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Topological indices of some families of nanostar dendrimers

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Abstract. A molecular graph is hydrogen depleted chemical structure in which vertices denote atoms and edges denote the bonds. Nanostar dendrimers, a type of chemical compound, have potential in fields such as chemistry, nanotechnology, electronics, optics, materials science and architecture. Nanostar dendrimers and their molecular descriptors are being widely used in QSAR/QSPR and these are studies in chemistry and drug designing as well as modeling of compounds. There are certain types of topological indices like distance based, degree based and counting related topological indices. In this article we gave exacts relationss for first and second Zagreb index, hyper Zagreb index, multiplicative Zagreb indices as well as first and second Zagreb polynomials for some families of nanostar dendrimers.

Keywords. hyper Zagreb index, first multiple Zagreb index, second multiple Zagreb index and Zagreb polynomials, inanostar dendrimers.

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1 Introduction

In mathematical chemistry, we discuss and predict some important properties of a chemical structure by using mathematical techniques. Chemical graph theory is a branch of mathematical Chemistry in which we apply tools from graph theory to mathematically model the chemical phenomenon. This theory plays a noticeable role in the fields of chemical sciences.

In last decade, graph theory has found a considerable use in this area of research. Graph theory has provided chemist with a variety of useful tools, such as topological indices.

Cheminformatics is new subject which is a combination of chemistry, mathematics and information science. It studies quantitative structure-activitys(QSAR) and structure-property (QSPR) relationships that are used to predict the biological activities and properties of chemical com-pounds. In the QSAR/QSPR study, physico-chemical propertiess and topological indices such as Hyper-Zagreb index, fFirst multiple Zagreb index, second multiple Zagreb index and Zagreb polynomials are iused to predict bioactivity of their chemical compounds.

The nanostar dendrimers are part of a new group of macromolecules that appear to be photon funnels like artificial antennas. These macromolecules and more precisely those containing phosphorus are used in the formation of nanotubes, micro and macro capsules, nanolatex, coloured glasses, chemical sensors, modified electrodes, etc. [1]. Nanostar dendrimers are one of the main objects of nano biotechnology. They possess a well defined molecular topology. Their step-wise growth follows a mathematical progression. Dendrimers are highly ordered branched macromolecules which have attracted much theoretical and experimental attention.

Let G be a simple graph, with set of vertices V and set of edges E. A molecular Graph is a simple connected graph where vertices denote atoms and edges denote bonds between atoms of the chemical compound. A molecular descriptor is a single numerical value which correlates the chemical structure with certain Physio chemical properties of the compound and is invariant under graph automorphisms. A large class of molecular descriptors depend on degree of vertices and are called degree based molecular descriptors. Degree of a vertex, say, v is number of vertices joined v by an edge of the graph, and is denoted by $deg(v)$.

Zagreb indices are one of the oldest known topological invariants which first appeared as terms in a formula for analysis of π-electron energy [5] and they grow with the branching of chemical graphs. Balaban et al. [2] named them "Zagreb group indices" which later on termed as first Zagreb index and second Zagreb index and are defined as:

$$M_1(G)=\sum_{uv\in E(G)}[deg(u)+deg(v)], \qquad M_2(G)=\sum_{uv\in E(G)}[deg(u)\times deg(v)].$$

In 2013, Shirdel et al. [12] introduced hyper-Zagreb index which is defined as

$$HM(G)=\sum_{uv\in E(G)}[deg(u)+deg(v)]^2.$$

Ghorbani and Azimi defined first multiple Zagreb index $PM_1(G)$ and second multiple Zagreb index $PM_2(G)$ of a graph G in 2012 [6]. These are given by the following formulae:

Table 1. (du,dv)-type edge partition of $NS_1[n]$.

(d_u, d_v)	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(4, 4)
No. of edges	$2^{n+2} - 6$	2^{n+2}	$2^{n+2} - 6$	$9 \times 2^{n+1} - 28$	2^{n+1}	$7 \times 2^{n} - 10$	2^{n}

$$PM_1(G) = \prod_{uv \in E(G)} [deg(u) + deg(v)], \qquad PM_2(G) = \prod_{uv \in E(G)} [deg(u) \times deg(v)].$$

The first Zagreb polynomial $M_1(G,x)$ and second Zagreb polynomial $M_2(G,x)$ are defined as:

$$M_1(G,x) = \sum_{uv \in E(G)} x^{[deg(u)+deg(v)]} \quad \text{and} \quad \mathrm{M_2(G,x)} = \sum_{\mathrm{uv \in E(G)}} \mathrm{x}^{[\mathrm{deg(u)+deg(v)}]}.$$

These new variants of Zagreb indices have been extensively studied recently [1-13].

2 Main Results

2. 1. First type of nanostar dendrimer $NS_1[n]$

Consider the graph G of first type of nanostar dendrimer $NS_1[n]$. The order and size of $NS_1[n]$ nanostar dendrimers are $9 \times 2^{n+2} - 44$ and $10 \times 2^{n+2} - 50$, respectively. See Figure 1.

