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EVALUATION OF WEIGHTED ENTROPIES BASED ON TOPOLOGICAL INDICES FOR POLY PROPYL ETHER IMINE DENDRIMERS

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Abstract

Dendrimers play a vital role in discovering drugs against the diseases such as Alzheimer's, HIV, and cancer. Because of their outstanding physical and chemical properties and a wide range of intriguing applications in numerous fields, dendrimers hold a prominent role in research. This paper introduces a variant of entropy measures based on distance-based topological indices for Poly Propyl ether imine (PETIM) dendrimers (PDL-Gn). A considerable spectrum of calculating entropies is accessible, among which entropies calculated based on topological indices are generally purposed in QSPR/QSAR studies. These entropies, along with topological indices, indicate different structural properties. In this manuscript, we compute the First (a, b) KA Index, Sombor Index, Modified Sombor Index, Reduced Sombor Index, Reduced modified Sombor Index, Reduced 1st (a, b) KA Index, Reduced 2nd (a, b) KA Index for PDG-G. Lately, We compute weighted entropies of PDL Gn based on some topological indices such as First Zagreb index, Second Zagreb index, Modified second Zagreb index, Augmented Zagreb Index, Hyper Zagreb 2nd Index, Redefined 1st Zagreb Index, Redefined 2nd Zagreb Index and Redefined 3rd Zagreb Index. Moreover, we presented our computed results numerically and graphically, leading to our contribution's good importance.

Keywords: *Entropy, First Zagreb Index, Second Zagreb Index, Modified Second Zagreb Index, Augmented Zagreb Index, Hyper Zagreb 2nd Index, Redefined 1st Zagreb Index, Redefined 2nd Zagreb Index, Redefined 3rd Zagreb Index, Weighted Entropies of PDL Gn, First (a, b) KA Index, Sombor Index, Modified Sombor Index, Reduced Sombor Index, Reduced Modified Sombor Index, Reduced 1st (a, b) KA Index, Reduced 2nd (a, b) KA Index for PDG-G, Dendrimers, PDL-Gn, PETIM Dendrimers.*

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1. Introduction

Graph theory was the first time it started when Leonhard Euler solved the seven-bridge problem. Leonhard Euler solved seven bridge problems in 1735. Graph theory is an important branch of applied mathematics that deals with graphs and structure. Any object that has connections and points is called a graph. If all connections are unidirectional, this type of graph is known as a digraph or directed graph. Graph Theory is used in different fields of life. For example, in computer science, graphs are used to construct and show a network of communication, computational devices, data organization, and the flow ofcomputation. It is also used to study the properties of molecules in chemistry, physics, and biology. In this chapter, we will discuss the basic definitions of Graph Theory [1]. An important branch of graph theory is Chemical Graph Theory. It deals with graphs related to chemistry. Here we also discuss the Topological indices and how to use them on Dendrimers. Our structure is related to $PDL\text{-}G_n$ Dendrimer.

In mathematics, graph theory means the study of graphs. In discrete mathematics, graphs are the major objects to study. In graph theory, a graph is denoted as vertices (nodes) attached by edges (lines). Graphs are mathematical structures that are used to investigate pairwise relations between objects. Their use is found in road map constellations when constructing schemes and drawings. To make modern communication and technological processes possible, we can use Graphsunderlie many computer programs. They donate to the development of thinking, both abstract and logical. For example, a famous game like connecting the dots on a piece of paper to make a figure, a cat, or a dog, those connections are also graphs.

Dendrimers are repetitively branched molecules [15, 30-44]. The word dendrimer drive from the word dendron, which means tree. Fritz Vogtle introduced the first dendrimer in 1978. Dendrimers are small-sized, symmetric, radially molecules. Dendrimers are monoids-persing, homogeneous and well-defined structures; Dendrimers consist of tree-like branches or arms[16].

Generally, Dendrimers have three elements that are

(i) a core
(ii) Branched Dendron's and
(iii) Terminal group [17].

A core is the main part of Dendrimers.

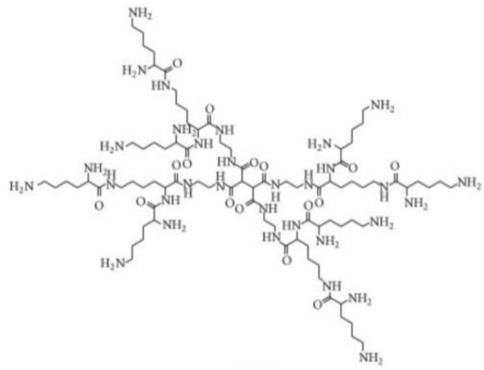

Figure 1: $PDL\text{-}G_n$ Dendrimer

Graph Theoretical (GT) applications in chemistry have recently undergone a dramatic revival. By using methods of statistics, graph theory, and set theory, its efforts to recognize structural types intricate in structure assets activity connection. In the half of the eighteenth century, Molecular graphs were introduced. The molecular graph represents the structural formula of a chemical compound; covalent bonds are described by lines (edges), and atoms depict by points (vertices). In the main branches of chemistry, we can use chemical graphs for a different aim. Correspondingly, a transform of the molecule can be envisioned by a reaction graph, whose edges (lines), reaction pathways, and vertices (nodes) are chemical species.

