On Van, R and S entropies of graphenylene

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Abstract

Applications in the disciplines of chemistry, pharmaceuticals, communication, physics, and aeronautics all heavily rely on graph theory. To examine the properties of chemical compounds, the molecules are modelled as a graph. A few physical characteristics of the substance, including its boiling point, enthalpy, pi-electron energy, and molecular weight, are related to its geometric shape. Through the resolution of one of the interdisciplinary problems characterizing the structures of benzenoid hydrocarbons and graphenylene, the essay seeks to ascertain the practical applicability of graph theory. The topological index, which displays the correlation of chemical structures using numerous physical, chemical, and biological processes, is an invariant of a molecular graph connected with the chemical structure. Shannon's concept of entropy served as the basis for the graph entropies with topological indices, which are now used to measure the structural information of chemical graphs. Using various graph entropy metrics, the theory of graphs can be used to establish the link between particular chemical structural features. This study uses the appropriate R, S, Van topological indices to introduce some unique degree-based entropy descriptors. Additionally, the graphenylene structure's entropy measurements indicated above were computed.

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

1. Introduction

Due to their use in quantitative structure-activity and quantitative structure-property relationships (QSPR) relationships, topological indices, which are structural invariants produced from molecular graphs and determine the fundamental connectivity of the molecular network, have received a lot of attention lately [1-4]. Degree-based topological indices, the focus of extensive study [1–5], have been used to predict the physicochemical features of molecular structures. The information complexity of complex chemical compounds like graphenylene can be determined using measures of information entropy. Shannon first introduced the concept of information entropy to examine and quantify the complexity of data and information transmission, but it has since been widely applied in a variety of scientific fields. One of the most important applications of information entropy is the study of the complexity of molecular structures

and associated quantum chemical electron densities [6]. Entropy is a phrase used to describe the quantity of energy that is scattered and the degree to which thermal energy is not used for work. Entropy was initially established by Shannon as a component of the communication theory [6,7]. He claims that a system made up of the three components source, channel, and receiver is how data is transmitted. In order to prove the entropy represents an absolute limit on how well data can be compressed from the source to reach the receiver in his famous coding theorem, Shannon used a variety of methods to encode, transmit, and compress the messages during his learning process. The entropy of a probability distribution is the indicator of uncertainty. In fact, the conclusion of an analysis can be predicted by using a number that represents the degree of uncertainty in the result of the analysis. In addition, numerous researchers looked into graph and network studies in the late 1950s. Graph invariants were used to conduct more research on entropy measurements, which was beneficial for understanding key graph features [8–11]. The complexity of the structural makeup of chemical compounds and complex networks has been studied using a variety of theoretical metrics and instruments. In order to investigate the entropies of relational systems, academics engage with the concept of entropy in a variety of ways by using a range of problems from many disciplines, such as discrete mathematics, discrete biology, discrete chemistry, and statistics, among others. A graph's structure can be described using graph entropy in mathematical chemistry [12–14]. A benzenoid is a class of chemical compounds that include at least one benzene ring.

They are highly chemically stable due to their bonds with specific molecules. Benzenoids are aromatic hydrocarbons that are widely used in the production of synthetic fibers, plastics, rubber-like goods, dry cleaning, and gasoline additives [15]. Their uses in industrial chemistry, notably in polymer-based products, are expanding quickly. Each hexagon in the cyclic hydrocarbon graphenylene has a square next to it. Biphenylenes are two such hexagons separated by a square. It is composed of two benzene rings sandwiched between a cyclobutadiene ring. The building block of graphenylene, which is a $110°$ C melting powder with a pale yellow color, is biphenylene. A hydrocarbon with the chemical formula $C_{12}H_8$, biphenylene. A 2D graphene is a potential substance with important uses in the upcoming electrical and optical systems. An intriguing precursor to Graphenylene, a 2D porous molecular network similar to graphene, is biphenylene. In the characterisation of the delocalized band, this novel material shows good dispersion and gap separation [16,17]. Researchers from all over the world have been drawn to several studies on graphene because of its amazing qualities and exciting prospective uses because of its distinctive 2D structure. Carbon nanotubes, fullerenes, and even graphene nanoribbon can be formed by wrapping graphene in a particular way. The family of carbon nanomaterials has been greatly enriched by these. Additionally, these investigations have sparked interest in using both experimental methods and theoretical computations to take advantage of novel 2D carbon allotropes [18]. The cyclotrimerization of graphene, a 2D network of hydrogen-free carbon atoms, produces biphenylene carbon.

This research's primary objectives are the introduction of novel entropy measures based on R, S, Van topological indices and the calculation of defined entropies of graphenylene structure.

Degree based and neighboring sum degree based entropies of the graphenylene have been calculted in the references [19-21].

In this work, we investigate the R, S, and Van topological indices and related entropy measures for the graphenylene 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; $van(v) = \frac{S_v}{M_v}$ [22]. Also, reverse Van degree of the vertex v, defined as; $rvan(v) = \frac{M_v}{S_v}$. Van topological indices defined as [22];

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; $r(v) = M_v + S_v$ [23]. Also, reverse R degree of the vertex v, defined as; $rr(v) = \frac{1}{M_v + S_v}$. R topological indices defined as [23]:

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; $s(v) = |M_v - S_v|$ [24]. Also, reverse S degree of the vertex v, defined as; $rs(v) = \frac{1}{|M_v - S_v| + 1}$. R topological indices defined as [24]:

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; $S^{1r}(G) = \sum_{v \in V(G)} rs(v)^2$.

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; $S^{3r}(G) = \sum_{uv \in E(G)} [rs(u) + rs(v)]$.

The graph entropy measurements, which are split into intrinsic and extrinsic measures, allow mathematicians to relate graph components like edges and vertices with probability distributions. Graph entropies are widely used in a variety of fields, including chemistry, ecology, sociology, and biology [25,26]. Dehmer created information functional-based graph entropies, examined their properties, and introduced them [27,28]. Estrada et al. [29] gave a physically valid definition of graph entropy in addition to studying the walk-based graph entropies.

Applications for entropy network measurements include deriving a quantitative definition of a molecular structure and analyzing the biological and chemical characteristics of molecular graphs [29]. Entropy metrics have many applications in the analysis of chemical graphs. They are employed to look at the chemical properties of intricate networks. According to the definition of Shannon's entropy for 2D networks based on the topological index T, defined as,

$$Entropy_T(G) = Ent_T(G)$$

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

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

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

3. Main results

In this section, we first determine the Van, R, and S topological indices for graphenylene families, followed by the associated entropies of these indices. Graphenylene can be viewed as the fundamental building block of these materials due to its structural resemblances to graphite, fullerene, carbon nanotubes, graphene, and other closely related materials such as amorphous carbon, carbon fiber, and charcoal. They all share the same structural makeup, although having incredibly varied sizes and shapes, hence they all share some traits. As a result, the structural study of graphenylene helps us understand the aforementioned materials.

