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Zagreb Polynomials and redefined Zagreb indices of nanostar dendrimers

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Abstract: Dendrimers are profoundly extended natural macromolecules with successive layers of branch units encompassing a central core. Topological indices are numbers related with graph of a compound to allow quantitative structureactivity/property/lethality connections. These topological indices relate certain physico-chemical properties like stability, boiling point, strain energy and so forth of a compound. In this report, there have been computed redefined first, second and third Zagreb indices of Nanostar dendrimers. The authors also analyzed some Zagreb polynomials of understudy dendrimers.

Keywords: Dendrimers, Zagreb index, Zagreb polynomial, topological index, redefined Zagreb index

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1 Introduction

Various studies have shown that there is a solid characteristic connection between synthetic properties of compounds and medications, (for example, melting point and boiling point) and their subatomic structure. The topological index characterized on the structure of these compound can enable scientists to guess physical attributes,

chemical reactivity and biological action [1, 2]. In this manner, the investigation of topological indices of compounds of medications can compensate for the absence of trials and give hypothetical premise to the arrangement of medications and synthetic substances [3]. In the previous two decades, a substantial number of graph invariants (topological indices) have been considered [4–14] and utilized for relationship examination in chemistry, pharmacology, toxicology and ecological science. The first and second Zagreb indices [14] are one of the most established and most understood topological indices characterized by Gutman and are given distinctive names in the literature, for example, the Zagreb group index, Sag, Loeb group and the most widely recognized as Zagreb indices. The Zagreb indices are one of the primary indices acquainted and have been utilized with concentrate sub-atomic intricacy, chirality, ZE isomers and heterogeneous systems [14–17]. Dendrimers are profoundly expanded natural macromolecules with progressive layers of branch units encompassing a central core [18–21]. These are key particles in nanotechnology and can be put to great use. Nanobiotechnology is a quickly propelling region of logical and innovative opportunity that applies the instruments and procedures of nanofabrication to construct gadgets for examining biosystems. Dendrimers are one of the primary objects of this new territory of science. A dendrimer is an artificially produced or synthesized molecule developed from extended units called monomers utilizing a nanoscale manufacture process. Dendrimers are perceived as one of the major commercially available nanoscale building blocks, complex and large particles with great characterized compound. From a polymer science perspective, dendrimers are almost impeccable monodisperse macromolecules with a customary and highly branched three dimensional design. They comprise of three major architectural components: core, branches and end groups. New branches emanating from a core center are included in steps until a tree-like structure is made. The nanostar dendrimer is a part of a new group of macroparticles that appear to be photon funnels just like artificial antennas. These macromolecules and all the more accurately those containing phosphorus are utilized in

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the development of nanotubes, micro and macrocapsules, nanolatex, shaded glasses, chemical sensors, modified electrodes, etc [22]. A k -polyomino framework is a limited 2-connected plane graph with the end goal that every inside face (likewise called cell) is encompassed by a normal 4k-cycle of length one. It is an edge-associated association of cells [23]. Dendrimer is a manufactured 3-dimensional macromolecule that is prepared in a step-wise fashion from straightforward branched monomer units see [24]. The nanostar dendrimer is a part of another gathering of macromolecules that appear to photon funnels simply like artificial antennas [25–28]. In this paper, the authors aim to analyze the Zagreb polynomials and redefined Zagreb indices of Nanostar dendrimers.

2 Basic definition

A graph is connected if there is a path between any two vertices of it. Throughout this paper G is a connected graph without multiple edges and loops, V is the set of vertices and E is the set of edges. The first topological index was defined by Wiener in 1947, when he was calculating boiling point of alkane [29]. Randic index is also one of the oldest topological index defined by Milan Randic [30], which has been studied extensively by both Chemists and Mathematicians due to its application in chemistry [31–35]. Gutman introduced the first and second Zagreb indices:

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

and

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

Considering the Zagreb indices, Fath-Tabar ([36–38]) defined first and the second Zagreb polynomials as

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

and

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

The properties of $M_1(G, x)$, $M_2(G, x)$ polynomials for some chemical structures can be seen in the work of Gutman [39].

G. H. Fath-Tabar et al. [38] defined the third Zagreb index

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

and the polynomial

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

In the year 2016, [40] following Zagreb type polynomials were defined

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

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

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

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

Ranjini et al. [41] redefines the Zagreb index, ie, the redefined first, second and third Zagreb indices of graph G . These indicators appear as

$$\text{ReZG}_1(G) = \sum_{uv \in E(PD_1)} \frac{d_u + d_v}{d_u \cdot d_v}$$

$$\text{ReZG}_2(G) = \sum_{uv \in E(PD_1)} \frac{d_u \cdot d_v}{d_u + d_v}$$

$$\text{ReZG}_3(G) = \sum_{uv \in E(PD_1)} (d_u \cdot d_v)(d_u + d_v).$$

3 Main results

We now consider two infinite classes $NS_1[n]$ and $NS_2[n]$ of nanostar dendrimers, see Figs. 1 and 2. Our aim is to compute the redefined Zagreb indices and Zagreb polynomials for two classes of these nanostar dendrimers. We consider the molecular graph of $NS_1[n]$ with four similar branches and three extra edges, where n is steps of growth in this type of nanostars dendrimer see Figure 1.