In 1988, around 500 articles were produced annually by several researchers, each on chemical graph theory. The most important topic in a large variety of articles was chemical indices in graph theory, which have their basis in the field of chemistry, and graph theory leads to results that chemists use. Some famous chemical indices are the first and second Zagreb index, multiplicative Zagreb indices, Wiener index, general hyper-Wiener index, Randic index, harmonic index, sum-connectivity index, general Randic index, general sum connectivity index, etc. [18-21]. Theoretical chemists recognized useful information in the middle of the last century about several things of organic material on molecular structure. These molecular structures can be found by observing appropriately created invariants of the fundamental molecular graph. Topological indices are defined as Graph invariants beneficial for chemical determinations. Many topological indices are important for Numerical structure-property relation, QSPR, and quantitative structure-activity relation, QSAR [22-29]. Property means some physical or chemical property, and structure means molecular structure.

Topological indices are real numbers for any graph of compounds and graph networks. The topological index is used to predict the properties of interesting compounds and remains invariant. In the field of hem informatics, if we want to study compounds' properties and chemical bioactivity, we need to utilize the quantitative structure-property relationship and structure-activity relationship, together with topological indices. In network theory, polynomials also support many applications like topological indices; for example, the Wiener polynomial or Hosoya polynomial [2] helps create distance-dependent topological indices. For deciding degree-dependent topological indices, the M-polynomial was introduced previously. "The valence and degreeare closely related in chemistry [3]. We can make a precise whole story that the topological index worked as a function that assigns each molecular structure to real number. Since the 1970s, the First and second Zagreb indices are degree-based graph invariants studied widely. Different types of graph indices are discussed below.

Definition 1.1. The First Zagreb index [4] is defined as

$$M_1(G) = \sum_{xy \in E(G)} (d_x + d_y)$$

Definition 1.2. The Second Zagreb index [4] is represented by $M_2(G)$ and it's defined as

$$M_2(G) = \sum_{xy \in E(G)} (d_x d_y)$$

Definition 1.3. The modified second Zagreb index [5] is denoted by $^{m}M_2(G)$ and is defined as

$$Modified\ M_2(G) = \sum_{xy \in E(G)} \frac{1}{d_x d_y}$$

Definition 1.4. The augmented Zagreb Index is represented by $AZI(G)$[6] and is defined as

$$AZI(G) = \sum_{xy \in E(G)} \left(\frac{d_x d_y}{d_x + d_y - 2} \right)^3$$

Definition 1.5. Hyper Zagreb 2nd Index [7] is denoted by $H_2(G)$ and its defined as

$$H_2(G) = \sum_{xy \in E(G)} (d_x d_y)^2$$

Definition 1.6. Redefined 1st zagreb Index [8] is denoted by $ReZG_1(G)$ and its defined as

$$ReZ\ G_1(G) = \sum_{xy \in E(G)} \frac{d_x + d_y}{d_x d_y}$$

Definition 1.7. Redefined 2nd Zagreb Index [9] is denoted by $ReZG_2(G)$ and it's defined as

$$ReZ\ G_2(G) = \sum_{xy \in E(G)} \frac{d_x d_y}{d_x + d_y}$$

Definition 1.8. Redefined 3rd Zagreb Index [9] is denoted by $ReZG_3(G)$ and it's defined as

$$ReZ\ G_3(G) = \sum_{xy \in E(G)} \left((d_x d_y)(d_x + d_y) \right)$$

Where d_x and d_y are the degree of vertices x and y, respectively, here, x and y are adjacentvertices.

Definition 1.9. Suppose that we have a probability density function

$$P_{ij} = \frac{w(xy)}{\sum W(xy)}$$

Then entropy[13] for any graph G is defined as

$$I(G,w) = -\sum P_{ij}\log(P_{ij})$$

Definition 1.10. The first (a,b)-*KA* Index is introduced in [10] and defined as

$$KA^1_{(a,b)}(G) = \sum_{xy\in E(G)} [d_G(x)^a + d_G(y)^a]^b$$

Where $a,b\in\mathbf{R}$ are chosen suitably.

Definition 1.11. The Sombor Index is introduced in [11] and defined as

$$SO(G) = \sum_{xy\in E(G)} \sqrt{d_G(x)^2 + d_G(y)^2}$$

If in First (a,b)-*KA* Index, we take value $a = 2$ and $b = \frac{1}{2}$ then we get sombor index.