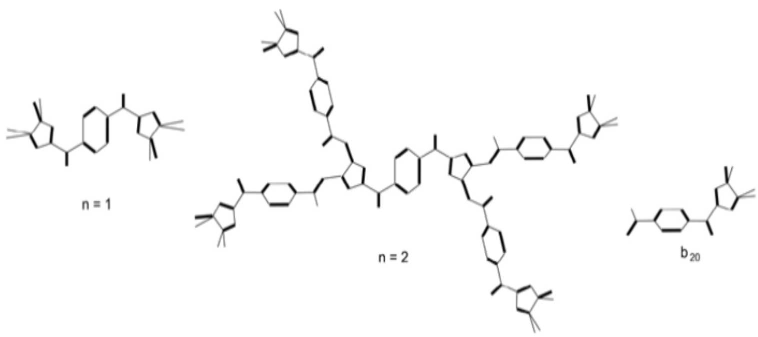

Figure 1. Graph of $NS_1[n]$ with $n = 1$, $n = 2$. The thick edges represent a matching. Here, b_{20} represents a branch of $NS_1[n]$ with 20 vertices.

The edge partition of $NS_1[n]$ with respect to the degrees of the end-vertices of edges given by Table 1.

We compute first Zagreb index, second Zagreb index, hyper-Zagreb index $HM(G)$, first multiple Zagreb index $PM_1(G)$, second multiple Zagreb index $PM_2(G)$, Zagreb polynomials $M_1(G,x)$, $M_2(G,x)$ for $NS_1[n]$ in the following theorem.

Theorem 2.1. *Consider the first type of nanostar dendrimer $NS_1[n]$, then its Zagreb indices and Zagreb polynomials are*

$$M_1(NS_1[n]) = 51 \times 2^{n+2} - 248\,.$$

$$M_2(NS_1[n]) = 247 \times 2^n - 300\ .$$
$$HM(NS_1[n]) = 533 \times 2^{n+1} - 1252.$$
$$PM_1(NS_1[n]) = 2^{19\times 2^n - 24} \times 5^{11\times 2^{n+1}-28} \times 6^{9\times 2^n - 10}\ .$$
$$PM_2(NS_1[n]) = 3^{9\times 2^{n+2}-44} \times 2^{11\times 2^{n+2}-40}.$$
$$M_1(NS_1[n],x) = 2^n x^8 + (9\times 2^n - 10)x^6 + \left(11\times 2^{n+1} - 28\right)x^5 + \left(2^{n+3} - 12\right)x^4.$$

$$M_2(NS_1[n],x) = 2^n x^{16} + (7\times 2^n - 10)x^9 + 2^{n+1}x^8 + \left(9\times 2^{n+1} - 28\right)x^6 + \left(2^{n+3} - 6\right)x^4 + \left(2^{n+3}\ - 6\right)x^3.$$

Proof. Let G be the graph of first type of nanostar dendrimer, $NS_1[n]$. The edge set is partitioned into seven sets, say, E_1, E_2, E_3, E_4, E_5, E_6, E_7 based on the degree of end vertices of each edge. E_1 contains $2^{n+2} - 6$ edges of type uv such that $\deg(u) = 1$, $\deg(v) = 3$, E_2 contains 2^{n+2} edges of type uv such that $\deg(u) = 1$, $\deg(v) = 4$, E_3 contains $2^{n+2} - 6$ edges of type uv such that $\deg(u) = \deg(v) = 2$, E_4 contains $9\times 2^{n+1} - 28$ edges of type uv such that deg(u) = 2, deg (v) = 3, E_5 contains 2^{n+1} edges of type uv such that deg(u) = 2, deg(v)=4, E_6 contains $7\times 2^n - 10$ edges of type uv such that deg(u) = deg(v) = 3 and E_7 contains 2^n edges of type uv such that deg(u) = deg(v) = 4.

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

$$\begin{aligned} M_1(NS_1[n]) = &\sum_{uv\in E_1}[d_u + d_v] + \sum_{uv\in E_2}[d_u + d_v] + \sum_{uv\in E_3}[d_u + d_v] + \sum_{uv\in E_4}[d_u + d_v] \\ &+ \sum_{uv\in E_5}[d_u + d_v] + \sum_{uv\in E_6}[d_u + d_v] + \sum_{uv\in E_7}[d_u + d_v] \\ &= 4|E_1(NS_1[n])| + 5\ |E_2(NS_1[n])| + 4|E_3(NS_1[n])| + 5|E_4(NS_1[n])| \\ &+ 6|E_5(NS_1[n])| + 6|E_6(NS_1[n])| + 8|E_7(NS_1[n])| \\ &= 4\left(2^{n+2} - 6\right) + 5\left(2^{n+2}\right) + 4\left(2^{n+2} - 6\right) + 5\left(9\times 2^{n+1} - 28\right) + 6\left(2^{n+1}\right) \\ &+\ 6(7\times 2^n - 10) + 8(2^n)\ = 51\times 2^{n+2} - 248. \end{aligned}$$

