Research Article

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Zagreb Polynomials and redefined Zagreb indices of Dendrimers and Polyomino Chains

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Abstract: Dendrimers have an incredibly strong potential because their structure allows multivalent frameworks, i.e. one dendrimer molecule has many possible destinations to couple to a functioning species. Researchers expected to utilize the hydrophobic conditions of the dendritic media to lead photochemical responses that make the things that are artificially tested. Carboxylic acid and phenol- terminated water-dissolvable dendrimers were joined to set up their utility in tranquilize conveyance and furthermore driving compound reactions in their inner parts. This may empower scientists to associate both concentrating on atoms and medication particles to the equivalent dendrimer, which could diminish negative manifestations of prescriptions on sound and health cells. Topological indices are numerical numbers associated with the graphs of dendrimers and are invariant up to graph isomorphism. These numbers compare certain physicochemical properties like boiling point, strain energy, stability, etc. of a synthetic compound. There are three main types of topological indices, i.e. degree-based, distance-based and spectrum-based. In this paper, our aim is to compute some degree-based indices and polynomials for some dendrimers and polyomino chains. We computed redefined first, second and third Zagreb indices of PAMAM dendrimers PD_1 , PD_2 , and DS_1 and linear Polyomino chain L_n , Zigzag Polyomino chain Z_n , polyomino chain with n squares and of m segments B_n^1

and B_n^2 . We also computed some Zagreb polynomials of understudy dendrimers and chains.

Keywords: Zagreb Index; Zagreb Polynomial; Dendrimers; Polyomino chain; Chemical graph theory.

1 Introduction

In medicine mathematical modelling is used to understand the structure of new drugs, usually as an undirected graph where each vertex exhibits a molecule and each edge addresses a bond between atoms. A huge number of new drugs are made each year which then requires significant work to choose the pharmacological, compound and organic qualities of these new drugs. This is challenging for countries, in for example South America, Southeast Asia, Africa and India where the cost for gauging the biochemical properties is prohibitive.

It has been proven in numerous studies that there is a strong link between the properties of compounds and drugs with their molecular structure. The topological index (TI) defined on the structure of these compounds can help researchers to develop an understanding of the physical characteristics, chemical reactivity and biological activity [1,2]. Therefore, the study of TIs of chemical structures of drugs can provide a theoretical basis for the preparation of new drugs [3].

In the past two decades many TIs have been defined and used in toxicology, environmental chemistry, pharmacology and theoretical chemistry [4-14].

The oldest degree-based TIs were defined by Gutman in [14] and are known by different names such as Sag. Loeb group parameters, Zagreb group index. Nowadays these indices are known as first Zagreb index and second Zagreb index. Zagreb indices are used to studying chirality, heterogeneity, ZE isomers and molecular complexity and have potential relevance with multiple linear regression models. For detailed survey we refer to [14-17].

The **Polyomino Chains** is a finite 2-connected floor plan, where each inner face (or a unit) is encompassed by

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a square of length one. It is a union of cells connected by edges in a planar square lattice [18-20]:

Dendrimer originates from the Greek word meaning “trees” [21,22] and are redundantly spread molecules. Dendrimers are commonly symmetrical about the center and generally display a circular three-dimensional morphology. The first dendrimer was made by Fritz Vögtle in [23] utilizing distinctive engineered techniques RG Denkewalter in Allied in [24,25] Donald Tomalia in Dow Chemical in [26] and [27,28] and in [29] by George R. Newkome 1990, Craig Hawker and Jean Fréchet presented a combination union strategy. The prevalence of dendrimers has significantly expanded and by 2005 there were in excess of 5,000 logical papers and patents. We aim to study some Zagreb polynomials and redefined Zagreb indices of Polyomino Chains and Dendrimers in this paper.

2 Basic Notions

In this section, we will give some definitions and basic theory of chemical graph theory.

Throughout this paper G means a connected simple graph, $V(G)$ and $E(G)$ represent the vertex set and edge set of G respectively. The degree of a vertex $v \in V(G)$ is the number of vertices attached to it. The formulae for the first and second Zagreb indices are (cf. [14])

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

and

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v).$$

After the success of Zagreb indices, the following first and second Zagreb polynomials were introduced [30]

$$M_1(G, x) = \sum_{uv \in E(G)} x^{d_u + d_v}$$

and

$$M_2(G, x) = \sum_{uv \in E(G)} x^{d_u \cdot d_v}.$$

These Zagreb polynomials find applications in chemistry due to their symmetric behaviour [31].