In the following theorem we compute Zagreb polynomials of $NS_1[n]$.

Theorem 1 Let $NS_1[n]$ be a polypropylenimineoctaamin dendrimer, then

1.

$$M_3(NS_1[n], x) = 4(2^n - 1)x^2 + 2(2^{n+3} - 7)x + (12 \cdot 2^n - 11).$$

2.

$$M_4(NS_1[n], x) = 2^{n+1}x^3 + 4(2^n - 1)x^4 + (12 \cdot 2^n - 11)x^8 + 14(2^n - 1)x^{10}.$$

Figure 1: $NS_1[1]$ and $NS_1[2]$ polypropylenimineoctaamin dendrimer

3.

$$M_5(NS_1[n], x) = 2^{n+1}x^6 + 4(2^n - 1)x^{12} + (12 \cdot 2^n - 11)x^8 + 14(2^n - 1)x^{15}.$$

4.

$$M_{a,b}(NS_1[n], x) = 4(2^n + 2^{n-1} - 1)x^a + (13 \cdot 2^{n+1} - 25)x^{2a} + (7 \cdot 2^{n+1} - 11)x^{2b} + 18(2^n - 1)x^{3b}.$$

5.

$$M'_{a,b}(NS_1[n], x) = 2^{n+1}x^{(1+a)(1+b)} + 4(2^n - 1)x^{(1+a)(3+b)} + (12 \cdot 2^n - 11)x^{(2+a)(2+b)} + 14(2^n - 1)x^{(2+a)(3+b)}.$$

Proof. From the structure of $NS_1[n]$, we can see that there are three partitions of vertices $V_1 = \{v \in V(NS_1[n]) \mid d_v = 1\}$, $V_2 = \{v \in V(NS_1[n]) \mid d_v = 2\}$, and $V_3 = \{v \in V(NS_1[n]) \mid d_v = 3\}$.

The edge set of the has following four partitions:

$$E_{\{1,2\}} = \{e = uv \in E(NS_1[n]) \mid d_u = 1, d_v = 2\},$$

$$E_{\{1,3\}} = \{e = uv \in E(NS_1[n]) \mid d_u = 1, d_v = 3\},$$

$$E_{\{2,2\}} = \{e = uv \in E(NS_1[n]) \mid d_u = 2, d_v = 2\},$$

$$E_{\{2,3\}} = \{e = uv \in E(NS_1[n]) \mid d_u = 2, d_v = 3\},$$

Now

$$\begin{aligned} |E_{\{1,2\}}| &= 2^{n+1} \\ |E_{\{1,3\}}| &= 4(2^n - 1) \\ |E_{\{2,2\}}| &= 12 \cdot 2^n - 11 \\ |E_{\{2,3\}}| &= 14(2^n - 1) \end{aligned}$$

1.

$$\begin{aligned} M_3(NS_1[n], x) &= \sum_{uv \in E(NS_1[n])} x^{d_u - d_v} = \sum_{uv \in E_{\{1,2\}}(NS_1[n])} x^{|2-1|} \\ &+ \sum_{uv \in E_{\{1,3\}}(NS_1[n])} x^{|3-1|} + \sum_{uv \in E_{\{2,2\}}(NS_1[n])} x^{|2-2|} \\ &+ \sum_{uv \in E_{\{2,3\}}(NS_1[n])} x^{|3-2|} = |E_{\{1,2\}}(NS_1[n])| x^1 \\ &+ |E_{\{1,3\}}(NS_1[n])| x^2 + |E_{\{2,2\}}(NS_1[n])| x^0 \\ &+ |E_{\{2,3\}}(NS_1[n])| x^1 = 4(2^n - 1)x^2 \\ &+ 2(2^{n+3} - 7)x + (12 \cdot 2^n - 11). \end{aligned}$$

2.