$$\begin{aligned} M_2(G) = &\sum_{uv\in E(G)}[d_u \times d_v]\ M_2(NS_1[n]) = \sum_{uv\in E_1}[d_u \times d_v] + \sum_{uv\in E_2}[d_u \times d_v] \\ &+ \sum_{uv\in E_3}[d_u \times d_v] + \sum_{uv\in E_4}[d_u \times d_v]\ + \sum_{uv\in E_5}[d_u \times d_v] + \sum_{uv\in E_6}[d_u \times d_v] \\ &+ \sum_{uv\in E_7}[d_u \times d_v]\ = 3\ |E_1(NS_1[n])| + 4\ |E_2(NS_1[n])| + 4|E_3(NS_1[n])| \\ &+ 6|E_4(NS_1[n])|\ + 8|E_5(NS_1[n])| + 9|E_6(NS_1[n])| + 16|E_7(NS_1[n])| \\ &= 3\left(2^{n+2} - 6\right) + 4\left(2^{n+2}\right) + 4\left(2^{n+2} - 6\right) + 6\left(9\times 2^{n+1} - 28\right) + 8\left(2^{n+1}\right) \\ &+\ 9(7\times 2^n - 10) + 16(2^n)\ \ 247\times 2^n - 300. \end{aligned}$$

$$HM(G) = \sum_{uv \in E(G)} [d_u + d_v]^2.$$

$$\begin{aligned} HM(NS_1[n]) &= \sum_{uv\in E_1} [d_u + d_v]^2 + \sum_{uv\in E_2} [d_u + d_v]^2 + \sum_{uv\in E_3} [d_u + d_v]^2 + \sum_{uv\in E_4} [d_u + d_v]^2 \\ &+ \sum_{uv\in E_5} [d_u + d_v]^2 + \sum_{uv\in E_6} [d_u + d_v]^2 + \sum_{uv\in E_7} [d_u + d_v]^2 \\ &= 16\ |E_1(NS_1[n])| + 25\ |E_2(NS_1[n])| + 16|E_3(NS_1[n])| + 25|E_4(NS_1[n])| \\ &+ 36|E_5(NS_1[n])| + 36|E_6(NS_1[n])| + 64|E_7(NS_1[n])| \\ &= 16\left(2^{n+2} - 6\right) + 25\left(2^{n+2}\right) + 16\left(2^{n+2} - 6\right) + 25\left(9 \times 2^{n+1} - 28\right) \\ &+ 36\left(2^{n+1}\right) + 36(7 \times 2^n - 10) + 64(2^n) = 533 \times 2^{n+1} - 1252. \end{aligned}$$

$$PM_1(G) = \prod_{uv\in E(G)} [d_u + d_v].$$

$$\begin{aligned} PM_1(NS_1[n]) &= \prod_{uv\in E_1} [d_u + d_v] \times \prod_{uv\in E_2} [d_u + d_v] \times \prod_{uv\in E_3} [d_u + d_v] \times \prod_{uv\in E_4} [d_u + d_v] \\ &\times \prod_{uv\in E_5} [d_u + d_v] \times \prod_{uv\in E_6} [d_u + d_v] \times \prod_{uv\in E_7} [d_u + d_v] = (1+3)^{|E_1(NS_1[n])|} \\ &\times (1+4)^{|E_2(NS_1[n])|} \times (2+2)^{|E_3(NS_1[n])|} \times (2+3)^{|E_4(NS_1[n])|} \\ &= 4^{2^{n+2}-6} \times 5^{2^{n+2}} \times 4^{2^{n+2}-6} \times 5^{9\times 2^{n+1}-28} \times 6^{2^{n+1}} \times 6^{7\times 2^n - 10} \times 8^{2^n} \\ &= 2^{19\times 2^n - 24} \times 5^{11\times 2^{n+1}-28} \times 6^{9\times 2^n - 10}. \end{aligned}$$

$$\begin{aligned} PM_2(G) &= \prod_{uv?E(G)} [d_u \times d_v] PM_2(NS_1[n]) = \prod_{uv\in E_1} [d_u \times d_v] \times \prod_{uv\in E_2} [d_u \times d_v] \\ &\times \prod_{uv\in E_3} [d_u \times d_v] \times \prod_{uv\in E_4} [d_u \times d_v] \times \prod_{uv\in E_5} [d_u \times d_v] \times \prod_{uv\in E_6} [d_u \times d_v] \\ &\times \prod_{uv\in E_7} [d_u \times d_v] = (1\times 3)^{|E_1(NS_1[n])|} \times (1\times 4)^{|E_2(NS_1[n])|} \times (2\times 2)^{|E_3(NS_1[n])|} \\ &\times (2\times 3)^{|E_4(NS_1[n])|} \times (2\times 4)^{|E_5(NS_1[n])|} \times (3\times 3)^{|E_6(NS_1[n])|} \times (4\times 4)^{|E_7(NS_1[n])|} \\ &= 3^{2^{n+2}-6} \times 4^{2^{n+2}} \times 4^{2^{n+2}-6} \times 6^{9\times 2^{n+1}-28} \times 8^{2^{n+1}} \times 9^{7\times 2^n - 10} \times 16^{2^n} \\ &= 3^{9\times 2^{n+2}-44} \times 2^{11\times 2^{n+2}-40}. \end{aligned}$$