The third Zagreb index is defined as [32]

$$M_3(G) = \sum_{uv \in E(G)} |d_u - d_v|.$$

and the third Zagreb polynomial is defined as:

$$M_3(G, x) = \sum_{uv \in E(G)} x^{|d_u - d_v|}.$$

Bindusree et al. [33] defined the following Zagreb type polynomials.

$$M_4(G, x) = \sum_{uv \in E(G)} x^{d_u(d_u + d_v)}$$

$$M_5(G, x) = \sum_{uv \in E(G)} x^{d_v(d_u + d_v)}$$

$$M_{a,b}(G, x) = \sum_{uv \in E(G)} x^{ad_u + bd_v}$$

$$M'_{a,b}(G, x) = \sum_{uv \in E(G)} x^{(d_u + a)(d_v + b)}.$$

The first, second and third redefined Zagreb indices were defined by Ranjini et al. in [34]. These indicators appear as

$$\text{Re}ZG_1(G) = \sum_{uv \in E(PD_1)} \frac{d_u + d_v}{d_u \cdot d_v}$$

$$\text{Re}ZG_2(G) = \sum_{uv \in E(PD_1)} \frac{d_u \cdot d_v}{d_u + d_v}$$

$$\text{Re}ZG_3(G) = \sum_{uv \in E(PD_1)} (d_u \cdot d_v)(d_u + d_v).$$

3 Main Results

3.1 Zagreb Polynomials and Redefined Zagreb indices of PAMAM Dendrimers

Polyamidoamine (PAMAM) dendrimers are hyperbranched polymers with unparalleled sub-atomic consistency, sub-atomic weight distribution, characterized size and shape qualities and a multifunctional terminal surface. These nanoscale polymers comprise an ethylenediamine center, a redundant fanning amidoamine inward structure and an essential amine terminal surface. Dendrimers are “grown” off a central core in an iterative assembling process, with each resulting venture speaking to another “generation” of dendrimer. Expanding generation (atomic weight) produce bigger sub-atomic measurements, double the quantity of responsive surface destinations, and around twofold the sub-atomic load of the first era. PAMAM dendrimers likewise expect a spheroidal, globular shape at Generation 4 or above. Their usefulness

is promptly custom fitted, and their consistency, measure and profoundly responsive “sub-atomic Velcro” surfaces is keys to their utilization. Here we study PD_1 which is PAMAM dendrimers with trifunctional center unit created by G_n dendrimer with n growth stages and the PAMAM dendrimers PD_2 with various centers produced by dendrimer generators with n growth stages. DS_1 is PAMAM dendrimers with n growth stages. The M-polynomials, first and second Zagreb indices, modified Zagreb index, generalized Randic index, inverse Randic index, symmetric division index, harmonic index, inverse sum index and augmented Zagreb index for some dendrimers and Polyomino chains were computed in [35]. In this paper we aim to compute Zagreb polynomials and redefined Zagreb indices of the same structures that were previously studied in [35].

Theorem 1. For the PAMAM dendrimers PD_1 , we have

$$1. M_3(PD_1, x) = 9(2^{n+1} - 1) + 3(2^{n+3} - 4)x^{-1} + 3(2^{n+1} - 1)x^{-2}.$$

$$2. M_4(PD_1, x) = 3 \cdot 2^n x^3 + 3(2^{n+1} - 1)x^4 + 9(2^{n+1} - 1)x^8 + 3(7 \cdot 2^n - 4)x^{10}.$$

$$3. M_5(PD_1, x) = 3 \cdot 2^n x^6 + 3(2^{n+1} - 1)x^{12} + 9(2^{n+1} - 1)x^8 + 3(7 \cdot 2^n - 4)x^{15}.$$

$$4. M_{a,b}(PD_1, x) = 3(3 \cdot 2^n - 1)x^a + 3(13 \cdot 2^n - 7)x^{2a} + 3(7 \cdot 2^n - 3)x^{2b} + 3(9 \cdot 2^n - 5)x^{3b}.$$

$$5. M'_{a,b}(PD_1, x) = 3 \cdot 2^n x^{(1+a)(1+b)} + 3(2^{n+1} - 1)x^{(1+a)(3+b)} + 9(2^{n+1} - 1)x^{(2+a)(2+b)} + 3(7 \cdot 2^n - 4)x^{(2+a)(3+b)}.$$

Proof. The edge set of the molecular graph of PD_1 PAMAM dendrimers has the following four classes depending on the degrees of end vertices.

$$E_{\{1,2\}} = \{uv \in E(PD_1) | d_u = 1, d_v = 2\},$$

$$E_{\{1,3\}} = \{uv \in E(PD_1) | d_u = 1, d_v = 3\},$$

$$E_{\{2,2\}} = \{uv \in E(PD_1) | d_u = 2, d_v = 2\},$$

$$E_{\{2,3\}} = \{uv \in E(PD_1) | d_u = 2, d_v = 3\}.$$

Now

$$\begin{aligned} |E_{\{1,2\}}| &= 3 \cdot 2^n, \\ |E_{\{1,3\}}| &= 6 \cdot 2^n - 3, \\ |E_{\{2,2\}}| &= 18 \cdot 2^n - 9, \end{aligned}$$