Each hexagon of the cyclic hydrocarbon graphenylene has a square next to it. Biphenylene is the name for two such hexagons that are spaced apart by a square. It is composed of two benzene rings sandwiched between a cyclobutadiene ring. The molecular graph of graphenylene is modeled, and the vertices, edges, and features are listed in Tables 1 and 4, based on the degrees and neighborhood degrees of the end vertices, respectively. According to Figure 1, Graphenylene has a total of *12mn* vertices and*18mn-2m-2n* edges, respectively.
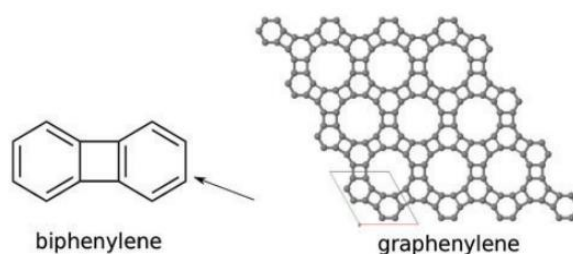

Figure 1 *A planar picture of biphenylene (graphenylene) supercells measuring 4 by 4.*

Graphenylene 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 graphenylene.

Cardinality	(S_u, S_v)	(M_u, M_v)
2	(4,4)	(4,4)
4	(4,5)	(4,6)
$2m + 2n - 4$	(5,5)	(6,6)
$18mn - 16m - 16n + 14$	(5,8)	(6,18)
$4m + 4n - 4$	(8,8)	(18,18)
4	(8,9)	(18,27)
$8m + 8n - 16$	(9,9)	(27,27)

With the help of Table 1, the Van, R and S edge end vertex degree partitions of graphenylene are calculated and given in Tables 2-4.

Table 2 Van edge end vertex degree partition of graphenylene

Cardinality	$(van(u), van(v))$	$(rvan(u), rvan(v))$
2	(1,1)	(1,1)
4	(1,5/6)	(1,6/5)
$2m + 2n - 4$	(5/6,5/6)	(6/5,6/5)
$18mn - 16m - 16n + 14$	(5/6,4/9)	(6/5, 9/4)
$4m + 4n - 4$	(4/9,4/9)	(9/4,9/4)
4	(4/9,1/3)	(9/4,3)
$8m + 8n - 16$	(1/3,1/3)	(3,3)

Table 3 S edge end vertex degree partition of graphenylene

Cardinality	$(s(u), s(v))$	$(rs(u), rs(v))$
2	(0,0)	(1,1)
4	(0,1)	(1,1/2)

$2m + 2n - 4$	(1,1)	(1/2,1/2)
$18mn - 16m$ $- 16n + 14$	(1,10)	(1/2,1/11)
$4m + 4n - 4$	(10,10)	(1/11,1/11)
4	(10,18)	(1/11,1/19)
$8m + 8n - 16$	(18,18)	(1/19,1/19)

Table 4 R edge end vertex degree partition of graphenylene

Cardinality	$(r(u), r(v))$	$(rr(u), rr(v))$
2	(8,8)	(1/8,1/8)
4	(8,11)	(1/8,1/11)
$2m + 2n - 4$	(11,11)	(1/11,1/11)
$18mn - 16m$ $- 16n + 14$	(11,26)	(1/11,1/26)
$4m + 4n - 4$	(26,26)	(1/26,1/26)
4	(26,36)	(1/27,1/36)
$8m + 8n - 16$	(36,36)	(1/36,1/36)

3.1 Topological indices graphenylene

The following theorems give the overall Van, R, and S indices representation of graphenylene.

Theorem 1. Let G(m,n) be a graphenylene network. Then, the second Van index of G(m,n) is;

$$Van^2(\text{G(m,n)}) = \frac{20}{3}mn - \frac{463}{162}m - \frac{463}{162}n + \frac{467}{81}$$

Proof. Considering that G(m,n) is a graphenylene network. By definition;

$$Van^2(\text{G(m,n)}) = \sum_{uv \in E(\text{G(m,n)})} van(u)van(v)$$

As a result by using Table 2;

$$Van^2(\text{G(m,n)}) = 2 \times 1 \times 1 + 4 \times 1 \times \frac{5}{6} + (2m + 2n - 4) \times \frac{5}{6} \times \frac{5}{6}$$

$$+(18mn - 16m - 16n + 14) \times \frac{5}{6} \times \frac{4}{9} + (4m + 4n - 4) \times \frac{4}{9} \times \frac{4}{9} + 4 \times \frac{4}{9} \times \frac{1}{3}$$

$$+(8m + 8n - 16) \times \frac{1}{3} \times \frac{1}{3}$$

the conclusion follows.

3D plot of the second Van index of graphenylene network, G(m,n), is shown in Figure 2.

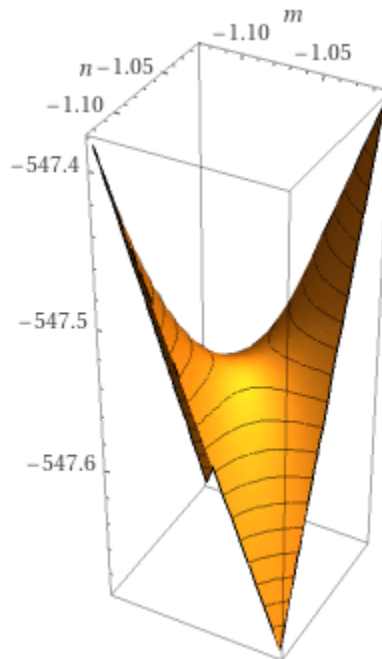**Theorem 2.** Let G(m,n) be a graphenylene network. Then, the second reverse Van index of G(m,n) is;

$$Van^{2r}(G(m, n)) = \frac{243}{5}mn + \frac{5193}{100}m + \frac{5193}{100}n - \frac{9841}{20}$$

Proof. Considering that G(m,n) is a graphenylene network. By definition;

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

As a result by using Table 2;

$$Van^{2r}(G(m, n)) = 2 \times 1 \times 1 + 4 \times 1 \times \frac{6}{5} + (2m + 2n - 4) \times \frac{6}{5} \times \frac{6}{5}$$

$$+(18mn - 16m - 16n + 14) \times \frac{6}{5} \times \frac{9}{4} + (4m + 4n - 4) \times \frac{9}{4} \times \frac{9}{4} + 4 \times \frac{9}{4} \times 3$$

$$+(8m + 8n - 16) \times 3 \times 3$$

the conclusion follows.