$$\begin{aligned} M_4(NS_1[n], x) &= \sum_{uv \in E(NS_1[n])} x^{d_u(d_u + d_v)} = \sum_{uv \in E_{\{1,2\}}(NS_1[n])} x^3 \\ &+ \sum_{uv \in E_{\{1,3\}}(NS_1[n])} x^4 + \sum_{uv \in E_{\{2,2\}}(NS_1[n])} x^8 \\ &+ \sum_{uv \in E_{\{2,3\}}(NS_1[n])} x^{10} = |E_{\{1,2\}}(NS_1[n])| x^3 \\ &+ |E_{\{1,3\}}(NS_1[n])| x^4 + |E_{\{2,2\}}(NS_1[n])| x^8 \\ &+ |E_{\{2,3\}}(NS_1[n])| x^{10} = 2^{n+1}x^3 + 4(2^n - 1)x^4 \\ &+ (12 \cdot 2^n - 11)x^8 + 14(2^n - 1)x^{10}. \end{aligned}$$

$$\begin{aligned} M_5(NS_1[n], x) &= \sum_{uv \in E(NS_1[n])} x^{d_v(d_u + d_v)} = \sum_{uv \in E_{\{1,2\}}(NS_1[n])} x^6 \\ &+ \sum_{uv \in E_{\{1,3\}}(NS_1[n])} x^{12} + \sum_{uv \in E_{\{2,2\}}(NS_1[n])} x^8 \\ &+ \sum_{uv \in E_{\{2,3\}}(NS_1[n])} x^{15} = |E_{\{1,2\}}(NS_1[n])| x^6 \\ &+ |E_{\{1,3\}}(NS_1[n])| x^{12} + |E_{\{2,2\}}(NS_1[n])| x^8 \\ &+ |E_{\{2,3\}}(NS_1[n])| x^{15} = 2^{n+1}x^6 + 4(2^n - 1)x^{12} \\ &+ (12 \cdot 2^n - 11)x^8 + 14(2^n - 1)x^{15}. \end{aligned}$$

4.

$$\begin{aligned} M_{a,b}(NS_1[n], x) &= \sum_{uv \in E(NS_1[n])} x^{(ad_u + bd_v)} = \\ &\sum_{uv \in E_{\{1,2\}}(NS_1[n])} x^{a+2b} + \sum_{uv \in E_{\{1,3\}}(NS_1[n])} x^{a+3b} \\ &+ \sum_{uv \in E_{\{2,2\}}(NS_1[n])} x^{2a+2b} + \sum_{uv \in E_{\{2,3\}}(NS_1[n])} x^{2a+3b} = \\ &|E_{\{1,2\}}(NS_1[n])| x^{a+2b} + |E_{\{1,3\}}(NS_1[n])| x^{a+3b} \\ &+ |E_{\{2,2\}}(NS_1[n])| x^{2a+2b} + |E_{\{2,3\}}(NS_1[n])| x^{2a+3b} = \\ &4(2^n + 2^{n-1} - 1)x^a + (13 \cdot 2^{n+1} - 25)x^{2a} + \\ &(7 \cdot 2^{n+1} - 11)x^{2b} + 318(2^n - 1)x^{3b}. \end{aligned}$$

Figure 2: $NS_2[n]$ polypropylenimine octaamin dendrimer

5.

$$\begin{aligned}
 M'_{a,b}(NS_1[n], x) &= \sum_{uv \in E(NS_1[n])} x^{(d_u+a)(d_v+b)} = \\
 &\sum_{uv \in E_{\{1,2\}}(NS_1[n])} x^{(1+a)(2+b)} + \sum_{uv \in E_{\{1,3\}}(NS_1[n])} x^{(1+a)(3+b)} \\
 &+ \sum_{uv \in E_{\{2,2\}}(NS_1[n])} x^{(2+a)(2+b)} + \sum_{uv \in E_{\{2,3\}}(NS_1[n])} x^{(2+a)(3+b)} = \\
 s |E_{\{1,2\}}(NS_1[n])| x^{(1+a)(2+b)} &+ |E_{\{1,3\}}(NS_1[n])| x^{(1+a)(3+b)} \\
 &+ |E_{\{2,2\}}(NS_1[n])| x^{(2+a)(2+b)} + |E_{\{2,3\}}(NS_1[n])| x^{(2+a)(3+b)} \\
 &= 2^{n+1} x^{(1+a)(2+b)} + 4(2^n - 1) x^{(1+a)(3+b)} \\
 &+ (12 \cdot 2^n - 11) x^{(2+a)(2+b)} + 14(2^n - 1) x^{(2+a)(3+b)}.
 \end{aligned}$$

First, second and third redefined Zagreb indices of $NS_1[n]$ has been computed in theorem 2. $\square$

Theorem 2 Let $NS_1[n]$ be a polypropylenimine octaamin dendrimer, then

1.

$$\text{Re}ZG_1(NS_1[n]) = 2^{n+5} - 28.$$

2.

$$\text{Re}ZG_2(NS_1[n]) = \frac{2^{n+2}}{3} + \left(\frac{159}{5}\right) 2^n - \frac{154}{5}.$$