And

$$|E_{\{2,3\}}| = 21 \cdot 2^n - 12.$$

$$\begin{aligned} 1. M_3(PD_1, x) &= \sum_{uv \in E(PD_1)} x^{d_u + d_v} \\ &= \sum_{uv \in E_{\{1,2\}}(PD_1)} x^{1+2} + \sum_{uv \in E_{\{1,3\}}(PD_1)} x^{1+3} + \sum_{uv \in E_{\{2,2\}}(PD_1)} x^{2+2} + \sum_{uv \in E_{\{2,3\}}(PD_1)} x^{2+3} \\ &= |E_{\{1,2\}}(PD_1)|x^{-1} + |E_{\{1,3\}}(PD_1)|x^{-2} + |E_{\{2,2\}}(PD_1)|x^0 + |E_{\{2,3\}}(PD_1)|x^{-1} \\ &= 9(2^{n+1} - 1) + 3(2^{n+3} - 4)x^{-1} + 3(2^{n+1} - 1)x^{-2}. \end{aligned}$$

$$\begin{aligned} 2. M_4(PD_1, x) &= \sum_{uv \in E(PD_1)} x^{d_u(d_u + d_v)} \\ &= \sum_{uv \in E_{\{1,2\}}(PD_1)} x^3 + \sum_{uv \in E_{\{1,3\}}(PD_1)} x^4 + \sum_{uv \in E_{\{2,2\}}(PD_1)} x^8 + \sum_{uv \in E_{\{2,3\}}(PD_1)} x^{10} \\ &= |E_{\{1,2\}}(PD_1)|x^3 + |E_{\{1,3\}}(PD_1)|x^4 + |E_{\{2,2\}}(PD_1)|x^8 + |E_{\{2,3\}}(PD_1)|x^{10} \\ &= 3 \cdot 2^n x^3 + 3(2^{n+1} - 1)x^4 + 9(2^{n+1} - 1)x^8 + 3(7 \cdot 2^n - 4)x^{10}. \end{aligned}$$

$$\begin{aligned} 3. M_5(PD_1, x) &= \sum_{uv \in E(PD_1)} x^{d_v(d_u + d_v)} \\ &= \sum_{uv \in E_{\{1,2\}}(PD_1)} x^6 + \sum_{uv \in E_{\{1,3\}}(PD_1)} x^{12} + \sum_{uv \in E_{\{2,2\}}(PD_1)} x^8 + \sum_{uv \in E_{\{2,3\}}(PD_1)} x^{15} \\ &= |E_{\{1,2\}}(PD_1)|x^6 + |E_{\{1,3\}}(PD_1)|x^{12} + |E_{\{2,2\}}(PD_1)|x^8 + |E_{\{2,3\}}(PD_1)|x^{15} \\ &= 3 \cdot 2^n x^6 + 3(2^{n+1} - 1)x^{12} + 9(2^{n+1} - 1)x^8 + 3(7 \cdot 2^n - 4)x^{15}. \end{aligned}$$

$$\begin{aligned} 4. M_{a,b}(PD_1, x) &= \sum_{uv \in E(PD_1)} x^{(ad_u + bd_v)} \\ &= \sum_{uv \in E_{\{1,2\}}(PD_1)} x^{a+2b} + \sum_{uv \in E_{\{1,3\}}(PD_1)} x^{a+3b} + \sum_{uv \in E_{\{2,2\}}(PD_1)} x^{2a+2b} + \sum_{uv \in E_{\{2,3\}}(PD_1)} x^{2a+3b} \\ &= |E_{\{1,2\}}(PD_1)|x^{a+2b} + |E_{\{1,3\}}(PD_1)|x^{a+3b} + |E_{\{2,2\}}(PD_1)|x^{2a+2b} + |E_{\{2,3\}}(PD_1)|x^{2a+3b} \\ &= 3(3 \cdot 2^n - 1)x^a + 3(13 \cdot 2^n - 7)x^{2a} + 3(7 \cdot 2^n - 3)x^{2b} + 3(9 \cdot 2^n - 5)x^{3b}. \end{aligned}$$