3D plot of the second reverse Van index of graphenylene network, G(m,n), is shown in Figure 3.
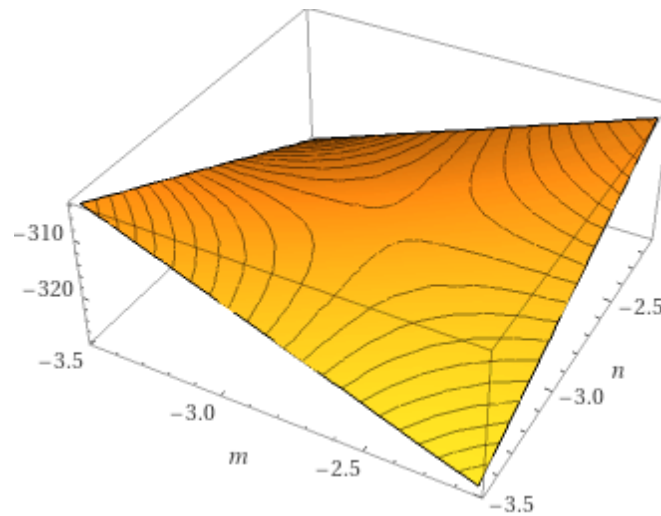

Figure 2 3D plot of second Van index of G(m,n)

Figure 3 3D plot of second reverse Van index of G(m,n)

Theorem 3. Let G(m,n) be a graphenylene network. Then, the third Van index of G(m,n) is;

$$Van^3\big(G(m,n)\big) = 23mn - \frac{74}{9}m - \frac{74}{9}n + \frac{103}{9}$$

Proof. Considering that G(m,n) is a graphenylene network. By definition;

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

As a result by using Table 2;

$$Van^3(G(m,n)\,) = 2 \times (1 + 1) + 4 \times \left(1 + \frac{5}{6}\right) + (2m + 2n - 4) \times \left(\frac{5}{6} + \frac{5}{6}\right)$$

$$+(18mn - 16m - 16n + 14) \times \left(\frac{5}{6} + \frac{4}{9}\right) + (4m + 4n - 4) \times \left(\frac{4}{9} + \frac{4}{9}\right) + 4 \times \left(\frac{4}{9} + \frac{1}{3}\right)$$

$$+(8m + 8n - 16) \times \left(\frac{1}{3} + \frac{1}{3}\right)$$

the conclusion follows.

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

Theorem 4. Let G(m,n) be a graphenylene network. Then, the third reverse Van index of G(m,n)is;

$$Van^{3r}(G(m,n)\,) = \frac{621}{10}mn + \frac{78}{5}m + \frac{78}{5}n - \frac{83}{5}$$

Proof. Considering that G(m,n) is a graphenylene network. By definition;

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

As a result by using Table 2;

$$Van^{3r}(G(m, n)) = 2 \times (1 + 1) + 4 \times \left(1 + \frac{6}{5}\right) + (2m + 2n - 4) \times \left(\frac{6}{5} + \frac{6}{5}\right)$$

$$+(18mn - 16m - 16n + 14) \times \left(\frac{6}{5} + \frac{9}{4}\right) + (4m + 4n - 4) \times \left(\frac{9}{4} + \frac{9}{4}\right) + 4 \times \left(\frac{9}{4} + 3\right)$$

$$+(8m + 8n - 16) \times (3 + 3)$$

the conclusion follows.

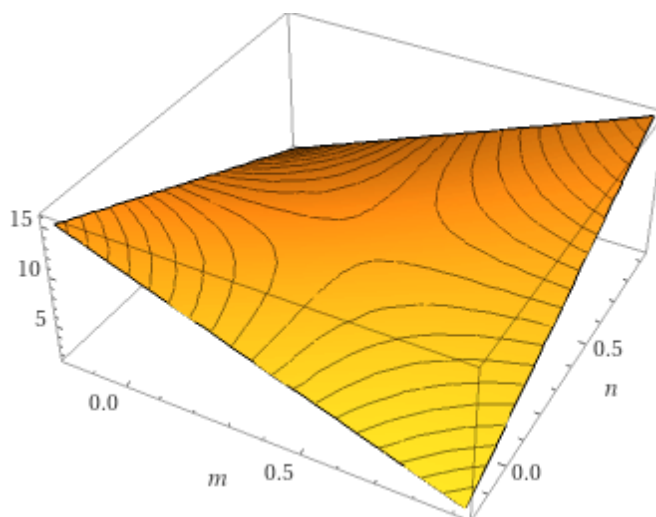3D plot of the third reverse Van index of graphenylene network, G(m,n), is shown in Figure 5.

Figure 4 3D plot of the third Van index of G(m,n)

Theorem 5. Let G(m,n)be a graphenylene network. Then, the second S index of G(m,n)is;

$$S^2(G(m, n)) = 180mn + 2834m + 2834n - 4728$$

Proof. Considering that G(m,n)is a graphenylene network. By definition;

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

As a result by using Table 3;

$$S^2(G(m, n)) = 2 \times 0 \times 0 + 4 \times 0 \times 1 + (2m + 2n - 4) \times 1 \times 1$$

$$+(18mn - 16m - 16n + 14) \times 1 \times 10 + (4m + 4n - 4) \times 10 \times 10 + 4 \times 10 \times 18$$

$$+(8m + 8n - 16) \times 18 \times 18$$

the conclusion follows.

3D plot of the second S index of graphenylene network, G(m,n), is shown in Figure 6.
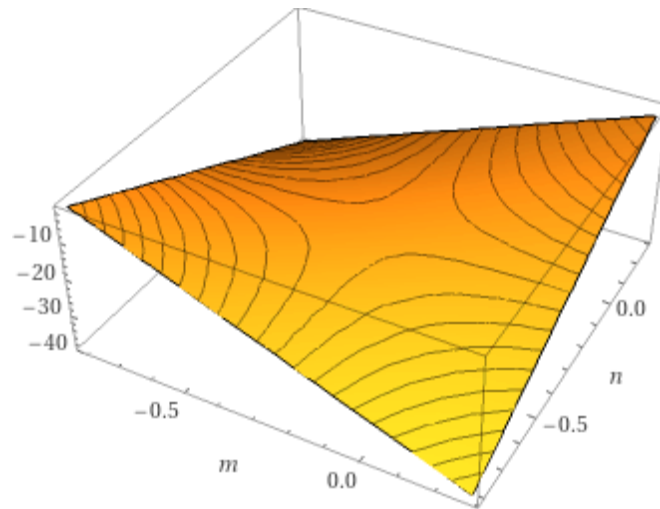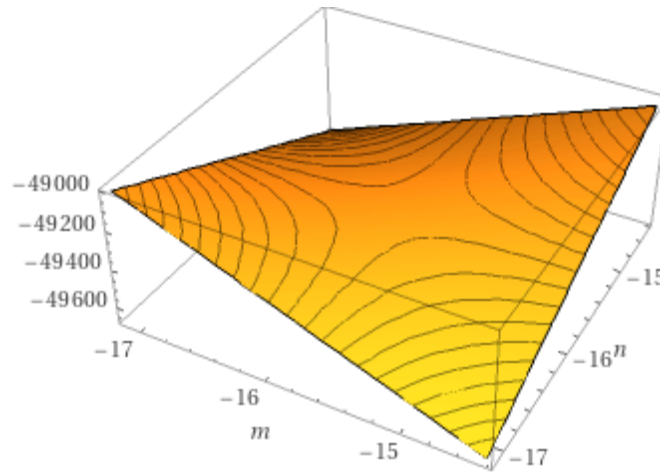
Figure 5 3D plot of the third reverse Van index of G(m,n)

