G)} f(uv)log\big(f(uv)\big)$$

As a result by using Theorem 10, the conclusion follows.

**Theorem 23.** Let G be a beta graphene network β-GN(m,n). Then, entropy of G which is based on the third R index of β-GN(m,n) is;

$$Ent_{R^3}(G) = log(1296mn - 342m + 368n - 276) - \frac{1}{1296mn-342m+368n-276}((4m+2n) \times 22 \times \log(22) + (4m+8) \times 30 \times \log(30) + (4m+4n-8) \times 37 \times \log(37)$$
$$+(2m+4) \times 45 \times \log(45) + (4m-8) \times 52 \times \log(52) + (8m+4n-12) \times 62 \times \log(62)$$
$$+(18mn - 21m - n + 10) \times 72 \times \log(72))$$

*Proof.* Considering that G is a beta graphene network. By definition;

$$Ent_{R^3}(G) = log(R^3(G)) - \frac{1}{R^3(G)}\sum_{uv\in E(G)} f(uv)log\big(f(uv)\big)$$

As a result by using Theorem 11, the conclusion follows.

**Theorem 24.** Let G be a beta graphene network β-GN(m,n). Then, entropy of G which is based on the third reverse R index of β-GN(m,n) is;

$$Ent_{R^3r}(G) = log\left(mn + \frac{120256}{73359}m + \frac{8377}{7722}n - \frac{895}{2223}\right) - \frac{1}{mn+\frac{120256}{73359}m+\frac{8377}{7722}n-\frac{895}{2223}}((4m+2n) \times \frac{2}{11} \times \log(\frac{2}{11}) + (4m+8) \times \frac{30}{209} \times \log(\frac{30}{209}) + (4m+4n-8) \times \frac{37}{286} \times \log(\frac{37}{286})$$
$$+(2m+4) \times \frac{55}{684} \times \log(\frac{55}{684}) + (4m-8) \times \frac{1}{13} \times \log(\frac{1}{13}) + (8m+4n-12) \times \frac{63}{972} \times \log(\frac{63}{972})$$
$$+(18mn - 21m - n + 10) \times \frac{1}{18} \times \log(\frac{1}{18}))$$

*Proof.* Considering that G is a beta graphene network. By definition;

$$Ent_{R^3r}(G) = log(R^{3r}(G)) - \frac{1}{R^{3r}(G)}\sum_{uv\in E(G)} f(uv)log\big(f(uv)\big)$$

As a result by using Theorem 12, the conclusion follows.

## 4. Conclusions

The generalized mathematical expression for R, S, and Van topological indices for structures of β-GN is described in this study. Information-theoretic entropy measurements of various phases of 2D materials of β-GN are provided by these generalized mathematical formulations. The structures examined here were shown to have very little variation in their entropies. These many phases of 2D materials made from graphite might be predicted in terms of their thermochemistry, physicochemical properties, electrical, optical, and mechanical characteristics using our proposed topological indices and entropy metrics. Additionally, these indices can be combined with metrics derived from quantum chemistry, such as molecular hardness, polarizability measures, atomic charges, etc., to create a platform that is robust in predicting molecular connectivity and electronic-based attributes. Numerous probabilistic entropy metrics are produced using the same indices that Shannon's formula uses to define the probability function. We create a connection between the degree-based entropies of and structures using their respective degree-based topological indices. By linking the architectures of and nanoribbons with a number of their physicochemical and optoelectronic properties, the results of this study could significantly advance QSAR and QSPR studies of these materials.

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