$$\begin{aligned} 5. M'_{a,b}(PD_1, x) &= \sum_{uv \in E(PD_1)} x^{(d_u + a)(d_v + b)} \\ &= \sum_{uv \in E_{\{1,2\}}(PD_1)} x^{(1+a)(2+b)} + \sum_{uv \in E_{\{1,3\}}(PD_1)} x^{(1+a)(3+b)} + \sum_{uv \in E_{\{2,2\}}(PD_1)} x^{(2+a)(2+b)} + \sum_{uv \in E_{\{2,3\}}(PD_1)} x^{(2+a)(3+b)} \\ &= |E_{\{1,2\}}(PD_1)|x^{(1+a)(2+b)} + |E_{\{1,3\}}(PD_1)|x^{(1+a)(3+b)} + |E_{\{2,2\}}(PD_1)|x^{(2+a)(2+b)} + |E_{\{2,3\}}(PD_1)|x^{(2+a)(3+b)} \\ &= 3 \cdot 2^n x^{(1+a)(2+b)} + 3(2^{n+1} - 1)x^{(1+a)(3+b)} + 9(2^{n+1} - 1)x^{(2+a)(2+b)} + 3(7 \cdot 2^n - 4)x^{(2+a)(3+b)}. \end{aligned}$$

Theorem 2. For the PAMAM dendrimers PD_1 , we have

$$1. \text{Re} ZG_1(PD_1) = 3 \cdot 2^{n+4} - 23.$$

$$2. \text{Re} ZG_2(PD_2) = \left(\frac{497}{10}\right)2^n - \frac{513}{20}.$$

$$3. \text{Re} ZG_3(PD_1) = 9(7 \cdot 2^n - 60).$$

Proof. From the edge partition given in Theorem 1, we have

$$\begin{aligned} 1. \text{Re} ZG_1(PD_1) &= \sum_{uv \in E(PD_1)} \frac{d_u + d_v}{d_u \cdot d_v} \\ &= \sum_{uv \in E_{\{1,2\}}(PD_1)} \frac{1+2}{1 \cdot 2} + \sum_{uv \in E_{\{1,3\}}(PD_1)} \frac{1+3}{1 \cdot 3} + \sum_{uv \in E_{\{2,2\}}(PD_1)} \frac{2+2}{2 \cdot 2} + \sum_{uv \in E_{\{2,3\}}(PD_1)} \frac{2+3}{2 \cdot 3} \\ &= |E_{\{1,2\}}(PD_1)|\frac{3}{2} + |E_{\{1,3\}}(PD_1)|\frac{4}{3} + |E_{\{2,2\}}(PD_1)|\frac{4}{4} + |E_{\{2,3\}}(PD_1)|\frac{5}{6} \\ &= 3 \cdot 2^{n+4} - 23. \end{aligned}$$

$$\begin{aligned}
2. \operatorname{ReZG}_2(PD_1) &= \sum_{uv \in E(PD_1)} \frac{d_u \cdot d_v}{d_u + d_v} \\
&= \sum_{uv \in E_{\{1,2\}}(PD_1)} \frac{1 \cdot 2}{1+2} + \sum_{uv \in E_{\{1,3\}}(PD_1)} \frac{1 \cdot 3}{1+3} + \sum_{uv \in E_{\{2,2\}}(PD_1)} \frac{2 \cdot 2}{2+2} + \sum_{uv \in E_{\{2,3\}}(PD_1)} \frac{2 \cdot 3}{2+3} \\
&= |E_{\{1,2\}}(PD_1)| \frac{2}{3} + |E_{\{1,3\}}(PD_1)| \frac{3}{4} + |E_{\{2,2\}}(PD_1)| \frac{4}{4} + |E_{\{2,3\}}(PD_1)| \frac{6}{5} \\
&= \left(\frac{497}{10}\right) 2^n - \frac{513}{20}.
\end{aligned}$$

$$\begin{aligned}
3. \operatorname{ReZG}_3(PD_1) &= \sum_{uv \in E(PD_1)} (d_u \cdot d_v)(d_u + d_v) \\
&= \sum_{uv \in E_{\{1,2\}}(PD_1)} (1 \cdot 2)(1+2) + \sum_{uv \in E_{\{1,3\}}(PD_1)} (1 \cdot 3)(1+3) + \sum_{uv \in E_{\{2,2\}}(PD_1)} (2 \cdot 2)(2+2) + \sum_{uv \in E_{\{2,3\}}(PD_1)} (2 \cdot 3)(2+3) \\
&= 6|E_{\{1,2\}}(PD_1)| + 12|E_{\{1,3\}}(PD_1)| + 16|E_{\{2,2\}}(PD_1)| + 30|E_{\{2,3\}}(PD_1)| \\
&= 9(7 \cdot 2^n - 60).
\end{aligned}$$