Figure 6 3D plot of the second S index of G(m,n)

Theorem 6. Let G(m,n) be a graphenylene network. Then, the second reverse S index of G(m,n)is;

$$S^{2r}(G(m,n)) = \frac{9}{11}mn - \frac{15031}{87362}m - \frac{15031}{87362}n + \frac{156296}{43681}$$

Proof. Considering that G(m,n)is a graphenylene network. By definition;

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

As a result by using Table 3;

$$S^{2r}(G(m,n)) = 2 \times 1 \times 1 + 4 \times 1 \times 1/2 + (2m + 2n - 4) \times 1/2 \times 1/2$$

$$+(18mn - 16m - 16n + 14) \times 1/2 \times 1/11 + (4m + 4n - 4) \times 1/11 \times 1/11 + 4 \times 1/11 \times 1/19$$

$$+(8m + 8n - 16) \times 1/19 \times 1/19$$

the conclusion follows.

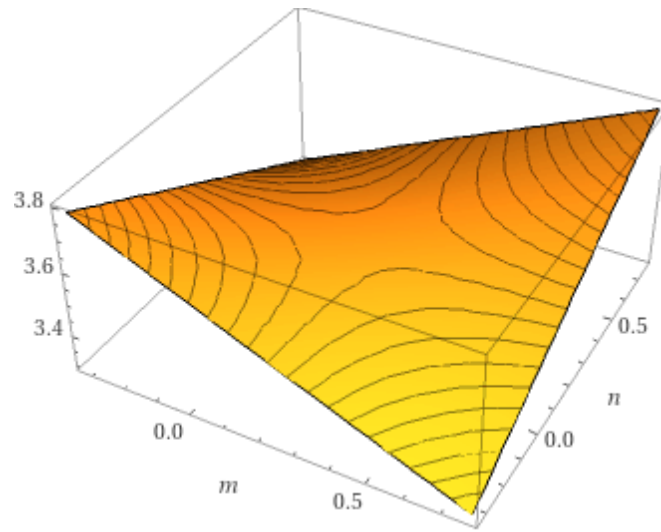3D plot of the second reverse S index of graphenylene network, G(m,n), is shown in Figure 7.

Figure 7 3D plot of the second reverse S index of G(m,n)

Theorem 7. Let G(m,n)be a graphenylene network. Then, the third S index of G(m,n)is;

$$S^3(G(m, n)) = 198mn + 196m + 196n - 394$$

Proof. Considering that G(m,n)is a graphenylene network. By definition;

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

As a result by using Table 3;

$$S^3(G(m, n)) = 2 \times (0 + 0) + 4 \times (0 + 1) + (2m + 2n - 4) \times (1 + 1)$$

$$+(18mn - 16m - 16n + 14) \times (1 + 10) + (4m + 4n - 4) \times (10 + 10) + 4 \times (10 + 18)$$

$$+(8m + 8n - 16) \times (18 + 18)$$

the conclusion follows.

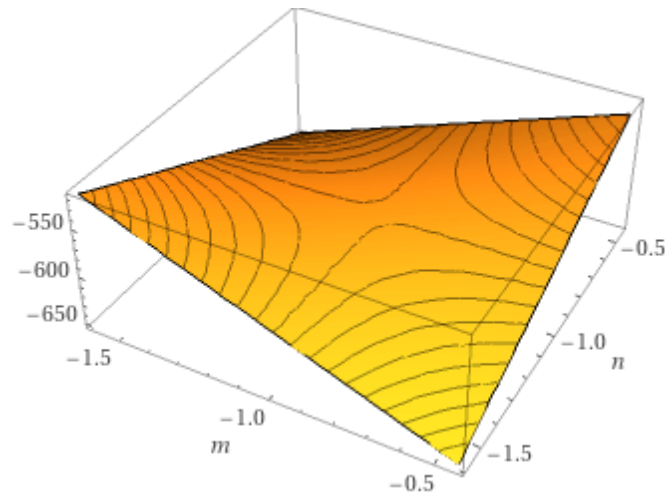3D plot of the third S index of graphenylene network, G(m,n), is shown in Figure 8.

Figure 8 3D plot of the third S index of G(m,n)

Theorem 8. Let G(m,n) be a graphenylene network. Then, the third reverse S index of G(m,n)is;

$$S^{3r}(G(m, n)) = \frac{117}{11}mn - \frac{1230}{209}m - \frac{1230}{209}n + \frac{2599}{209}$$

Proof. Considering that G(m,n)is a graphenylene network. By definition;

$$S^{3r}(G(m, n)) = \sum_{uv \in E(G(m,n))} (rs(u) + rs(v))$$

As a result by using Table 3;

$$S^{3r}(G(m, n)) = 2 \times (1 + 1) + 4 \times \left(1 + \frac{1}{2}\right) + (2m + 2n - 4) \times \left(\frac{1}{2} + \frac{1}{2}\right)$$

$$+(18mn - 16m - 16n + 14) \times \left(\frac{1}{2} + \frac{1}{11}\right) + (4m + 4n - 4) \times \left(\frac{1}{11} + \frac{1}{11}\right) + 4 \times \left(\frac{1}{11} + \frac{1}{19}\right)$$

$$+(8m + 8n - 16) \times \left(\frac{1}{19} + \frac{1}{19}\right)$$

the conclusion follows.