3. $\text{Re}ZG_3(NS_1[n]) = 7(3 \cdot 2^{n+5} - 92).$

Proof. From the edge partition given in theorem 2 and using definitions, we have

1.

$$\begin{aligned} \text{ReZG}_1(NS_1[n]) &= \sum_{uv \in E(NS_1[n])} \frac{d_u + d_v}{d_u \cdot d_v} \\ &= \sum_{uv \in E_{\{1,2\}}(NS_1[n])} \frac{1+2}{1 \cdot 2} + \sum_{uv \in E_{\{1,3\}}(NS_1[n])} \frac{1+3}{1 \cdot 3} \\ &\quad + \sum_{uv \in E_{\{2,2\}}(NS_1[n])} \frac{2+2}{2 \cdot 2} + \sum_{uv \in E_{\{2,3\}}(NS_1[n])} \frac{2+3}{2 \cdot 3} \\ &= |E_{\{1,2\}}(NS_1[n])| \frac{3}{2} + |E_{\{1,3\}}(NS_1[n])| \frac{4}{3} \\ &\quad + |E_{\{2,2\}}(NS_1[n])| \frac{4}{4} + |E_{\{2,3\}}(NS_1[n])| \frac{5}{6} = 2^{n+5} - 28. \end{aligned}$$

2.

$$\begin{aligned} \text{ReZG}_2(NS_1[n]) &= \sum_{uv \in E(NS_1[n])} \frac{d_u \cdot d_v}{d_u + d_v} \\ &= \sum_{uv \in E_{\{1,2\}}(NS_1[n])} \frac{1 \cdot 2}{1+2} + \sum_{uv \in E_{\{1,3\}}(NS_1[n])} \frac{1 \cdot 3}{1+3} \\ &\quad + \sum_{uv \in E_{\{2,2\}}(NS_1[n])} \frac{2 \cdot 2}{2+2} + \sum_{uv \in E_{\{2,3\}}(NS_1[n])} \frac{2 \cdot 3}{2+3} \\ &= |E_{\{1,2\}}(NS_1[n])| \frac{2}{3} + |E_{\{1,3\}}(NS_1[n])| \frac{3}{4} \\ &\quad + |E_{\{2,2\}}(NS_1[n])| \frac{4}{4} + |E_{\{2,3\}}(NS_1[n])| \frac{6}{5} \\ &= \frac{2^{n+2}}{3} + \left(\frac{159}{5}\right) 2^n - \frac{154}{5}. \end{aligned}$$

3.

$$\begin{aligned} \text{ReZG}_3(NS_1[n]) &= \sum_{uv \in E(NS_1[n])} (d_u \cdot d_v)(d_u + d_v) \\ &= \sum_{uv \in E_{\{1,2\}}(NS_1[n])} (1 \cdot 2)(1+2) \\ &\quad + \sum_{uv \in E_{\{1,3\}}(NS_1[n])} (1 \cdot 3)(1+3) \\ &\quad + \sum_{uv \in E_{\{2,2\}}(NS_1[n])} (2 \cdot 2)(2+2) \\ &\quad + \sum_{uv \in E_{\{2,3\}}(NS_1[n])} (2 \cdot 3)(2+3) = 6 |E_{\{1,2\}}(NS_1[n])| \\ &\quad + 12 |E_{\{1,3\}}(NS_1[n])| + 16 |E_{\{2,2\}}(NS_1[n])| \\ &\quad + 30 |E_{\{2,3\}}(NS_1[n])| = 7 \left(3 \cdot 2^{n+5} - 92\right). \end{aligned}$$

We consider the second class of nanostar dendrimers $NS_2[n]$, where n is steps of growth. Since the molecular graph of G has four similar branches and five extra edges (see Figure 2). Next theorem is about the Zagreb polynomials of $NS_2[n]$. $\square$

Theorem 3 Let $NS_2[n]$ be the polypropylenimineoctaamin dendrimer, then

1.

$$M_3(NS_2[n], x) = 2 \left(2^{n+2} - 3\right) x + (8 \cdot 2^n - 5).$$

2.

$$M_4(NS_2[n], x) = 2^{n+1} x^3 + (8 \cdot 2^n - 5) x^8 + 6 (2^n - 1) x^{10}.$$

3.

$$M_5(NS_2[n], x) = 2^{n+1} x^6 + (8 \cdot 2^n - 5) x^8 + 6 (2^n - 1) x^{15}.$$

4.

$$\begin{aligned} M_{a,b}(NS_2[n], x) &= 2^{n+1} x^a + (7 \cdot 2^{n+1} - 11) x^{2a} \\ &\quad + (2^{n+3} + 2^{n+1} - 5) x^{2b} + 6 (2^n - 1) x^{3b}. \end{aligned}$$

