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INVESTIGATING TOPOLOGICAL DESCRIPTORS OF α-GRAPHDIYNE BY EMPLOYING REVAN INDICES AND ENTROPY ANALYSIS THROUGH LINEAR REGRESSION

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Abstract

Graphdiyne Nanoribbons have considerable potential across several applications. In electronics, they offer distinctive electrical characteristics for high-performance nanoscale devices, while in catalysis, their superior surface area and reactivity render them useful catalyst supports. Various chemical processes, facilitating advancements in sustainable energy and environmental restoration. Topological indices (TIs) are numerical invariants that provide significant information on the molecular topology of a certain molecular graph. Linear regression model is employed to ascertain relationships among these indices, entropy, and other relevant chemical descriptors. These results elucidate the structural and chemical characteristics of these nanoribbons and advance the creation of novel materials for diverse applications, thereby enhancing comprehension of the material's potential uses across various scientific and technological domains. This work examines the computation of degree-based entropies for alpha Graphdiyne to ascertain the association between indices, employing entropies and a linear regression model. The findings enhance comprehension of the material's potential applications across several scientific and technical domains.

Math. Subject Classification: 05C09, 05C92, 92E10

Key Words and Phrases: Graphdiyne, revan indices, entropies, linear regression.

1. Introduction:

Chemical graph theory is a branch of mathematical chemistry that contributes significantly to the advancement of the chemical sciences which deals with the application of graph theory in which the atoms are represented by the vertices, and the bonds are represented by the edges. When calculating a molecular graph of chemical events, a specific type of molecular descriptor is called a topological index. Numerical invariants known as topological indices (TIs) offer essential information on the molecular topology of a particular molecular graph. In Molecular graphs topology and graph invariants are studied using topological indices. In 1736, Leonhard Euler established the principles of graph theory and anticipated the concept

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of topology. In 1947, Wiener developed the notion of topological indices, addressing both their functional uses and theoretical prominence.

For a simple, finite, undirected and connected graph G with vertex set V(G) and edge set E(G). A vertex degree $d_G(V)$ in relation to the number of vertices that are adjacent to V. Let ($\delta(G)$) represent the minimum degree among the vertices of G and $\Delta(G)$ represent the maximum degree. Refer [8] for undetermined terms and notation. The expression $r_G(v) = \Delta(G) + \delta(G) - d_G(v)$ is used to determine the Revan vertex degree of a vertex v in G. Also uv stand for the revan edge that connects the revan vertices u and v. Revan indices have been introduced by V.R. Kulli and it was examined for oxides and honeycomb network in [8]. Analytical and statistical studies of Revan indices on graph was explored in [9]. The first and second Revan indices of certain graphs are studied and examined in [5]. Computation of square snake graph using revan indices including their polynomials has been discussed in [7]. Using the molecule of alkanes with double graph and strong double graph by applying revan indices generic formula has been computed in [6].

Graphdiyne is a derivative of garaphene. Graphdiyne, often known as graphyne-2, signifies that the benzene rings have been bound by two consecutive acetylene molecules, forming a diacetylenic structure. The graphdiyne Nanoribbons provide significant potential for a variety of uses. Their exceptional surface area and reactivity generate them with essential catalyst supports for a variety of chemical reactions in catalysis, which advances environmentally friendly and sustainable energy. This distinctive material is highly promising for use in modern microelectronics due to its unique and sophisticated characteristics. In electronics, they provide distinctive electronic properties for high-performance nanoscale devices. Graphdiyne, characterized by its band gap and magnetic properties, holds considerable potential for employing in nanoelectronics and spintronics. Graphdiyne (GDY), characterized by its highly conjugated and adaptable molecular architecture, exhibits significant potential in several sensing applications owing to its distinctive physicochemical properties, including a high specific surface area, variable band gap, exceptional conductivity, and remarkable stability.

The graphdiyne structure is extracted from [2]. Degree based entropies using shannon's approach was studied in [3]. In this work molecular graph of graphdiyne structure has been employed in revan topological indices with various types. Based on the materials and synthesis Graphdiyne has been discussed in [4]. Reduced reverse degree based TI using Graphdiyne with its chemical analysis have been explored in [10]. Also computed an entropy measurement that corresponds to degree based topological indices and linear regression model has been defined using the applied topological indices and entropy measurements.

2. Methodology

Topological Indices	**Notation**	**Expression**
First Revan Index	$R_1(G)$	$\sum_{uv \in E(G)} (r_u + r_v)$

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Second Revan Index	$R_2(G)$	$\sum_{uv\in E(G)} (r_u.r_v)$
Third Revan Index	$R_3(G)$	$\sum_{uv\in E(G)} \lvert(r_u - r_v)\rvert$
First Hyper Revan Index	$HR_1(G)$	$\sum_{uv\in E(G)} (r_u + r_v)^2$
Second Hyper Revan Index	$H\ R_2(G)$	$\sum_{uv\in E(G)} (r_u.r_v)^2$
First Modified Revan Index	$^{m}R_1(G)$	$\sum_{uv\in E(G)} \frac{1}{(r_u + r_v)}$
Second Modified Revan Index	$^{m}R_2(G)$	$\sum_{uv\in E(G)} \frac{1}{(r_u.r_v)}$
Sum Connectivity Revan Index	SR(G)	$\sum_{uv\in E(G)} \frac{1}{\sqrt{(r_u + r_v)}}$
Product Connectivity Revan Index	PR(G)	$\sum_{uv\in E(G)} \frac{1}{\sqrt{(r_u.r_v)}}$
Harmonic Revan Index	HR(G)	$\sum_{uv\in E(G)} \left(\frac{2}{r_u + r_v}\right)$
Inverse Sum Revan Index	ISR(G)	$\sum_{uv\in E(G)} \left(\frac{r_u.r_v}{r_u + r_v}\right)$
Geometric Arithmetic Revan Index	GAR(G)	$\sum_{uv\in E(G)} \left(\frac{2\sqrt{(r_u.r_v)}}{r_u + r_v}\right)$
Arithmetic Geometric Revan Index	AGR(G)	$\sum_{uv\in E(G)} \left(\frac{r_u + r_v}{2\sqrt{(r_u.r_v)}}\right)$
Atom Bond Connectivity Revan Index	ABCR(G)	$\sum_{uv\in E(G)} \sqrt{\left(\frac{r_u + r_v - 2}{r_u.r_v}\right)}$
First Gourava Revan Index	$RGO_1(G)$	$\sum_{uv\in E(G)} [(r_u + r_v) + (r_u.r_v)]$
Redefined First Revan Index	$ReR_1(G)$	$\sum_{uv\in E(G)} \left(\frac{r_u + r_v}{r_u.r_v}\right)$

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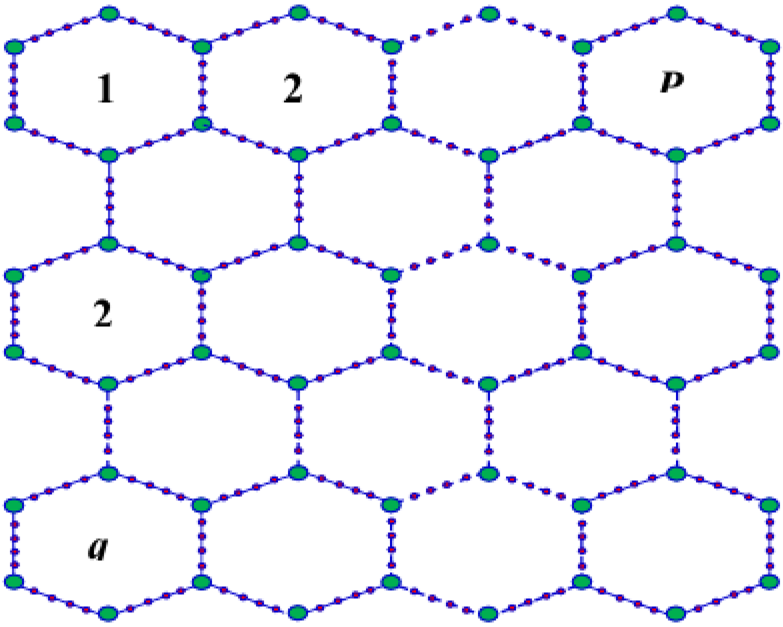
Table 1: Notations and expressions for various Revan-based topological indices.