Definition 1.12. We define the modified sombor Index as ${}^{m}SO(G)$ [12] for a graph G as

$$Modified\ SO(G) = \sum_{xy\in E(G)} \frac{1}{\sqrt{d_G(x)^2 + d_G(y)^2}}$$

Definition 1.13. We define the reduced sombor Index [12] for a graph G as

$$RSO(G) = \sum_{xy\in E(G)} \sqrt{(d_G(x)-1)^2 + (d_G(y)-1)^2}$$

Definition 1.14. We define the reduced modified sombor Index for a graph G as

$$Modified\ RSO(G) = \sum_{xy\in E(G)} \frac{1}{\sqrt{(d_G(x)-1)^2 + (d_G(y)-1)^2}}$$

Definition 1.15. We define Reduced 1st (a,b)-*KA* Index for a graph G as

$$RKA^1_{(a,b)}(G) = \sum_{xy\in E(G)} [(d_G(x)-1)^a + (d_G(y)-1)^a]^b$$

Definition 1.16. We define the Reduced 2nd (a,b)-*KA* Index for a graph G as

$$RKA^2_{(a,b)}(G) = \sum_{xy\in E(G)} [(d_G(x)-1)^a (d_G(y)-1)^a]^b$$

Table 1: Edge Partition of $PDL - G_n$

(d_s, d_t)	Frequency	Set of Edges
(1,2)	2^{n+1}	E_1
(2,2)	$7(2^{n+1}) - 4$	E_2
(2,3)	$5(2^{n+1}) - 8$	E_3
(3,3)	$2(2^{n+1}) + 1$	E_4
(1,3)	$3(2^{n+1})$	E_5

The general result for PDL-G_n are given in below.

2. Main Results

Theorem 1. The weighted entropy of PDL-G_n with the first Zagrab Index is

$$I(PDL - G_n, M_1) = \log[5(2^{n+5} - 10)] - \frac{1}{5(2^{n+5} - 10)}[(40.10110863435)2^{n+1} - 32.92285253239]$$

Proof. By definition, 1.1. We have

$$M_1(PDG - G_n) = 5(2^{n+5} - 10)$$

By definition, 1.9. We have

$$I(PDG-G_n,M_1)=\log[5(2^{n+5}-10)]-\frac{1}{5(2^{n+5}-10)}\begin{bmatrix}(1+2)|E_1|\log(1+2)+(2+2)|E_2|\log(2+2)+\\(2\ +\ 3)|E_3|\log(2+3)+(3+3)|E_4|\log(3+3)+\\(1+3)|E_5|\log(1+3)\end{bmatrix}$$

$$I(PDG-G_n,M_1)=\log[5(2^{n+5}-10)]-\frac{1}{5(2^{n+5}-10)}[3|E_1|\log 3+4|E_2|\log4+5||E_3|\log5\ +6|E_4|\log6+4|E_5|\log4]$$

$$I(PDG-G_n,M_1)=\log[5(2^{n+5}-10)]-\frac{1}{5(2^{n+5}-10)}\begin{bmatrix}\log2(68.2^{n+1}-26)+\ \log3(15.2^{n+1}\ +6)+\\\log5(25.2^{n+1}-40)\end{bmatrix}$$

$$I(PDL-G_n,M_1)=\log[5(2^{n+5}-10)]-\frac{1}{5(2^{n+5}-10)}[(40.10110863435)2^{n+1}-32.92285253239]$$

Theorem 2. The weighted entropy of PDL-G_n with the second Zagreb Index is

$$I(PDL-G_n,M_2)=\log[11(7.2^{n+1}-5)]-\frac{1}{[11(7.2^{n+1}-5)]}[62.27473372241)2^{n+1}-126.00410622224]$$

Proof. By definition 1.2, we have

$$M_2(PDG-G_n)=[11(7.2^{n+1}-5)]$$

By definition 1.9, we have

$$I(PDG-G_n,M_2)=\log[11(7.2^{n+1}-5)]-\frac{1}{[11(7.2^{n+1}-5)]}[(1.2)|E_1|\log(1.2)+(2.2)|E_2|\log(2.2)$$
$$+(2.3)|E_3|\log(2.3)\ +(3.3)|E_4|\log(3.3)+(1.3)|E_5|\log(1.3)]$$

$$I(PDG-G_n,M_2)=\log[11(7.2^{n+1}-5)]-\frac{1}{[11(7.2^{n+1}-5)]}[2|E_1|\log\ 2+8|E_2|\log2+6|E_3|\log6\ +18|E_4|\log3+3|E_5|\log3]$$

$$I(PDG-G_n,M_2)=\log[11(7.2^{n+1}-5)]-\frac{1}{[11(7.2^{n+1}-5)]}[\ \log2(88.2^{n+1}-80)\ +\ \log3(75.2^{n+1}\ +18)$$

$$I(PDL-G_n,M_2)=\log[11(7.2^{n+1}-5)]-\frac{1}{[11(7.2^{n+1}-5)]}[62.27473372241)2^{n+1}-126.00410622224]$$