First and second Zagreb polynomial of $NS_1[n]$ are computed as:

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

$$M_1(NS_1[n],x) = \sum_{uv\in E_1} x^{[d_u+d_v]} + \sum_{uv\in E_2} x^{[d_u+d_v]} + \sum_{uv\in E_3} x^{[d_u+d_v]} + \sum_{uv\in E_4} x^{[d_u+d_v]} + \sum_{uv\in E_5} x^{[d_u+d_v]} + \sum_{uv\in E_6} x^{[d_u+d_v]} + \sum_{uv\in E_7} x^{[d_u+d_v]}.$$

$$M_1(NS_1[n],x) = (|E_1(NS_1[n])|)x^{1+3} + (|E_2(NS_1[n])|)x^{1+4} + (|E_3(NS_1[n])|)x^{2+2} + (|E_4(NS_1[n])|)x^{2+3} + (|E_5(NS_1[n])|)x^{2+4} + (|E_6(NS_1[n])|)x^{3+3} + (|E_7(NS_1[n])|)x^{4+4} = \left(2^{n+2}-6\right)x^4 + \left(2^{n+2}\right)x^5 + \left(2^{n+2}-6\right)x^4 + \left(9\times 2^{n+1}-28\right)x^5 + \left(2^{n+1}\right)x^6 + (7\times 2^n-10)x^6 + (2^n)x^8 = 2^n x^8 + (9\times 2^n-10)x^6 + \left(11\times 2^{n+1}-28\right)x^5 + \left(2^{n+3}-12\right)x^4.$$

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

$$M_2(NS_1[n],x) = \sum_{uv\in E_1} x^{[d_u\times d_v]} + \sum_{uv\in E_2} x^{[d_u\times d_v]} + \sum_{uv\in E_3} x^{[d_u\times d_v]} + \sum_{uv\in E_4} x^{[d_u\times d_v]} + \sum_{uv\in E_5} x^{[d_u\times d_v]} + \sum_{uv\in E_6} x^{[d_u\times d_v]} + \sum_{uv\in E_7} x^{[d_u\times d_v]}.$$

$$M_2(NS_1[n],x) = (|E_1(NS_1[n])|)x^{1\times 3} + (|E_2(NS_1[n])|)x^{1\times 4} + (|E_3(NS_1[n])|)x^{2\times 2} + (|E_4(NS_1[n])|)x^{2\times 3} + (|E_5(NS_1[n])|)x^{2\times 4} + (|E_6(NS_1[n])|)x^{3\times 3} + (|E_7(NS_1[n])|)x^{4\times 4} = \left(2^{n+2}-6\right)x^3 + \left(2^{n+2}\right)x^4 + \left(2^{n+2}-6\right)x^4 + \left(9\times 2^{n+1}-28\right)x^6 + \left(2^{n+1}\right)x^8 + (7\times 2^n-10)x^9 + (2^n)x^{16} = 2^n x^{16} + (7\times 2^n-10)x^9 + 2^{n+1}x^8 + \left(9\times 2^{n+1}-28\right)x^6 + \left(2^{n+3}-6\right)x^4 + \left(2^{n+3}-6\right)x^3.$$

2. 2. Second type of nanostar dendrimer $NS_2[n]$

We denote the molecular graph of polyphenylene nanostar dendrimer by $NS_2[n]$. The order and size of $NS_2[n]$ nanostar dendrimers are $15\times 2^{n+3}-95$ and $35\times 2^{n+2}-112$, respectively. See Figure 2.

The edge partition of $NS_2[n]$ with respect to the degrees of the end-vertices of edges given by Table 2.

We compute first Zagreb index, second Zagreb index, hyper-Zagreb index $HM(G)$, first multiple Zagreb index $PM_1(G)$, second multiple Zagreb index $PM_2(G)$, Zagreb polynomials $M_1(G,x)$, $M_2(G,x)$ for $NS_2[n]$ in the following theorem.

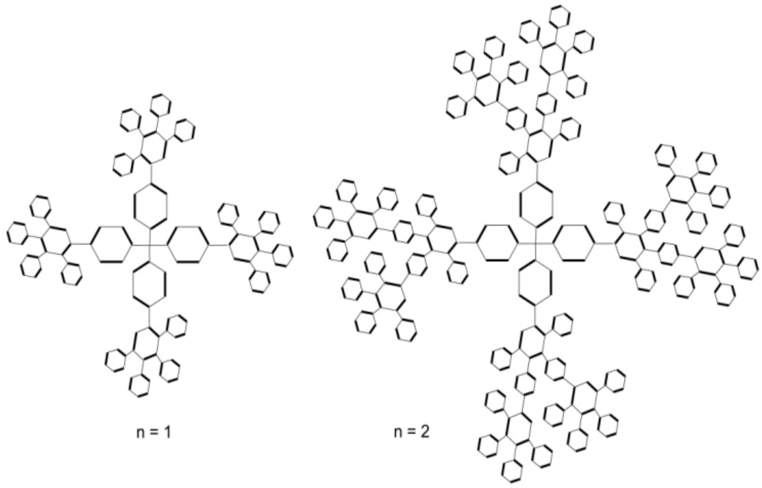

Figure 2. Graph of $NS_2[n]$ with $n = 1$, $n = 2$. $NS_2[n]$ is also known as Polyphenylene dendrimer. The thick edges represent a matching.