Structure of $\alpha -$ graphdiyne

(d(u),d(v))	**Frequency**	**d(e)**	**r_u**	**r_v**
(2,2)	18mn+m+11n	2	3	3
(2,3)	12mn-6m-6n	3	3	2

Table 2: Edge Partition of $\alpha -$ Graphdiyne

Using entropy [4], Chen et al. emerged up with an idea of a connected graph T with edge e = pq. They defined it as

$$ENT_g(T) = -\sum_{i=1}^{m} \frac{g(e_i)}{\sum_{i=1}^{m} g(e_i)} log\left(\frac{g(e_i)}{\sum_{i=1}^{m} g(e_i)}\right)$$

By expanding this equation, we arrive at

$$ENT_g(T) = log\left(\sum_{i=1}^{m} g(e_i)\right) - \frac{1}{\sum_{i=1}^{m} g(e_i)} \sum_{i=1}^{m} g(e_i) log\big(g(e_i)\big)$$

Now, replacing $\sum_{i=1}^{m} g(e_i)$by the topological indices in the above equation, we get the respective index entropy.

Definition 2.1: First revan index entropy

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If $g_1(e) = (r_u + r_v)$ and $\sum_{pq\in E(T)} g_1(e) = \sum_{pq\in E(T)}(r_u + r_v) = R_1(T)$, then the first revan index entropy is given by

$$ENT\big(R_1(T)\big) = log\big(R_1(T)\big) - \frac{1}{\big(R_1(T)\big)}\sum_{pq\in E(T)} g_1(e)log\big(g_1(e)\big)$$

Definition 2.2: Second revan index entropy

If $g_2(e) = (r_u . r_v)$ and $\sum_{pq\in E(T)} g_2(e) = \sum_{pq\in E(T)}(r_u . r_v) = R_2(T)$, then the second revan index entropy is given by

$$ENT\big(R_2(T)\big) = log\big(R_2(T)\big) - \frac{1}{\big(R_2(T)\big)}\sum_{pq\in E(T)} g_2(e)log\big(g_2(e)\big)$$

Definition 2.3: Third revan index entropy

If $g_3(e) = |(r_u - r_v)|$ and$\sum_{pq\in E(T)} g_3(e) = \sum_{pq\in E(T)}|(r_u - r_v)| = R_3(T)$, then the third revan index entropy is given by

$$ENT\big(R_3(T)\big) = log\big(R_3(T)\big) - \frac{1}{\big(R_3(T)\big)}\sum_{pq\in E(T)} g_3(e)log\big(g_3(e)\big)$$

Definition 2.4: First hyper revan index entropy

If $g_4(e) = (r_u + r_v)^2$ and$\sum_{pq\in E(T)} g_4(e) = \sum_{pq\in E(T)}(r_u + r_v)^2 = HR_1(T)$, then the first hyper revan index entropy is given by

$$ENT(HR_1(T)) = log(HR_1(T)) - \frac{1}{HR_1(T)}\sum_{pq\in E(T)} g_4(e)log\big(g_4(e)\big)$$

Definition 2.5: Second hyper revan index entropy

If $g_5(e) = (r_u . r_v)^2$ and$\sum_{pq\in E(T)} g_5(e) = \sum_{pq\in E(T)}(r_u . r_v)^2 = HR_2(T)$, then the second hyper revan index entropy is given by

$$ENT(HR_2(T)) = log(HR_2(T)) - \frac{1}{HR_2(T)}\sum_{pq\in E(T)} g_5(e)log\big(g_5(e)\big)$$

Definition 2.6: First modified revan index entropy

If $g_6(e) = \frac{1}{(r_u+r_v)}$ and$\sum_{pq\in E(T)} g_6(e) = \sum_{pq\in E(T)}\frac{1}{(r_u+r_v)} = mR_1(T)$, then the first modified revan index entropy is given by

$$ENT(mR_1(T)) = log(mR_1(T)) - \frac{1}{mR_1(T)}\sum_{pq\in E(T)} g_6(e)log\big(g_6(e)\big)$$

Definition 2.7: Second modified revan index entropy

If $g_7(e) = \frac{1}{(r_u\,.\,r_v)}$ and$\sum_{pq\in E(T)} g_7(e) = \sum_{pq\in E(T)}\frac{1}{(r_u\,.\,r_v)} = mR_2(T)$, then the second modified revan index entropy is given by

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$$ENT(mR_2(T)) = log(mR_2(T)) - \frac{1}{mR_2(T)} \sum_{pq \in E(T)} g_7(e) log\big(g_7(e)\big)$$

Definition 2.8: Sum connectivity revan index entropy

If $g_8(e) = \frac{1}{\sqrt{r_u + r_v}}$ and $\sum_{pq \in E(T)} g_8(e) = \sum_{pq \in E(T)} \frac{1}{\sqrt{r_u + r_v}} = SR(T)$, then the sum connectivity revan index entropy is given by

$$ENT(SR(T)) = log(SR(T)) - \frac{1}{SR(T)} \sum_{pq \in E(T)} g_8(e) log\big(g_8(e)\big)$$

Definition 2.9: Product connectivity revan index entropy

If $g_9(e) = \frac{1}{\sqrt{r_u \cdot r_v}}$ and $\sum_{pq \in E(T)} g_9(e) = \sum_{pq \in E(T)} \frac{1}{\sqrt{r_u \cdot r_v}} = PR(T)$, then the product connectivity revan index entropy is given by

$$ENT(PR(T)) = log(PR(T)) - \frac{1}{PR(T)} \sum_{pq \in E(T)} g_9(e) log\big(g_9(e)\big)$$

Definition 2.10: Harmonic connectivity revan index entropy

If $g_{10}(e) = \frac{2}{r_u + r_v}$ and $\sum_{pq \in E(T)} g_{10}(e) = \sum_{pq \in E(T)} \frac{2}{r_u + r_v} = HR(T)$, then the harmonic connectivity revan index entropy is given by

$$ENT(HR(T)) = log(HR(T)) - \frac{1}{HR(T)} \sum_{pq \in E(T)} g_{10}(e) log\big(g_{10}(e)\big)$$

Definition 2.11: Inverse sum revan index *entropy*

If $g_{11}(e) = \left(\frac{r_u \cdot r_v}{r_u + r_v}\right)$ and $\sum_{pq \in E(T)} g_{11}(e) = \sum_{pq \in E(T)} \left(\frac{r_u \cdot r_v}{r_u + r_v}\right) = ISR(T)$, then the harmonic connectivity revan index entropy is given by

$$ENT(ISR(T)) = log(ISR(T)) - \frac{1}{ISR(T)} \sum_{pq \in E(T)} g_{11}(e) log\big(g_{11}(e)\big)$$

Definition 2.12: Geometric arithmetic revan index entropy

If $g_{12}(e) = \left(\frac{2\sqrt{(r_u \cdot r_v)}}{r_u + r_v}\right)$ and $\sum_{pq \in E(T)} g_{12}(e) = \sum_{pq \in E(T)} \left(\frac{2\sqrt{(r_u \cdot r_v)}}{r_u + r_v}\right) = GAR(T)$, then the harmonic connectivity revan index entropy is given by

$$ENT(GAR(T)) = log(GAR(T)) - \frac{1}{GAR(T)} \sum_{pq \in E(T)} g_{12}(e) log\big(g_{12}(e)\big)$$

Definition 2.13: Arithmetic geometric revan index entropy

If $g_{13}(e) = \left(\frac{r_u + r_v}{2\sqrt{(r_u \cdot r_v)}}\right)$ and $\sum_{pq \in E(T)} g_{13}(e) = \sum_{pq \in E(T)} \left(\frac{r_u + r_v}{2\sqrt{(r_u \cdot r_v)}}\right) = AGR(T)$, then the harmonic connectivity revan index entropy is given by

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$$ENT(AGR(T)) = log(AGR(T)) - \frac{1}{AGR(T)} \sum_{pq \in E(T)} g_{13}(e) log\big(g_{13}(e)\big)$$

Definition 2.14: Atom bond connectivity revan index entropy

If $g_{14}(e) = \sqrt{\left(\frac{r_u + r_v - 2}{r_u \cdot r_v}\right)}$ and$\sum_{pq \in E(T)} g_{14}(e) = \sum_{pq \in E(T)} \sqrt{\left(\frac{r_u + r_v - 2}{r_u \cdot r_v}\right)} = ABC(T)$, then the atom bond connectivity revan index entropy is given by

$$ENT(ABC(T)) = log(ABC(T)) - \frac{1}{ABC(T)} \sum_{pq \in E(T)} g_{14}(e) log\big(g_{14}(e)\big)$$

Definition 2.15: First gourava revan index entropy

If $g_{15}(e) = [(r_u + r_v) + (r_u . r_v)]$ and$\sum_{pq \in E(T)} g_{15}(e) = \sum_{pq \in E(T)} [(r_u + r_v) + (r_u . r_v)] = RGO_1(T)$, then the first gourava revan index entropy is given by

$$ENT(RGO_1(T)) = log(RGO_1(T)) - \frac{1}{RGO_1(T)} \sum_{pq \in E(T)} g_{15}(e) log\big(g_{15}(e)\big)$$