Theorem 3. The entropy of PDL-G_n with modified 2nd Zagreb weight is

$$\mathrm{I}\ (\mathrm{PDL}\text{-}G_n,{}^{m}M_2)=\log\left[\frac{1}{18}(155.2^n-40)\right]-\frac{18}{(155.2^n-40)}[2.27389571589)2^n-1.53356804778]$$

Proof. By definition 1.3, we have

$${}^{m}\mathrm{M}_2(PDG-G_n)=\frac{1}{18}(155.2^n-40)$$

By definition 1.9, we have

$$\mathrm{I}\ (\mathrm{PDL}\text{-}G_n,{}^{m}M_2)=\log\left[\frac{1}{18}(155.2^n-40)\right]-\frac{18}{(155.2^n-40)}\left[\frac{1}{1.2}|E_1|log\frac{1}{1.2}+\frac{1}{2.2}|E_2|log\frac{1}{2.2}+\frac{1}{2.3}|E_3|log\frac{1}{2.3}+\right.$$
$$\left.\frac{1}{3.3}|E_4|log\frac{1}{3.3}+\frac{1}{1.3}|E_5|log\frac{1}{1.3}\right]$$

$$\mathrm{I}\ (\mathrm{PDL}\text{-}G_n,{}^{m}M_2)=\log\left[\frac{1}{18}(155.2^n-40)\right]-\frac{18}{(155.2^n-40)}\left[\frac{1}{2}|E_1|log2+\frac{1}{2}|E_2|log2+\frac{1}{6}|E_3|log2+\right.$$
$$\left.\frac{1}{6}|E_3|log3+\ \frac{2}{9}|E_4|log3+\frac{1}{3}|E_3|log3\right]$$

$$\mathrm{I}\ (\mathrm{PDL}\text{-}G_n,{}^{m}M_2)=\log\left[\frac{1}{18}(155.2^n-40)\right]-\frac{18}{(155.2^n-40)}\left[\left(\frac{29.2^n-10}{3}\right)log2+\left(\frac{41.2^n-10}{9}\right)log3\right]$$

$$\mathrm{I}\ (\mathrm{PDL}\text{-}G_n,{}^{m}M_2)=\log\left[\frac{1}{18}(155.2^n-40)\right]-\frac{18}{(155.2^n-40)}[2.27389571589)2^n-1.53356804778]$$

Theorem 4. *The* entropy *of PDL-Gn with Augmented Zagreb weight is*

$$I(PDL-G_n,AZI)=\log(17524.2^n-5415)-\frac{1}{17524.2^n-5415}[(246.697209).2^n-72.182125]$$

Proof. By definition 1.4, we have

$$AZI(G_n)=(17524.2^n-5415)$$

By definition 1.9, we have

$$I(PDL-G_n,AZI) = log(17524.2^n-5415)-\frac{1}{17524.2^n-5415}\begin{bmatrix} \left(\frac{1.2}{1+2-2}\right)^3 |E_1| log\left(\frac{1.2}{1+2-2}\right)^3 + \\ \left(\frac{2.2}{2+2-2}\right)^3 |E_2| log\left(\frac{2.2}{2+2-2}\right)^3 \\ +\left(\frac{2.3}{2+3-2}\right)^3 |E_3| log\left(\frac{2.3}{2+3-2}\right)^3 + \\ \left(\frac{3.3}{3+3-2}\right)^3 |E_4| log\left(\frac{3.3}{3+3-2}\right)^3 \\ +\left(\frac{1.3}{1+3-2}\right)^3 |E_5| log\left(\frac{1.3}{1+3-2}\right)^3 \end{bmatrix}$$

$$I(PDL-G_n,AZI) = log(17524.2^n-5415)-\frac{1}{17524.2^n-5415}\begin{bmatrix} 24|E_1|log2+24|E_2|log2+24|E_3|log2+ \\ \frac{4374}{64}|E_4|log3-\frac{4374}{64}|E_4|log2 + \\ \frac{81}{8}|E_5|log3-\frac{81}{8}|E_5|log2 \end{bmatrix}$$

$$I(PDL-G_n,AZI) = log(17524.2^n-5415)-\frac{1}{17524.2^n-5415}\begin{bmatrix} \begin{pmatrix} 48.2^n+336.2^n-96+240.2^n- \\ 192-(273.375).2^n \end{pmatrix} log2+ \\ log3((273.375).2^n+ \\ (60.75)2^n+68.34375) \end{bmatrix}$$

$$I(PDL-G_n,AZI) = log(17524.2^n-5415)-\frac{1}{17524.2^n-5415}[(246.697209).2^n-72.182125]$$

Theorem 5. *The entropy of PDL-Gn with hyper Zagrab second weight is*

$$I(PDL-G_n,H_2) = \log\big((934)2^n-271\big)-\frac{1}{(934)2^n-271}[(370.6915125879)-(1504.68649794818)2^n]$$

