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# ENTROPY OF BENZENOID HYDROCARBON CHAINS USING REVERSE TOPOLOGICAL INDICES

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**Abstract:** In this paper, we have computed the reverse degree based topological indices like the reverse Randić index, reverse geometric arithmetic index, reverse Zagreb indices, reverse forgotten index, reverse arithmetic geometric index, reverse symmetric division degree index, reverse atom bond sum connectivity index, reverse hyper Zagreb indices, reverse redefined Zagreb indices using edge partition method and also obtained the entropy of above computed indices on hexagonal hydrocarbon chains using Shannon's entropy model.

**Keywords:** benzenoid hydrocarbon chains; topological indices; reverse topological indices; entropy of graphs.

**AMS subject classification:** 2020: 05C92, 05C90, 68R10, 68P30, 05C09.

## 1. INTRODUCTION

Topological indices are the numerical values that provide information about the molecular structure of chemical compounds. Topological indices are used in the field of cheminformatics and quantitative structure activity/ property relationship (QSAR/QSPR) studies to predict various properties of molecules, such as their biological activities, physical properties and toxicity parameters. Wiener introduced the first topological index [1] way back in 1947, which is well

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known by his name now that describes a correlation between chemical /physical property [2]-[4] of a molecule and its structure. Many of its forms are used in mathematical, combinatorial chemistry [5]-[20]. Several papers have been written [21]-[28] which help in getting many properties of a molecule with the help of its structure.

Hexagonal chain is a chain like structure composed of hexagonal rings. This hexagonal chain and its derivatives are well known organic compounds known for their sensitivity, durability and availability in nature. Formally speaking, benzenoid hydrocarbons are condensed polycyclic unsaturated fully conjugated hydrocarbons composed exclusively of six membered rings. A segment [29] of a hexagonal chain is its maximal sub chain in which all rings are linearly annihilated. A segment including a terminal hexagon is a terminal segment. The number of hexagons in a segment $s$ is called its length and is denoted by $l(s)$. In particular, if length of each segment is 2, then it is called a fibonacene, denoted by $\boldsymbol{F_h}$, $h$ being number of hexagonal rings. In this paper we determine exact value of degree based topological indices (Table1) and entropy based on reverse degree-based indices for hexagonal chains with $n$ segments of length $l$, that is $\boldsymbol{G_{n,l}}$ as well as linear polyacenes ($\boldsymbol{L_h}$).

## 2. Materials and Methods

Kulli [30] introduced reverse vertex degree as $\boldsymbol{\mathcal{R}(u) = \Delta(G) - \lambda(u) + 1}$, where $\Delta(\boldsymbol{G})$ is the maximum degree of a graph and $\boldsymbol{\lambda(u)}$is the degree of vertex $u$. Wei et al. [31] introduced some reverse topological indices namely, the reverse general Randić index, the reverse atom bond connectivity index, the reverse geometric arithmetic index, the reverse forgotten index and the reverse Zagreb type indices etc. Many of these indices are used in treatment of corona virus (COVID 19). Jung et al.[32] introduced first and second reverse Zagreb indices, first and second reverse hyper Zagreb indices, reverse atomic-bond connectivity index and reverse geometric-arithmetic index for TUC4[$m$, $n$]. The expression for these indices is given below in Table1.

**Table 1:** Topological indices, reverse topological indices of graphs

| TIs | Formula | Reverse TIs |
|---|---|---|
| [33]Randic index | $R(G)=\sum_{uv\epsilon E(G)}\frac{1}{\sqrt{\lambda(u)\lambda(v)}}$ | [32]$\mathcal{R}R_{\alpha}(G)=\sum_{uv\in E(G)}[\mathcal{R}\lambda(u)\times\mathcal{R}\lambda(v)]^{\alpha}$ |
| [33] Inverse Randic index | $IR(G)=\sum_{uv\epsilon E(G)}\sqrt{\lambda(u)\lambda(v)}$ | [32]$\mathcal{R}IR(G)=\sum_{uv\epsilon E(G)}\sqrt{\mathcal{R}\lambda(u)\mathcal{R}\lambda(v)}$ |
| [34]Geometric Arithmetic index | $GA(G)=\sum_{uv\epsilon E(G)}\frac{2\sqrt{\lambda(u)\lambda(v)}}{\lambda(u)+\lambda(v)}$ | [32] $\mathcal{R}GA(G)=\sum_{uv\epsilon E(G)}\frac{2\sqrt{\mathcal{R}\lambda(u)\times\mathcal{R}\lambda(v)}}{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}$ |
| [36] Symmetric division deg index | $SSD(G)=\sum_{uv\epsilon E(G)}\frac{\lambda(u)}{\lambda(v)}+\frac{\lambda(v)}{\lambda(u)}$ | [35]$\mathcal{R}SSD(G)=\sum_{uv\epsilon E(G)}\frac{\mathcal{R}\lambda(u)}{\mathcal{R}\lambda(v)}+\frac{\mathcal{R}\lambda(v)}{\mathcal{R}\lambda(u)}$ |
| [6]First Zagreb index | $M_1=\sum_{uv\epsilon E(G)}\lambda(u)+\lambda(v)$ | [32] $\mathcal{R}M_1(G)=\sum_{uv\in E(G)}\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)$ |
| [37]Second Zagreb index | $M_2=\sum_{uv\epsilon E(G)}\lambda(u)\lambda(v)$ | [32] $\mathcal{R}M_2(G)=\sum_{uv\in E(G)}\mathcal{R}\lambda(u)\mathcal{R}\lambda(v)$ |
| [38]Harmonic index | $HI=\sum_{uv\in E(G)}\frac{2}{\lambda(u)+\lambda(v)}$ | [35]$\mathcal{R}HI=\sum_{uv\in E(G)}\frac{2}{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}$ |
| [39]First hyper Zagreb index | $HM1(G)=\sum_{uv\epsilon E(G)}[\lambda(u)+\lambda(v)]^2$ | [31] $\mathcal{R}HM1(G)=\sum_{uv\in E(G)}[\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)]^2$ |
| [39]Second hyper Zagreb index | $HM_2(G)=\sum_{uv\epsilon E(G)}[\lambda(u)\times\lambda(v)]^2$ | [35]$\mathcal{R}HM2(G)=\sum_{uv\epsilon E(G)}[\mathcal{R}\lambda(u)\times\mathcal{R}\lambda(v)]^2$ |
| [40]Sum connectivity | $SCI=\sum_{uv\epsilon E(G)}\frac{1}{\sqrt{\lambda(u)+\lambda(v)}}$ | [35]$\mathcal{R}SCI=\sum_{uv\epsilon E(G)}\frac{1}{\sqrt{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}}$ |
| [41]Inverse sum index | $ISI=\sum_{uv\in E(G)}\frac{\lambda(u)\lambda(v)}{\lambda(u)+\lambda(v)}$ | [35]$\mathcal{R}ISI=\sum_{uv\in E(G)}\frac{\mathcal{R}\lambda(u)\mathcal{R}\lambda(v)}{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}$ |
| [43]Atom Bond Connectivity | $ABC(G)=\sum_{uv\epsilon E(G)}\sqrt{\frac{\lambda(u)+\lambda(v)-2}{\lambda(u)\lambda(v)}}$ | [32]$\mathcal{R}ABC(G)=\sum_{uv\epsilon E(G)}\sqrt{\frac{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)-2}{\mathcal{R}\lambda(u)\mathcal{R}\lambda(v)}}$ |
| [44]Atom Bond Sum connectivity index | $ABS(G)=\sum_{uv\epsilon E(G)}\sqrt{\frac{\lambda(u)+\lambda(v)-2}{\lambda(u)+\lambda(v)}}$ | [35]$\mathcal{R}ABS(G)=\sum_{uv\epsilon E(G)}\sqrt{\frac{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)-2}{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}}$ |
| [16]Arithmetic Geometric index | $AG(G)=\sum_{uv\epsilon E(G)}\frac{\lambda(u)+\lambda(v)}{2\sqrt{\lambda(u)\lambda(v)})}$ | [35]$\mathcal{R}AG(G)=\sum_{uv\epsilon E(G)}\frac{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}{2\sqrt{\mathcal{R}\lambda(u)\mathcal{R}\lambda(v)})}$ |
| [37]Forgotten index | $F(G)=\sum_{uv\in E(G)}(\lambda(u))^2+(\lambda(v))^2$ | [32] $\mathcal{R}F(G)=\sum_{uv\in E(G)}(\mathcal{R}\lambda(u))^2+(\mathcal{R}\lambda(v))^2$ |
| [42]First redefined Zagreb index | $ReZG_1(G)=\sum_{uv\in E(G)}\frac{\lambda(u)+\lambda(v)}{\lambda(u)\times\lambda(v)}$ | [31] $\mathcal{R}ReZG_1(G)=\sum_{uv\in E(G)}\frac{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}{\mathcal{R}\lambda(u)\times\mathcal{R}\lambda(v)}$ |
| [42]Second redefined Zagreb index | $ReZG_2(G)=\sum_{uv\in E(G)}\frac{\lambda(u)\times\lambda(v)}{\lambda(u)+\lambda(v)}$ | [31] $\mathcal{R}ReZG_2(G)=\sum_{uv\in E(G)}\frac{\mathcal{R}\lambda(u)\times\mathcal{R}\lambda(v)}{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}$ |
| [42]Third redefined Zagreb index | $ReZG_3(G)=\sum_{uv\in E(G)}\big(\lambda(u)+\lambda(v)\big)(\lambda(u)\lambda(v))$ | [31] $\mathcal{R}ReZG_3(G)=\sum_{uv\in E(G)}\big(\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)\big)(\mathcal{R}\lambda(u)\mathcal{R}\lambda(v))$ |

We consider the following basic concepts, which will be applied throughout the paper. Let *G* be connected, simple graph. *V(G)* be the set of vertices belonging to the graph *G*, let *u*, *v* be the vertices belongs to *V*(*G*). *E(G)* be the edge set of a graph (*G*). Degree of vertex *u* is represented by $\boldsymbol{\lambda}(\mathbf{u})$. Let *e* =*uv* belong to edge set of G. Reverse vertex degree of a vertex u is given by $\boldsymbol{\mathcal{R}}(\mathbf{u}) = \Delta(\mathbf{G}) - \boldsymbol{\lambda}(\mathbf{u}) + \mathbf{1}$, where $\Delta$ is the maximum degree of a graph and $\boldsymbol{\lambda}(\boldsymbol{u})$is the degree of vertex *u*. Then Reverse Topological index can be written as $\boldsymbol{\psi}(\boldsymbol{G}) = \sum_{\boldsymbol{e}\in\boldsymbol{E}(\boldsymbol{G})}(\boldsymbol{f}(\boldsymbol{e}))$ where *f* is a structural-functional that characterizes the bond- additive reverse topological index.