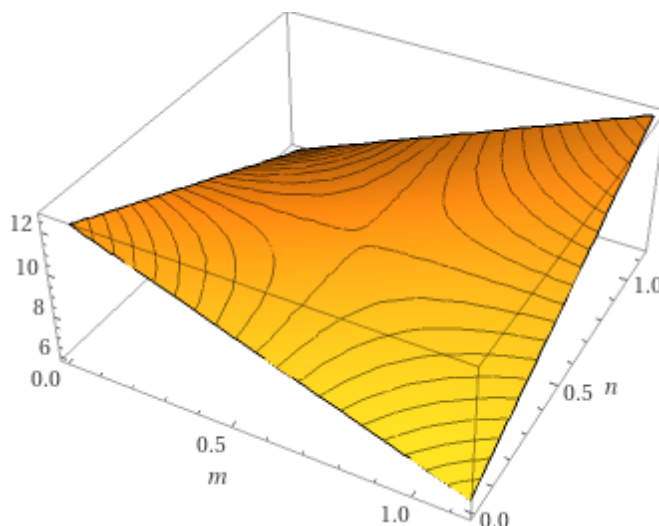3D plot of the third reverse S index of graphenylene network, G(m,n), is shown in Figure 9.

Figure 9 3D plot of the third reverse S index of G(m,n)

Theorem 9. Let G(m,n)be a graphenylene network. Then, the second R index of G(m,n)is;

$$R^2(\text{G(m, n)}) = 5148mn + 8738m + 8738n - 15696$$

Proof. Considering that G(m,n)is a graphenylene network. By definition;

$$R^2(\text{G(m, n)}) = \sum_{uv \in E(\text{G(m,n)})} r(u)r(v)$$

As a result by using Table 4;

$$R^2(\text{G(m, n)}) = 2 \times 8 \times 8 + 4 \times 8 \times 11 + (2m + 2n - 4) \times 11 \times 11$$

$$+(18mn - 16m - 16n + 14) \times 11 \times 26 + (4m + 4n - 4) \times 26 \times 26 + 4 \times 26 \times 36$$

$$+(8m + 8n - 16) \times 36 \times 36$$

the conclusion follows.

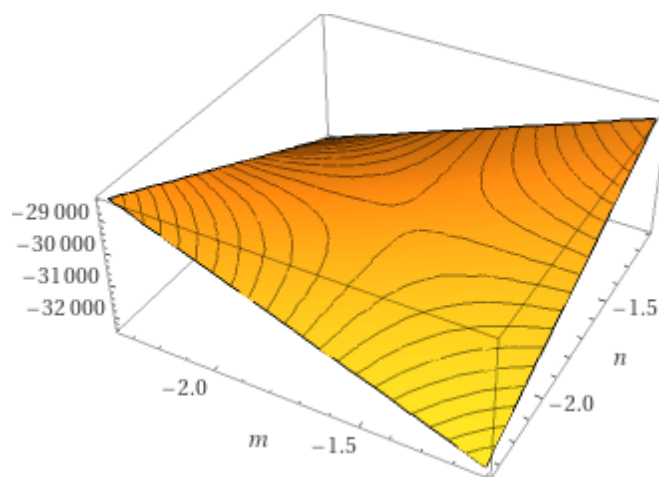3D plot of the second R index of graphenylene network, G(m,n), is shown in Figure 10.

Figure 10 3D plot of the second R index of G(m,n)

Theorem 10. Let G(m,n) be a graphenylene network. Then, the second reverse R index of G(m,n)is;

$$R^{2r}(\text{G(m, n)}) = \frac{9}{143}mn - \frac{90521}{3312738}m - \frac{90521}{3312738}n + \frac{4166545}{53003808}$$

Proof. Considering that G(m,n)is a graphenylene network. By definition;

$$R^{2r}(G(\text{m, n})) = \sum_{uv \in E(\text{G(m,n)})} rr(u)rr(v)$$

As a result by using Table 4;

$$R^{2r}(\text{G(m, n)}) = 2 \times 1/8 \times 1/8 + 4 \times 1/8 \times 1/11 + (2m + 2n - 4) \times 1/11 \times 1/11$$

$$+(18mn - 16m - 16n + 14) \times 1/11 \times 1/26 + (4m + 4n - 4) \times 1/26 \times 1/26 + 4 \times 1/26 \times 1/36$$

$$+(8m + 8n - 16) \times 1/36 \times 1/36$$

the conclusion follows.

3D plot of the second reverse R index of graphenylene network, G(m,n), is shown in Figure 11.

Theorem 11. Let G(m,n) be a graphenylene network. Then, the third R index of G(m,n) is;

$$R^3(\text{G(m, n)}) = 666mn + 236m + 236n - 574$$

Proof. Considering that G(m,n) is a graphenylene network. By definition;

$$R^3(G(\text{m, n})) = \sum_{uv \in E(\text{G(m,n)})} (r(u) + r(v))$$

As a result by using Table 4;

$$R^3(\text{G(m, n)}) = 2 \times (8 + 8) + 4 \times (8 + 11) + (2m + 2n - 4) \times (11 + 11)$$

$$+(18mn - 16m - 16n + 14) \times (11 + 26) + (4m + 4n - 4) \times (26 + 26) + 4 \times (26 + 36)$$

$$+(8m + 8n - 16) \times (36 + 36)$$

the conclusion follows.

3D plot of the third R index of graphenylene network, G(m,n), is shown in Figure 12.
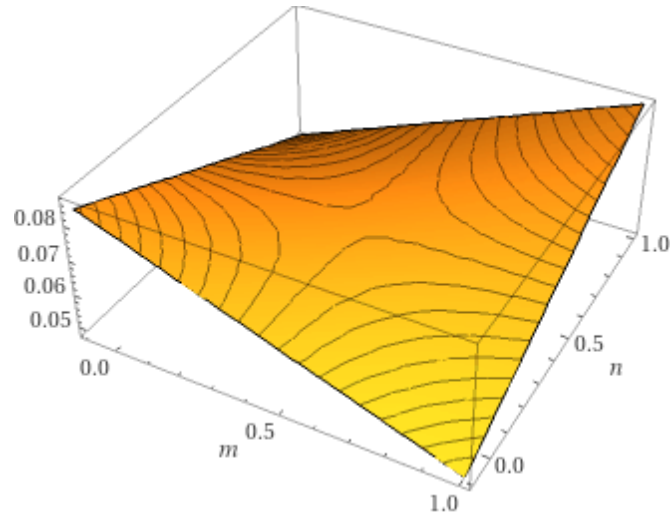

Figure 11 3D plot of the second reverse R index of G(m,n)
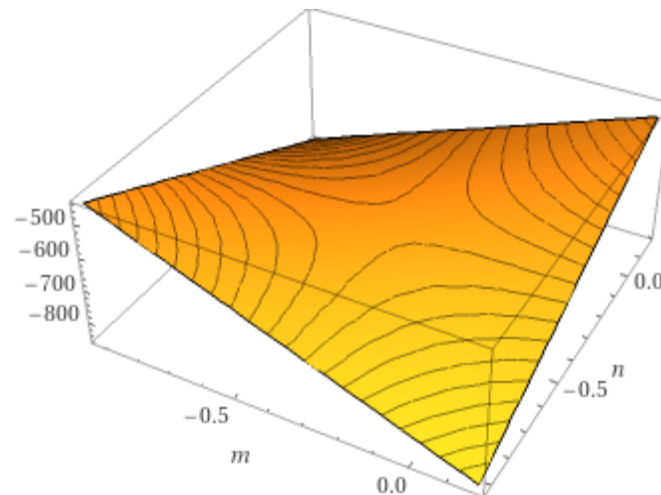