Table 2. (du,dv)-type edge partition of $NS_2[n]$.

(d_u, d_v)	(2, 2)	(2, 3)	(3, 3)	(3, 4)
No. of edges	$7 \times 2^{n+3} - 40$	$11 \times 2^{n+2} - 32$	$10 \times 2^{n+2} - 44$	4

Theorem 2.2. *Consider the first type of nanostar dendrimers $NS_2[n]$, then its Zagreb indices and Zagreb polynomials are*

$$M_1(NS_2[n]) = 7 \times 2^{n+5} + 115 \times 2^{n+2} - 556\,.$$

$$M_2(NS_2[n]) = 7 \times 2^{n+5} + 78 \times 2^{n+3} - 700\,.$$

$$HM(NS_2[n]) = 7 \times 2^{n+7} + 45 \times 2^{n+5} + 275 \times 2^{n+2} - 2828.$$

$$PM_1(NS_2[n]) = 2^{19 \times 2^{n+3} - 124} \times 3^{5 \times 2^{n+3} - 44} \times 5^{11 \times 2^{n+2} - 32} \times 7^4.$$

$$PM_2(NS_2[n]) = 2^{67 \times 2^{n+2} - 104} \times 3^{31 \times 2^{n+2} - 116}\,.$$

$$M_1(NS_2[n], x) = 7x^7 + \left(5 \times 2^{n+3} - 44\right)x^6 + \left(11 \times 2^{n+2} - 32\right)x^5 + \left(7 \times 2^{n+3} - 40\right)x^4 M_2.$$

$$(NS_2[n], x) = 4x^{12} + \left(5 \times 2^{n+3} - 44\right)x^9 + \left(11 \times 2^{n+2} - 32\right)x^6 + \left(7 \times 2^{n+3} - 40\right)x^4.$$

Proof. Let G be the graph of first type of nanostar dendrimers, $NS_2[n]$. The edge set is partitioned into four sets, say, E_1, E_2, E_3, E_4 based on the degree of end vertices of each edge. E_1 contains $7 \times 2^{n+3} - 40$ edges of type uv such that $\deg(u) = \deg(v) = 2$, E_2 contains

$11 \times 2^{n+2} - 32$ edges of type uv such that $\deg(u) = 2$, $\deg(v) = 3$, E_3 contains $10 \times 2^{n+2} - 44$ edges of type uv such that $\deg(u) = 3$, $\deg(v) = 3$, E_4 contains 4 edges of type uv such that deg (u) = 3, deg (v) = 4.

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

$$\begin{aligned} M_1(NS_2[n]) &= \sum_{uv \in E_1} [d_u + d_v] + \sum_{uv \in E_2} [d_u + d_v] + \sum_{uv \in E_3} [d_u + d_v] + \sum_{uv \in E_4} [d_u + d_v] \\ &= 4\ |E_1(NS_2[n])| + 5\ |E_2(NS_2[n])| + 6|E_3(NS_2[n])| + 7|E_4(NS_2[n])| \\ &= 4(7 \times 2^{n+3} - 40) + 5(11 \times 2^{n+2} - 32) + 6(10 \times 2^{n+2} - 44) + 7(4) \\ &= 7 \times 2^{n+5} + 115 \times 2^{n+2} - 556. \end{aligned}$$

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

$$\begin{aligned} M_2(NS_2[n]) &= \sum_{uv \in E_1} [d_u \times d_v] + \sum_{uv \in E_2} [d_u \times d_v] + \sum_{uv \in E_3} [d_u \times d_v] + \sum_{uv \in E_4} [d_u \times d_v] \\ &= 4\ |E_1(NS_2[n])| + 6\ |E_2(NS_2[n])| + 9|E_3(NS_2[n])| + 12|E_4(NS_2[n])| \\ &= 4(7 \times 2^{n+3} - 40) + 6(11 \times 2^{n+2} - 32) + 9(10 \times 2^{n+2} - 44) + 12(4) \\ &= 7 \times 2^{n+5} + 78 \times 2^{n+3} - 700. \end{aligned}$$

$$HM(G) = \sum_{uv \in E(G)} [d_u + d_v]^2.$$

$$\begin{aligned} HM(NS_2[n]) &= \sum_{uv \in E_1} [d_u + d_v]^2 + \sum_{uv \in E_2} [d_u + d_v]^2 + \sum_{uv \in E_3} [d_u + d_v]^2 + \sum_{uv \in E_4} [d_u + d_v]^2 \\ &= 16\ |E_1(NS_2[n])| + 25\ |E_2(NS_2[n])| + 36|E_3(NS_2[n])| + 49|E_4(NS_2[n])| \\ &= 16(7 \times 2^{n+3} - 40) + 25(11 \times 2^{n+2} - 32) + 36(10 \times 2^{n+2} - 44) + 49(4) \\ &= 7 \times 2^{n+7} + 45 \times 2^{n+5} + 275 \times 2^{n+2} - 2828. \end{aligned}$$