Proof*. By definition 1.5, we have*

$$H_2(G_n) = (934)2^n-271$$

By definition 1.9, we have

$$I(PDL-G_n,H_2) = log\big((934)2^n-271\big)-\frac{1}{(934)2^n-271}\begin{bmatrix} (1.2)^2|E_1|log(1.2)^2+(2.2)^2|E_2|log(2.2)^2+ \\ (2.3)^2|E_3|log(2.3)^3 \\ +(3.3)^2|E_4|log(3.3)^2+ \\ (1.3)^2|E_5|log(1.3)^2 \end{bmatrix}$$

$$I(PDL-G_n,H_2) = log\big((934)2^n-271\big)-\frac{1}{(934)2^n-271}\begin{bmatrix} 8|E_1|log2-64|E_2|log2- \\ 72|E_3|log3-72|E_3|log2 \\ -384|E_4|log3-18|E_5|log3 \end{bmatrix}$$

$$I(PDL-G_n,H_2) = log\big((934)2^n-271\big)-\frac{1}{(934)2^n-271}\begin{bmatrix} -log2(8|E_1|+64|E_2|+72|E_3|)- \\ log3(72|E_3|+384|E_4|+18|E_5|) \end{bmatrix}$$

$$I(PDL-G_n,H_2) = log\big((934)2^n-271\big)-\frac{1}{(934)2^n-271}[-log2(1631.2^n-832)-log3(2124.2^n-252)]$$

$$I(PDL-G_n,H_2) = log\big((934)2^n-271\big)-\frac{1}{(934)2^n-271}[(370.6915125879)-(1504.68649794818)2^n]$$

Theorem 6. *The* entropy *of PDL-Gn with redefined first Zagreb weight is*

$$I(PDL-G_n,ReZ(G_1)) = \log(108.2^n-30)-\frac{1}{108.2^n-30}[(3.59128916574)-(3.57764719384)2^n]$$

Proof. By definition1.6,we have

$$ReZ(G_1) = 108.2^n-30$$

By definition 1.9, we have

$$I(PDL-G_n,ReZ(G_1)) = \log(108.2^n-30)-\frac{1}{108.2^n-30}\begin{bmatrix} \frac{1+2}{1.2}|E_1|log\frac{1+2}{1.2}+\frac{2+2}{2.2}|E_2|log\frac{2+2}{2.2}+ \\ \frac{2+3}{2.3}|E_3|log\frac{2+3}{2.3}+\frac{3+3}{3.3}|E_4|log\frac{3+3}{3.3}+ \\ \frac{1+3}{1.3}|E_5|log\frac{1+3}{1.3} \end{bmatrix}$$

$$I(PDL-G_n,ReZ(G_1))=\log(108.2^n-30)-\frac{1}{108.2^n-30}\begin{bmatrix}\frac{3}{2}|E_1|log3-\frac{3}{2}|E_1|log2+\frac{5}{6}|E_3|log5-\frac{5}{6}|E_3|log2- \\ \frac{5}{6}|E_3|log3+\frac{2}{3}|E_4|log2-\frac{2}{3}|E_4|log3+\frac{8}{3}|E_5|log2 \\ -\frac{4}{3}|E_5|log3\end{bmatrix}$$

$$I(PDL-G_n,ReZ(G_1))=\log(108.2^n-30)-\frac{1}{108.2^n-30}\begin{bmatrix}log2\left(-\frac{3}{2}|E_1|-\frac{5}{6}|E_3|+\frac{2}{3}|E_4|+\frac{8}{3}|E_5|\right)+ \\ log3\left(\frac{3}{2}|E_1|-\frac{5}{6}|E_3|-\frac{2}{3}|E_4|-\frac{4}{3}|E_5|\right)+log5(\frac{5}{6}|E_3|)\end{bmatrix}$$

$$I(PDL-G_n,ReZ(G_1))=\log(108.2^n-30)-\frac{1}{108.2^n-30}\begin{bmatrix}log2\left(\frac{22}{3}2^n+\frac{22}{3}\right)+log3\left(\frac{-73}{3}2^n+\frac{38}{3}\right)+ \\ log5(\frac{25}{3}2^n-\frac{20}{3})\end{bmatrix}$$

$$I(PDL-G_n,ReZ(G_1))=\log(108.2^n-30)-\frac{1}{108.2^n-30}[(3.59128916574)-(3.57764719384)2^n]$$

Theorem 7. *The entropy of PDL-Gn with redefined second zagrab weight is*

$$I(PDL-G_n,ReZ(G_2))=\log\left(\frac{105}{6}2^n-\frac{121}{10}\right)-\frac{1}{\left(\frac{105}{6}2^n-\frac{121}{10}\right)}[(3.356755493)2^n-0.49600307347]$$