Figure 12 3D plot of the third R index of GN(m,n)

Theorem 12. Let G(m,n)be a graphenylene network. Then, the third reverse R index of G(m,n) is;

$$R^{3r}(\text{G(m,n)}) = \frac{333}{143}mn - \frac{1228}{1287}m - \frac{1228}{1287}n + \frac{1951}{1287}$$

Proof. Considering that G(m,n)is a graphenylene network. By definition;

$$R^{3r}(G\text{G(m,n)}) = \sum_{uv \in E(\text{G(m,n)})} (rr(u) + rr(v))$$

As a result by using Table 4;

$$R^{3r}(G(m,n)) = 2 \times \left(\frac{1}{8} + \frac{1}{8}\right) + 4 \times \left(\frac{1}{8} + \frac{1}{11}\right) + (2m + 2n - 4) \times \left(\frac{1}{11} + \frac{1}{11}\right)$$

$$+(18mn - 16m - 16n + 14) \times \left(\frac{1}{11} + \frac{1}{26}\right) + (4m + 4n - 4) \times \left(\frac{1}{26} + \frac{1}{26}\right) + 4 \times \left(\frac{1}{26} + \frac{1}{36}\right)$$

$$+(8m + 8n - 16) \times \left(\frac{1}{36} + \frac{1}{36}\right)$$

the conclusion follows.

3D plot of the third reverse R index of graphenylene network, G(m,n), is shown in Figure 13.
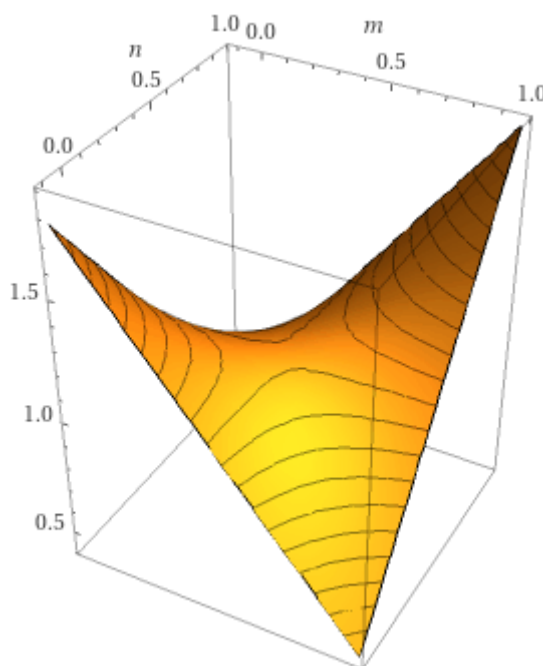

Figure 13 3D plot of the third reverse R index of G(m,n)

3.2 Entropies of grapenylene

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

Theorem 13. Let G be a graphenylene network G(m,n). Then, entropy of G which is based on the second Van index of G(m,n)is;

$$Ent_{Van^2}(G) = \log\left(\frac{20}{3}mn - \frac{463}{162}m - \frac{463}{162}n + \frac{467}{81}\right) - \frac{1}{\frac{20}{3}mn - \frac{463}{162}m - \frac{463}{162}n + \frac{467}{81}}(2m + 2n$$

$$- 4) \times \frac{25}{36} \times \log\frac{25}{36}$$

$$+(18mn - 16m - 16n + 14) \times \frac{10}{27} \times \log\frac{10}{27} + (4m + 4n - 4) \times \frac{16}{81} \times \log\frac{16}{81} + 4 \times \frac{4}{27} \times \log\frac{4}{27}$$

$$+(8m + 8n - 16) \times \frac{1}{9} \times log\frac{1}{9})$$

Proof. Considering that G is a graphenylene network. By definition;

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

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

Theorem 14. Let G be a graphenylene network G(m,n). Then, entropy of G which is based on the second reverse Van index of G(m,n)is;

$$Ent_{Van^{2r}}(G) = log\left(\frac{243}{5}mn + \frac{5193}{100}m + \frac{5193}{100}n - \frac{9841}{20}\right) - \frac{1}{\frac{243}{5}mn+\frac{5193}{100}m+\frac{5193}{100}n-\frac{9841}{20}}(4 \times \frac{6}{5} \times log\frac{6}{5} +$$

$$(2m + 2n - 4) \times \frac{36}{25} \times log\frac{36}{25}$$

$$+(18mn - 16m - 16n + 14) \times \frac{27}{10} \times log\frac{27}{10} + (4m + 4n - 4) \times \frac{81}{16} \times log\frac{81}{16} + 27 \times log\frac{27}{4}$$

$$+(8m + 8n - 16) \times 18 \times log3)$$

Proof. Considering that G is a graphenylene network. By definition;

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

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

Theorem 15. Let G be a graphenylene network G(m,n). Then, entropy of G which is based on the third Van index of G(m,n)is;

$$Ent_{Van^3}(G) = log\left(23mn - \frac{74}{9}m - \frac{74}{9}n + \frac{103}{9}\right) - \frac{1}{23mn-\frac{74}{9}m-\frac{74}{9}n+\frac{103}{9}}(4 \times log2 + 4 \times \frac{11}{6} \times log\frac{11}{6} +$$

$$(2m + 2n - 4) \times \frac{5}{3} \times log\frac{5}{3}$$

$$+(18mn - 16m - 16n + 14) \times \frac{23}{18} \times log\frac{23}{18} + (4m + 4n - 4) \times \frac{8}{9} \times log\frac{8}{9} + 4 \times \frac{7}{9} \times log\frac{7}{9}$$

$$+(8m + 8n - 16) \times \frac{2}{3} \times log\frac{2}{3})$$

Proof. Considering that G is a graphenylene network. By definition;