$$PM_1(G) = \prod_{uv \in E(G)} [d_u + d_v].$$

$$\begin{aligned} PM_1(NS_2[n]) &= \prod_{uv \in E_1} [d_u + d_v] \times \prod_{uv \in E_2} [d_u + d_v] \times \prod_{uv \in E_3} [d_u + d_v] \times \prod_{uv \in E_4} [d_u + d_v] \\ &= (2+2)^{|E_1(NS_2[n])|} \times (2+3)^{|E_2(NS_2[n])|} \times (3+3)^{|E_3(NS_2[n])|} \\ &\times (3+4)^{|E_4(NS_2[n])|} = 4^{7 \times 2^{n+3} - 40} \times 5^{11 \times 2^{n+2} - 32} \times 6^{10 \times 2^{n+2} - 44} \times 7^4 \\ &= 2^{19 \times 2^{n+3} - 124} \times 3^{5 \times 2^{n+3} - 44} \times 5^{11 \times 2^{n+2} - 32} \times 7^4. \end{aligned}$$

$$PM_2(G) = \prod_{uv?E(G)} [d_u \times d_v].$$

$$\begin{aligned}PM_2(NS_2[n]) &= \prod_{uv\in E_1}[d_u \times d_v] \times \prod_{uv\in E_2}[d_u \times d_v] \times \prod_{uv\in E_3}[d_u \times d_v] \times \prod_{uv\in E_4}[d_u \times d_v]\\ &= (2\times 2)^{|E_1(NS_2[n])|} \times (2\times 3)^{|E_2(NS_2[n])|} \times (3\times 3)^{|E_3(NS_2[n])|}\\ &\times (3\times 4)^{|E_4(NS_2[n])|} = 4^{7\times 2^{n+3}-40} \times 6^{11\times 2^{n+2}-32} \times 9^{10\times 2^{n+2}-44} \times 12^4\\ &= 2^{67\times 2^{n+2}-104} \times 3^{31\times 2^{n+2}-116}.\end{aligned}$$

First and second Zagreb polynomial of $NS_2[n]$ are computed as:

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

$$\begin{aligned}M_1(NS_2[n],x) &= \sum_{uv\in E_1} x^{[d_u+d_v]} + \sum_{uv\in E_2} x^{[d_u+d_v]} + \sum_{uv\in E_3} x^{[d_u+d_v]} + \sum_{uv\in E_4} x^{[d_u+d_v]}\\ &= (|E_1(NS_2[n])|)\,x^{2+2} + (|E_2(NS_2[n])|)\,x^{2+3} + (|E_3(NS_2[n])|)\,x^{3+3}\\ &+ (|E_4(NS_2[n])|)\,x^{3+4} = (7\times 2^{n+3}-40)x^4 + (11\times 2^{n+2}-32)x^5\\ &+ (10\times 2^{n+2}-44)x^6 + (4)x^7.\end{aligned}$$

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

$$M_2(NS_2[n],x) = \sum_{uv\in E_1} x^{[d_u\times d_v]} + \sum_{uv\in E_2} x^{[d_u\times d_v]} + \sum_{uv\in E_3} x^{[d_u\times d_v]} + \sum_{uv\in E_4} x^{[d_u\times d_v]}.$$

$$\begin{aligned}M_2(NS_2[n],x) &= (|E_1(NS_2[n])|)\,x^{2\times 2} + (|E_2(NS_2[n])|)\,x^{2\times 3} + (|E_3(NS_2[n])|)\,x^{3\times 3}\\ &+ (|E_4(NS_2[n])|)\,x^{3\times 4}\\ &= (7\times 2^{n+3}-40)x^4 + (11\times 2^{n+2}-32)x^6 + (10\times 2^{n+2}-44)x^9 + (4)x^{12}.\end{aligned}$$

2. 3. Third type of nanostar dendrimer $NS_3[n]$

Consider the graph G of first type of nanostardendrimers, $NS_3[n]$. Since $NS_3[n]$ is a unicyclic graph, its order and size are same and are equal to $3 \times 2^{n+1} + 3$. See Figure 3.

The edge partition of $NS_3[n]$ with respect to the degrees of the end-vertices of edges given by Table 3.

We compute first Zagreb index, second Zagreb index, hyper-Zagreb index $HM(G)$, first multiple Zagreb index $PM_1(G)$, second multiple Zagreb index $PM_2(G)$, Zagreb polynomials $M_1(G,x)$, $M_2(G,x)$ for $NS_3[n]$ in the following theorem.