Entropy was first introduced by Claude Shannon in relation to information theory. As researchers looked for ways to evaluate the uncertainty, unpredictability or information content in network architecture and connectivity patterns, it turned out that entropy measure is a very effective tool which can be applied to complex networks. This advancement is a component of network science's larger progress. Later graph entropy was introduced by Rashevsky [45] , which is used to characterize the structural complexity of graphs. Currently, graph entropy is a very effective tool for determining how information theoretical techniques can be employed in applied mathematical chemistry [2], [46]-[51]. An extensive overview on graph entropy measures can be found in [49]. There are several ways to define and calculate graph entropy, and the choice of a specific measure often depends on the aspect of the graph under consideration. Shannon's model [4], [52] is the most widely used method for calculating probabilistic entropy, and we employed it for our computations. In this paper we are obtaining the entropy of linear poly-acene and hexagonal chain of equal segment lengths using reversed degree-based indices. Shannon's entropy (*H*) of a discrete random variable $X = \{x_1, x_2, x_3 \ldots.. x_n\}$ is defined as

$$\boldsymbol{H}(\boldsymbol{X}) = -\sum_{i=1}^{n} \boldsymbol{p}(\boldsymbol{x_i})\, \boldsymbol{ln}\big(\boldsymbol{p}(\boldsymbol{x_i})\big)$$

where $\boldsymbol{p}(\boldsymbol{x_i})$ is the probability of the $i^{th}$ outcome, *n* is the total number of random variables. This entropy is modified in the case of chemical graphs in order to describe their structural characteristics. The edges of a chemical graph are regarded as elements and reverse topological indices are used to assign probability values to each edge. The entropy [42] measured using a topological index $\boldsymbol{\psi}$ of a graph *G* is defined as,

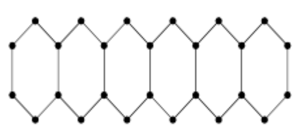
$$E_{\psi}(G) = -\sum_{e\in E(G)} \frac{f(e)}{\psi(G)} ln\left(\frac{f(e)}{\psi(G)}\right) = -\sum_{e\in E(G)} \frac{f(e)}{\psi(G)} ln(f(e) - \psi(G))$$

$$E_{\psi}(G) = ln\,(\psi(G)) - \frac{1}{\psi(G)} \sum_{e\in E(G)} (f(e)\, ln(f(e)) \ldots\ldots\ldots\ldots\ldots\ldots \quad (1)$$

The above equation (1) is used to compute the graph entropies of reverse topological indices.

## 3. RESULTS AND DISCUSSION

Poly-acenes are a class of benzenoid hydrocarbon chains, that consist of linearly arranged benzene rings. Generally speaking, substances with several benzene rings joined in a linear form are referred to as "poly-acenes." These compounds have intriguing optical and electrical characteristics and are aromatic. We usually refer them as linear poly-acenes and represented as $L_h$, with $h$ number of hexagons. Graphically it is represented as shown in Figure 1(a), which will have 4$h$+2 number of vertices and 5$h$+1 number of edges. A hexagonal chain's longest sub-chain, where every ring is linearly annealed, is called a segment ($s$). Its length, represented by $l$, is the total number of hexagons in a segment $s$. Specifically, if every segment has a length 2, it is referred to as a fibonacene, represented by the symbol $F_h$, where $h$ is the number of hexagonal rings, given by $h = n(l-1)+1$. In this paper we are considering $n$ segments of length $l$ denoted by $G_{n,l}$, with two segments of any pattern like zigzag, non-zigzag etc



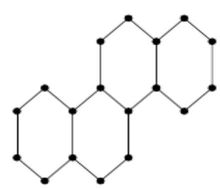


Fig. 1(a): Linear poly-acene ($L_6$)      Fig. 1(b): Hexagonal chain with 3 segments of length 2 ($G_{3,2}$).

Here we establish results related to hexagonal hydrocarbon chains mainly based on reverse degree-based indices. We use edge partition method for both of them that help in proving our results. The edge partition of linear poly-acene based on degrees and corresponding reverse degrees of each edge is given in Table 2(a) and 2(b), of end vertices respectively for $L_h$ and $G_{n,l}$.

Table 2(a): Reverse degree edge partitions of $L_h$

| $\lambda(u), \lambda(v)$ | $\mathcal{R}\lambda(u), \mathcal{R}\lambda(v)$ | Frequency |
|---|---|---|
| (2,2) | (2,2) | 6 |
| (2,3) | (2,1) | 4(*h*-1) |
| (3,3) | (1,1) | (*h*-1) |

Table 2(b): Reverse degree edge partitions of $G_{n,l}$

| $\lambda(u), \lambda(v)$ | $\mathcal{R}\lambda(u), \mathcal{R}\lambda(v)$ | Frequency |
|---|---|---|
| (2,2) | (2,2) | *n*+5 |
| (2,3) | (2,1) | *n* (4*l*- 5) +1 |
| (3,3) | (1,1) | *n*(*l*-1) |

**Theorem 1**. *The values of reverse degree-based indices of linear poly-acene having h number of hexagons is given as follows:*

(1) $\mathcal{R}R_1(L_h) = 9h + 15$,

$\mathcal{R}R_{-1}(L_h) = \frac{3}{2} + 3(h-1)$,

$\mathcal{R}R_{\frac{1}{2}}(L_h) = 12 + (4\sqrt{2} + 1)(h-1)$,

$\mathcal{R}R_{\frac{-1}{2}}(L_h) = 3 + (2\sqrt{2} + 1)(h-1)$.

(2) $\mathcal{R}IR(L_h) = 12 + (4\sqrt{2} + 1)(h-1)$.

(3) $\mathcal{R}M_1(L_h) = 14h + 10$, $\mathcal{R}M_2(L_h) = 9h + 15$.

(4) $\mathcal{R}HI(L_h) = 3 + \frac{11}{3}(h-1)$.

(5) $\mathcal{R}SCI(L_h) = 3 + \left(\frac{4}{\sqrt{3}} + \frac{1}{\sqrt{2}}\right)(h-1)$.

(6) $\mathcal{R}ISI(L_h) = 6 + \left(\frac{19}{6}\right)(h-1)$.

(7) $\mathcal{R}ABC(L_h) = 2\sqrt{2}h - \sqrt{2}$.

(8) $\mathcal{R}ABS(L_h) = 3\sqrt{2} + \left(\frac{4}{\sqrt{3}}\right)(h-1)$.

(9) $\mathcal{R}GA(L_h) = 6 + \left(\frac{8\sqrt{2}}{3} + 1\right)(h-1)$.

(10) $\mathcal{R}AG(L_h) = 6 + (3\sqrt{2} + 1)(h-1)$.

(11) $\mathcal{R}SSD(L_h) = 12h$.

(12) $\mathcal{R}F(L_h) = 22h + 26$.

(13) $\mathcal{R}HM_1(L_h) = 40h + 56,\ \mathcal{R}HM_2(L_h) = 17h + 79.$

(14) $\mathcal{R}ReZG_1(L_h) = 8h - 2,\ \mathcal{R}ReZG_2(L_h) = 6 + \frac{19}{6}(h-1)\ ,\ \mathcal{R}ReZG_3(L_h) = 26h + 70.$

*Proof:* Here we calculate reverse topological indices of linear poly-acene $L_h$ as follows:

(1) From Table 1, using definition of Randić index and reverse Randić index, we get

$\mathcal{R}R_\alpha(G) = \sum_{uv\in E(G)} [\mathcal{R}\lambda(u) \times \mathcal{R}\lambda(v)]^\alpha$. Substituting different values of $\propto$ as follows we get,

For $\propto = 1,\ \mathcal{R}R_1(G) = 6 * 4 + 4(h-1) * 2 + (h-1) = 9h + 15.$

For $\propto = -1,\ \mathcal{R}R_{-1}(G) = \frac{6}{2\times 2} + \frac{4(h-1)}{2\times 1} + \frac{h-1}{1\times 1} = \frac{3}{2} + 3(h-1),$

For $\propto = \frac{1}{2},\ \mathcal{R}R_{\frac{1}{2}}(G) = 6 * \sqrt{4} + 4(h-1) * \sqrt{2} + (h-1) = 12 + (4\sqrt{2}+1)(h-1).$

For $\propto = \frac{-1}{2},\ \mathcal{R}R_{\frac{-1}{2}}(G) = \frac{6}{\sqrt{2\times 2}} + \frac{4(h-1)}{\sqrt{2\times 1}} + \frac{h-1}{\sqrt{1\times 1}} = 3 + (2\sqrt{2}+1)(h-1).$

(2) The Reverse inverse Randić index is given by

$$\mathcal{R}IR(L_h) = \sum_{uv\epsilon E(G)} \sqrt{\mathcal{R}\lambda(u)\mathcal{R}\lambda(v)} = 6 * \sqrt{4} + 4(h-1) * \sqrt{2} + (h-1)$$

$$= 12 + (4\sqrt{2}+1)(h-1).$$

(3) The Reverse first Zagreb index is given by $\mathcal{R}M_1(L_h) = \sum_{uv\in E(G)} \mathcal{R}\lambda(u) + \mathcal{R}\lambda(v)$

$= 6(2+2) + 4(h-1)(2+1) + (h-1)(1+1) = 14h + 10.$

The Reverse second Zagreb index is given by $M_2(L_h) = \sum_{uv\in E(G)} \mathcal{R}\lambda(u) \times \mathcal{R}\lambda(v)$

$= 6(2\times 2) + 4(h-1)(2\times 1) + (h-1)(1\times 1) = 9h + 15.$

(4) The Reverse harmonic index is given by

$$\mathcal{R}HI\ (L_h) = \sum_{uv\in E(G)} \frac{2}{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)} = 6\left(\frac{2}{2+2}\right) + 4(h-1)\left(\frac{2}{2+1}\right) + (h-1)\left(\frac{2}{1+1}\right)$$

$$= 3 + \frac{11}{3}(h-1).$$

(5) The Reverse Sum Connectivity index is given by

$$\mathcal{R}SCI(L_h) = \sum_{uv\epsilon E(G)} \frac{1}{\sqrt{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}} = 3 + \left(\frac{4}{\sqrt{3}} + \frac{1}{\sqrt{2}}\right)(h-1).$$

(6) The Reverse Inverse sum index is given by

$$\mathcal{R}ISI(L_h) = \sum_{uv\in E(G)} \frac{\mathcal{R}\lambda(u)\mathcal{R}\lambda(v)}{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)} = 6\left(\frac{2.2}{2+2}\right) + 4(h-1)\left(\frac{2.1}{2+1}\right) + (h-1)\left(\frac{1.1}{1+1}\right)$$

$$= \mathbf{6} + \left(\frac{\mathbf{19}}{\mathbf{6}}\right)(\boldsymbol{h} - \mathbf{1}).$$

(7) The Reverse Atom Bond Connectivity index is given by

$$\mathcal{R}ABC(L_h) = \sum_{uv\epsilon E(G)} \sqrt{\frac{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)-2}{\mathcal{R}\lambda(u)\mathcal{R}\lambda(v)}} = 6 * \sqrt{\frac{2}{4}} + 4(h-1) * \sqrt{\frac{1}{2}} = 2\sqrt{2}h - \sqrt{2}.$$