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

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

Theorem 16. Let G be a graphenylene network G(m,n). Then, entropy of G which is based on the third reverse Van index of G(m,n)is;

$$Ent_{Van^{3r}}(G) = log\left(\frac{621}{10}mn + \frac{78}{5}m + \frac{78}{5}n - \frac{83}{5}\right) - \frac{1}{\frac{621}{10}mn + \frac{78}{5}m + \frac{78}{5}n - \frac{83}{5}}(4 \times log2 + 4 \times \frac{11}{5} \times log\frac{11}{5} +$$

$$(2m + 2n - 4) \times \frac{12}{5} \times log\frac{12}{5}$$

$$+(18mn - 16m - 16n + 14) \times \frac{69}{20} \times log\frac{69}{20} + (4m + 4n - 4) \times \frac{9}{2} \times log\frac{9}{2} + 21 \times log\frac{21}{4}$$

$$+(8m + 8n - 16) \times 6 \times log6)$$

Proof. Considering that G is a graphenylene network. By definition;

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

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

Theorem 17. Let G be a graphenylene network G(m,n). Then, entropy of G which is based on the second S index of G(m,n)is;

$$Ent_{S^2}(G) = log(180mn + 2834m + 2834n - 4728) - \frac{1}{180mn + 2834m + 2834n - 4728}((18mn - 16m -$$

$$16n + 14) \times 10 \times log10 + (4m + 4n - 4) \times 10 \times 10 + 4 \times 180 \times log180$$

$$+(8m + 8n - 16) \times 648 \times log18))$$

Proof. Considering that G is a graphenylene network. By definition;

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

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

Theorem 18. Let G be a graphenylene network G(m,n). Then, entropy of G which is based on the second reverse S index of G(m,n)is;

$$Ent_{S^{2r}}(G) = log\left(\frac{9}{11}mn - \frac{15031}{87362}m - \frac{15031}{87362}n + \frac{156296}{43681}\right) - \frac{1}{\frac{9}{11}mn - \frac{15031}{87362}m - \frac{15031}{87362}n + \frac{156296}{43681}}(4 \times log1/2 +$$

$$(2m + 2n - 4) \times \frac{1}{4} \times log\frac{1}{4} + (18mn - 16m - 16n + 14) \times \frac{1}{22} \times log\frac{1}{22} + (4m + 4n - 4) \times \frac{1}{121} \times$$

$$log\frac{1}{121} + 4 \times \frac{1}{209} \times log\frac{1}{209} + (8m + 8n - 16) \times \frac{1}{361} \times log\frac{1}{361})$$

Proof. Considering that G is a graphenylene 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 graphenylene network G(m,n). Then, entropy of G which is based on the third S index of G(m,n)is;

$Ent_{S^3}(G) = log(198mn + 196m + 196n - 394) - \frac{1}{198mn+196m+196n-394}((2m + 2n - 4) \times 2 \times$
$log2 + (18mn - 16m - 16n + 14) \times 11 \times log11 + (4m + 4n - 4) \times 20 \times log20 + 112 \times log28 +$
$(8m + 8n - 16) \times 72 \times log6)$

Proof. Considering that G is a graphenylene network. By definition;

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

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

Theorem 20. Let G be a graphenylene network G(m,n). Then, entropy of G which is based on the third reverse S index of G(m,n)is;

$Ent_{S^{3r}}(G) = log\left(\frac{117}{11}mn - \frac{1230}{209}m - \frac{1230}{209}n + \frac{2599}{209}\right) - \frac{1}{\frac{117}{11}mn-\frac{1230}{209}m-\frac{1230}{209}n+\frac{2599}{209}}(4 \times log2 + 6 \times$
$log\frac{3}{2} + (18mn - 16m - 16n + 14) \times \frac{13}{22} \times log\frac{13}{22} + (4m + 4n - 4) \times \frac{2}{11} \times log\frac{2}{11} + 4 \times \frac{30}{209} \times$
$log\frac{30}{209} + (8m + 8n - 16) \times \frac{2}{19} \times log\frac{2}{19})$

Proof. Considering that G is a graphenylene network. By definition;

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

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

Theorem 21. Let G be a graphenylene network G(m,n). Then, entropy of G which is based on the second R index of G(m,n)is;

$Ent_{R^2}(G) = log(5148mn + 8738m + 8738n - 15696) - \frac{1}{5148mn+8738m+8738n-15696}(768 \times$
$log2 + 352 \times log88 + (2m + 2n - 4) \times 242 \times log11 + (18mn - 16m - 16n + 14) \times 286 \times$
$log286 + (4m + 4n - 4) \times 1352 \times log26 + 3744 \times log936 + (8m + 8n - 16) \times 2612 \times log6)$

Proof. Considering that G is a graphenylene network. By definition;

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

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

Theorem 22. Let G be a graphenylene network G(m,n). Then, entropy of G which is based on the second reverse R index of G(m,n)is;

$$Ent_{R^{2r}}(G) = log\left(\frac{9}{143}mn - \frac{90521}{3312738}m - \frac{90521}{3312738}n + \frac{4166545}{53003808}\right) - \frac{1}{\frac{9}{143}mn - \frac{90521}{3312738}m - \frac{90521}{3312738}n + \frac{4166545}{53003808}}(2 \times$$

$$\frac{1}{64} \times log\frac{1}{64} + 4 \times \frac{1}{88} \times log\frac{1}{88} + (2m + 2n - 4) \times \frac{1}{121} \times log\frac{1}{121}$$

$$+(18mn - 16m - 16n + 14) \times \frac{1}{286} \times log\frac{1}{286} + (4m + 4n - 4) \times \frac{1}{676} \times log\frac{1}{676}$$

$$+ 4 \times \frac{1}{936} \times log\frac{1}{936}$$

$$+(8m + 8n - 16) \times \frac{1}{1296} \times log\frac{1}{1296})$$

Proof. Considering that G is a graphenylene network. By definition;

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

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

Theorem 23. Let G be a graphenylene network G(m,n). Then, entropy of G which is based on the third R index of G(m,n)is;

$$Ent_{R^3}(G) = log(666mn + 236m + 236n - 574) - \frac{1}{666mn+236m+236n-574}(64 \times log2 + 76 \times log19 + (2m + 2n - 4) \times 22 \times log22$$

$$+(18mn - 16m - 16n + 14) \times 37 \times log37 + (4m + 4n - 4) \times 52 \times log \times log52$$
$$+ 4 \times 62 \times log62$$

$$+(8m + 8n - 16) \times 72 \times log72)$$

Proof. Considering that G is a graphenylene network. By definition;

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

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

Theorem 24. Let G be a graphenylene network G(m,n). Then, entropy of G which is based on the third reverse R index of G(m,n)is;

$$Ent_{R^{3r}}(G) = log\left(\frac{333}{143}mn - \frac{1228}{1287}m - \frac{1228}{1287}n + \frac{1951}{1287}\right) - \frac{1}{\frac{333}{143}mn - \frac{1228}{1287}m - \frac{1228}{1287}n + \frac{1951}{1287}}(2 \times \frac{1}{4} \times log\frac{1}{4} + 4 \times$$

$$\frac{19}{88} \times log\frac{19}{88} + (2m + 2n - 4) \times \frac{2}{11} \times log\frac{2}{11}$$

$$+(18mn - 16m - 16n + 14) \times \frac{37}{286} \times log\frac{37}{286} + (4m + 4n - 4) \times \frac{1}{13} \times log\frac{1}{13}$$

$$+ 4 \times \frac{31}{468} \times log\frac{31}{468}$$

$$+(8m + 8n - 16) \times \frac{1}{18} \times log\frac{1}{18})$$

Proof. Considering that G is a graphenylene network. By definition;

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

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 graphenylene is described in this study. Information-theoretic entropy measurements of various phases of 2D materials of graphenylenes 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 graphenylene with a number of their physicochemical and optoelectronic properties, the results of this study could significantly advance QSAR and QSPR studies of these materials.