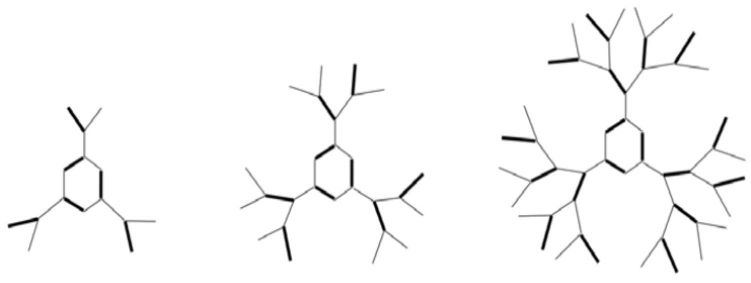

Figure 3. Graph of $NS_3[n]$ with $n = 1,2,3$. The thick edges represent a matching.

Table 3. (du,dv)-type edge partition of $NS_3[n]$.

(d_u, d_v)	$(1,3)$	$(2,3)$	$(3,3)$
No. of edges	3×2^n	6	$3\times 2^n - 3$

Theorem 2.3. *Consider the first type of nanostardendrimers $NS_3[n]$, then its Zagreb indices and Zagreb polynomials are*

$$M_1(NS_3[n]) = 15\times 2^{n+1} + 12\,.$$

$$M_2(NS_3[n]) = 9\times 2^{n+2} + 9\,.$$

$$HM(NS_3[n]) = 39\times 2^{n+2} + 42.$$

$$PM_1(NS_3[n]) = 2^{9\times 2^n - 3}\times 3^{3\times 2^n - 3}\times 5^6.$$

$$PM_2(NS_3[n]) = 3^{9\times 2^n}\times 2^6.$$

$$M_1(NS_3[n],x) = (3\times 2^n - 3)\,x^6 + 6x^5 + (3\times 2^n)\,x^4.$$

$$M_2(NS_3[n],x) = (3\times 2^n - 3)\,x^9 + 6x^6 + (3\times 2^n)\,x^3.$$

Proof. Let G be the graph of first type of nanostardendrimers, $NS_3[n]$. The edge set is partitioned into three sets, say, E_1, E_2, E_3 based on the degree of end vertices of each edge. E_1 contains 3×2^n edges of type uv such that $\deg(u) = 1$, $\deg(v) = 3$, E_2 contains 6 edges of type uv such that $\deg(u) = 2$, $\deg(v) = 3$, E_3 contains $3\times 2^n - 3$ edges of type uv such that $\deg(u) = \deg(v) = 3$.

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

$$\begin{aligned} M_1(NS_3[n]) &= \sum_{uv\in E_1} [d_u + d_v] + \sum_{uv\in E_2} [d_u + d_v] + \sum_{uv\in E_3} [d_u + d_v] \\ &= 4\,|E_1(NS_3[n])| + 5\,|E_2(NS_3[n])| + 6|E_3(NS_3[n])| \\ &= 4(3\times 2^n) + 5(6) + 6(3\times 2^n - 3) = 15\times 2^{n+1} + 12. \end{aligned}$$

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

$$\begin{aligned} M_2(NS_3[n]) &= \sum_{uv \in E_1} [d_u \times d_v] + \sum_{uv \in E_2} [d_u \times d_v] + \sum_{uv \in E_3} [d_u \times d_v] \\ &= 3\ |E_1(NS_3[n])| + 6\ |E_2(NS_3[n])| + 9|E_3(NS_3[n])| \\ &= 3(3 \times 2^n) + 6(6) + 9(3 \times 2^n - 3) = 9 \times 2^{n+2} + 9. \end{aligned}$$

$$HM(G) = \sum_{uv \in E(G)} [d_u + d_v]^2.$$

$$\begin{aligned} HM(NS_3[n]) &= \sum_{uv \in E_1} [d_u + d_v]^2 + \sum_{uv \in E_2} [d_u + d_v]^2 + \sum_{uv \in E_3} [d_u + d_v]^2 \\ &= 16\ |E_1(NS_3[n])| + 25\ |E_2(NS_3[n])| + 36|E_3(NS_3[n])| \\ &= 16(3 \times 2^n) + 25(6) + 36(3 \times 2^n - 3) = 39 \times 2^{n+2} + 42. \end{aligned}$$

$$PM_1(G) = \prod_{uv \in E(G)} [d_u + d_v].$$

$$\begin{aligned} PM_1(NS_3[n]) &= \prod_{uv \in E_1} [d_u + d_v] \times \prod_{uv \in E_2} [d_u + d_v] \times \prod_{uv \in E_3} [d_u + d_v] \\ &= (1+3)^{|E_1(NS_3[n])|} \times (2+3)^{|E_2(NS_3[n])|} \times (3+3)^{|E_3(NS_3[n])|} \\ &= 4^{3 \times 2^n} \times 5^6 \times 6^{3 \times 2^n - 3} = 2^{9 \times 2^n - 3} \times 3^{3 \times 2^n - 3} \times 5^6. \end{aligned}$$

$$PM_2(G) = \prod_{uv?E(G)} [d_u \times d_v]$$

$$\begin{aligned} PM_2(NS_3[n]) &= \prod_{uv \in E_1} [d_u \times d_v] \times \prod_{uv \in E_2} [d_u \times d_v] \times \prod_{uv \in E_3} [d_u \times d_v] \\ &= (1 \times 3)^{|E_1(NS_3[n])|} \times (2 \times 3)^{|E_2(NS_3[n])|} \times (3 \times 3)^{|E_3(NS_3[n])|} \\ &= 3^{3 \times 2^n} \times 6^6 \times 9^{3 \times 2^n - 3} = 3^{9 \times 2^n} \times 2^6. \end{aligned}$$