(8) The Reverse Atom Bond Sum connectivity index is given by

$$\mathcal{R}ABS(L_h) = \sum_{uv\epsilon E(G)} \sqrt{\frac{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)-2}{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}} = 6\sqrt{\frac{2}{4}} + 4(h-1)\sqrt{\frac{1}{3}} = 3\sqrt{2} + \left(\frac{4}{\sqrt{3}}\right)(h-1).$$

(9) The Reverse geometric index is

$$\mathcal{R}GA(L_h) = \sum_{uv\in E(G)} \frac{2\sqrt{\mathcal{R}\lambda(u)\times\mathcal{R}\lambda(v)}}{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)} = 6 + \left(\frac{8\sqrt{2}}{3} + 1\right)(h-1).$$

(10) The Reverse Arithmetic Geometric index is given by

$$\mathcal{R}AG(L_h) = \sum_{uv\epsilon E(G)} \frac{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}{2\sqrt{\mathcal{R}\lambda(u)\mathcal{R}\lambda(v)})} = 6 + \left(3\sqrt{2} + 1\right)(h-1).$$

(11) The Reverse Symmetric division degree index is

$$\mathcal{R}SSD(L_h) = \sum_{uv\epsilon E(G)} \frac{\mathcal{R}\lambda(u)}{\mathcal{R}\lambda(v)} + \frac{\mathcal{R}\lambda(v)}{\mathcal{R}\lambda(u)} = 6\left(\frac{2.}{2} + \frac{2}{2}\right) + 4(h-1)\left(\frac{2}{1} + \frac{1}{2}\right) + (h-1)2 = 12h.$$

(12) The Reverse Forgotten index is given by

$$\mathcal{R}F(L_h) = \sum_{uv\in E(G)} \left(\mathcal{R}\lambda(u)\right)^2 + \left(\mathcal{R}\lambda(v)\right)^2 = 6(4+4) + 4(h-1)(4+1) +$$

$$(h-1)(1+1) = 22h + 26.$$

(13) The Reverse first hyper Zagreb index is given by

$$\mathcal{R}HM_1(L_h) = \sum_{uv\in E(G)} [\mathcal{R}\lambda(u) + \mathcal{R}\lambda(v)]^2$$

$$= 6(2+2)^2 + 4(h-1)(2+1)^2 + (h-1)(1+1)^2 = 40h + 56.$$

The Reverse second hyper Zagreb index is given by

$$\mathcal{R}HM_2(L_h) = \sum_{uv\epsilon E(G)} [\mathcal{R}\lambda(u) \times \mathcal{R}\lambda(v)]^2$$

$$= 6(4)^2 + 4(h-1)(2)^2 + (h-1)(1)^2 = 17h + 79.$$

(14) The Reverse first redefined Zagreb index is given by

$$\mathcal{R}ReZG_1(L_h) = \sum_{uv\in E(G)} \frac{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}{\mathcal{R}\lambda(u)\times\mathcal{R}\lambda(v)}$$

$$= 6\left[\frac{2+2}{2\times2}\right] + 4(h-1)\left[\frac{2+1}{2\times1}\right] + (h-1)\left[\frac{2+2}{2\times2}\right] = 6 + 8(h-1)$$

The Reverse second redefined Zagreb index is given by

$$\mathcal{R}ReZG_2(L_h) = \sum_{uv\in E(G)} \frac{\mathcal{R}\lambda(u)\times\mathcal{R}\lambda(v)}{\mathcal{R}\lambda(u)+\mathcal{R}\lambda(v)}$$

$$= 6\left(\frac{2\times2}{2+2}\right) + 4(h-1)\left(\frac{2\times1}{2+1}\right) + (h-1)\left(\frac{1\times1}{1+1}\right) = 6 + \frac{19}{6}(h-1).$$

The Reverse third redefined Zagreb index is given by

$$\mathcal{R}ReZG_3(G) = \sum_{uv\in E(G)} (\mathcal{R}\lambda(u) + \mathcal{R}\lambda(v)) \times (\mathcal{R}\lambda(u) \times \mathcal{R}\lambda(v))$$

$$= 6(2\times 2)(2+2) + 4(h-1)(2\times1)(2+1) + (h-1)(1\times1)(1+1)$$

$$= 48 + 26(h-1).$$ ■

**Theorem 2**. *The values of reverse degree-based indices of hexagonal chain of n segments of length l are given as follows:*

(1). $\mathcal{R}R_1(G_{n,l}) = 9nl - 7n + 22,\ \ \mathcal{R}R_{-1}(G_{n,l}) = 3nl - \frac{13n}{4} + \frac{7}{4},$

$\mathcal{R}R_{\frac{1}{2}}(G_{n,l}) = (4\sqrt{2}+1)nl + (1-5\sqrt{2})n + 10,$

$\mathcal{R}R_{\frac{-1}{2}}(G_{n,l}) = (2\sqrt{2}+1)nl - \left(\frac{1+5\sqrt{2}}{2}\right)n + \left(\frac{5+\sqrt{2}}{2}\right).$

(2). $\mathcal{R}IR(G_{n,l}) = (4\sqrt{2}+1)nl + (1-5\sqrt{2})n + 10.$

(3). $\mathcal{R}HI(G_{n,l}) = \frac{11nl}{3} - \frac{23n}{6} + \frac{19}{6}.$

(4). $\mathcal{R}M_1(G_{n,l}) = 14nl - 13n + 23,\ \ \mathcal{R}M_2(G_{n,l}) = 9nl - 7n + 22.$

(5) $\mathcal{R}SCI(G_{n,l}) = \left(\frac{4}{\sqrt{3}} + \frac{1}{\sqrt{2}}\right)nl + n\left(\frac{1}{2} - \frac{5}{\sqrt{3}} - \frac{1}{\sqrt{2}}\right) + \left(\frac{1}{\sqrt{3}} + \frac{5}{2}\right).$

(6). $\mathcal{R}ISI(G_{n,l}) = \frac{19nl}{6} - \frac{17}{6}n + \frac{17}{3}.$

(7). $\mathcal{R}ABC(G_{n,l}) = 2\sqrt{2}(nl-n) + 3\sqrt{2}.$

(8) . $\mathcal{R}ABS(G_{n,l}) = \frac{4\sqrt{2}nl}{\sqrt{3}} + n\left(\frac{1}{\sqrt{2}} - \frac{5\sqrt{2}}{\sqrt{3}}\right) + \left(\frac{5}{\sqrt{2}} + \frac{\sqrt{2}}{\sqrt{3}}\right).$

(9). $\mathcal{R}GA(G_{n,l}) = \left(\frac{8\sqrt{2}}{3} + 1\right)nl - \frac{10\sqrt{2}}{3} + \frac{(15+2\sqrt{2})}{3}.$

(10) $\mathcal{R}AG(G_{n,l}) = (3\sqrt{2}+1)nl - \frac{15\sqrt{2}}{4} + \frac{(20+3\sqrt{2})}{4}.$

(11) $\mathcal{R}SSD(G_{n,l}) = 12nl - \frac{25n}{2} + \frac{25}{2}.$

(12) $\mathcal{R}F(G_{n,l}) = 22nl - 19n + 45$.

(13). $\mathcal{R}HM_1(G_{n,l}) = 40nl - 33n + 89$, $\mathcal{R}HM_2(G_{n,l}) = 17nl - 5n + 84$.

(14) $\mathcal{R}ReZG_1(G_{n,l}) = 8nl - \frac{17n}{2} + \frac{13}{2}$, $\mathcal{R}ReZG_2(G_{n,l}) = \frac{19nl}{6} - \frac{17n}{6} + \frac{17}{3}$ ,

$\mathcal{R}ReZG_3(G_{n,l}) = 26nl - 16n + 86$.

*Proof:* Proof is similar to the above Theorem 1, depending on the values of indices as defined in Table 1 and edge partitions as given in Table 2(b) and the values are as given in the statement of the theorem. ■

**Theorem 3.** *The entropy of reverse degree-based indices of linear poly-acene* $L_h$ *having h number of hexagons are as follows:*

(1). $E_{\mathcal{R}R_1}(L_h) = ln(9h + 15) - \frac{1}{9h+15}\{24\, ln(4) + 8(h - 1)\, ln(2)\}$.

$E_{\mathcal{R}R_{-1}}(L_h) = \ln\left(\frac{3}{2} + 3(h - 1)\right) - \frac{1}{\frac{3}{2}+3(h-1)}\left\{\frac{3}{2}\, ln\left(\frac{1}{4}\right) + 2(h - 1)\, ln\left(\frac{1}{2}\right)\right\}$.

$E_{\mathcal{R}R_{\frac{1}{2}}}(L_h) = ln\left(12 + (4\sqrt{2} + 1)(h - 1)\right) - \frac{1}{12+(4\sqrt{2}+1)(h-1)}\{12\, ln(2) + 4\sqrt{2}(h -$

$1)\, ln(\sqrt{2})\}$.

$E_{\mathcal{R}R_{\frac{-1}{2}}}(L_h) = ln\left(3 + (2\sqrt{2} + 1)(h - 1)\right) - \frac{1}{3+(2\sqrt{2}+1)(h-1)}\left\{3\, ln\left(\frac{1}{2}\right) + 2\sqrt{2}(h - 1)\, ln\left(\frac{1}{\sqrt{2}}\right)\right\}$.

*(2)* $E_{\mathcal{R}IR}(L_h) = ln\,(12 + (4\sqrt{2} + 1)(h - 1)) - \frac{1}{12+(4\sqrt{2}+1)(h-1)}\{12\, ln(2) + 4\sqrt{2}(h - 1)\, ln(\sqrt{2})\}$.

*(3)* $E_{\mathcal{R}M_1}(L_h) = ln\,(14h + 10) - \frac{1}{14h+10}\{24\, ln(4) + 12(h - 1)\, ln(3) + 2(h - 1) ln\,(2)\}$.

$E_{\mathcal{R}M_2}(L_h) = ln(9h + 15) - \frac{1}{9h+15}\{24\, ln(4) + 8(h - 1)\, ln(2)\}$.

*(4)* $E_{\mathcal{R}HI}(L_h) = ln\left(3 + \frac{11}{3}(h - 1)\right) - \frac{1}{3+\frac{11}{3}(h-1)}\left\{3\, ln\left(\frac{1}{2}\right) + \frac{8}{3}(h - 1)\, ln\left(\frac{2}{3}\right)\right\}$.

*(5)* $E_{\mathcal{R}SCI}(L_h) = ln(\mathcal{R}SCI) - \frac{1}{3+\left(\frac{4}{\sqrt{3}}+\frac{1}{\sqrt{2}}\right)(h-1)}\left\{3\, ln\left(\frac{1}{2}\right) + \frac{4}{\sqrt{3}}(h - 1)\, ln\left(\frac{1}{\sqrt{3}}\right) + \frac{1}{\sqrt{2}}(h - 1)\, ln\left(\frac{1}{\sqrt{2}}\right)\right\}$.