Proof. By definition 1.7, we have

$$ReZ(G_2)=\frac{105}{6}2^n-\frac{121}{10}$$

By definition 1.9, we have

$$I(PDL-G_n,ReZ(G_2))=\log\left(\frac{105}{6}2^n-\frac{121}{10}\right)-\frac{1}{\left(\frac{105}{6}2^n-\frac{121}{10}\right)}\begin{bmatrix}\frac{1.2}{1+2}|E_1|log\frac{1.2}{1+2}+\frac{2.2}{2+2}|E_2|log\frac{2.2}{2+2}+ \\ \frac{2.3}{2+3}|E_3|log\frac{2.3}{2+3}+\frac{3.3}{3+3}|E_4|log\frac{3.3}{3+3}+\frac{1.3}{1+3}|E_5|log\frac{1.3}{1+3}\end{bmatrix}$$

$$I(PDL-G_n,ReZ(G_2))=\log\left(\frac{105}{6}2^n-\frac{121}{10}\right)-\frac{1}{\left(\frac{105}{6}2^n-\frac{121}{10}\right)}\begin{bmatrix}\frac{2}{3}|E_1|log2-\frac{2}{3}|E_1|log+\frac{6}{5}|E_3|log2+ \\ \frac{6}{5}|E_3|log3-\frac{6}{5}|E_3|log5+\frac{3}{2}|E_4|log3- \\ \frac{3}{2}|E_4|log2+\frac{3}{4}|E_5|log3-\frac{3}{2}|E_5|log2\end{bmatrix}$$

$$I(PDL-G_n,ReZ(G_2))=\log\left(\frac{105}{6}2^n-\frac{121}{10}\right)-\frac{1}{\left(\frac{105}{6}2^n-\frac{121}{10}\right)}\begin{bmatrix}log2\left(\frac{2}{3}|E_1|+\frac{6}{5}|E_3|-\frac{3}{2}|E_4|-\frac{3}{2}|E_5|\right)+ \\ log3\left(-\frac{2}{3}|E_1|+\frac{6}{5}|E_3|+\frac{3}{2}|E_4|+\frac{3}{4}|E_5|\right)+log5(-\frac{6}{5}|E_3|)\end{bmatrix}$$

$$I(PDL-G_n,ReZ(G_2))=\log\left(\frac{105}{6}2^n-\frac{121}{10}\right)-\frac{1}{\left(\frac{105}{6}2^n-\frac{121}{10}\right)}\left[log2\left(\frac{-5}{3}2^n-\frac{111}{10}\right)+log3\left(\frac{77}{3}2^n-\frac{81}{10}\right)+log5(-12.2^n+\frac{48}{5})\right]$$

$$I(PDL-G_n,ReZ(G_2))=\log\left(\frac{105}{6}2^n-\frac{121}{10}\right)-\frac{1}{\left(\frac{105}{6}2^n-\frac{121}{10}\right)}[(3.356755493)2^n-0.49600307347]$$

Theorem 8. *The* entropy *of PDL-Gn with redefined third zagrab weight is*

$$I(PDL-G_n,ReZ(G_3))=\log(824.2^n-254)-\frac{1}{(824.2^n-254)}[(1174.09516937262)2^n-338.02351699226]$$

Proof. By definition 1.8, we have

$$ReZ(G_3)=(824.2^n-254)$$

By definition 1.9, we have

$$I(PDG-G_n,ReZ(G_3))=\log[824.2^n-254]-\frac{1}{[824.2^n-254]}\begin{bmatrix}(1.2)(1+2)|E_1|\log(1.2)(1+2)+ \\ (2.2)(2+2)|E_2|\log(2.2)(2+2)+ \\ (2.3)(2+3)|E_3|\log(2.3)(2+3)+ \\ (3.3)(3+3)|E_4|\log(3.3)(3+3)+ \\ (1.3)(1+3)|E_5|\log(1.3)(1+3)\end{bmatrix}$$

$$I(PDG-G_n,ReZ(G_3))=\log[824.2^n-254]-\frac{1}{[824.2^n-254]}\begin{bmatrix}6|E_1|\log 6+16|E_2|\log 16+30|E_3|\log 30+ \\ 54|E_4|\log 54+12|E_5|\log 12\end{bmatrix}$$

$$I(PDG-G_n, ReZ(G_3)) = \log[824.2^n - 254] - \frac{1}{[824.2^n - 254]}\begin{bmatrix} (12.2^n)\log 6 + (224.2^n - 64)\log 16 + \\ (300.2^n - 240)\log 30 + (216.2^n + 54)\log 54 \\ +(72.2^n)\log 12 \end{bmatrix}$$

$$I(PDL-G_n, ReZ(G_3)) = \log(824.2^n - 254) - \frac{1}{(824.2^n - 254)}[(1174.09516937262)2^n - 338.02351699226]$$

Theorem 9. The First (a,b)-KA index of PDL-G_n is

$$\mathrm{KA}^1(\mathrm{a,b})[\mathrm{PDL}-\mathrm{G_n}] = \begin{bmatrix} 2^{n+1}[1+2^a]^b + (7(2^{n+1})-4)[2(2^a)]^b + 3(2^{n+1})[1+3^a]^b + \\ (5(2^{n+1})-8)[2^a+3^a]^b + [2(3^a)^b](2^{n+1}+1) \end{bmatrix}$$