References

[1]Balasubramanian, K. (2021). Computational and artificial intelligence techniques for drug discovery and administration. *Reference Module in Biomedical Sciences*.
[2]Balasubramanian, K. (2018). Mathematical and computational techniques for drug discovery: promises and developments. *Current Topics in Medicinal Chemistry*, *18*(32), 2774-2799.
[3]Huilgol, M. I., Sriram, V., & Balasubramanian, K. (2022). Structure–activity relations for antiepileptic drugs through omega polynomials and topological indices. *Molecular Physics*, *120*(3), e1987542.
[4]Balasubramanian, K. (2021). Combinatorics, big data, neural network & AI for medicinal chemistry & drug administration. *Letters in Drug Design & Discovery*, *18*(10), 943-948.
[5]Gao, W., Younas, M., Farooq, A., Mahboob, A., & Nazeer, W. (2018). M-polynomials and degree-based topological indices of the crystallographic structure of molecules. *Biomolecules*, *8*(4), 107.
[6]Sabirov, D. S., & Shepelevich, I. S. (2021). Information entropy in chemistry: An overview. *Entropy*, *23*(10), 1240.

[7]Shannon, C. E. (1948). A mathematical theory of communication. *The Bell system technical journal*, *27*(3), 379-423.

[8] Bonchev, D. (1983). Information theoretic indices for characterization of chemical structures. New York: Wiley. 21.

[9]Dehmer, M., Mowshowitz, A. (2011). A history of graph entropy measures. Information Sciences, 181(1), 57–78. https://doi.org/10.1016/j.ins.2010.08.041

[10]   Kazemi, R. (2016). Entropy of weighted graphs with the degree-based topological indices as weights. MATCH Communications in Mathematical and in Computer Chemistry, 76(1), 69–80.

[11]   Manzoor, S., Siddiqui, M. K., Ahmad, S. (2020). On entropy measures of molecular graphs using topological indices. Arabian Journal of Chemistry, 13(8), 6285–6298.

[12]   Cao, S., Dehmer, M. (2015). Degree-based entropies of networks revisited. Applied Mathematics and Computation, 261(1), 141–147. https://doi.org/10.1016/j.amc.2015.03.046

[13]   Dehmer, M., Grabner, M. (2013). The discrimination power of molecular identification numbers revisited. MATCH Communications in Mathematical and in Computer Chemistry, 69(3), 785–794.

[14]   Manzoor, S., Siddiqui, M. K., Ahmad, S. (2021). On physical analysis of degree-based entropy measures for metal organic superlattices. The European Physical Journal Plus, 136(3), 1–22. https://doi.org/10. 1140/epjp/s13360-021-01275-5

[15]   Hayat, S., Khan, S., Imran, M. (2021). Quality testing of spectrum-based distance descriptors for polycyclic aromatic hydrocarbons with applications to carbon nanotubes and nanocones. Arabian Journal of Chemistry, 14(3), 102994.

[16]   De La Pierre, M., Karamanis, P., Baima, J., Orlando, R., Pouchan, C. et al. (2013). Ab initio periodic simulation of the spectroscopic and optical properties of novel porous graphene phases. The Journal of Physical Chemistry C, 117(5), 2222–2229. https://doi.org/10.1021/jp3103436

[17]   Zhang, T. (2018). Synchrotron radiation studies of molecular building blocks for functional materials (Ph.D. Thesis). Uppsala University, Uppsala.

[18]   Rong, J., Dong, H., Feng, J., Wang, X., Zhang, Y. et al. (2018). Planar metallic carbon allotrope from graphene-like nanoribbons. Carbon, 135(3B), 21–28. https://doi.org/10.1016/j.carbon.2018.04.033

[19]   Rahul, M. P., Clement, J., Junias, J. S., Arockiaraj, M., & Balasubramanian, K. (2022). Degree-based entropies of graphene, graphyne and graphdiyne using Shannon's approach. *Journal of Molecular Structure*, *1260*, 132797.

[20]   Yang, J., Konsalraj, J., & Raja S, A. A. (2022). Neighbourhood Sum Degree-Based Indices and Entropy Measures for Certain Family of Graphene Molecules. *Molecules*, *28*(1), 168.

[21]   Shanmukha, M. C., Lee, S., Usha, A., Shilpa, K. C., & Azeem, M. (2023). Degree-based entropy descriptors of graphenylene using topological indices. *Comput. Model. Eng. Sci*, *2023*, 1-25.

[22]   Ediz S., Semiz M. (2017), On Van Degrees of Vertices and Van Indices of Graphs, Mathematics and Computer Science 2(4), 35-38.

[23]   Ediz, S. (2017), On R Degrees of Vertices and R Indices of Graphs International Journal of Advanced Chemistry 5(2), 70-73

[24]   Ediz, S. (2017) , On S Degrees of Vertices and S Indices of Graphs, Science Journal of Analytical Chemistry 5(5), 86-89

[25]   Dehmer, M., & Grabner, M. (2013). The discrimination power of molecular identification numbers revisited. *MATCH Commun. Math. Comput. Chem*, *69*(3), 785-794.

[26]   Ulanowicz, R. E. (2004). Quantitative methods for ecological network analysis. Computational biology and chemistry, 28(5-6), 321-339.

[27]   Dehmer, M. (2008). Information processing in complex networks: Graph entropy and information functionals. *Applied Mathematics and Computation*, *201*(1-2), 82-94.

[28]Dehmer, M., & Kraus, V. (2012). On extremal properties of graph entropies. *MATCH Commun. Math. Comput. Chem*, *68*(3), 889-912.

[29]   Estrada, E. (2010). Generalized walks-based centrality measures for complex biological networks. *Journal of theoretical biology*, *263*(4), 556-565.

[30]   Kazemi, R. (2016). Entropy of weighted graphs with the degree-based topological indices as weights. *MATCH Commun. Math. Comput. Chem*, *76*(1), 69-80.