Definition 2.16: Redefined 1st revan index entropy

If $g_{16}(e) = \left(\frac{r_u + r_v}{r_u \cdot r_v}\right)$ and$\sum_{pq \in E(T)} g_{16}(e) = \sum_{pq \in E(T)} \left(\frac{r_u + r_v}{r_u \cdot r_v}\right) = R_e R_1(T)$, then the first gourava revan index entropy is given by

$$ENT(R_e R_1(T)) = log(R_e R_1(T)) - \frac{1}{R_e R_1(T)} \sum_{pq \in E(T)} g_{16}(e) log\big(g_{16}(e)\big)$$

3. Main Results and Analysis

3.1 *Main Results*

Theorem 3.1: Let G be the graph α −graphdiyne nanosheet, the various molecular descriptor of G are examined as follows

$R_1(G)$ = 168mn-24m+36n

$R_2(G)$ = 234mn-27m+63n

$R_3(G)$ = 12mn+6m-6n

$HR_1(G)$ = 948mn-114m+246n

$HR_2(G)$ = 1890mn-135m+675n

$mR_1(G)$ = 5.4mn-1.03m+0.63n

$mR_2(G)$ = 4mn-0.89m+0.22n

SR(G) = 12.78mn -2.29m + 1.81n

PR(G) = 10.86mn – 2.13m + 1.17n

HR(G) = 10.74mn -2.07m + 1.23n

ISR(G) = 41.4mn – 5.7m + 9.3n

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$GAR(G) = 29.76mn – 4.88m + 5.12n$

$AGR(G) = 79.2mn – 29.6m-19.6n$

$ABC(G) = 21.3mn – 3.95m + 2.75n$

$RGO(G) = 402mn – 51m + 99n$

$ReR_1(G) = 22.02mn - 4.31m + 2.39n$

Proof: Using table 1 and table 2, we get the topological index of the various revan index are computed as follows

(i) ***The First Revan Index***

$$R_1(G) = \sum_{uv\in E(G)} (r_u + r_v)$$

$R_1(G) = (18mn+m+11n)(3+3)+(12mn-6m-6n)(3+2)$

$= 108mn+6m+66n+60mn-30m-30n$

$R_1(G) = 168mn-24m+36n$ (1)

- ***The Second Revan Index***

$$R_2(G) = \sum_{uv\in E(G)} (r_u . r_v)$$

$R_2(G) = (18mn+m+11n)(3*3)+(12mn-6m-6n)(3*2)$

$= 162mn+9m+99n+72mn-36m-36n$

$R_2(G) = 234mn-27m+63n$ (2)

- ***The Third Revan Index***

$$R_3(G) = \sum_{uv\in E(G)} |(r_u - r_v)|$$

$R_3(G) = |(18mn+m+11n)(3-3)+(12mn-6m-6n)(3-2)|$

$R_3(G) = 12mn+6m-6n$ (3)

- ***The First Hyper Revan Index***

$$HR_1(G) = \sum_{uv\in E(G)} (r_u + r_v)^2$$

$HR_1(G) = (18mn+m+11n)(3+3)^2+(12mn-6m-6n)(3+2)^2$

$= 648mn+36m+396n+300mn-150m-150n$

$HR_1(G) = 948mn-114m+246n$ (4)

- ***The Second Hyper Revan Index***

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$$HR_2(G) = \sum_{uv \in E(G)} (r_u . r_v)^2$$

$HR_2(G) = (18mn+m+11n)(3*3)^2+(12mn-6m-6n)(3*2)^2$

$= 1458mn+81m+891n+432mn-216m-216n$

$HR_2(G) = 1890mn-135m+675n$ (5)

- ***The First modified Revan Index***

$$mR_1(G) = \sum_{uv \in E(G)} \frac{1}{r_u + r_v}$$

$mR_1(G) = (18mn+m+11n)\left(\frac{1}{3+3}\right)^2+(12mn-6m-6n)\left(\frac{1}{3+2}\right)$

$mR_1(G) = 5.4mn-1.03m+0.63n$ (6)

- ***The Second modified Revan Index***

$$mR_2(G) = \sum_{uv \in E(G)} \frac{1}{(r_u . r_v)}$$

$mR_2(G) = (18mn+m+11n)\left(\frac{1}{3.3}\right)^2+(12mn-6m-6n)\left(\frac{1}{3.2}\right)$

$mR_2(G) = 4mn-0.89m+0.22n$ (7)

- ***Sum Connectivity Revan Index***

$$SR(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{r_u + r_v}}$$

$SR(G) = (18mn+m+11n)\left(\frac{1}{\sqrt{3+3}}\right)+(12mn-6m-6n)\left(\frac{1}{\sqrt{3+2}}\right)$

$= 7.38mn + 0.41m + 4.51n + 5.4mn - 2.7m - 2.7n$

$SR(G) = 12.78mn -2.29m + 1.81n$ (8)

- ***Product Connectivity Revan Index***

$$PR(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{r_u . r_v}}$$

$PR(G) = (18mn+m+11n)\left(\frac{1}{\sqrt{3.3}}\right)+(12mn-6m-6n)\left(\frac{1}{\sqrt{3.2}}\right)$

$= 5.94mn + 0.33m + 3.63n + 4.92mn - 2.46m - 2.46n$

$PR(G) = 10.86mn – 2.13m + 1.17n$ (9)

- ***Harmonic Revan Index***

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$$HR(G) = \sum_{uv \in E(G)} \frac{2}{r_u + r_v}$$

HR(G) = (18mn+m+11n)$\left(\frac{2}{3+3}\right)$+(12mn-6m-6n) $\left(\frac{2}{3+2}\right)$

= 5.94mn + 0.33m + 3.63n + 4.8mn - 2.4m - 2.4n

HR(G) = 10.74mn -2.07m + 1.23n (10)

In similar way the solutions for other indices are

Inverse sum Revan Index

ISR(G) = 41.4mn – 5.7m + 9.3n (11)

Geometric Arithmetic Revan Index

GAR(G) = 29.76mn – 4.88m + 5.12n (12)

Arithmetic Geometric Revan Index

AGR(G) = 79.2mn – 29.6m-19.6n (13)

Atom Bond Connectivity Revan Index

ABC(G) = 21.3mn – 3.95m + 2.75n (14)

First Gourava Revan Index

$RGO_1(G)$ = 402mn – 51m + 99n (15)

Redefined 1st Revan Index

$ReR_1(G)$ = 22.02mn - 4.31m + 2.39n (16)

n values	**$R_1(G)$**	**$R_2(G)$**	**$R_3(G)$**	**$HR_1(G)$**	**$HR_2(G)$**	**$^mR_1(G)$**	**$^mR_2(G)$**	**SR(G)**
2	696	1008	24	4056	8640	20.8	14.66	50.16
3	1548	2214	72	8928	18630	47.4	33.99	113.58
4	2736	3888	144	15696	32400	84.8	61.32	202.56
5	4260	6030	240	24360	49950	133	96.65	317.1
6	6120	8640	360	34920	71280	192	139.98	457.2
7	8316	11718	504	47376	96390	261.8	191.31	622.86
8	10848	15264	672	61728	125280	342.4	250.64	814.08
9	13716	19278	864	77976	157950	433.8	317.97	1030.86
10	16920	23760	1080	96120	194400	536	393.3	1273.2

Table 3: Numerical Computation of TI for $\alpha -$ Graphdyine

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n values	PR	HR	ISR	GAR	AGR	ABC	RGO	ReR_1
2	41.52	41.28	172.8	119.52	218.4	82.8	1704	84.24
3	94.86	94.14	383.4	268.56	565.2	188.1	3762	192.42
4	169.92	168.48	676.8	477.12	1070.4	336	6624	344.64
5	266.7	264.3	1053	745.2	1734	526.5	10290	540.9
6	385.2	381.6	1512	1072.8	2556	759.6	14760	781.2
7	525.42	520.38	2053.8	1459.92	3536.4	1035.3	20034	1065.54
8	687.36	680.64	2678.4	1906.56	4675.2	1353.6	26112	1393.92
9	871.02	862.38	3385.8	2412.72	5972.4	1714.5	32994	1766.34
10	1076.4	1065.6	4176	2978.4	7428	2118	40680	2182.8