*(6)* $E_{\mathcal{R}ISI}(L_h) = ln\left(6 + \left(\frac{19}{6}\right)(h - 1)\right) - \frac{1}{6+\left(\frac{19}{6}\right)(h-1)}\left\{6\, ln(1) + \frac{8}{3}(h - 1)\, ln\left(\frac{2}{3}\right) +\right.$

$\left.\frac{1}{2}(h - 1)\, ln\left(\frac{1}{2}\right)\right\}$.

*(7)* $E_{\mathcal{R}ABC}(L_h) = ln(2\sqrt{2}h - \sqrt{2}) - \frac{1}{2\sqrt{2}h-\sqrt{2}}\left\{3\sqrt{2}\, ln\left(\frac{1}{\sqrt{2}}\right) + 2\sqrt{2}(h - 1)\, ln\left(\frac{1}{\sqrt{2}}\right)\right\}$.

*(8)* $$E_{\mathcal{R}ABS}(L_h) = ln\left(3\sqrt{2} + \left(\frac{4}{\sqrt{3}}\right)(h-1)\right) - \frac{1}{3\sqrt{2}+\left(\frac{4}{\sqrt{3}}\right)(h-1)}\left\{3\sqrt{2}\, ln\left(\frac{1}{\sqrt{2}}\right) + \frac{4}{\sqrt{3}}(h-1)\, ln\left(\frac{1}{\sqrt{3}}\right)\right\}.$$

*(9)* $$E_{\mathcal{R}GA}(L_h) = ln\left(6 + \left(\frac{8\sqrt{2}}{3} + 1\right)(h-1)\right) - \frac{1}{6+\left(\frac{8\sqrt{2}}{3}+1\right)(h-1)}\left\{\frac{8\sqrt{2}}{3}(h-1)\, ln\left(\frac{2\sqrt{2}}{3}\right)\right\}.$$

*(10)* $$E_{\mathcal{R}AG}(L_h) = ln\,(6 + (3\sqrt{2}+1)(h-1)) - \frac{1}{6+(3\sqrt{2}+1)(h-1)}\left\{3\sqrt{2}(h-1)\, ln\left(\frac{3}{2\sqrt{2}}\right)\right\}.$$

*(11)* $$E_{\mathcal{R}SSD}(L_h) = ln(12h) - \frac{1}{12h}\left\{12\, ln(2) + 10(h-1)\, ln\left(\frac{5}{2}\right) + 2(h-1)\, ln(2))\right\}.$$

*(12)* $$E_{\mathcal{R}F}(L_h) = ln(22h+26) - \frac{1}{22h+26}\{48\, ln(8) + 20(h-1)\, ln(5) + 2(h-1)\, ln(2)\}.$$

*(13)* $$E_{\mathcal{R}HM_1}(L_h) = ln(40h+56) - \frac{1}{40h+56}\{96\, ln(16) + 36(h-1)\, ln(9) + 4(h-1)\, ln(4)\}.$$

$$E_{\mathcal{R}HM_2}(L_h) = ln(17h+79) - \frac{1}{17h+79}\{96\, ln(16) + 16(h-1)\, ln(4))\}.$$

*(14)* $$E_{\mathcal{R}ReZG_1}(L_h) = ln(8h-2) - \frac{1}{8h-2}\left\{6(h-1)\, ln\left(\frac{3}{2}\right) + 2(h-1)\ln(2)\right\}.$$

$$E_{\mathcal{R}ReZG_2}(L_h) = ln\left(6 + \frac{19}{6}(h-1)\right) - \frac{1}{\left(6+\frac{19}{6}(h-1)\right)}\left\{\frac{8}{3}(h-1)\, ln\left(\frac{2}{3}\right) + \frac{1}{2}(h-1)\, ln\left(\frac{1}{2}\right)\right\}.$$

$$E_{\mathcal{R}ReZG_3}(L_h) = ln(26h+70) - \frac{1}{26h+70}\{48\, ln(8) + 20(h-1)\, ln(5) + 3(h-1) ln\,(3)\}.$$

Proof: The Reverse Randić index entropy for linear poly-acene is obtained as $E_{\mathcal{R}R_\alpha}(L_h) = ln\,(\mathcal{R}R_\alpha) - \frac{1}{\mathcal{R}R_\alpha} ln\,\{\prod(\,[\mathcal{R}\lambda(u)\times\mathcal{R}\lambda(v)]^\alpha)^{[\mathcal{R}\lambda(u)\times\mathcal{R}\lambda(v)]^\alpha}\}$, by substituting in the definition of entropy as given in Equation (1) and reverse Randić index value obtained in Theorem 1, above. For $\alpha = 1$, we get by substitution $\mathcal{R}R_1(T[p,q]) = 9h + 15$ value and using reverse degree edge partitions in Table 4 we get

$$E_{\mathcal{R}R_1}(L_h) = ln\,(9h+15) - \frac{1}{9h+15}\{6\times 4\, ln(4) + 4\times 2(h-1)\, ln(2) + 1\times 1(h-)\, ln(1)\}$$

$$= ln\,(9h+15) - \frac{1}{9h+15}\{24 ln\,(4) + 8(h-1)\, ln(2)\}.$$

Similarly, for all the reverse topological indices, we get the respective entropy value using Equation (1), Table 2(a), 2(b) and Theorem 1 and are given as in the statement of the theorem.

■

**Theorem 4**. *The entropy of reverse degree- based indices of hexagonal chain of n segments of length l* $G_{n,l}$ *having h number of hexagons are as follows*:

(1). $E_{\mathcal{R}R_1}(G_{n,l}) = ln(9nl-7n+22) - \frac{1}{9nl-7n+22}\{4(n+5)\,ln(4) + 2(4nl-5n+1)\,ln(2\,)\}.$

$E_{\mathcal{R}R_{-1}}(G_{n,l}) = ln\left(3nl - \frac{13n}{4} + \frac{7}{4}\right) - \frac{1}{3nl-\frac{13n}{4}+\frac{7}{4}}\left\{\frac{(n+5)}{4}\,ln\left(\frac{1}{4}\right) + \frac{1}{2}(4nl-5n+1)\,ln\left(\frac{1}{2}\right)\right\}.$

$E_{\mathcal{R}R_{\frac{1}{2}}}(G_{n,l}) = ln\left((4\sqrt{2}+1)nl + (1-5\sqrt{2})n + 10\right) - \frac{1}{(4\sqrt{2}+1)nl+(1-5\sqrt{2})n+10} *$

$\{2(n+\ 5)\,ln(2) + \sqrt{2}(4nl-5n+1)\,ln(\sqrt{2})\}.$

$E_{\mathcal{R}R_{\frac{-1}{2}}}(G_{n,l}) = ln\left((2\sqrt{2}+1)nl - \left(\frac{1+5\sqrt{2}}{2}\right)n + \left(\frac{5+\sqrt{2}}{2}\right)\right) - \frac{1}{(2\sqrt{2}+1)nl-\left(\frac{1+5\sqrt{2}}{2}\right)n+\left(\frac{5+\sqrt{2}}{2}\right)}$

$\left\{\frac{1}{2}(n+5)ln\left(\frac{1}{2}\right) + \frac{1}{\sqrt{2}}(4nl-5n+1)\,ln\left(\frac{1}{\sqrt{2}}\right)\right\}.$

*(2).*$E_{\mathcal{R}IR}(G_{n,l}) = ln\left((4\sqrt{2}+1)nl + (1-5\sqrt{2})n + 10\right) - \frac{1}{(4\sqrt{2}+1)nl+(1-5\sqrt{2})n+10}$

$\{2\,(n+5)ln(2) + \sqrt{2}(4nl-5n+1)\,ln(\sqrt{2})\}.$

*(4)* $E_{\mathcal{R}M_1}(G_{n,l}) = ln\,(14nl-13n+23) - \frac{1}{14nl-13n+23}\{4(n+5)\,log(4) + 3(4nl-5n+$

$1)\,ln(3) + \ 2(nl-n)ln\,(2)\}.$

$E_{\mathcal{R}M_2}(G_{n,l}) = ln(9nl-7n+22) - \frac{1}{9nl-7n+22}\{4\,(n+5)ln(4) + 2(4nl-5n+1)\,ln(2)\}.$

*(4).* $E_{\mathcal{R}HI}(G_{n,l}) = ln\left(\frac{11nl}{3} - \frac{23n}{6} + \frac{19}{6}\right) - \frac{1}{\frac{11nl}{3}-\frac{23n}{6}+\frac{19}{6}}\left\{\frac{1}{2}(n+5)\,ln\left(\frac{1}{2}\right) + \frac{2}{3}(4nl-5n+\right.$

$\left.1)\,ln\left(\frac{2}{3}\right)\right\}.$

*(5)* $E_{\mathcal{R}SCI}(G_{n,l}) = ln\left(\left(\frac{4}{\sqrt{3}} + \frac{1}{\sqrt{2}}\right)nl + n\left(\frac{1}{2} - \frac{5}{\sqrt{3}} - \frac{1}{\sqrt{2}}\right) + \left(\frac{1}{\sqrt{3}} + \frac{5}{2}\right)\right) - \frac{1}{\left(\frac{4}{\sqrt{3}}+\frac{1}{\sqrt{2}}\right)nl+n\left(\frac{1}{2}-\frac{5}{\sqrt{3}}-\frac{1}{\sqrt{2}}\right)+\left(\frac{1}{\sqrt{3}}+\frac{5}{2}\right)}$

$\left\{\frac{1}{2}(n+5)\,ln\left(\frac{1}{2}\right) + \frac{1}{\sqrt{3}}(4nl-5n+1)\,ln\left(\frac{1}{\sqrt{3}}\right) + \frac{1}{\sqrt{2}}(nl-n)\,ln\left(\frac{1}{\sqrt{2}}\right)\right\}.$

*(6).* $E_{\mathcal{R}ISI}(G_{n,l}) = ln\left(\frac{19nl}{6} - \frac{17}{6}n + \frac{17}{3}\right) - \frac{1}{\frac{19nl}{6}-\frac{17}{6}n+\frac{17}{3}}\left\{\frac{2}{3}(4nl-5n+1)\,log\left(\frac{2}{3}\right) + \frac{1}{2}(nl-\right.$

$\left.n)\,ln\left(\frac{1}{2}\right)\right\}.$

*(7)*$E_{\mathcal{R}ABC}(G_{n,l}) = l\,n(2\sqrt{2}(nl-n) + 3\sqrt{2}) - \frac{1}{2\sqrt{2}(nl-n)+3\sqrt{2}}\left\{\frac{1}{\sqrt{2}}(n+5)\,ln\left(\frac{1}{\sqrt{2}}\right) +\right.$