Proof. By using table 1 and the definition of first (a, b)-KA index

$$\mathrm{KA}^1(\mathrm{a,b})[\mathrm{PDL}-\mathrm{G_n}] = \sum_{xy\in E(G)} [d_G(u)^a + d_G(v)^a]^b$$

$$\mathrm{KA}^1(\mathrm{a,b})[\mathrm{PDL}-\mathrm{G_n}] = 2^{n+1}[1^a+2^a]^b + (7(2^{n+1})-4)[2^a+2^a]^b + 3(2^{n+1})[1^a+3^a]^b + (5(2^{n+1})-8)[2^a+3^a]^b + [(3^a+3^a)^b](2^{n+1}+1)$$

$$\mathrm{KA}^1(\mathrm{a,b})[\mathrm{PDL}-\mathrm{G_n}] = 2^{n+1}[1+2^a]^b + (7(2^{n+1})-4)[2(2^a)]^b + 3(2^{n+1})[1+3^a]^b + (5(2^{n+1})-8)[2^a+3^a]^b + [2(3^a)^b](2^{n+1}+1)$$

Corollary *10.* The sombor index of PDL-Gn is

$$\mathrm{SO}[\mathrm{PDL}-\mathrm{G_n}] = \sum_{xy\in E(G)} \sqrt{d_G(u^2) + d_G(v^2)}$$

$$SO[\mathrm{PDL}-\mathrm{G_n}] = 2^{n+1}\sqrt{5} + (7(2^{n+1})-4)\sqrt{8} + (5(2^{n+1})-8)\sqrt{13} + (2^{n+1}+1)\sqrt{18} + 3(2^{n+1})\sqrt{10}$$

$$SO[\mathrm{PDL}-\mathrm{G_n}] = 2^{n+1}\sqrt{5} + (14(2^{n+1})-4)\sqrt{2} + (5(2^{n+1})-8)\sqrt{13} + 3(2^{n+1}+1)\sqrt{2} + 3(2^{n+1})\sqrt{10}$$

Corollary *11.* The Modified sombor index of PDL-Gn is

$$^{\mathrm{m}}\mathrm{SO}[\mathrm{PDL}-\mathrm{G_n}] = \frac{2(2^n)}{\sqrt{5}} + \frac{14(2^n)-4}{2\sqrt{2}} + \frac{6(2^n)}{\sqrt{10}} + \frac{10(2^n)-8}{\sqrt{13}} + \frac{4(2^n)+1}{3\sqrt{2}}$$

$$^{\mathrm{m}}SO[\mathrm{PDL}-\mathrm{G_n}] = \left(\frac{2\sqrt{5}}{5} + \frac{7}{2} + \frac{3\sqrt{10}}{5} + \frac{10\sqrt{13}}{13} + \frac{2\sqrt{2}}{3}\right)2^n - \left(\sqrt{2} + \frac{8\sqrt{13}}{13} - \frac{\sqrt{2}}{6}\right)$$

$$^{\mathrm{m}}\mathrm{SO}[\mathrm{PDL}-\mathrm{G_n}] = \left(\frac{156\sqrt{5}+1365+234\sqrt{10}+300\sqrt{13}+260\sqrt{2}}{390}\right)2^n - \left(\frac{65\sqrt{2}+48\sqrt{13}}{78}\right)$$

Theorem 12. The First Reduced (a,b)-KA index of PDL-G_n is

$$\mathrm{RKA}^1(\mathrm{a,b})[\mathrm{PDL}-\mathrm{G_n}] = \begin{bmatrix} 2^{n+1}[1+7(2^b)+3(2^a)^b+5(1+2^a)^b + \\ 2(2(2)^a)^b - 4[2^b+2(1+2^a)^b] \end{bmatrix}$$

Proof. By using table 1 and the definition of first reduced (a, b)-KA index

$$\mathrm{RKA}^1(\mathrm{a,b})[\mathrm{PDL}-\mathrm{G_n}] = \begin{bmatrix} 2(2^n)[(1-1)^a+(2-1)^a]^b + \\ [(2-1)^a+(2-1)^a]^b[14(2^n)-4)] + \\ 6(2^n)[(1-1)^a+(3-1)^a]^b + \\ [10(2^n-8)][(2-1)^a+(3-1)^a]^b + \\ [4(2^n+1)][(2)^a+(2)^a]^b \end{bmatrix}$$

$$\mathrm{RKA}^1(\mathrm{a,b})[\mathrm{PDL}-\mathrm{G_n}] = \begin{bmatrix} 2(2^n) + 2^b[14(2^n)-4)] + \\ 6(2^n)[(2)^a]^b + \\ [10(2^n-8)][1+(2)^a]^b \\ +[4(2^n+1)] \\ [2(2)^a]^b \end{bmatrix}$$

$$\mathrm{R\ KA}^1(\mathrm{a,b})[\mathrm{PDL}-\mathrm{G_n}] = \begin{bmatrix} 2^{n+1}[1+7(2^b)+3(2^a)^b+5(1+2^a)^b + \\ 2(2(2)^a)^b - 4[2^b+2(1+2^a)^b] \end{bmatrix}$$