Table 4: Numerical Computation of TI for $\alpha -$ Graphdyine

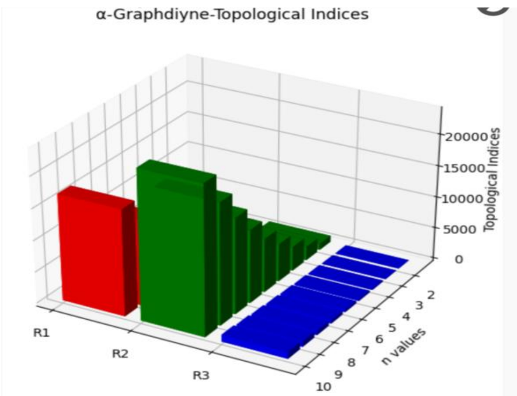

Figure 1: TI of R_1, R_2 and R_3

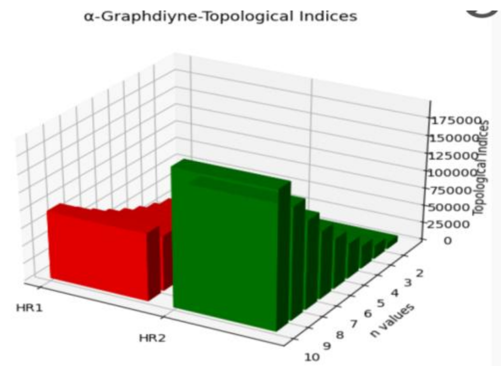

Figure 2: TI of HR_1 and HR_2

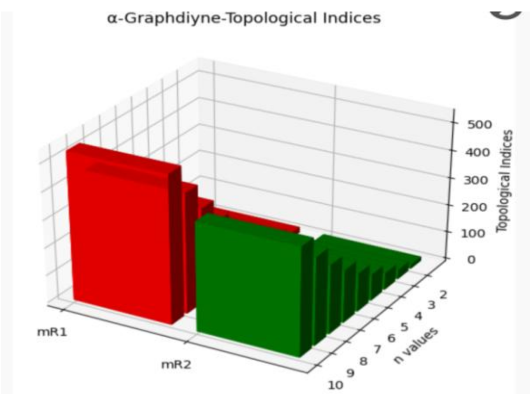

Figure 3: TI of $^mR_1$ and $^mR_2$

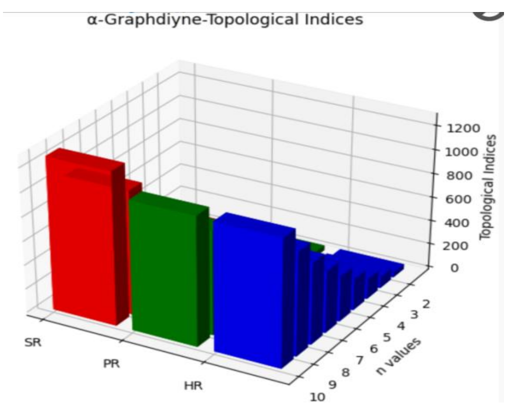

Figure 4: TI of SR, PR and HR

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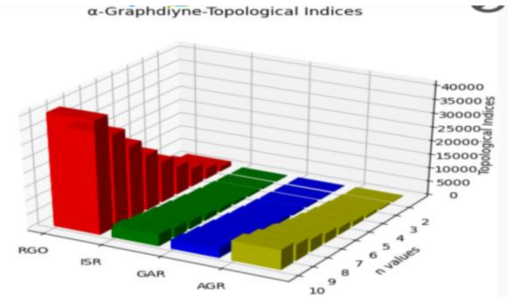

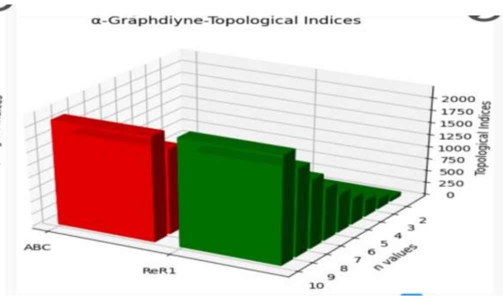

Figure 5: TI of ISR, GRA, AGR, RGO

Figure 6: TI of ABC, R_eR_1

Theorem 3.2: The entropy of the graph α −graphdiyne nanosheet, for the various molecular descriptor of G are examined

Proof: The index entropies of α −graphdiyne nanosheet is

- ***The First Revan Entropy***
  The First Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.1 is

$$ENT(R_1(T)) = log(R_1(T)) - \frac{1}{(R_1(T))} \sum_{pq \in E(T)} g_1(e) log(g_1(e))$$

Using table 2 and equation in (1) in theorem 3.1 the First Revan entropy is examined as follows

$$ENT(R_1(T)) = log(168mn - 24m + 36n) - \frac{1}{(168mn-24m+36n)} \times \{[(3+3)log(3+3)](18mn + m + 11n) + [(3+2)log(3+2)](12mn - 6m - 6n)\}$$

$$= log(168mn - 24m + 36n) - \frac{1}{(168mn-24m+36n)}$$

$$\times \{[(6)log(6)](18mn + m + 11n) + [(5)log(5)](12mn - 6m - 6n)\}$$

$$ENT(R_1(T)) = log(168mn - 24m + 36n)$$

$$- \frac{4.669(18mn + m + 11n)}{(168mn - 24m + 36n)} - \frac{3.495(12mn - 6m - 6n)}{(168mn - 24m + 36n)}$$

- ***The Second Revan Entropy***
  The Second Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.2 is

$$ENT(R_2(T)) = log(R_2(T)) - \frac{1}{(R_2(T))} \sum_{pq \in E(T)} g_2(e) log(g_2(e))$$

Using table 2 and equation in (2) in theorem 3.1 the Second Revan entropy is examined as follows

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$$ENT\big(R_2(T)\big) = log(234mn - 27m + 63n) - \frac{1}{(234mn-27m+63n)}$$

$$\times \{[(3*3)log(3*3)](18mn + m + 11n) + [(3*2)log(3*2)]$$

$$(12mn - 6m - 6n)\}$$

$$= log(234mn - 27m + 63n) - \frac{1}{(234mn-27m+63n)}$$

$$\times \{[(9)log(9)](18mn + m + 11n) + [(6)log(6)](12mn - 6m - 6n)\}$$

$$ENT\big(R_2(T)\big) = log(234mn - 27m + 63n)$$

$$-\frac{8.588(18mn + m + 11n)}{(168mn - 24m + 36n)} - \frac{4.669(12mn - 6m - 6n)}{(168mn - 24m + 36n)}$$

- ***The Third Revan Entropy***

The third Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.3 is

$$ENT\big(R_3(T)\big) = log\big(R_3(T)\big) - \frac{1}{\big(R_3(T)\big)} \sum_{pq \in E(T)} g_3(e) log\big(g_3(e)\big)$$

Using table 2 and equation in (3) in theorem 3.1 the third Revan entropy is examined as follows

$$ENT\big(R_3(T)\big) = log(12mn - 6m - 6n) - \frac{1}{(12mn-6m-6n)}$$

$$\times \{[|(3-3)|log|(3-3)|](18mn + m + 11n) + [|(3-2)|log|(3-2)|]$$

$$(12mn - 6m - 6n)\}$$

$$= log(12mn - 6m - 6n) - \frac{1}{(12mn-6m-6n)}$$

$$\times \{[(0)log(0)](18mn + m + 11n) + [(1)log(1)](12mn - 6m - 6n)\}$$

$$ENT\big(R_3(T)\big) = log(12mn - 6m - 6n)$$

- ***The First Hyper Revan Entropy***

The First Hyper Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.4 is

$$ENT\big(HR_1(T)\big) = log\big(HR_1(T)\big) - \frac{1}{\big(HR_1(T)\big)} \sum_{pq \in E(T)} g_4(e) log\big(g_4(e)\big)$$

Using table 2 and equation in (4) in theorem 3.1 the First Hyper Revan entropy is examined as follows

$$ENT\big(HR_1(T)\big) = log(948mn - 114m + 246n) - \frac{1}{(948mn-114m+246n)}$$

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$$\times \{[(3+3)^2 log(3+3)^2\ ](18mn+m+11n)+[(3+2)^2 log(3+2)^2\ ]$$
$$(12mn-6m-6n)\ \}$$

$$ENT\big(HR_1(T)\big) = \ log(948mn-114m+246n)$$
$$-\frac{56.027(18mn+m+11n)}{948mn-114m+246n}-\frac{34.949(12mn-6m-6n)}{948mn-114m+246n}$$

- ***The Second Hyper Revan Entropy***

The Second Hyper Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.5 is

$$ENT\big(HR_2(T)\big) = \ log\big(HR_2(T)\big) - \frac{1}{\big(HR_2(T)\big)} \sum_{pq\in E(T)} g_5(e) log\big(g_5(e)\big)$$