$\left.\frac{1}{\sqrt{2}}(4nl-\ 5n+1)\,ln\left(\frac{1}{\sqrt{2}}\right)\right\}.$

(8). $E_{\mathcal{R}ABS}(G_{n,l}) = ln\left(\frac{4\sqrt{2}nl}{\sqrt{3}} + n\left(\frac{1}{\sqrt{2}} - \frac{5\sqrt{2}}{\sqrt{3}}\right) + \left(\frac{5}{\sqrt{2}} + \frac{\sqrt{2}}{\sqrt{3}}\right)\right) - \frac{1}{\frac{4\sqrt{2}nl}{\sqrt{3}} + n\left(\frac{1}{\sqrt{2}} - \frac{5\sqrt{2}}{\sqrt{3}}\right) + \left(\frac{5}{\sqrt{2}} + \frac{\sqrt{2}}{\sqrt{3}}\right)}\left\{\frac{1}{\sqrt{2}}(n + 5)\, ln\left(\frac{1}{\sqrt{2}}\right) + \frac{1}{\sqrt{3}}(4nl - 5n + 1)\, ln\left(\frac{1}{\sqrt{3}}\right)\right\}.$

(9). $E_{\mathcal{R}GA}(G_{n,l}) = ln\left(\left(\frac{8\sqrt{2}}{3} + 1\right)nl - \frac{10\sqrt{2}}{3} + \frac{(15+2\sqrt{2})}{3}\right) - \frac{1}{\left(\frac{8\sqrt{2}}{3}+1\right)nl - \frac{10\sqrt{2}}{3} + \frac{(15+2\sqrt{2})}{3}}\left\{\frac{2\sqrt{2}}{3}(4nl - 5n + 1)\, log\left(\frac{2\sqrt{2}}{3}\right)\right\}.$

(10). $E_{\mathcal{R}AG}(G_{n,l}) = ln\left((3\sqrt{2} + 1)nl - \frac{15\sqrt{2}}{4} + \frac{(20+3\sqrt{2})}{4}\right) - \frac{1}{(3\sqrt{2}+1)nl - \frac{15\sqrt{2}}{4} + \frac{(20+3\sqrt{2})}{4}}\left\{\frac{3}{2\sqrt{2}}(4nl - 5n + 1)\, log\left(\frac{3}{2\sqrt{2}}\right)\right\}.$

(11). $E_{\mathcal{R}SSD}(G_{n,l}) = ln\left(12nl - \frac{25n}{2} + \frac{25}{2}\right) - \frac{1}{12nl - \frac{25n}{2} + \frac{25}{2}}\left\{2(n + 5)\, ln(2) + \frac{5}{2}(4nl - 5n + 1)\, ln\left(\frac{5}{2}\right) + 2(nl - n)\, ln(2))\right\}.$

(12). $E_{\mathcal{R}F}(G_{n,l}) = ln\,(22nl - 19n + 45) - \frac{1}{22nl - 19n + 45}\{8(n + 5)\, ln(8) + 5(4nl - 5n + 1)\, ln(5) + 2(nl - n)\, ln(2)\}.$

(13). $E_{\mathcal{R}HM_1}(G_{n,l}) = ln\,(40nl - 33n + 89) - \frac{1}{40nl - 33n + 89}\{16\,(n + 5) ln(16) + 9(4nl - 5n + 1)\, ln(9) + 4(nl - n)\, ln(4)\}$

$E_{\mathcal{R}HM_2}(G_{n,l}) = ln\,(17nl - 5n + 84) - \frac{1}{17nl - 5n + 84}\{16\,(n + 5) ln(16) + 4(4nl - 5n + 1)\, ln(4)\}$

(14). $E_{\mathcal{R}ReZG_1}(G_{n,l}) = ln\left(8nl - \frac{17n}{2} + \frac{13}{2},\ \right) - \frac{1}{8nl - \frac{17n}{2} + \frac{13}{2},}\left\{\frac{3}{2}(4nl - 5n + 1)\, ln\left(\frac{3}{2}\right) + 2(nl - n)\, ln(2\,)\right\}.$

$E_{\mathcal{R}ReZG_2}(G_{n,l}) = ln\left(\frac{19}{6}nl - \frac{17n}{6} + \frac{17}{3}\right) - \frac{1}{\left(\frac{19}{6}nl - \frac{17n}{6} + \frac{17}{3}\right)}\left\{\frac{2}{3}(4nl - 5n + 1)\, ln\left(\frac{2}{3}\right) + \frac{1}{2}(nl - n)\, ln\left(\frac{1}{2}\right)\right\}.$

$E_{\mathcal{R}ReZG_3}(G_{n,l}) = ln(26nl - 16n + 86) - \frac{1}{26nl - 16n + 86}\{8(n + 5)\, ln(8) + 5(4nl - 5n + 1)\, ln(5) + 3(nl - n) ln\,(3)\}.$

*Proof:* Proof is similar to the above Theorem 3.

**3.2. Analysis:** Numerical values for reverse degree-based indices and respective entropy of linear poly-acene $(\boldsymbol{L_h})$ and hexagonal chain of equal segment length $(\boldsymbol{G_{n,l}})$ are given in the following tables: Table 3-4. Graphical representations of entropies for the different *h* values of linear poly-acene and different *n, l* values of hexagonal chain of equal segments are shown below in Figure 2(a) and Figure 2(b).

## TABLE 3: REVERSE TOPOLOGICAL INDICES AND ITS ENTROPY OF LINEAR POLYACENE ($L_h$)

| *h* | $\mathcal{R}$ $R_1$ | $\mathcal{R}$ $R_{-1}$ | $\mathcal{R}$ $R_{1/2}$ | $\mathcal{R}$ $R_{-1/2}$ | $\mathcal{R}$ IR | $\mathcal{R}$ $M_1$ | $\mathcal{R}$ $M_2$ | $\mathcal{R}$ HI | $\mathcal{R}$ SCI | $\mathcal{R}$ ISI | $\mathcal{R}$ ABC | $\mathcal{R}$ ABS | $\mathcal{R}$ GA | $\mathcal{R}$ AG | $\mathcal{R}$ SSD | $\mathcal{R}$ F | $\mathcal{R}$ $HM_1$ | $\mathcal{R}$ $HM_2$ | $\mathcal{R}$ $ReZG_1$ | $\mathcal{R}$ $ReZG_2$ | $\mathcal{R}$ $ReZG_3$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 51 | 10.5 | 31.97 | 14.49 | 31.97 | 66 | 51 | 14 | 12.05 | 15.50 | 12.73 | 11.17 | 20.31 | 21.73 | 48 | 114 | 216 | 147 | 30 | 15.50 | 174 |
| 5 | 60 | 13.5 | 38.63 | 18.31 | 38.63 | 80 | 60 | 17.67 | 15.07 | 18.67 | 15.56 | 13.48 | 25.08 | 26.97 | 60 | 136 | 256 | 164 | 38 | 18.67 | 200 |
| 6 | 69 | 16.5 | 45.28 | 22.14 | 45.28 | 94 | 69 | 21.33 | 18.08 | 21.83 | 18.38 | 15.79 | 29.86 | 32.21 | 72 | 158 | 296 | 181 | 46 | 21.83 | 226 |
| 7 | 78 | 19.5 | 51.94 | 25.97 | 51.94 | 108 | 78 | 25 | 21.10 | 25 | 21.21 | 18.10 | 34.63 | 37.46 | 84 | 180 | 336 | 198 | 54 | 25 | 252 |
| 8 | 87 | 22.5 | 58.60 | 29.80 | 58.60 | 122 | 87 | 28.67 | 24.12 | 28.17 | 24.04 | 20.41 | 39.40 | 42.70 | 96 | 202 | 376 | 215 | 62 | 28.17 | 278 |
| 9 | 96 | 25.5 | 65.25 | 33.63 | 65.25 | 136 | 96 | 32.33 | 27.13 | 31.33 | 26.87 | 22.72 | 44.17 | 47.94 | 108 | 224 | 416 | 232 | 70 | 31.33 | 304 |
| 10 | 105 | 28.5 | 71.91 | 37.46 | 71.91 | 150 | 105 | 36 | 30.15 | 34.50 | 29.70 | 25.03 | 48.94 | 53.18 | 120 | 246 | 456 | 249 | 78 | 34.50 | 330 |
| 11 | 114 | 31.5 | 78.57 | 41.28 | 78.57 | 164 | 114 | 39.67 | 33.17 | 37.67 | 32.53 | 27.34 | 53.71 | 58.43 | 132 | 268 | 496 | 266 | 86 | 37.67 | 356 |
| 12 | 123 | 34.5 | 85.23 | 45.11 | 85.23 | 178 | 123 | 43.33 | 36.18 | 40.83 | 35.36 | 29.65 | 58.48 | 63.67 | 144 | 290 | 536 | 283 | 94 | 40.83 | 382 |
| 13 | 132 | 37.5 | 91.88 | 48.94 | 91.88 | 192 | 132 | 47 | 39.20 | 44 | 38.18 | 31.96 | 63.25 | 68.91 | 156 | 312 | 576 | 300 | 102 | 44 | 408 |
| 14 | 141 | 40.5 | 98.54 | 52.77 | 98.54 | 206 | 141 | 50.67 | 42.21 | 47.17 | 41.01 | 34.26 | 68.03 | 74.15 | 168 | 334 | 616 | 317 | 110 | 47.17 | 434 |
| 15 | 150 | 43.5 | 105.2 | 56.60 | 105.2 | 220 | 150 | 54.33 | 45.23 | 50.33 | 43.84 | 36.57 | 72.80 | 79.40 | 180 | 356 | 656 | 334 | 118 | 50.33 | 460 |