Theorem 3. For the PAMAM dendrimers PD_2 , we have

$$1. M_3(PD_2, x) = (3 \cdot 2^{n+3} - 11) + (2^{n+5} - 14)x^{-1} + 4(2^{n+1} - 1)x^{-2}.$$

$$2. M_4(PD_2, x) = 2^{n+2}x^3 + 4(2^{n+1} - 1)x^4 + (24 \cdot 2^n - 11)x^8 + 14(2^{n+1} - 1)x^{10}.$$

$$3. M_5(PD_2, x) = 2^{n+2}x^6 + 4(2^{n+1} - 1)x^{12} + (24 \cdot 2^n - 11)x^8 + 14(2^{n+1} - 1)x^{15}.$$

$$4. M_{a,b}(PD_2, x) = 4(3 \cdot 2^n - 1)x^a + (13 \cdot 2^{n+2} - 25)x^{2a} + (7 \cdot 2^{n+2} - 11)x^{2b} + 18(2^{n+1} - 1)x^{3b}.$$

$$5. M'_{a,b}(PD_2, x) = 2^{n+2}x^{(1+a)(1+b)} + 4(2^{n+1} - 1)x^{(1+a)(3+b)} + (24 \cdot 2^n - 11)x^{(2+a)(2+b)} + 14(2^{n+1} - 1)x^{(2+a)(3+b)}.$$

Proof. The edge set of the molecular graph of PD_2 PAMAM dendrimers can be divided into the following four types by mean of degree of end vertices.

$$E_{\{1,2\}} = \{uv \in E(PD_2) | d_u = 1, d_v = 2\},$$

$$E_{\{1,3\}} = \{uv \in E(PD_2) | d_u = 1, d_v = 3\},$$

$$E_{\{2,2\}} = \{uv \in E(PD_2) | d_u = 2, d_v = 2\},$$

$$E_{\{2,3\}} = \{uv \in E(PD_2) | d_u = 2, d_v = 3\}.$$

Now

$$|E_{\{1,2\}}| = 4 \cdot 2^n,$$

$$|E_{\{1,3\}}| = 8 \cdot 2^n - 4,$$

$$|E_{\{2,2\}}| = 24 \cdot 2^n - 11,$$

And

$$|E_{\{2,3\}}| = 28 \cdot 2^n - 14.$$

The remaining proof of our results follows similarly as in Theorem 1.

Theorem 4. For the PAMAM dendrimers PD_2 , we have

$$1. \operatorname{ReZG}_1(PD_2) = 4(2^{n+4} - 7).$$

$$2. \operatorname{ReZG}_2(PD_2) = \left(\frac{497}{15}\right) 2^{n+1} - \frac{154}{5}.$$

$$3. \operatorname{ReZG}_3(PD_2) = 7(3 \cdot 2^{n+6} - 92).$$

Proof. Using the edge partition given in theorem 3 and definitions of the first, second and third redefined Zagreb indices, we get our desired results as in theorem 2.

Theorem 5: For the PAMAM dendrimers DS_1 , we have

$$1. M_3(DS_1, x) = 10(3^n - 1) + 4(3^n - 1)x^{-2} + 4 \cdot 3^n x^{-3}.$$

$$2. M_4(DS_1, x) = 4 \cdot 3^n x^5 + 10(3^n - 1)x^8 + 4(3^n - 1)x^{12}.$$

$$3. M_5(DS_1, x) = 10(3^n - 1)x^8 + 4 \cdot 3^n x^{20} + 4(3^n - 1)x^{24}.$$

$$4. M_{a,b}(DS_1, x) = 4 \cdot 3^n x^a + 14(3^n - 1)x^{2a} + 10(3^n - 1)x^{2b} + 4(2 \cdot 3^n - 1)x^{4b}.$$

$$5. M'_{a,b}(DS_1, x) = 4 \cdot 3^n x^{(1+a)(4+b)} + 10(3^n - 1)x^{(2+a)(2+b)} + 4(3^n - 1)x^{(2+a)(4+b)}.$$

Proof. The edge set of the molecular graph of DS_1 PAMAM dendrimers can be divided into the following three classes,

$$E_{\{1,4\}} = \{uv \in E(DS_1) | d_u = 1, d_v = 4\},$$

$$E_{\{2,2\}} = \{uv \in E(DS_1) | d_u = 2, d_v = 2\},$$

$$E_{\{2,4\}} = \{uv \in E(DS_1) | d_u = 2, d_v = 4\}.$$

Now

$$|E_{\{1,4\}}| = 4 \cdot 3^n,$$

$$|E_{\{2,2\}}| = 10 \cdot 3^n - 10,$$

And

$$|E_{\{2,4\}}| = 4 \cdot 3^n - 4.$$

The remaining proof follows directly as in Theorem 1.

Theorem 6. For the PAMAM dendrimers DS_1 , we have

$$1. \operatorname{ReZG}_1(DS_1) = 18 \cdot 3^n - 13.$$

2. $\text{Re } ZG_2(DS_1) = \left(\frac{278}{15}\right)3^n - \frac{46}{3}$.
3. $\text{Re } ZG_3(DS_1) = 16(3^{n+3} - 22)$.