Using table 2 and equation in (5) in theorem 3.1 the Second Hyper Revan entropy is examined as follows

$$ENT\big(HR_2(T)\big) = \ log(1890mn-135m+675n) - \frac{1}{1890mn-135m+675n}$$
$$\times \{[(3*3)^2 log(3*3)^2\ ](18mn+m+11n)+[(3*2)^2 log(3*2)^2\ ]$$
$$(12mn-6m-6n)\ \}$$

$$ENT\big(HR_2(T)\big) = \ log(1890mn-135m+675n) -$$
$$\frac{154.587(18mn+m+11n)}{1890mn-135m+675n}-\frac{56.027(12mn-6m-6n)}{1890mn-135m+675n}$$

- ***The First Modified Revan Entropy***

The First Modified Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.6 is

$$ENT\big(mR_1(T)\big) = \ log\big(mR_1(T)\big) - \frac{1}{\big(mR_1(T)\big)} \sum_{pq\in E(T)} g_6(e) log\big(g_6(e)\big)$$

Using table 2 and equation in (6) in theorem 3.1 the first modified Revan entropy is examined as follows

$$ENT\big(mR_1(T)\big) = \ log(5.4mn-1.03m+0.63n) - \frac{1}{5.4mn-1.03m+0.63n}$$
$$\times \left\{\left[\left(\frac{1}{3+3}\right) log\left(\frac{1}{3+3}\right)\right](18mn+m+11n)+\left[\left(\frac{1}{3+2}\right) log\left(\frac{1}{3+2}\right)\right](12mn-6m-6n\right\}$$

$$ENT\big(mR_1(T)\big) = \ log(5.4mn-1.03m+0.63n) -$$
$$\frac{(-0.130)(18mn+m+11n)}{5.4mn-1.03m+0.63n}-\frac{(-0.140)(12mn-6m-6n)}{5.4mn-1.03m+0.63n}$$

- ***The Second Modified Revan Entropy***

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The Second Modified Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.7 is

$$ENT\big(mR_2(T)\big) = log\big(mR_2(T)\big) - \frac{1}{\big(mR_2(T)\big)} \sum_{pq\in E(T)} g_7(e) log\big(g_7(e)\big)$$

Using table 2 and equation in (7) in theorem 3.1 the second modified Revan entropy is examined as follows

$$ENT\big(mR_2(T)\big) = log(4mn - 0.89m + 0.22n) - \frac{1}{4mn-0.89m+0.22n}$$

$$\times \left\{\left[\left(\frac{1}{3*3}\right) log\left(\frac{1}{3*3}\right)\right](18mn + m + 11n) + \left[\left(\frac{1}{3*2}\right) log\left(\frac{1}{3*2}\right)\right](12mn - 6m - 6n\right\}$$

$$ENT\big(mR_2(T)\big) = log(4mn - 0.89m + 0.22n) -$$

$$\frac{(-0.105)(18mn + m + 11n)}{4mn - 0.89m + 0.22n} - \frac{(-0.130)(12mn - 6m - 6n)}{4mn - 0.89m + 0.22n}$$

- ***The Sum Connectivity Revan Entropy***

The Sum Connectivity Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.8 is

$$ENT\big(SR(T)\big) = log\big(SR(T)\big) - \frac{1}{\big(SR(T)\big)} \sum_{pq\in E(T)} g_8(e) log\big(g_8(e)\big)$$

Using table 2 and equation in (8) in theorem 3.1 the Sum Connectivity Revan entropy is examined as follows

$$ENT\big(SR(T)\big) = log(12.78mn - 2.29m + 1.81n) - \frac{1}{12.78mn-2.29m+1.81n}$$

$$\times \left\{\left[\left(\frac{1}{\sqrt{6}}\right) log\left(\frac{1}{\sqrt{6}}\right)\right](18mn + m + 11n) + \left[\left(\frac{1}{\sqrt{5}}\right) log\left(\frac{1}{\sqrt{5}}\right)\right](12mn - 6m - 6n\right\}$$

$$ENT\big(SR(T)\big) = log(12.78mn - 2.29m + 1.81n) -$$

$$\frac{(-0.160)(18mn + m + 11n)}{12.78mn - 2.29m + 1.81n} - \frac{(-0.156)(12mn - 6m - 6n)}{12.78mn - 2.29m + 1.81n}$$

- ***The Product Connectivity Revan Entropy***

The Product Connectivity Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.9 is

$$ENT\big(PR(T)\big) = log\big(PR(T)\big) - \frac{1}{\big(PR(T)\big)} \sum_{pq\in E(T)} g_9(e) log\big(g_9(e)\big)$$

Using table 2 and equation in (9) in theorem 3.1 the Product Connectivity Revan entropy is examined as follows

$$ENT\big(PR(T)\big) = log(10.86mn - 2.13m + 1.17n) - \frac{1}{10.86mn-2.13m+1.17n}$$

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$$\times\left\{\left[\left(\frac{1}{\sqrt{9}}\right) log\left(\frac{1}{\sqrt{9}}\right)\right](18mn+m+11n)+\left[\left(\frac{1}{\sqrt{6}}\right) log\left(\frac{1}{\sqrt{6}}\right)\right](12mn-6m-6n\right\}$$

$$ENT\big(PR(T)\big) = log(10.86mn-2.13m+1.17n) - \frac{(-0.159)(18mn+m+11n)}{10.86mn-2.13m+1.17n} - \frac{(-0.159)(12mn-6m-6n)}{10.86mn-2.13m+1.17n}$$

- ***The Harmonic Revan Entropy***

The Harmonic Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.10 is

$$ENT\big(HR(T)\big) = log\big(HR(T)\big) - \frac{1}{\big(HR(T)\big)}\sum_{pq\in E(T)} g_{10}(e) log\big(g_{10}(e)\big)$$

Using table 2 and equation in (10) in theorem 3.1 the Harmonic Revan entropy is examined as follows

$$ENT\big(HR(T)\big) = log(10.74mn-2.07m+1.23n) - \frac{1}{10.74mn-2.07m+1.23n}$$

$$\times\left\{\left[\left(\frac{2}{3+3}\right) log\left(\frac{2}{3+3}\right)\right](18mn+m+11n)+\left[\left(\frac{2}{3+2}\right) log\left(\frac{2}{3+2}\right)\right](12mn-6m-6n\right\}$$

$$ENT\big(HR(T)\big) = log(10.74mn-2.07m+1.23n) - \frac{(-0.1589)(18mn+m+11n)}{10.74mn-2.07m+1.23n} - \frac{(-0.1591)(12mn-6m-6n)}{10.74mn-2.07m+1.23n}$$

- ***The Inverse Sum Revan Entropy***

The Inverse Sum Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.11 is

$$ENT\big(ISR(T)\big) = log\big(ISR(T)\big) - \frac{1}{\big(ISR(T)\big)}\sum_{pq\in E(T)} g_{11}(e) log\big(g_{11}(e)\big)$$

Using table 2 and equation in (11) in theorem 3.1 the Inverse Sum Revan entropy is examined as follows

$$ENT\big(ISR(T)\big) = log(41.4mn-5.7m+9.3n) - \frac{1}{41.4mn-5.7m+9.3n}$$

$$\times\left\{\left[\left(\frac{3.3}{3+3}\right) log\left(\frac{3.3}{3+3}\right)\right](18mn+m+11n)+\left[\left(\frac{3.2}{3+2}\right) log\left(\frac{3.2}{3+2}\right)\right](12mn-6m-6n\right\}$$

$$ENT\big(ISR(T)\big) = log(41.4mn-5.7m+9.3n) - \frac{(0.264)(18mn+m+11n)}{41.4mn-5.7m+9.3n} - \frac{(0.095)(12mn-6m-6n)}{41.4mn-5.7m+9.3n}$$

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- ***The Geometric Arithmetic Revan Entropy***

The Geometric Arithmetic Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.12 is

$$ENT\big(GAR(T)\big) = log\big(GAR(T)\big) - \frac{1}{\big(GAR(T)\big)} \sum_{pq \in E(T)} g_{12}(e) log\big(g_{12}(e)\big)$$

Using table 2 and equation in (12) in theorem 3.1 the Geometric Arithmetic Revan entropy is examined as follows

$$ENT\big(GAR(T)\big) = log(29.76mn - 4.88m + 5.12n) - \frac{1}{29.76mn-4.88m+5.12n}$$

$$\times \left\{ \left[\left(\frac{2\sqrt{3.3}}{3+3} \right) log \left(\frac{2\sqrt{3.3}}{3+3} \right) \right] (18mn + m + 11n) + \left[\left(\frac{2\sqrt{3.2}}{3+2} \right) log \left(\frac{2\sqrt{3.2}}{3+2} \right) \right] (12mn - 6m - 6n) \right\}$$

$$ENT\big(GAR(T)\big) = log(29.76mn - 4.88m + 5.12n) - \frac{(0)(18mn + m + 11n)}{29.76mn - 4.88m + 5.12n} - \frac{(-0.0086)(12mn - 6m - 6n)}{29.76mn - 4.88m + 5.12n}$$