5.

$$\begin{aligned} M'_{a,b}(NS_2[n], x) &= 2^{n+1} x^{(1+a)(2+b)} + (8 \cdot 2^n - 5) x^{(2+a)(2+b)} \\ &\quad + 6 (2^n - 1) x^{(2+a)(3+b)}. \end{aligned}$$

Proof. From the structure of $NS_2[n]$, we can see that there are three partitions of vertices

$$V_2 = \{v \in V(NS_2[n]) \mid d_v = 2\},$$

and

$$V_3 = \{v \in V(NS_2[n]) \mid d_v = 3\},$$

The edge set of the $NS_2[n]$ has following four partitions;

$$E_{\{1,2\}} = \{e = uv \in E(NS_2[n]) \mid d_u = 1, d_v = 2\},$$

$$E_{\{2,2\}} = \{e = uv \in E(NS_2[n]) \mid d_u = 2, d_v = 2\},$$

$$E_{\{2,3\}} = \{e = uv \in E(NS_2[n]) \mid d_u = 2, d_v = 3\},$$

Now

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

$$|E_{\{2,2\}}| = 8 \cdot 2^n - 5$$

1.

$$\begin{aligned} M_3(NS_2[n], x) &= \sum_{uv \in E(NS_2[n])} x^{|d_u - d_v|} = \sum_{uv \in E_{\{1,2\}}(NS_2[n])} x^{|2-1|} \\ &\quad + \sum_{uv \in E_{\{2,2\}}(NS_2[n])} x^{|2-2|} + \sum_{uv \in E_{\{2,3\}}(NS_2[n])} x^{|2-3|} \\ &= |E_{\{1,2\}}(NS_2[n])| x^1 \\ &\quad + |E_{\{2,2\}}(NS_2[n])| x^0 + |E_{\{2,3\}}(NS_2[n])| x^1 \\ &= 2 \left(2^{n+2} - 3\right) x + (8 \cdot 2^n - 5). \end{aligned}$$

2.

$$\begin{aligned}
M_4(NS_2[n], x) &= \sum_{uv \in E(NS_2[n])} x^{d_u + d_v} = \sum_{uv \in E_{\{1,2\}}(NS_2[n])} x^3 \\
&+ \sum_{uv \in E_{\{2,2\}}(NS_2[n])} x^8 + \sum_{uv \in E_{\{2,3\}}(NS_2[n])} x^{10} \\
&= |E_{\{1,2\}}(NS_2[n])| x^3 + |E_{\{2,2\}}(NS_2[n])| x^8 \\
&+ |E_{\{2,3\}}(NS_2[n])| x^{10} = 2^{n+1} x^3 + (8 \cdot 2^n - 5) x^8 \\
&+ 6(2^n - 1) x^{10}.
\end{aligned}$$

3.

$$\begin{aligned}
M_5(NS_2[n], x) &= \sum_{uv \in E(NS_2[n])} x^{d_u + d_v} = \sum_{uv \in E_{\{1,2\}}(NS_2[n])} x^6 \\
&+ \sum_{uv \in E_{\{2,2\}}(NS_2[n])} x^8 + \sum_{uv \in E_{\{2,3\}}(NS_2[n])} x^{15} \\
&= |E_{\{1,2\}}(NS_2[n])| x^6 + |E_{\{2,2\}}(NS_2[n])| x^8 \\
&+ |E_{\{2,3\}}(NS_2[n])| x^{15} = 2^{n+1} x^6 + (8 \cdot 2^n - 5) x^8 \\
&+ 6(2^n - 1) x^{15}.
\end{aligned}$$

4.

$$\begin{aligned}
M_{a,b}(NS_2[n], x) &= \sum_{uv \in E(NS_2[n])} x^{ad_u + bd_v} \\
&= \sum_{uv \in E_{\{1,2\}}(NS_2[n])} x^{a+2b} + \sum_{uv \in E_{\{2,2\}}(NS_2[n])} x^{2a+2b} \\
&+ \sum_{uv \in E_{\{2,3\}}(NS_2[n])} x^{2a+3b} = |E_{\{1,2\}}(NS_2[n])| x^{a+2b} \\
&+ |E_{\{2,2\}}(NS_2[n])| x^{2a+2b} + |E_{\{2,3\}}(NS_2[n])| x^{2a+3b} \\
&= 2^{n+1} x^a + (7 \cdot 2^{n+1} - 11) x^{2a} + (2^{n+3} + 2^{n+1} - 5) x^{2b} \\
&+ 6(2^n - 1) x^{3b}.
\end{aligned}$$

5.