**Respective entropy values**

| *h* | $\mathcal{R}$ $R_1$ | $\mathcal{R}$ $R_{-1}$ | $\mathcal{R}$ $R_{1/2}$ | $\mathcal{R}$ $R_{-1/2}$ | $\mathcal{R}$ IR | $\mathcal{R}$ $M_1$ | $\mathcal{R}$ $M_2$ | $\mathcal{R}$ HI | $\mathcal{R}$ SCI | $\mathcal{R}$ ISI | $\mathcal{R}$ ABC | $\mathcal{R}$ ABS | $\mathcal{R}$ GA | $\mathcal{R}$ AG | $\mathcal{R}$ SSD | $\mathcal{R}$ F | $\mathcal{R}$ $HM_1$ | $\mathcal{R}$ $HM_2$ | $\mathcal{R}$ $ReZG_1$ | $\mathcal{R}$ $ReZG_2$ | $\mathcal{R}$ $ReZG_3$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 2.95 | 2.95 | 3.02 | 3.02 | 3.02 | 3.02 | 2.95 | 3.02 | 3.04 | 3.02 | 2.89 | 2.89 | 3.04 | 3.04 | 3.04 | 2.98 | 2.97 | 2.73 | 3.02 | 3.02 | 2.86 |
| 5 | 3.17 | 3.17 | 3.24 | 3.24 | 3.24 | 3.24 | 3.17 | 3.23 | 3.25 | 3.23 | 3.09 | 3.09 | 3.26 | 3.26 | 3.25 | 3.19 | 3.18 | 2.94 | 3.24 | 3.23 | 3.08 |
| 6 | 3.35 | 3.35 | 3.41 | 3.41 | 3.41 | 3.41 | 3.35 | 3.41 | 3.43 | 3.41 | 3.26 | 3.25 | 3.43 | 3.43 | 3.43 | 3.37 | 3.36 | 3.12 | 3.41 | 3.41 | 3.26 |
| 7 | 3.50 | 3.50 | 3.56 | 3.56 | 3.56 | 3.56 | 3.50 | 3.56 | 3.58 | 3.56 | 3.40 | 3.40 | 3.58 | 3.58 | 3.58 | 3.52 | 3.51 | 3.27 | 3.56 | 3.56 | 3.42 |
| 8 | 3.64 | 3.64 | 3.69 | 3.69 | 3.69 | 3.70 | 3.64 | 3.69 | 3.71 | 3.69 | 3.53 | 3.52 | 3.71 | 3.71 | 3.71 | 3.65 | 3.65 | 3.41 | 3.70 | 3.69 | 3.55 |
| 9 | 3.76 | 3.76 | 3.81 | 3.81 | 3.81 | 3.81 | 3.76 | 3.81 | 3.82 | 3.81 | 3.64 | 3.63 | 3.83 | 3.83 | 3.82 | 3.77 | 3.76 | 3.53 | 3.81 | 3.81 | 3.67 |
| 10 | 3.86 | 3.86 | 3.91 | 3.91 | 3.91 | 3.91 | 3.86 | 3.91 | 3.93 | 3.91 | 3.74 | 3.73 | 3.93 | 3.93 | 3.93 | 3.87 | 3.87 | 3.65 | 3.92 | 3.91 | 3.78 |
| 11 | 3.96 | 3.96 | 4.01 | 4.01 | 4.01 | 4.01 | 3.96 | 4.01 | 4.02 | 4.01 | 3.83 | 3.83 | 4.02 | 4.03 | 4.02 | 3.97 | 3.96 | 3.75 | 4.01 | 4.01 | 3.88 |
| 12 | 4.05 | 4.04 | 4.09 | 4.09 | 4.09 | 4.09 | 4.05 | 4.09 | 4.11 | 4.09 | 3.91 | 3.91 | 4.11 | 4.11 | 4.11 | 4.05 | 4.05 | 3.84 | 4.10 | 4.09 | 3.97 |
| 13 | 4.13 | 4.12 | 4.17 | 4.17 | 4.17 | 4.17 | 4.13 | 4.17 | 4.19 | 4.17 | 3.99 | 3.99 | 4.19 | 4.19 | 4.19 | 4.13 | 4.13 | 3.93 | 4.18 | 4.17 | 4.05 |
| 14 | 4.20 | 4.20 | 4.25 | 4.25 | 4.25 | 4.25 | 4.20 | 4.24 | 4.26 | 4.25 | 4.06 | 4.06 | 4.26 | 4.26 | 4.26 | 4.21 | 4.20 | 4.01 | 4.25 | 4.25 | 4.13 |
| 15 | 4.27 | 4.27 | 4.32 | 4.32 | 4.32 | 4.32 | 4.27 | 4.31 | 4.33 | 4.32 | 4.13 | 4.13 | 4.33 | 4.33 | 4.33 | 4.27 | 4.27 | 4.08 | 4.32 | 4.32 | 4.20 |

## TABLE 4: REVERSE TOPOLOGICAL INDICES AND ITS ENTROPY OF HEXAGONAL CHAIN OF EQUAL SEGMENT LENGTH $(G_{n,l})$

| $n$ | $l$ | $\mathcal{R}$ $R_1$ | $\mathcal{R}$ $R_{1/2}$ | $\mathcal{R}$ $R_{-1/2}$ | $\mathcal{R}$ IR | $\mathcal{R}$ $M_1$ | $\mathcal{R}$ $M_2$ | $\mathcal{R}$ HI | $\mathcal{R}$ SCI | $\mathcal{R}$ ISI | $\mathcal{R}$ ABC | $\mathcal{R}$ ABS | $\mathcal{R}$ GA | $\mathcal{R}$ AG | $\mathcal{R}$ SSD | $\mathcal{R}$ F | $\mathcal{R}$ $HM_1$ | $\mathcal{R}$ $HM_2$ | $\mathcal{R}$ $ReZG_1$ | $\mathcal{R}$ $ReZG_2$ | $\mathcal{R}$ $ReZG_3$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 2 | 66 | 40.38 | 17.69 | 40.38 | 83 | 66 | 17.17 | 14.83 | 19.67 | 15.56 | 16.98 | 25.26 | 26.79 | 58.5 | 145 | 277 | 200 | 36.5 | 19.67 | 230 |
| 5 | 2 | 77 | 47.63 | 21.31 | 47.63 | 98 | 77 | 20.67 | 17.77 | 23.17 | 18.38 | 20.14 | 30.08 | 31.97 | 70 | 170 | 324 | 229 | 44 | 23.17 | 266 |
| 6 | 2 | 88 | 54.87 | 24.94 | 54.87 | 113 | 88 | 24.17 | 20.71 | 26.67 | 21.21 | 23.29 | 34.91 | 37.15 | 81.5 | 195 | 371 | 258 | 51.5 | 26.67 | 302 |
| 7 | 2 | 99 | 62.11 | 28.56 | 62.11 | 128 | 99 | 27.67 | 23.65 | 30.17 | 24.04 | 26.45 | 39.74 | 42.33 | 93 | 220 | 418 | 287 | 59 | 30.17 | 338 |
| 8 | 2 | 110 | 69.36 | 32.18 | 69.36 | 143 | 110 | 31.17 | 26.59 | 33.67 | 26.87 | 29.60 | 44.57 | 47.52 | 104.5 | 245 | 465 | 316 | 66.5 | 33.67 | 374 |
| 9 | 2 | 121 | 76.60 | 35.80 | 76.60 | 158 | 121 | 34.67 | 29.53 | 37.17 | 29.70 | 32.76 | 49.40 | 52.70 | 116 | 270 | 512 | 345 | 74 | 37.17 | 410 |
| 10 | 2 | 132 | 83.84 | 39.42 | 83.84 | 173 | 132 | 38.17 | 32.47 | 40.67 | 32.53 | 35.92 | 54.23 | 57.88 | 127.5 | 295 | 559 | 374 | 81.5 | 40.67 | 446 |
| 11 | 2 | 143 | 91.08 | 43.04 | 91.08 | 188 | 143 | 41.67 | 35.41 | 44.17 | 35.36 | 39.07 | 59.06 | 63.06 | 139 | 320 | 606 | 403 | 89 | 44.17 | 482 |
| 12 | 2 | 154 | 98.33 | 46.66 | 98.33 | 203 | 154 | 45.17 | 38.35 | 47.67 | 38.18 | 42.23 | 63.88 | 68.24 | 150.5 | 345 | 653 | 432 | 96.5 | 47.67 | 518 |
| 13 | 2 | 165 | 105.57 | 50.28 | 105.57 | 218 | 165 | 48.67 | 41.29 | 51.17 | 41.01 | 45.39 | 68.71 | 73.43 | 162 | 370 | 700 | 461 | 104 | 51 | 554 |
| 14 | 2 | 176 | 112.81 | 53.91 | 112.81 | 233 | 176 | 52.17 | 44.23 | 54.67 | 43.84 | 48.54 | 73.54 | 78.61 | 174 | 395 | 747 | 490 | 112 | 55 | 590 |
| 15 | 2 | 187 | 120.05 | 57.53 | 120.05 | 248 | 187 | 55.67 | 47.16 | 58.17 | 46.67 | 51.70 | 78.37 | 83.79 | 185 | 420 | 794 | 519 | 119 | 58 | 626 |
| **Respective entropy values** | | | | | | | | | | | | | | | | | | | | | |
| $n$ | l | $E\mathcal{R}$ $R_1$ | $E\mathcal{R}$ $R_{1/2}$ | $E\mathcal{R}$ $R_{-1/2}$ | $E\mathcal{R}$ IR | $E\mathcal{R}$ $M_1$ | $E\mathcal{R}$ $M_2$ | $E\mathcal{R}$ HI | $E\mathcal{R}$ SCI | $E\mathcal{R}$ ISI | $E\mathcal{R}$ ABC | $E\mathcal{R}$ ABS | $E\mathcal{R}$ GA | $E\mathcal{R}$ AG | $E\mathcal{R}$ SSD | $E\mathcal{R}$ F | $E\mathcal{R}$ $HM_1$ | $E\mathcal{R}$ $HM_2$ | $E\mathcal{R}$ $ReZG_1$ | $E\mathcal{R}$ $ReZG_2$ | $E\mathcal{R}$ $ReZG_3$ |
| 4 | 2 | 3.16 | 3.23 | 3.23 | 3.23 | 3.23 | 3.16 | 3.23 | 3.25 | 3.23 | 3.09 | 3.09 | 3.258 | 3.26 | 3.25 | 3.18 | 3.17 | 2.94 | 3.23 | 3.23 | 3.07 |
| 5 | 2 | 3.34 | 3.41 | 3.41 | 3.41 | 3.41 | 3.34 | 3.41 | 3.43 | 3.40 | 3.26 | 3.26 | 3.434 | 3.43 | 3.43 | 3.36 | 3.35 | 3.11 | 3.41 | 3.40 | 3.24 |
| 6 | 2 | 3.48 | 3.56 | 3.56 | 3.56 | 3.56 | 3.48 | 3.56 | 3.58 | 3.55 | 3.40 | 3.40 | 3.583 | 3.58 | 3.58 | 3.51 | 3.50 | 3.25 | 3.56 | 3.55 | 3.39 |
| 7 | 2 | 3.61 | 3.69 | 3.69 | 3.69 | 3.69 | 3.61 | 3.69 | 3.71 | 3.68 | 3.53 | 3.52 | 3.713 | 3.71 | 3.71 | 3.64 | 3.63 | 3.38 | 3.69 | 3.68 | 3.52 |
| 8 | 2 | 3.73 | 3.80 | 3.80 | 3.80 | 3.80 | 3.73 | 3.80 | 3.82 | 3.80 | 3.64 | 3.64 | 3.828 | 3.83 | 3.82 | 3.75 | 3.74 | 3.49 | 3.80 | 3.80 | 3.63 |
| 9 | 2 | 3.83 | 3.91 | 3.91 | 3.91 | 3.91 | 3.83 | 3.90 | 3.93 | 3.90 | 3.74 | 3.74 | 3.931 | 3.93 | 3.93 | 3.86 | 3.85 | 3.59 | 3.91 | 3.90 | 3.74 |
| 10 | 2 | 3.93 | 4.00 | 4.00 | 4.00 | 4.00 | 3.93 | 4.00 | 4.02 | 4.00 | 3.83 | 3.83 | 4.025 | 4.02 | 4.02 | 3.95 | 3.94 | 3.69 | 4.00 | 4.00 | 3.83 |
| 11 | 2 | 4.01 | 4.09 | 4.08 | 4.09 | 4.09 | 4.01 | 4.08 | 4.10 | 4.08 | 3.91 | 3.91 | 4.110 | 4.11 | 4.10 | 4.03 | 4.03 | 3.77 | 4.08 | 4.08 | 3.92 |
| 12 | 2 | 4.09 | 4.16 | 4.16 | 4.16 | 4.17 | 4.09 | 4.16 | 4.18 | 4.16 | 3.99 | 3.99 | 4.189 | 4.19 | 4.18 | 4.11 | 4.10 | 3.85 | 4.16 | 4.16 | 3.99 |
| 13 | 2 | 4.16 | 4.24 | 4.24 | 4.24 | 4.24 | 4.16 | 4.24 | 4.26 | 4.23 | 4.06 | 4.06 | 4.26 | 4.26 | 4.26 | 4.19 | 4.18 | 3.92 | 4.24 | 4.23 | 4.07 |
| 14 | 2 | 4.23 | 4.31 | 4.30 | 4.31 | 4.31 | 4.23 | 4.30 | 4.32 | 4.30 | 4.13 | 4.13 | 4.33 | 4.33 | 4.32 | 4.25 | 4.25 | 3.99 | 4.31 | 4.30 | 4.14 |
| 15 | 2 | 4.30 | 4.37 | 4.37 | 4.37 | 4.37 | 4.30 | 4.37 | 4.39 | 4.37 | 4.19 | 4.19 | 4.39 | 4.39 | 4.39 | 4.32 | 4.31 | 4.05 | 4.37 | 4.37 | 4.20 |