- ***The Arithmetic Geometric Revan Entropy***

The Arithmetic Geometric Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.13 is

$$ENT\big(AGR(T)\big) = log\big(AGR(T)\big) - \frac{1}{\big(AGR(T)\big)} \sum_{pq \in E(T)} g_{13}(e) log\big(g_{13}(e)\big)$$

Using table 2 and equation in (13) in theorem 3.1 the Arithmetic Geometric Revan entropy is examined as follows

$$ENT\big(AGR(T)\big) = log(79.2mn - 29.6m - 19.6n) - \frac{1}{79.2mn-29.6m-19.6n}$$

$$\times \left\{ \left[\left(\frac{3+3}{2\sqrt{3.3}} \right) log \left(\frac{3+3}{2\sqrt{3.3}} \right) \right] (18mn + m + 11n) + \left[\left(\frac{3+2}{2\sqrt{3.2}} \right) log \left(\frac{3+2}{2\sqrt{3.2}} \right) \right] (12mn - 6m - 6n) \right\}$$

$$ENT\big(AGR(T)\big) = log(79.2mn - 29.6m - 19.6n) - \frac{(0)(18mn + m + 11n)}{79.2mn - 29.6m - 19.6n} - \frac{(3.609)(12mn - 6m - 6n)}{79.2mn - 29.6m - 19.6n}$$

- ***The Atom Bond Connectivity Revan Entropy***

The Atom Bond Connectivity Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.14 is

$$ENT\big(ABC(T)\big) = log\big(ABC(T)\big) - \frac{1}{\big(ABC(T)\big)} \sum_{pq \in E(T)} g_{14}(e) log\big(g_{14}(e)\big)$$

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Using table 2 and equation in (14) in theorem 3.1 the Atom Bond Connectivity Revan entropy is examined as follows

$$ENT(ABC(T)) = log(21.3mn - 3.95m + 2.75n) - \frac{1}{21.3mn-3.95m+2.75n}$$

$$\times \left\{ \left[\left(\sqrt{\frac{3+3-2}{3.3}} \right) log \left(\sqrt{\frac{3+3-2}{3.3}} \right) \right] (18mn + m + 11n) + \left[\left(\sqrt{\frac{3+2-2}{3.2}} \right) log \left(\sqrt{\frac{3+2-2}{3.2}} \right) \right] (12mn - 6m - 6n) \right\}$$

$$ENT(ABC(T)) = log(21.3mn - 3.95m + 2.75n) - \frac{(-0.117)(18mn + m + 11n)}{21.3mn - 3.95m + 2.75n} - \frac{(-0.087)(12mn - 6m - 6n)}{21.3mn - 3.95m + 2.75n}$$

- ***The First Gourava Revan Entropy***

The First Gourava Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.15 is

$$ENT(RGO_1(T)) = log(RGO_1(T)) - \frac{1}{(RGO_1(T))} \sum_{pq \in E(T)} g_{14}(e) log(g_{14}(e))$$

Using table 2 and equation in (15) in theorem 3.1 the First Gourava Revan entropy is examined as follows

$$ENT(RGO_1(T)) = log(402mn - 51m + 99n) - \frac{1}{402mn-51m+99n}$$

$$\times \{ [((3+3) + (3.3)) log((3+3) + (3.3))](18mn + m + 11n) + [((3+2) + (3.2)) log((3+2) + (3.2))](12mn - 6m - 6n) \}$$

$$ENT(RGO_1(T)) = log(402mn - 51m + 99n) - \frac{(17.641)(18mn + m + 11n)}{402mn - 51m + 99n} - \frac{(11.455)(12mn - 6m - 6n)}{402mn - 51m + 99n}$$

- ***The Redefined First Revan Entropy***

The Redefined First Revan entropy for the α −graphdiyne nanosheet is computed by Definition 2.15 is

$$ENT(R_eR_1(T)) = log(R_eR_1(T)) - \frac{1}{(R_eR_1(T))} \sum_{pq \in E(T)} g_{14}(e) log(g_{14}(e))$$

Using table 2 and equation in (16) in theorem 3.1 the Redefined First Revan entropy is examined as follows

$$ENT(R_eR_1(T)) = log(22.02mn - 4.31m + 2.39n) - \frac{1}{22.02mn-4.31m+2.39n}$$

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$$\times\left\{\left[\left(\frac{3+3}{3.3}\right)log\left(\frac{3+3}{3.3}\right)\right](18mn+m+11n)+\left[\left(\frac{3+2}{3.2}\right)log\left(\frac{3+2}{3.2}\right)\right](12mn-6m-6n)\right\}$$

$$ENT\big(R_eR_1(T)\big)= log(22.02mn-4.31m+2.39n)-\frac{(-0.117)(18mn+m+11n)}{22.02mn-4.31m+2.39n}-\frac{(-0.067)(12mn-6m-6n)}{22.02mn-4.31m+2.39n}$$

n values	ENT R1	ENT R2	ENT R3	ENT HR1	ENT HR2	ENT mR1	ENT mR2	ENT SR
2	2.078092	2.074389	1.380211	2.075216	2.06325	2.079602	2.066543	2.081219
3	2.430015	2.425308	1.857332	2.426373	2.41073	2.431475	2.418377	2.433115
4	2.679783	2.674627	2.158362	2.675801	2.658412	2.681226	2.668228	2.682857
5	2.873543	2.868138	2.380211	2.869373	2.850971	2.874979	2.862077	2.876598
6	3.031869	3.026305	2.556303	3.027579	3.008518	3.033301	3.020477	3.034909
7	3.165738	3.160065	2.702431	3.161366	3.141842	3.167168	3.154405	3.168767
8	3.281704	3.275951	2.827369	3.277272	3.257407	3.283132	3.27042	3.284724
9	3.383995	3.378182	2.936514	3.379518	3.35939	3.385422	3.372751	3.387008
10	3.4755	3.469639	3.033424	3.470987	3.45065	3.476926	3.464289	3.478506

Table 5: Numerical Computation of Entropy for $\alpha-$ Graphdyine

n values	ENT PR	ENT HR	ENT ISR	ENT GAR	ENT AGR	ENT ABC	ENT RGO	ENT R_eR_1
2	2.077795	2.077775	2.077683	2.079159	1.942659	2.0789	2.076272	2.07794
3	2.429645	2.429663	2.429474	2.431336	2.292457	2.430848	2.427711	2.429713
4	2.679397	2.679426	2.679184	2.681211	2.54403	2.680625	2.677265	2.679427

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5	2.873155	2.873187	2.872913	2.87503	2.739534	2.87439	2.870908	2.873161
6	3.031481	3.031514	3.031218	3.033391	2.899251	3.032718	3.02916	3.031472
7	3.165351	3.165384	3.165073	3.167284	3.034215	3.166588	3.162977	3.165331
8	3.281318	3.281352	3.28103	3.283268	3.151053	3.282554	3.278906	3.28129
9	3.383612	3.383645	3.383314	3.385572	3.254051	3.384846	3.38117	3.383577
10	3.475118	3.475151	3.474812	3.477087	3.346138	3.476351	3.472652	3.475078