$$\begin{aligned}
M'_{a,b}(NS_2[n], x) &= \sum_{uv \in E(NS_2[n])} x^{(d_u+a)(d_v+b)} \\
&= \sum_{uv \in E_{\{1,2\}}(NS_2[n])} x^{(1+a)(2+b)} + \sum_{uv \in E_{\{2,2\}}(NS_2[n])} x^{(2+a)(2+b)} \\
&+ \sum_{uv \in E_{\{2,3\}}(NS_2[n])} x^{(2+a)(3+b)} = |E_{\{1,2\}}(NS_2[n])| x^{(1+a)(2+b)} \\
&+ |E_{\{2,2\}}(NS_2[n])| x^{(2+a)(2+b)} + |E_{\{2,3\}}(NS_2[n])| x^{(2+a)(3+b)} \\
&= 2^{n+1} x^{(1+a)(2+b)} + (8 \cdot 2^n - 5) x^{(2+a)(2+b)} \\
&+ 6(2^n - 1) x^{(2+a)(3+b)}.
\end{aligned}$$

Next theorem is about the first, second and third redefined Zagreb indices. $\square$

Theorem 4 Let $NS_2[n]$ be the polypropylenimine octaamin dendrimer, then

1.

$$\text{ReZG}_1(NS_2[n]) = 2^{n+4} - 10.$$

2.

$$\text{ReZG}_2(NS_2[n]) = \left(\frac{31}{15}\right) 2^{n+3} - \frac{61}{5}.$$

3.

$$\text{ReZG}_3(NS_2[n]) = 5 \cdot 2^{n+6} - 260.$$

Proof. From the edge partition given in theorem 3 and using definitions, we have 1.

$$\begin{aligned}
\text{ReZG}_1(NS_2[n]) &= \sum_{uv \in E(NS_2[n])} \frac{d_u + d_v}{d_u \cdot d_v} \\
&= \sum_{uv \in E_{\{1,2\}}(NS_2[n])} \frac{1+2}{1 \cdot 2} + \sum_{uv \in E_{\{2,2\}}(NS_2[n])} \frac{2+2}{2 \cdot 2} \\
&+ \sum_{uv \in E_{\{2,3\}}(NS_2[n])} \frac{2+3}{2 \cdot 3} = |E_{\{1,2\}}(NS_2[n])| \frac{3}{2} \\
&+ |E_{\{1,3\}}(NS_2[n])| + |E_{\{2,2\}}(NS_2[n])| \frac{5}{6} = 2^{n+4} - 10.
\end{aligned}$$

2.

$$\begin{aligned}
\text{ReZG}_2(NS_2[n]) &= \sum_{uv \in E(NS_2[n])} \frac{d_u \cdot d_v}{d_u + d_v} \\
&= \sum_{uv \in E_{\{1,2\}}(NS_2[n])} \frac{1 \cdot 2}{1+2} + \sum_{uv \in E_{\{2,2\}}(NS_2[n])} \frac{2 \cdot 2}{2+2} \\
&+ \sum_{uv \in E_{\{2,3\}}(NS_2[n])} \frac{2 \cdot 3}{2+3} = |E_{\{1,2\}}(NS_2[n])| \frac{2}{3} \\
&+ |E_{\{2,2\}}(NS_2[n])| + |E_{\{2,3\}}(NS_2[n])| \frac{6}{5} \\
&= \left(\frac{31}{15}\right) 2^{n+3} - \frac{61}{5}.
\end{aligned}$$

3.

$$\begin{aligned}
\text{ReZG}_3(NS_2[n]) &= \sum_{uv \in E(NS_2[n])} (d_u \cdot d_v)(d_u + d_v) \\
&= \sum_{uv \in E_{\{1,2\}}(NS_2[n])} (1 \cdot 2)(1+2) \\
&+ \sum_{uv \in E_{\{2,2\}}(NS_2[n])} (2 \cdot 2)(2+2) \\
&+ \sum_{uv \in E_{\{2,3\}}(NS_2[n])} (2 \cdot 3)(2+3) = 6 |E_{\{1,2\}}(NS_2[n])| \\
&+ 16 |E_{\{2,2\}}(NS_2[n])| + 30 |E_{\{2,3\}}(NS_2[n])| \\
&= 5 \cdot 2^{n+6} - 260.
\end{aligned}$$

Next, we compute Zagreb polynomials and redefined Zagreb indices of $D[n]$ shown in Figures 3 and 4. $\square$

Figure 3: $D[1]$ Nanostar dendrimer

Theorem 5 Let D_n be the nanostar dendrimer, then

1.

$$M_3(D_n, x) = 6 \left(5 \cdot 2^{n-1} - 4 \right) x + 3 \left(3 \cdot 2^{n+1} - 7 \right).$$

2.