## TABLE 5: ENTROPY COMPARISON OF HEXAGONAL CHAINS FOR DIFFERENT VALUES OF *h*

| *h* | *G* | ℛ $R_1$ | ℛ $R_{-1}$ | ℛ $R_{1/2}$ | ℛ $R_{-1/2}$ | ℛ IR | ℛ $M_1$ | ℛ $M_2$ | ℛ HI | ℛ SCI | ℛ ISI | ℛ ABC | ℛ ABS | ℛ GA | ℛ AG | ℛ SSD | ℛ F | ℛ $HM_1$ | ℛ $HM_2$ | ℛ $ReZG_1$ | ℛ $ReZG_2$ | ℛ $ReZG_3$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 5 | $L_5$ | 3.17 | 3.17 | 3.24 | 3.24 | 3.24 | 3.24 | 3.17 | 3.23 | 3.25 | 3.23 | 3.09 | 3.09 | 3.26 | 3.26 | 3.25 | 3.19 | 3.18 | 2.94 | 3.24 | 3.23 | 3.08 |
| | $G_{4,2}$ | 3.16 | 3.14 | 3.23 | 3.23 | 3.23 | 3.23 | 3.16 | 3.23 | 3.25 | 3.23 | 3.09 | 3.09 | 3.26 | 3.26 | 3.25 | 3.18 | 3.17 | 2.94 | 3.23 | 3.23 | 3.07 |
| | $G_{2,3}$ | 3.17 | 3.16 | 3.23 | 3.23 | 3.23 | 3.24 | 3.17 | 3.23 | 3.25 | 3.23 | 3.09 | 3.09 | 3.26 | 3.26 | 3.25 | 3.19 | 3.18 | 2.93 | 3.23 | 3.23 | 3.07 |
| 6 | $L_6$ | 3.35 | 3.35 | 3.41 | 3.41 | 3.41 | 3.41 | 3.35 | 3.41 | 3.43 | 3.41 | 3.26 | 3.25 | 3.43 | 3.43 | 3.43 | 3.37 | 3.36 | 3.12 | 3.41 | 3.41 | 3.26 |
| | $G_{5,2}$ | 3.34 | 3.32 | 3.41 | 3.41 | 3.41 | 3.41 | 3.34 | 3.41 | 3.43 | 3.40 | 3.26 | 3.26 | 3.43 | 3.43 | 3.43 | 3.36 | 3.35 | 3.11 | 3.41 | 3.40 | 3.24 |
| 7 | $L_7$ | 3.50 | 3.50 | 3.56 | 3.56 | 3.56 | 3.56 | 3.50 | 3.56 | 3.58 | 3.56 | 3.40 | 3.40 | 3.58 | 3.58 | 3.58 | 3.52 | 3.51 | 3.27 | 3.56 | 3.56 | 3.42 |
| | $G_{4,2}$ | 3.48 | 3.47 | 3.56 | 3.56 | 3.56 | 3.56 | 3.48 | 3.56 | 3.58 | 3.55 | 3.40 | 3.40 | 3.58 | 3.58 | 3.58 | 3.51 | 3.50 | 3.25 | 3.56 | 3.55 | 3.39 |
| | $G_{3,3}$ | 3.49 | 3.49 | 3.56 | 3.56 | 3.56 | 3.56 | 3.49 | 3.56 | 3.58 | 3.56 | 3.40 | 3.40 | 3.58 | 3.58 | 3.58 | 3.51 | 3.51 | 3.25 | 3.56 | 3.56 | 3.40 |
| | $G_{2,4}$ | 3.50 | 3.50 | 3.56 | 3.56 | 3.56 | 3.56 | 3.50 | 3.56 | 3.58 | 3.56 | 3.40 | 3.40 | 3.58 | 3.58 | 3.58 | 3.52 | 3.51 | 3.26 | 3.56 | 3.56 | 3.41 |
| 8 | $L_8$ | 3.64 | 3.64 | 3.69 | 3.69 | 3.69 | 3.70 | 3.64 | 3.69 | 3.71 | 3.69 | 3.53 | 3.52 | 3.71 | 3.71 | 3.71 | 3.65 | 3.65 | 3.41 | 3.70 | 3.69 | 3.55 |
| | $G_{7,2}$ | 3.61 | 3.61 | 3.69 | 3.69 | 3.69 | 3.69 | 3.61 | 3.69 | 3.71 | 3.68 | 3.53 | 3.52 | 3.71 | 3.71 | 3.71 | 3.64 | 3.63 | 3.38 | 3.69 | 3.68 | 3.52 |
| 9 | $L_9$ | 3.76 | 3.76 | 3.81 | 3.81 | 3.81 | 3.81 | 3.76 | 3.81 | 3.82 | 3.81 | 3.64 | 3.63 | 3.83 | 3.83 | 3.82 | 3.77 | 3.76 | 3.53 | 3.81 | 3.81 | 3.67 |
| | $G_{8,2}$ | 3.73 | 3.72 | 3.80 | 3.80 | 3.80 | 3.80 | 3.73 | 3.80 | 3.82 | 3.80 | 3.64 | 3.64 | 3.83 | 3.83 | 3.82 | 3.75 | 3.74 | 3.49 | 3.80 | 3.80 | 3.63 |
| | $G_{4,3}$ | 3.74 | 3.74 | 3.81 | 3.81 | 3.81 | 3.81 | 3.74 | 3.80 | 3.82 | 3.80 | 3.64 | 3.64 | 3.83 | 3.83 | 3.82 | 3.76 | 3.75 | 3.50 | 3.81 | 3.80 | 3.65 |
| | $G_{2,5}$ | 3.75 | 3.75 | 3.81 | 3.81 | 3.81 | 3.81 | 3.75 | 3.81 | 3.82 | 3.81 | 3.64 | 3.64 | 3.83 | 3.83 | 3.82 | 3.76 | 3.76 | 3.52 | 3.81 | 3.81 | 3.66 |
| 10 | $L_{10}$ | 3.86 | 3.86 | 3.91 | 3.91 | 3.91 | 3.91 | 3.86 | 3.91 | 3.93 | 3.91 | 3.74 | 3.73 | 3.93 | 3.93 | 3.93 | 3.87 | 3.87 | 3.65 | 3.92 | 3.91 | 3.78 |
| | $G_{9,2}$ | 3.83 | 3.83 | 3.91 | 3.91 | 3.91 | 3.91 | 3.83 | 3.90 | 3.93 | 3.90 | 3.74 | 3.74 | 3.93 | 3.93 | 3.93 | 3.86 | 3.85 | 3.59 | 3.91 | 3.90 | 3.74 |
| | $G_{3,4}$ | 3.85 | 3.85 | 3.91 | 3.91 | 3.91 | 3.91 | 3.85 | 3.91 | 3.93 | 3.91 | 3.74 | 3.74 | 3.93 | 3.93 | 3.93 | 3.87 | 3.86 | 3.62 | 3.91 | 3.91 | 3.76 |
| 11 | $L_{11}$ | 3.96 | 3.96 | 4.01 | 4.01 | 4.01 | 4.01 | 3.96 | 4.01 | 4.02 | 4.01 | 3.83 | 3.83 | 4.02 | 4.03 | 4.02 | 3.97 | 3.96 | 3.75 | 4.01 | 4.01 | 3.88 |
| | $G_{10,2}$ | 3.93 | 3.92 | 4.00 | 4.00 | 4.00 | 4.00 | 3.93 | 4.00 | 4.02 | 4.00 | 3.83 | 3.83 | 4.02 | 4.02 | 4.02 | 3.95 | 3.94 | 3.69 | 4.00 | 4.00 | 3.83 |
| | $G_{5,3}$ | 3.94 | 3.94 | 4.00 | 4.00 | 4.00 | 4.01 | 3.94 | 4.00 | 4.02 | 4.00 | 3.83 | 3.83 | 4.02 | 4.02 | 4.02 | 3.96 | 3.95 | 3.70 | 4.01 | 4.00 | 3.85 |
| | $G_{2,6}$ | 3.95 | 3.95 | 4.01 | 4.01 | 4.01 | 4.01 | 3.95 | 4.00 | 4.02 | 4.01 | 3.83 | 3.83 | 4.02 | 4.02 | 4.02 | 3.96 | 3.96 | 3.73 | 4.01 | 4.01 | 3.87 |

The following two figures Figure 2(a), 2(b) show the behavior of reverse topological indices of linear poly-acene ($L_h$), hexagonal chain with *n* segments of length *2* ($G_{n,2}$) respectively with respect to their entropy values.