Table 6: Numerical Computation of Entropy for $\alpha -$ Graphdyine

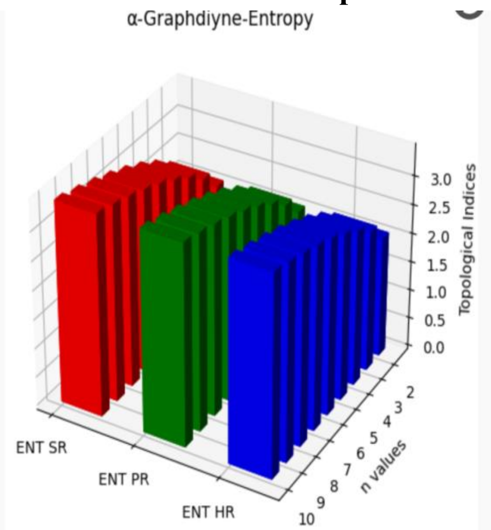

Figure 1: Entropy of SR, PR, HR

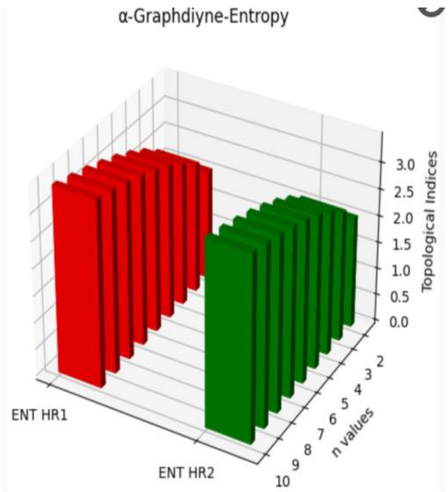

Figure 2: Entropy of HR_1, HR_2

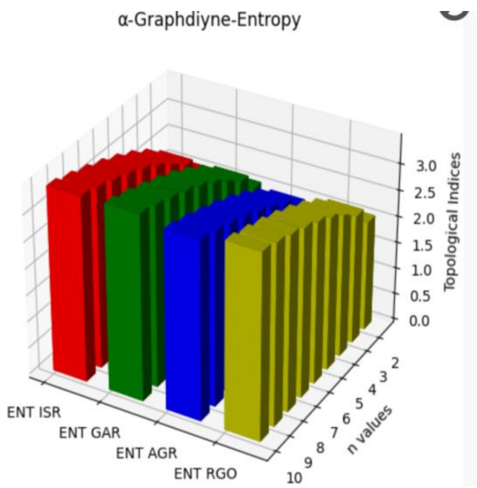

Figure 3: Entropy of ISR, GAR, AGR, RGO

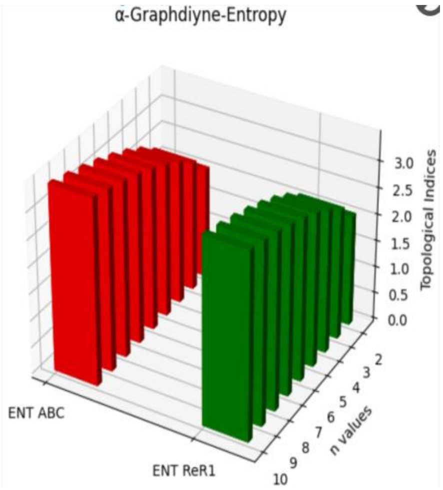

Figure 1: Entropy of ABC, ReR_1

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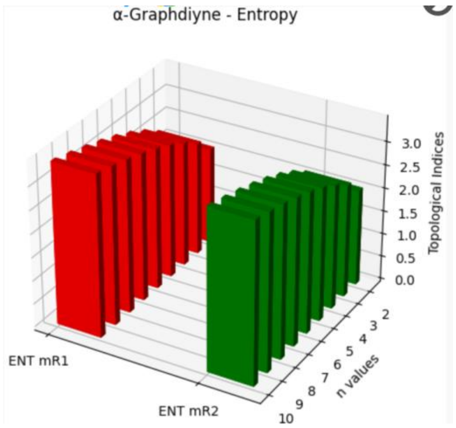

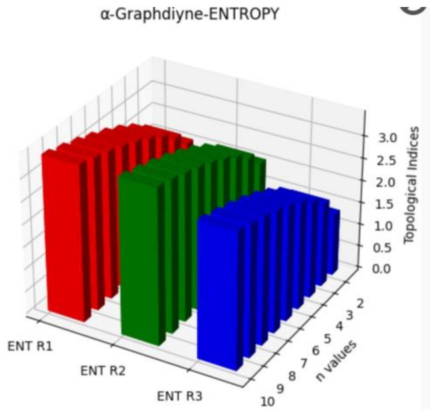

Figure 5: Entropy of mR_1, mR_2

Figure 6: Entropy of R_1, R_2, R_3

3.2 Linear Regression Analysis

This section examines the application of topological indices and regression models to analyze the correlation between calculated topological indices and one or more interpretative variables. The statistical technique known as regression analysis is used to provide a simulation of the relationship between a dependent variable and one or more independent variables. One of the most important objectives of regression analysis is to identify the curve or line that best reflects the degree of connection that exists between the variables. Its objective is to forecast the dependent variable's value using data from the independent variables.

$Y=a + bx$

where Y is dependent variable, a is the regression model constant, **x** is the independent variable, and b is the coefficients for descriptor. The SPSS software is used for determining the results.

Linear Model	A	B	R	R^2	S_E	F	Significant
$ENT[R_1(T)]$	0.00007537	2.385	0.919	0.844	0.19633	38.004	<0.001
$ENT[R_2(T)]$	0.00005397	2.378	0.92	0.846	0.19532	38.343	<0.001
$ENT[R_3(T)]$	0.001	1.845	0.894	0.799	0.26094	27.878	<0.001
$ENT[HR_1(T)]$	0.00001334	2.379	0.919	0.845	0.19552	38.278	<0.001

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ENT[HR_2(T)]	0.000006587	2.359	0.921	0.848	0.19282	39.03	<0.001
ENT[$^{m}R_1$(T)]	0.002	2.394	0.918	0.843	0.19731	37.554	<0.001
ENT[$^{m}R_2$(T)]	0.003	2.382	0.918	0.842	0.198	37.275	<0.001
ENT[SR (T)]	0.001	2.392	0.918	0.843	0.19706	37.665	<0.001
ENT[PR(T)]	0.001	2.391	0.918	0.843	0.19741	37.512	<0.001
ENT[HR(T)]	0.001	2.39	0.918	0.843	0.19735	37.54	<0.001
ENT[ISR(T)]	0	2.384	0.919	0.845	0.19617	38.063	<0.001
ENT[GAR(T)]	0	2.389	0.919	0.844	0.19688	37.786	<0.001
ENT[AGR(T)]	0	2.275	0.915	0.838	0.20166	36.134	<0.001
ENT[ABC(T)]	0.001	2.391	0.918	0.843	0.19722	37.603	<0.001
ENT[RGO(T)]	0.00003152	2.381	0.919	0.845	0.19579	38.193	<0.001
ENT[ReR1(T)]	0.001	2.391	0.918	0.843	0.19736	37.522	<0.001

Table 7: Statistical Values for linear regression Model

This part has been dealt with the relationship between the topological values and the measure of entropy that correlates with every individual one.

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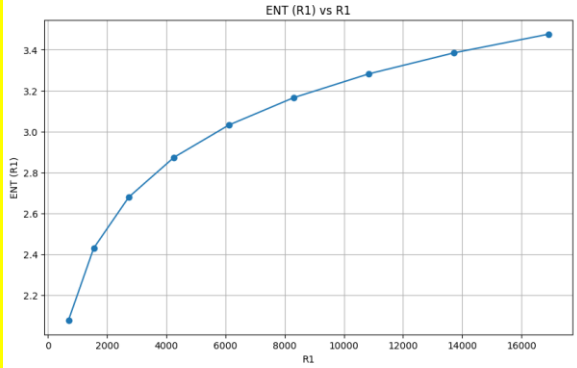