Corollary *13.* *The* Reduced *sombor index of PDL-Gn is*

$$RSO[PDL-G_n] = \begin{bmatrix} 2(2^n)\sqrt{1^2} + (14(2^n)-4)\sqrt{2} + \left(6(2^n)\right)\sqrt{4} + \\ \left(10(2^n)-8\right)\sqrt{5} + (4(2^n)+1)\sqrt{8} \end{bmatrix}$$

$$RSO[PDL-G_n]=\begin{bmatrix}2(2^n)\ +\left(14(2^n)\sqrt{2}-4\sqrt{2}\right)+\ \left(12(2^n)\right)+\\ \left(10(2^n)\sqrt{5}-8\sqrt{5}\right)+(8(2^n)\sqrt{2}+1\sqrt{8})\end{bmatrix}$$

$$RSO[PDL-G_n]=\begin{bmatrix}2^{n+1}\left(7+11\sqrt{2}+5\sqrt{5}\right)-\\ 2(4\sqrt{5}+\sqrt{2})\end{bmatrix}$$

Corollary *14.* The *Reduced, modified sombor index of PDL-Gn is*

$${}^{\mathrm{m}}RSO[PDL-G_n]=\left[\frac{2(2^n)}{\sqrt{1}}+\frac{14(2^n)-4}{\sqrt{2}}+3(2^n)+\frac{10(2^n)-8}{\sqrt{5}}+\frac{4(2^{n+1})}{2\sqrt{2}}\right]$$

$${}^{\mathrm{m}}RSO[PDL-G_n]=\begin{bmatrix}2(2^n)+7\sqrt{2}(2^n)-2\sqrt{2}+3(2^n)+\\ 2\sqrt{5}(2^n)-\frac{8}{\sqrt{5}}+\sqrt{2}(2^n)+\frac{1}{2\sqrt{2}}\end{bmatrix}$$

$${}^{\mathrm{m}}RSO[PDL-G_n]=\left[(2^n)\left(5+2\sqrt{5}+8\sqrt{2}\right)-\frac{32\sqrt{5}+35\sqrt{2}}{20}\right]$$

Theorem 15. The Second Reduced (a,b)-KA index of PDL-G_n is

$$\mathrm{RKA}^2(\mathrm{a},\mathrm{b})[\mathrm{PDL}-\mathrm{G_n}]=\begin{bmatrix}2^n\left[7+5(2^a)^b+\left(2(2^a)\right)^b\right]+\\ (2(2)^a)^b-8(2^a)^b-4\end{bmatrix}$$

***Proof*.** By using table 1 and the definition of second reduced (a, b)-KA index

$$\mathrm{RKA}^2(\mathrm{a},\mathrm{b})[\mathrm{PDL}-\mathrm{G_n}]=\begin{bmatrix}2(2^n)[(1-1)^a(2-1)^a]^b+\\ [(2-1)^a(2-1)^a]^b[14(2^n)-4)]+\\ 6(2^n)[(1-1)^a(3-1)^a]^b+\\ [10(2^n-8)][(2-1)^a(3-1)^a]^b+\\ [4(2^n+1)][2(2)^a]^b\end{bmatrix}$$

$$\mathrm{RKA}^2(\mathrm{a},\mathrm{b})[\mathrm{PDL}-\mathrm{G_n}]=\begin{bmatrix}[14(2^n)-4)]+\\ 10(2^n)[(2)^a]^b-\\ [(2)^a]^b\\ +[4(2^n)[2(2)^a]^b]+\\ [2(2)^a]^b\end{bmatrix}$$

$$\mathrm{RKA}^2(\mathrm{a},\mathrm{b})[\mathrm{PDL}-\mathrm{G_n}]=\begin{bmatrix}2^n[7+5(2^a)^b+\left(2(2^a)\right)^b]+\\ (2(2)^a)^b-8(2^a)^b-4\end{bmatrix}$$

3. Conclusion

We studied peptide (PDL-G_n) Dendrimers and their properties. We compute topological indices such as the First zagreb index, second zagreb index, Modified second zagreb index, Augmented zagreb Index, Hyper zagreb 2nd Index, Redefined 1st zagreb Index, Redefined 2nd zagreb Index and Redefined 3rd zagreb Index, and using these result we compute weighted entropies of PDL-G_n. Also, we compute the First (a;b)KA Index, Sombor Index, Modified Sombor Index, Reduced Sombor Index, Reduced modified Sombor Index, Reduced 1st (a;b)KA Index, Reduced 2nd (a;b)KA Index for nth generation of PDL.".

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