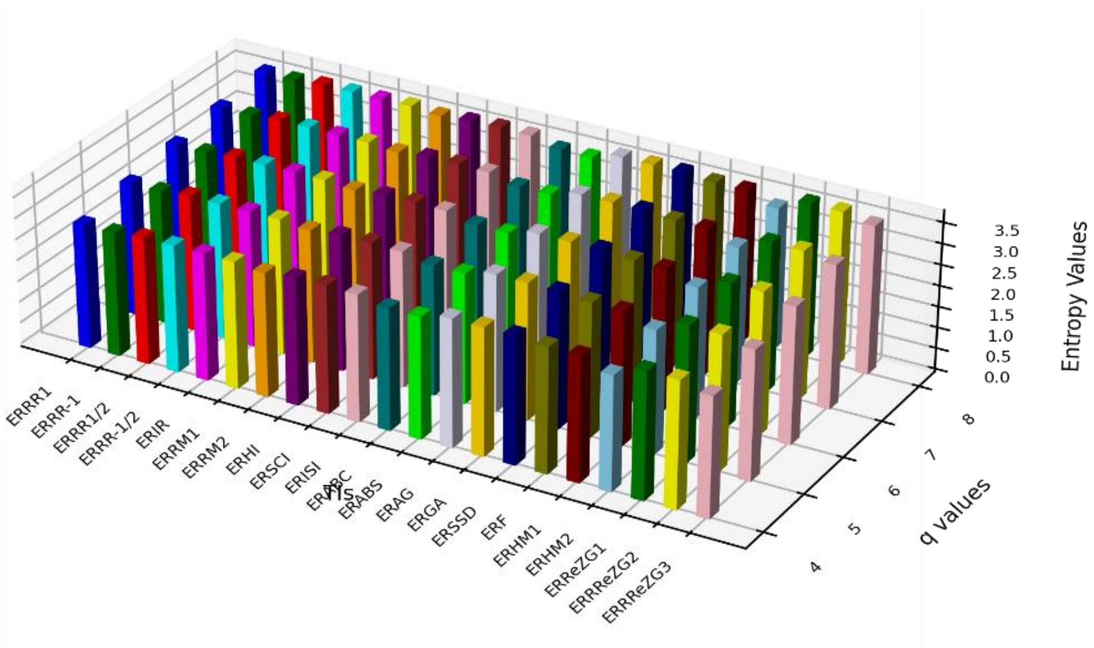



**Fig 2(a)**: Entropy based on reverse TIs for $L_h$

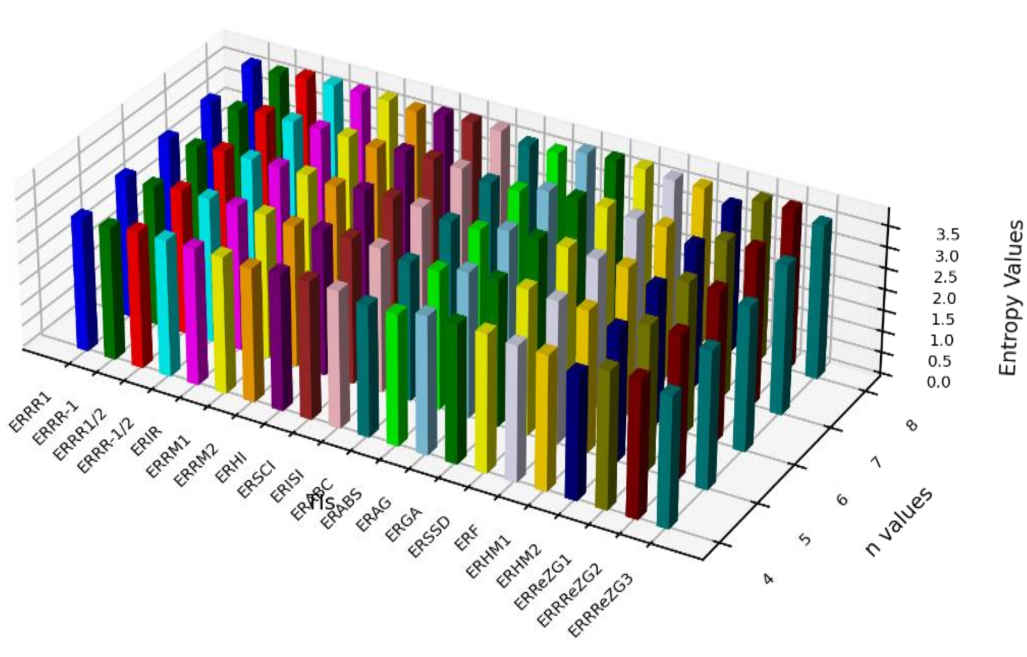



**Fig 2(b):** Entropy based on reverse TIs for $G_{n,2}$

Entropies of a hexagonal chain with $n$ segments of length $l$ and a linear poly-acene have been compared for specific values of $h$, which are listed in TABLE 5. And the comparison of these plots is are shown in Figure 3(a), 3(b).

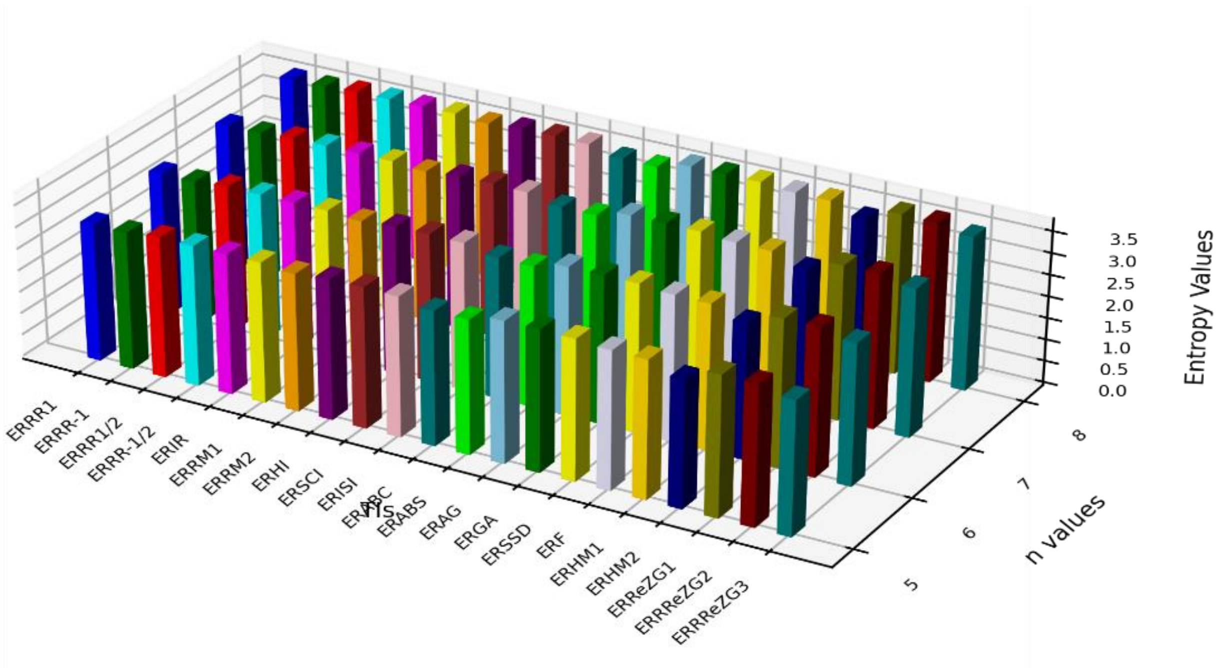



**Fig 3 (a):** Entropy of $G_{n,l}$ for different values of $h$

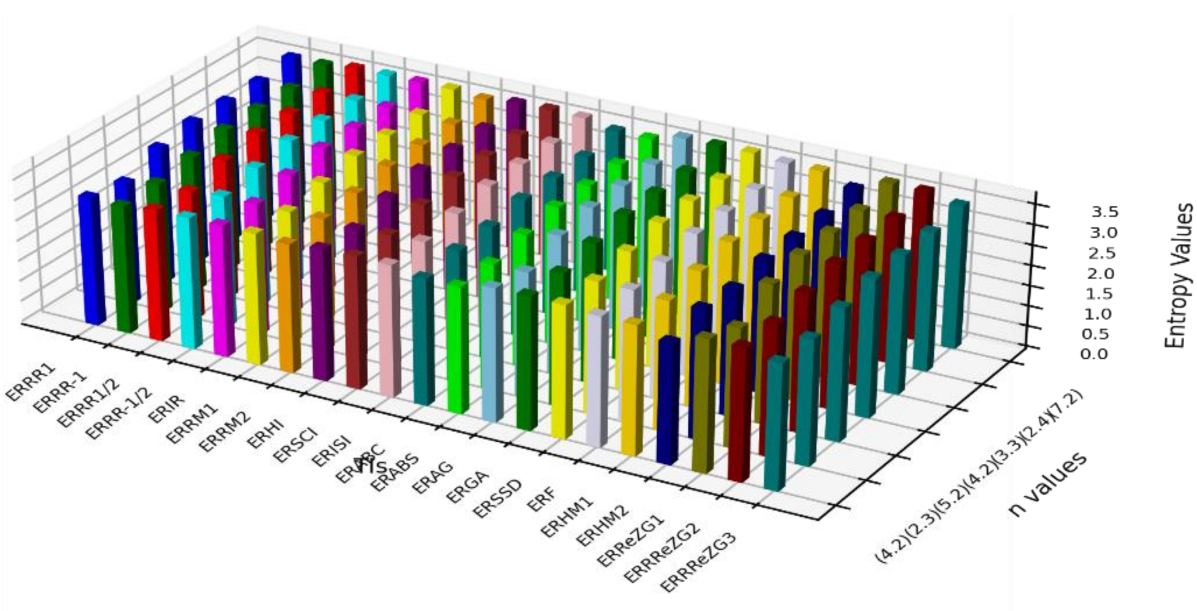



**Fig 3 (b):** Entropy of $L_h$ for different values of $h$

## 4. Conclusion

As various topological indices help in investigating properties of chemical molecules, in this paper, we have computed generalized expressions for reverse degree based topological indices, namely the reverse Randićindex, reverse geometric arithmetic index, reverse Zagreb indices, reverse forgotten index, reverse arithmetic geometric index, reverse symmetric division degree index, reverse atom bond sum connectivity index, reverse hyper Zagreb indices, reverse redefined Zagreb indices of two structures of benzenoid hydrocarbon chains, namely linear poly-acene $L_h$and hexagonal chain of equal segment length $G_{n,l}$. Information-theoretic entropy measurement is obtained by these generalised analytical formulations of linear poly-acene $L_h$ and hexagonal chain of segment length $l$ ($G_{n,l}$) for any arbitrary values of $h$. We have compared the entropies of two different structure $L_h$ and $G_{n,l}$, for specific values of $h$ and we have seen that their entropies show very little variation., implying that the structural transition between the above considered structure results in small change of disorder. Reverse degree based topological indices and entropies of these benzenoid hydrocarbon chains find applications in thermodynamic modelling/ process optimization, predicting the spontaneity of chemical reactions, helps in assessing the efficiency of combustion process, phase transitions, etc. They also, help in predicting Quantitative Structural Activity Properties, Chemo-informatics, Material Science, Chemical reactivity, Machine learning etc. in chemistry. Our findings in this paper, provide a very helpful contribution in developing QSAR/QSPR analysis.

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## Conflicts of Interest

The authors declare no conflict of interest

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