3.2 Zagreb Polynomials and Redefined Zagreb indices of Polyomino Chains

The Polyomino system is a finite graph which is 2-connected plane in which each inner cell is encircled by a square. In simple words, the Polyomino system is an edge-connected union of cells within the planar square lattice. Polyomino chain is an example of Polyomino system [35].

Let B_n be the Polyomino chains having n squares. There exist $2n+1$ number of edges in every $B_n \in B_n$, where B_n is a linear chain and is denoted by L_n in the subgraph of B_n formed by the vertices having $d(v)=3$ is the molecular graph with exactly $n-2$ squares. Also, B_n can be called a zigzag chain and labelled as Z_n if the subgraph of B_n is induced by the vertices with $d(v)>2$ is P_n .

The link of Polyomino chain is angularly connected squares. The segment of Polyomino chain can be defined as the maximum linear chain in the Polyomino chains. Let $l(S)$ denote the length of S which is equal to the number of squares contains in S . For any segment S of a Polyomino chain, we have $l(S) \in \{2, 3, 4, \dots, n\}$. Moreover, we deduce $l_1 = n$ and $m=1$ for a linear chain L_n having n squares and $l_i = 2$ and $m=n-1$ for a zigzag chain Z_n having n squares.

From now to onward, we consider that the Polyomino chain consists of a sequence of segments $S_1, S_2, S_3, \dots, S_n$ and $l(S_i) = l_i$, where $m \geq 1$ and $i \in \{2, 3, 4, \dots, m\}$. We derive that

$$\sum_{i=1}^m l_i = n + m - 1.$$

Theorem 7: For a linear Polyomino chain L_n , we have

1. $M_3(L_n, x) = 3(n-1) + 4x^{-1}$.
2. $M_4(L_n, x) = 2x^8 + 4x^{10} + (3n-5)x^{18}$.
3. $M_5(L_n, x) = 2x^8 + 4x^{15} + (3n-5)x^{18}$.
4. $M_{a,b}(L_n, x) = 6x^{2a} + 2x^{2b} + (3n-5)x^{3a} + (3n-1)x^{3b}$.
5. $M'_{a,b}(L_n, x) = 2x^{(2+a)(2+b)} + 4x^{(2+a)(3+b)} + (3n-5)x^{(3+a)(3+b)}$.

Proof

Let L_n be the Polyomino chain with n squares where $l_1 = n$ and $m=1$. L_n is called the linear chain.

The edge set of L_n Polyomino chain can be divided into following three classes

$$\begin{aligned} E_{\{2,2\}} &= \{e = uv \in E(L_n) | d_u = 2, d_v = 2\}, \\ E_{\{2,3\}} &= \{e = uv \in E(L_n) | d_u = 2, d_v = 3\}, \\ E_{\{3,3\}} &= \{e = uv \in E(L_n) | d_u = 3, d_v = 3\}, \end{aligned}$$

Now

$$\begin{aligned} |E_{\{2,2\}}| &= 2, \\ |E_{\{2,3\}}| &= 4, \\ |E_{\{3,3\}}| &= 3n-5. \end{aligned}$$

The remaining proof is similar to Theorem 1.

Theorem 8. For a linear Polyomino chain L_n , we have

1. $\text{Re } ZG_1(L_n) = 2(n+1)$
2. $\text{Re } ZG_2(L_n) = \frac{9}{2}n - \frac{7}{10}$.
3. $\text{Re } ZG_3(L_n) = 2(81n - 59)$.

Theorem 9. For the Zigzag Polyomino chain Z_n for $n \geq 2$, we have

1. $M_3(Z_n, x) = (3n-2m-3) + 6x^{-1} + 2(m-1)x^{-2}$.
2. $M_4(Z_n, x) = 2x^8 + 4x^{10} + 2(m-1)x^{12} + 2x^{21} + (3n-2m-5)x^{32}$.
3. $M_5(Z_n, x) = 2x^8 + 4x^{15} + 2(m-1)x^{24} + 2x^{28} + (3n-2m-5)x^{32}$.
4. $M_{a,b}(Z_n, x) = 2(m+2)x^{2a} + 2x^{2b} + 2x^{3a} + 4x^{3b} + (3n-2m-5)x^{4a} + (3n-5)x^{4b}$.
5. $M'_{a,b}(Z_n, x) = 2x^{(2+a)(2+b)} + 4x^{(2+a)(3+b)} + 2(m-1)x^{(2+a)(4+b)} + 2x^{(3+a)(4+b)} + (3n-2m-5)x^{(4+a)(4+b)}$.