First and second Zagreb polynomial of $NS_3[n]$ are computed as:

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

$$M_1(NS_3[n], x) = \sum_{uv \in E_1} x^{[d_u + d_v]} + \sum_{uv \in E_2} x^{[d_u + d_v]} + \sum_{uv \in E_3} x^{[d_u + d_v]}.$$

$$M_1\left(NS_3\left[n\right],x\right)=\left(\left|E_1\left(NS_3\left[n\right]\right)\right|\right)x^{1+3}+\left(\left|E_2\left(NS_3\left[n\right]\right)\right|\right)x^{2+3}+\left(\left|E_3\left(NS_3\left[n\right]\right)\right|\right)x^{3+3}$$
$$=\left(3\times 2^n\right)x^4+6x^5+\left(3\times 2^n-3\right)x^6=\left(3\times 2^n-3\right)x^6+6x^5+\left(3\times 2^n\right)x^4.$$

$$M_2\left(G,x\right)=\sum_{uv\in E(G)}x^{[d_u\times\, d_v]}.$$

$$M_2\left(NS_3\left[n\right],x\right)=\sum_{uv\in\, E_1}x^{[d_u\times\, d_v]}+\sum_{uv\in\, E_2}x^{[d_u\times\, d_v]}+\sum_{uv\in\, E_3}x^{[d_u\times\, d_v]}.$$

$$M_2\left(NS_3\left[n\right],x\right)=\left(\left|E_1\left(NS_3\left[n\right]\right)\right|\right)x^{1\times 3}+\left(\left|E_2\left(NS_3\left[n\right]\right)\right|\right)x^{2\times 3}+\left(\left|E_3\left(NS_3\left[n\right]\right)\right|\right)x^{3\times 3}$$
$$=\left(3\times 2^n\right)x^3+6x^6+\left(3\times 2^n-3\right)x^9=\left(3\times 2^n-3\right)x^9+6x^6+\left(3\times 2^n\right)x^3.$$

3 Conclusion

In this paper, we consider some infinite families of nanostar dendrimers. Different variants of Zagreb indices and Zagreb polynomials are analysed for nanostar dendrimers using edge partition based on degree of vertices of the edges of the corresponding chemical graphs. We found exact relations of First Zagreb index, second Zagreb index, hyper Zagreb index, multiplicative Zagreb indices as well as Zagreb polynomials for nanostar dendrimers. In future, we are interested to found some new chemical compound and then study their topological indices which will be quite helpful to understand their underlying topologies.

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References

[1] A. R. Ashrafi and M. Mirzargar, PI Szeged and edge Szeged indices of an infinite family of nanostar dendrimers, Indian J. Chem. 47 (2008) 538 -541.
[2] A. T. Balaban, I. Motoc, D. Bonchev and O. Mekenyan, Topological indices for structure- activity correlations, Topics Curr. Chem. 114 (1983) 21–55.
[3] M. Eliasi, A. Iranmanesh and I. Gutman, Multiplicative version of first Zagreb index, MATCH Commun. Math. Comput. Chem. 68 (2012) 217–230.
[4] B. Furtula, I. Gutman and M. Dehmer, On structure-sensitivity of degree-based topological indices, Appl. Math. Comput. 219 (2013) 8973–8978.
[5] I. Gutman and N. Trinajstic, Graph theory and molecular orbitals total ϕ-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535–538.
[6] M. Ghorbani and N. Azimi, Note on multiple Zagreb indices, Iranian. J. Math. Chem. 3 (2) (2012) 137–143.
[7] I. Gutman and K. C. Das, Some Properties of the Second Zagreb Index, MATCH Commun. Math. Comput. Chem. 50 (2004) 103–112.

[8] I. Gutman, B. Furtula, Z. K. Vukicevic and G. Popivoda, On Zagreb Indices and Coindices, MATCH Commun. Math. Comput. Chem. 74 (1) (2015) 5–16.
[9] I. Gutman, Degree-based topological indices, Croat. Chem. Acta. 86 (2013) 351–361.
[10] S. Hayat and M. Imran, Computation of topological indices of certain networks, Appl. Math. Comput. 240 (2014) 213–228.
[11] J. Rada, R. Cruz and I. Gutman, Benzenoid systems with extremal vertex-degree-based topological indices, MATCH Commun. Math. Comput. Chem. 72 (2014) 125–136.
[12] G. H. Shirdel, H. R. Pour and A. M. Sayadi, The Hyper-Zagreb index of graph operations, Iranian. J. Math. Chem. 4 (2) (2013) 213–220.
[13] M. K. Siddiqui, M. Imran and A. Ali, On Zagreb indices, Zagreb polynomials of some nanostar dendrimers, Appl. Math. Comput. 280 (2016) 132-139.