$$M_5(D_n, x) = 12 \left(2^n - 1 \right) x^8 + 6 \left(5 \cdot 2^{n-1} - 4 \right) x^{15} + 3 \left(2^{n+1} - 3 \right) x^{18}.$$

3.

$$M_{a,b}(D_n, x) = 9 \left(3 \cdot 2^n - 4 \right) x^{2a} + 12 \left(2^n - 1 \right) x^{2b} + 3 \left(2^{n+1} - 3 \right) x^{3a} + 3 \left(7 \cdot 2^n - 11 \right) x^{3b}.$$

4.

$$M'_{a,b}(D_n, x) = 12 \left(2^n - 1 \right) x^{(2+a)(2+b)} + 6 \left(5 \cdot 2^{n-1} - 4 \right) x^{(2+a)(3+b)} + 3 \left(2^{n+1} - 3 \right) x^{(3+a)(3+b)}.$$

Proof. From the structure of D_n , we can see that there are three partitions of vertices

$$V_2 = \{v \in V(D_n) \mid d_v = 2\},$$

and

$$V_3 = \{v \in V(D_n) \mid d_v = 3\},$$

The edge set of the D_n has following four partitions;

$$E_{\{1,2\}} = \{e = uv \in E(D_n) \mid d_u = 2, d_v = 2\},$$

$$E_{\{2,2\}} = \{e = uv \in E(D_n) \mid d_u = 2, d_v = 3\},$$

$$E_{\{2,3\}} = \{e = uv \in E(D_n) \mid d_u = 3, d_v = 3\},$$

Now

$$|E_{\{1,2\}}| = 12 \left(2 \cdot 2^{n-1} - 1 \right)$$

$$|E_{\{2,3\}}| = 12 \cdot 2^{n-1} - 9$$

1.

$$\begin{aligned} M_3((D_n), x) &= \sum_{uv \in E(D_n)} x^{|d_u - d_v|} = \sum_{uv \in E_{\{1,2\}}(D_n)} x^{|2-1|} \\ &+ \sum_{uv \in E_{\{2,2\}}(D_n)} x^{|2-2|} + \sum_{uv \in E_{\{2,3\}}(D_n)} x^{|2-3|} \\ &= |E_{\{1,2\}}(D_n)| x^1 + |E_{\{2,2\}}(D_n)| x^0 \\ &+ |E_{\{2,3\}}(D_n)| x^1 = 6 \left(5 \cdot 2^{n-1} - 4 \right) x \\ &+ 3 \left(3 \cdot 2^{n+1} - 7 \right). \end{aligned}$$

2.

$$\begin{aligned} M_4((D_n), x) &= \sum_{uv \in E(D_n)} x^{d_u(d_u + d_v)} = \sum_{uv \in E_{\{1,2\}}(D_n)} x^3 \\ &+ \sum_{uv \in E_{\{2,2\}}(D_n)} x^8 + \sum_{uv \in E_{\{2,3\}}(D_n)} x^{10} = |E_{\{1,2\}}(D_n)| x^3 \\ &+ |E_{\{2,2\}}(D_n)| x^8 + |E_{\{2,3\}}(D_n)| x^{10} \\ &= 12 \left(2^n - 1 \right) x^8 + \left(5 \cdot 2^{n-1} - 4 \right) x^{10} \\ &+ 3 \left(2^{n+1} - 3 \right) x^{18}. \end{aligned}$$

3.

$$\begin{aligned} M_5((D_n), x) &= \sum_{uv \in E(D_n)} x^{d_v(d_u + d_v)} = \sum_{uv \in E_{\{1,2\}}(D_n)} x^6 \\ &+ \sum_{uv \in E_{\{2,2\}}(D_n)} x^8 + \sum_{uv \in E_{\{2,3\}}(D_n)} x^{15} = |E_{\{1,2\}}(D_n)| x^6 \\ &+ |E_{\{2,2\}}(D_n)| x^8 + |E_{\{2,3\}}(D_n)| x^{15} = 12 \left(2^n - 1 \right) x^8 \\ &+ 6 \left(5 \cdot 2^{n-1} - 4 \right) x^{15} + 3 \left(2^{n+1} - 3 \right) x^{18}. \end{aligned}$$

4.

$$\begin{aligned} M_{a,b}((D_n), x) &= \sum_{uv \in E(D_n)} x^{(ad_u + bd_v)} = \sum_{uv \in E_{\{1,2\}}(D_n)} x^{a+2b} \\ &+ \sum_{uv \in E_{\{2,2\}}(D_n)} x^{2a+2b} + \sum_{uv \in E_{\{2,3\}}(D_n)} x^{2a+3b} \\ &= |E_{\{1,2\}}(D_n)| x^{a+2b} + |E_{\{2,2\}}(D_n)| x^{2a+2b} \\ &+ |E_{\{2,3\}}(D_n)| x^{2a+3b} = 9 \left(3 \cdot 2^n - 4 \right) x^{2a} \\ &+ 12 \left(2^n - 1 \right) x^{2b} + 3 \left(2^{n+1} - 3 \right) x^{3a} \\ &+ 3 \left(7 \cdot 2^n - 11 \right) x^{3b}. \end{aligned}$$