Proof. Let Z_n be zigzag Polyomino chain with n squares such that $l_i = 2$ and $m = n-1$. Polyomino chain consists of a sequence of segments $S_1, S_2, \dots, S_m$ and $l(S_i) = l_i$ where $m \geq 1$ and $i \in \{1, 2, \dots, m\}$.

The edge set of Z_n has following five partitions,

$$\begin{aligned} E_{\{2,2\}} &= \{e = uv \in E(Z_n) | d_u = 2, d_v = 2\}, \\ E_{\{2,3\}} &= \{e = uv \in E(Z_n) | d_u = 2, d_v = 3\}, \end{aligned}$$

$$E_{\{2,4\}} = \{e = uv \in E(Z_n) | d_u = 2, d_v = 4\},$$

$$E_{\{3,4\}} = \{e = uv \in E(Z_n) | d_u = 3, d_v = 4\},$$

$$E_{\{4,4\}} = \{e = uv \in E(Z_n) | d_u = 4, d_v = 4\}.$$

Now

$$|E_{\{2,2\}}| = 2,$$

$$|E_{\{2,3\}}| = 4,$$

$$|E_{\{2,4\}}| = 2(m-1),$$

$$|E_{\{3,4\}}| = 2,$$

And

$$|E_{\{4,4\}}| = 3n - 2m - 5.$$

Theorem 10. For the Zigzag Polyomino chain Z_n for $n \geq 2$, we have

$$1. \operatorname{Re} ZG_1(Z_n) = \frac{3}{2}n + \frac{1}{2}m + \frac{5}{2}$$

$$2. \operatorname{Re} ZG_2(Z_n) = 6n - \frac{4}{3}m - \frac{256}{105}.$$

$$3. \operatorname{Re} ZG_3(Z_n) = 32(12n - 5m - 13).$$

Theorem 11. For the Polyomino chain with n squares and of m segments S_1 and S_2 satisfy $l_1 = 2$ and $l_2 = n-1$, $B_n^1 (n \geq 3)$, we have

$$1. M_3(B_n^1, x) = (3n-8) + 8x^{-1} + x^{-2}.$$

$$2. M_4(B_n^1, x) = 2x^8 + 5x^{10} + x^{12} + (3n-10)x^{28} + 3x^{21}.$$

$$3. M_5(B_n^1, x) = 2x^8 + 5x^{15} + x^{24} + (3n-10)x^{18} + 3x^{28}.$$

$$4. M_{a,b}(B_n^1, x) = 8x^{2a} + 2x^{2b} + (3n-7)x^{3a} + (3n-5)x^{3b} + 4x^{4b}.$$

$$5. M'_{a,b}(B_n^1, x) = 2x^{(2+a)(2+b)} + 5x^{(2+a)(3+b)} + x^{(2+a)(4+b)} + (3n-10)x^{(3+a)(3+b)} + 3x^{(3+a)(4+b)}.$$

Proof. Let $B_n^1 (n \geq 3)$ be the Polyomino chain with n squares and of m segments S_1 and S_2 satisfy $l_1 = 2$ and $l_2 = n-1$. The edge set of $B_n^1 (n \geq 3)$ has following five partitions,

$$E_{\{2,2\}} = \{e = uv \in E(B_n^1) | d_u = 2, d_v = 2\},$$

$$E_{\{2,3\}} = \{e = uv \in E(B_n^1) | d_u = 2, d_v = 3\},$$

$$E_{\{2,4\}} = \{e = uv \in E(B_n^1) | d_u = 2, d_v = 4\},$$

$$E_{\{3,3\}} = \{e = uv \in E(B_n^1) | d_u = 3, d_v = 3\},$$

$$E_{\{3,4\}} = \{e = uv \in E(B_n^1) | d_u = 3, d_v = 4\}.$$

Now

$$|E_{\{2,2\}}| = 2,$$

$$|E_{\{2,3\}}| = 5,$$

$$|E_{\{2,4\}}| = 1,$$

$$|E_{\{3,3\}}| = 3n - 10,$$

$$|E_{\{3,4\}}| = 3.$$

Theorem 12. For the Polyomino chain with n squares and of m segments S_1 and S_2 satisfy $l_1 = 2$ and $l_2 = n-1$, $B_n^1 (n \geq 3)$, we have

$$1. \operatorname{Re} ZG_1(B_n^1) = 2(n+1)$$

$$2. \operatorname{Re} ZG_2(B_n^1) = \frac{9}{2}n - \frac{107}{21}.$$

$$3. \operatorname{Re} ZG_3(B_n^1) = 2(81n - 29).$$

Theorem 13. For Polyomino chain with n squares and m segments $S_1, S_2, \dots, S_m (m \geq 3)$ satisfy $l_1 = l_m = 2$ and $l_2, \dots, l_{m-1} \geq 3$, $B_n^2 (n \geq 4)$, we have