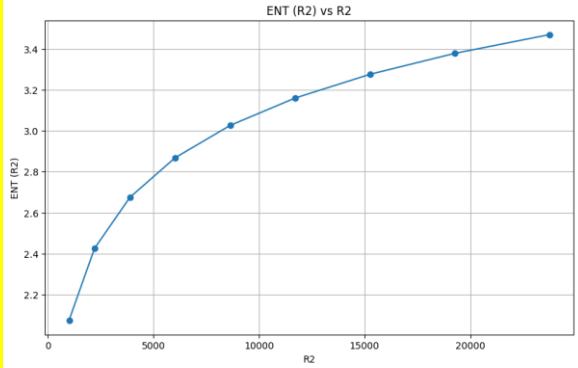

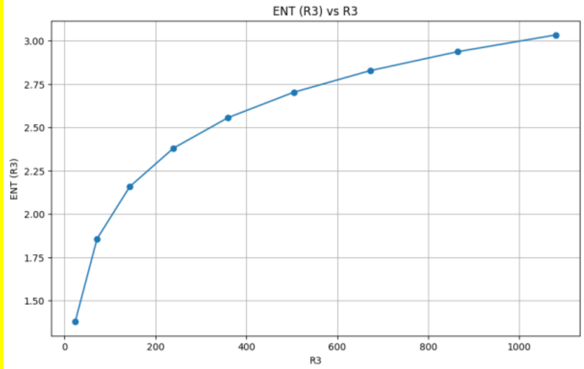

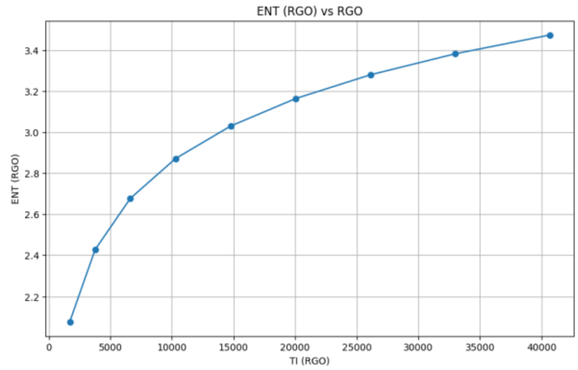

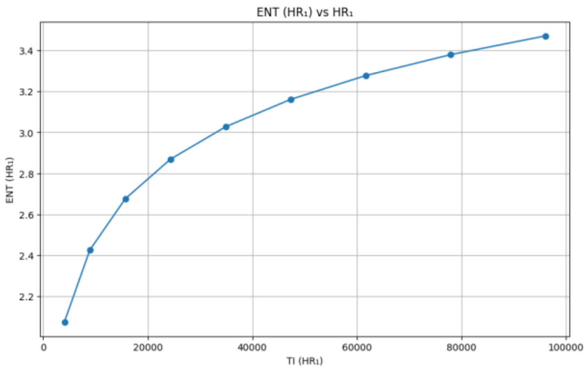

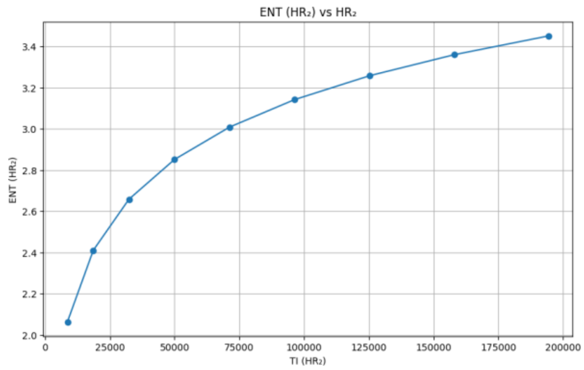

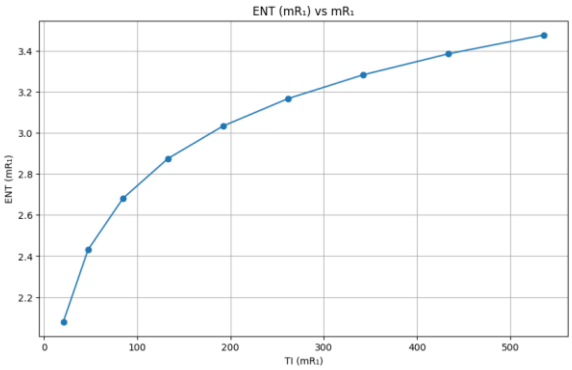

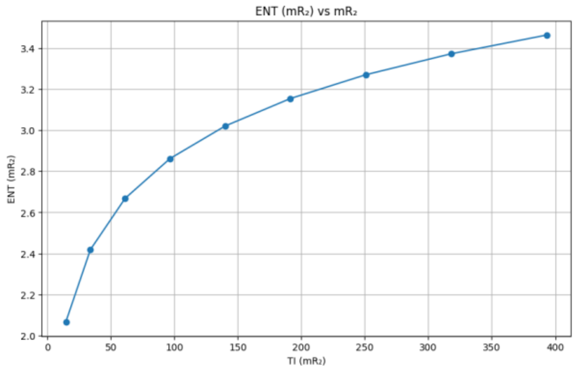

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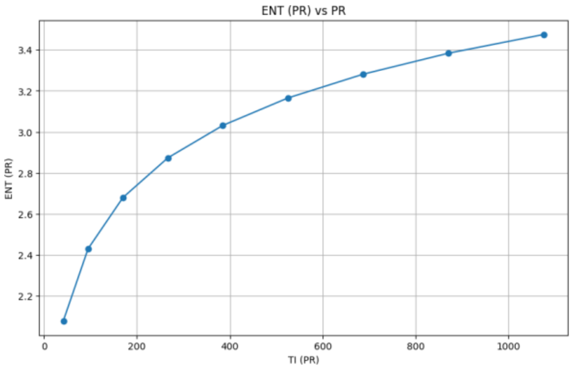

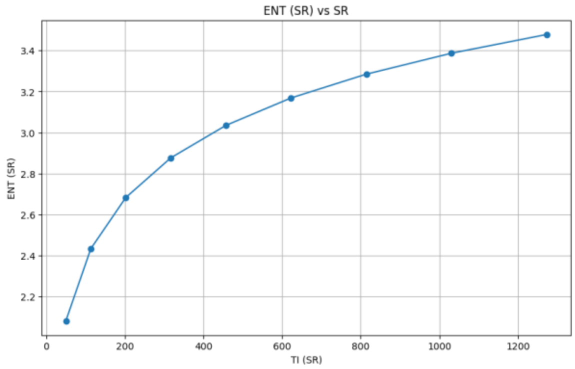

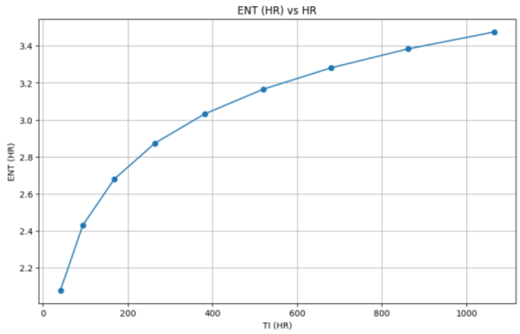

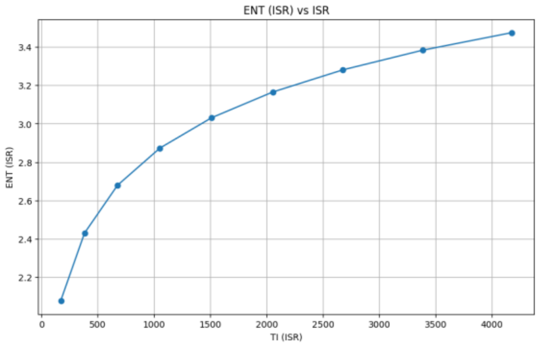

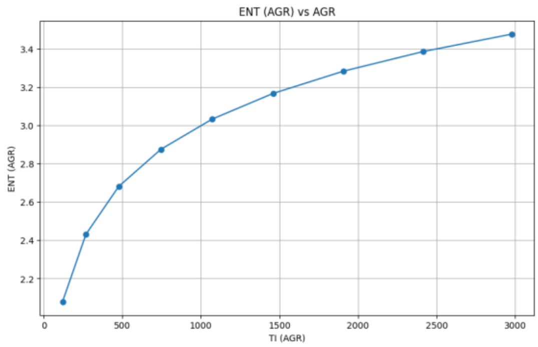

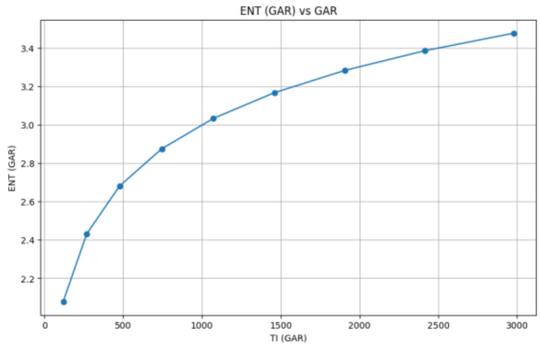

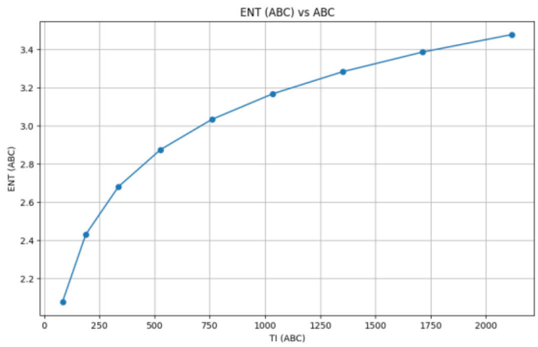

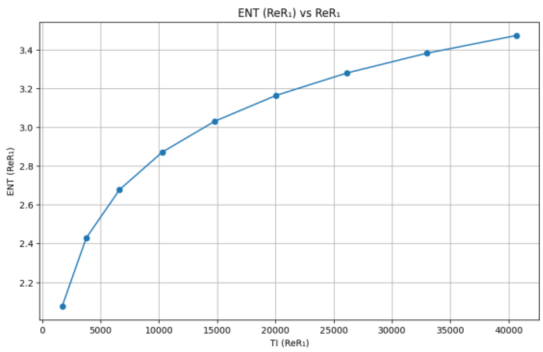

4. Conclusion

Calculating entropy is important for assessing the molecular structures' complexity. This work analyzed many entropies that included various revan indices alongside several

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numerical graph invariants of certain molecular graphs of alpha graphdiyne. The HR2 index has a substantially stronger correlation with its associated entropy alpha graphdiyne than the other topological indices. The highest values are R = 0.921, $R2$ = 0.848, and F = 39.03 for alpha graphdiyne, while the lowest values are SE = 0.19282 for the other TI Thus, it can be concluded that, among all the considered indices, the HR_2 index of alpha graphdiyne proves to be the most accurate indicator of complexity.

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