Figure 4: $D[2]$ Nanostar dendrimer

5.

$$\begin{aligned}
 M'_{a,b}(D_n, x) &= \sum_{uv \in E(D_n)} x^{(d_u+a)(d_v+b)} \\
 &= \sum_{uv \in E_{\{1,2\}}(D_n)} x^{(1+a)(2+b)} + \sum_{uv \in E_{\{2,2\}}(D_n)} x^{(2+a)(2+b)} \\
 &\quad + \sum_{uv \in E_{\{2,3\}}(D_n)} x^{(2+a)(3+b)} = |E_{\{1,2\}}(D_n)| x^{(1+a)(2+b)} \\
 &\quad + |E_{\{2,2\}}(D_n)| x^{(2+a)(2+b)} + |E_{\{2,3\}}(D_n)| x^{(2+a)(3+b)} \\
 &= 12(2^n - 1) x^{(2+a)(2+b)} + 6(5 \cdot 2^{n-1} - 4) x^{(2+a)(3+b)} \\
 &\quad + 3(2^{n+1} - 3) x^{(3+a)(3+b)}.
 \end{aligned}$$

□

Theorem 6 Let D_n be the nanostar dendrimer, then

1.

$$\text{ReZG}_2(D_n) = 3 \cdot 2^{n+2} + 27 \cdot 2^n - \frac{423}{10}.$$

$$2. \quad \text{ReZG}_3(D_n) = 3 \cdot 2^{n+6} + 387 \cdot 2^{n+1} - 1398.$$

Proof. From the edge partition given in theorem 5 and using definitions, we have

1.

$$\begin{aligned}
 \text{ReZG}_1(D_n) &= \sum_{uv \in E(D_n)} \frac{d_u + d_v}{d_u \cdot d_v} = \sum_{uv \in E_{\{1,2\}}(D_n)} \frac{1+2}{1 \cdot 2} \\
 &\quad + \sum_{uv \in E_{\{2,2\}}(D_n)} \frac{2+2}{2 \cdot 2} + \sum_{uv \in E_{\{2,3\}}(D_n)} \frac{2+3}{2 \cdot 3} \\
 &= |E_{\{1,2\}}(D_n)| \frac{3}{2} + |E_{\{1,3\}}(D_n)| + |E_{\{2,2\}}(D_n)| \frac{5}{6} \\
 &= 3 \cdot 2^{n+2} + 33 \cdot 2^{n-1} - 38.
 \end{aligned}$$

2.

$$\begin{aligned}
\text{ReZG}_2(D_n) &= \sum_{uv \in E(D_n)} \frac{d_u \cdot d_v}{d_u + d_v} = \sum_{uv \in E_{\{1,2\}}(D_n)} \frac{1 \cdot 2}{1 + 2} \\
&+ \sum_{uv \in E_{\{2,2\}}(D_n)} \frac{2 \cdot 2}{2 + 2} + \sum_{uv \in E_{\{2,3\}}(D_n)} \frac{2 \cdot 3}{2 + 3} \\
&= |E_{\{1,2\}}(D_n)| \frac{2}{3} + |E_{\{2,2\}}(D_n)| + |E_{\{2,3\}}(D_n)| \frac{6}{5} \\
&= 3 \cdot 2^{n+2} + 27 \cdot 2^n - \frac{423}{10}.
\end{aligned}$$

□

4 Conclusion

QSARs speak to prescient models got from utilization of measurable devices connecting natural action (counting attractive remedial impact and bothersome reactions) of synthetic activities (drugs/toxicants/ecological contaminations) with descriptors illustrative of atomic structure as well as properties. QSARs are being connected in numerous orders for instance hazard evaluation, lethality expectation, and administrative choices notwithstanding drug revelation and lead improvement. For instance, ETA index have been connected in the advancement of prescient QSAR/QSPR/QSTR models. Dendrimers have lot of application in biology [42], drugs [43], chemistry [44], etc. In this paper, the authors computed the first, second and third redefined Zagreb indices of nanostar dendrimers and $D(n)$. The authors also analyzed Zagreb polynomials of under study nanostar dendrimers. Topological indices computed in this paper can help to understand the structure of dendrimers and with the help of these topological indices we can guess many physicochemical properties of Nanostar dendrimers. See [45-47] for more application.

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