$$1. M_3(B_n^2, x) = (3n-6m+1) + 6(m-1)x^{-1} + 2x^{-2}.$$

$$2. M_4(B_n^2, x) = 2x^8 + 2mx^{10} + 2x^{12} + 3(n-2m+1)x^{18} + 2(2m-3)x^{21}.$$

$$3. M_5(B_n^2, x) = 2x^8 + 2mx^{15} + 2x^{24} + 3(n-2m+1)x^{18} + 2(2m-3)x^{28}.$$

$$4. M_{a,b}(B_n^2, x) = 2(m+2)x^{2a} + 2x^{2b} + (3n-2m-3)x^{3a} + (3n-4m+3)x^{3b} + 4(m-1)x^{4b}.$$

$$5. M'_{a,b}(B_n^2, x) = 2x^{(2+a)(2+b)} + 2mx^{(2+a)(3+b)} + 2x^{(2+a)(4+b)} + (3n-6m+3)x^{(3+a)(3+b)} + 2(2m-3)x^{(3+a)(4+b)}.$$

Proof. Let B_n^2 ($n \geq 4$) be a Polyomino chain with n squares and m segments $S_1, S_2, \dots, S_m$ ($m \geq 3$) satisfy $l_1 = l_m = 2$ and $l_2, \dots, l_{m-1} \geq 3$. Then the edge set of B_n^2 ($n \geq 4$) has following five partitions,

$$\begin{aligned} E_{\{2,2\}} &= \left\{ e = uv \in E(B_n^2) \mid d_u = 2, d_v = 2 \right\}, \\ E_{\{2,3\}} &= n \left\{ e = uv \in E(B_n^2) \mid d_u = 2, d_v = 3 \right\}, \\ E_{\{2,4\}} &= \left\{ e = uv \in E(B_n^2) \mid d_u = 2, d_v = 4 \right\}, \\ E_{\{3,3\}} &= \left\{ e = uv \in E(B_n^2) \mid d_u = 3, d_v = 3 \right\}, \\ E_{\{3,4\}} &= \left\{ e = uv \in E(B_n^2) \mid d_u = 3, d_v = 4 \right\}. \end{aligned}$$

Now

$$\begin{aligned} |E_{\{2,2\}}| &= 2, \\ |E_{\{2,3\}}| &= 2m, \\ |E_{\{2,4\}}| &= 2, \\ |E_{\{3,3\}}| &= 3n - 6m + 3, \end{aligned}$$

And

$$|E_{\{4,4\}}| = 4m - 6.$$

Theorem 14. For Polyomino chain with n squares and m segments $S_1, S_2, \dots, S_m$ ($m \geq 3$) satisfy $l_1 = l_m = 2$ and $l_2, \dots, l_{m-1} \geq 3$, B_n^2 ($n \geq 4$), we have

1. $\text{Re } ZG_1(B_n^2) = 2(n+1)$
2. $\text{Re } ZG_2(B_n^2) = \frac{9}{2}n + \frac{9}{35}m - \frac{47}{42}$.
3. $\text{Re } ZG_3(B_n^2) = 2(81n + 36m - 107)$.

4 Conclusion

Dendrimers are polymeric materials that given its structure in the form of branched molecules can benefit of mathematical arguments such as Polyomino chains, making this manuscript highly relevant for this type of molecules [36,37]. It is important to calculate topological indices of dendrimers, because it is proven fact that

topological indices help to predict many properties without requiring experimental work. For example, the first and second Zagreb indices were found to happen for the calculation of the π -electron energy of dendrimers, the Randic index corresponds with boiling point, the atomic bond connectivity (ABC) index gives an exceptionally decent relationship to understanding the strain energy of dendrimers and augmented Zagreb index is a good tool to predict the heat of formation of dendrimers, etc. There are round about 148 topological indices [38-40] but none of them can completely describe all properties of a chemical compound. Therefore there is always room to define and study new topological indices. Redefined Zagreb indices are one step in this direction and are very close to Zagreb indices. Zagreb indices are very well studied by chemists and mathematician due to its huge applications in chemistry [41]. In this paper, we calculated first, second and third redefined Zagreb indices for of PAMAM dendrimers PD_1 , PD_2 , and DS_1 and linear Polyomino chain L_n , Zigzag Polyomino chain Z_n , polyomino chain with n squares and of m segments B_n^1 and B_n^2 . We also computed Zagreb polynomials for the above mentioned dendrimers and Polyomino chains. Our results together with QSPR and QSAR can predict properties of understudy materials and are helpful in formulation of new drugs. It is interesting to compute distance-based indices and polynomials for the materials studied in this paper.

Ethical approval: The conducted research is not related to either human or animal use.

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