THE (a,b)-ZAGREB INDEX OF NANOSTAR DENDRIMERS

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In chemical graph theory, the structure of any chemical compound can be represented as a graph whose vertices correspond to the atoms and edges correspond to bonds between them. In this work, we study one generalized Zagreb index called (a; b)-Zagreb index of some nanostar dendrimers, which are generally large, complex and highly branched well-defined chemical structure.

Keywords: Degree-based topological indices, Generalized Zagreb index, Nanostar dendrimers

1. Introduction

Let $G = (V(G), E(G))$ be a simple graph, where $V(G)$ and $E(G)$ are the vertex and edge sets of G, n and m represent the number of vertices and edges of G respectively. The degree of a vertex $v \in V(G)$ is defined as the number of adjacent vertices of v in G and is denoted as $d_G(v)$. A topological index is a real number related to a chemical constitution for correlation of a chemical structure with various physicochemical properties. Quantitative structure-activity relationships (QSAR) and quantitative structure-properties relationships (QSPR) are mathematical correlation between a specified biological activity and one or more physicochemical properties, known as descriptors as they describe the activity or property under examination. Different topological indices are correlate with biological and physicochemical properties of chemical compounds. Therefore, they are useful descriptors in QSAR and QSPR that are used for predictive purposes, such as prediction of the toxicity of a chemical or the potency of a drug for future release in the market. In chemical graph theory, there are various topological indices were introduced by different researchers, among which the Zagreb indices are oldest and extremely studied vertex degree-based topological indices and were introduced by Gutman and Trinajestić in 1972 [1], to study the total π-electron energy (ϵ) of carbon atoms. The present authors studied these indices for new operations related to different subdivision related

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graphs [2], double join related to the total graph [3], double corona based on total graph [4] and are defined as

$$M_1(G) = \sum_{v\in V(G)} d_G(v)^2 = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]$$

and

$$M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v).$$

The "forgotten topological index" or F-index of a graph was introduced in the same paper [1], where Zagreb indices were introduced. This index is defined as

$$\boldsymbol{F(G) = \sum_{v\in V(G)} d_G(v)^3 = \sum_{uv\in E(G)} [d_G(u)^2 + d_G(v)^2]}.$$

One of the redefined version of the Zagreb index is defined as

$$ReZM(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)[d_G(u) + d_G(v)].$$

and was first introduced by Ranjini et al. in 2013 [5]. Li and Zheng in [6], generalised the first Zagreb index and F-index as follows

$$M^\alpha(G) = \sum_{u\in V(G)} d_G(u)^\alpha$$

where, $\alpha \neq 0, 1$ and $\alpha \in R$. Clearly, when $\alpha = 2$ we get first Zagreb index and when $\alpha = 3$ it gives the F-index. Gutman and Lepovic$'$ generalized the Randic$'$ index in [7], and is defined as

$$R_a = \sum_{uv\in E(G)} \{d_G(u)d_G(v)\}^a.$$

Where, $a \neq 0,$ $a \in R.$ The Symmetric division deg index of a graph is defined as

$$SDD(G) = \sum_{uv\in E(G)} [\frac{d_G(u)}{d_G(v)} + \frac{d_G(v)}{d_G(u)}].$$

We refer our reader to [8, 9], for further study about this index. Based on Zagreb indices Azari et al. [10], introduced the $(a; b)$ −Zagreb index in 2011 and is defined as

$$Z_{a,b}(G) = \sum_{uv\in E(G)} [d_G(u)^a d_G(v)^b + d_G(u)^b d_G(v)^a].$$

Recently, Sarkar et al. [11], studied this index for some derived networks, Farahani and Kanna studied this index for V-phenylenic nanotubes and nanotori molecules [12], Farahani himself studied this index for circum-coronene series of benzenoid [13].

It is clear that, for some particular values of a and b we can derive some other topological indices directly as a special case of (a,b)-Zagreb index as shown in table 1.

In this work, we study the mathematical property of (a,b) −Zagreb index for five types of infinite nanostar dendrimers namely $NS_1[n]$, $NS_2[n]$, $NS_3[n]$, $NS_4[n]$ and $NS_5[n]$.

Table 1

Relations between (a,b) −Zagreb index with some other topological indices

Topological index	**Corresponding (a,b) −Zagreb index**
First Zagreb index $M_1(G)$	$Z_{1,0}(G)$
Second Zagreb index $M_2(G)$	$\frac{1}{2}Z_{1,1}(G)$
Forgotten topological index F(G)	$Z_{2,0}(G)$
Redefined Zagreb index ReZM(G)	$Z_{2,1}(G)$
General first Zagreb index $M^a(G)$	$Z_{a-1,0}(G)$
General Randic′index $R_a(G)$	$\frac{1}{2}Z_{a,a}(G)$
Symmetric division deg index SDD(G)	$Z_{1,-1}(G)$

In general, dendrimers are synthesized from monomers by iterative growth and activation steps. The structure of nanostar dendrimers is mainly depended on the three parts namely core, branches and end groups. In molecular graph theory, there are various applications of nanostar dendrimers for formations of nano tubes, chemical sensors, electrodes, colored glasses and many more. The study about dendrimers received a great attention in the chemical and mathematical literature. Recently, various researchers studied the different topological indices of nanostar dendrimers. Graovac et al. [14], studied the fifth geometric-arithmetic index, De et al. in [15], studied the F-index of nanostar dendrimers, Siddiqui et al. studied the Zagreb indices for different nanostar dendrimers in [16], Madanshekaf found Randic′ index for some different classes nanostar dendrimers in [17, 18].

2. Main Results

In this section we derived (a,b)-Zagreb index of some nanostar dendrimers. First, we consider $NS_1[n]$. The edge sets of $NS_1[n]$ are divided into four parts and the degree of all the vertex are shown as follows:

$$E_1(NS_1[n]) = \{e = uv \in E(NS_1[n]): d_{NS_1[n]}(u) = 1 \text{ and } d_{NS_1[n]}(v) = 2\}$$

$$E_2(NS_1[n]) = \{e = uv \in E(NS_1[n]): d_{NS_1[n]}(u) = 1 \text{ and } d_{NS_1[n]}(v) = 3\}$$

$$E_3(NS_1[n]) = \{e = uv \in E(NS_1[n]): d_{NS_1[n]}(u) = 2 \text{ and } d_{NS_1[n]}(v) = 2\}$$

$$E_4(NS_1[n]) = \{e = uv \in E(NS_1[n]): d_{NS_1[n]}(u) = 2 \text{ and } d_{NS_1[n]}(v) = 3\}$$

note that, $|E_1(NS_1[n])| = 2^{n+1}$, $|E_2(NS_1[n])| = 4(2^n - 1)$, $|E_3(NS_1[n])| = (12.2^n - 11)$,

$|E_4(NS_1[n])| = (14.2^n - 14)$. The figure of $NS_1[n]$ is shown in Fig. 1.

Theorem 2.1. The (a,b)-Zagreb index of nanostar $NS_1[n]$ is

$$Z_{a,b}(NS_1[n]) = 2^{n+1}(2^a + 2^b) + 4(2^n - 1)(3^a + 3^b) + (12.2^n - 11).2^{a+b+1}$$
$$+(14.2^n - 14)(2^a.3^b + 2^b.3^a). \quad (1)$$

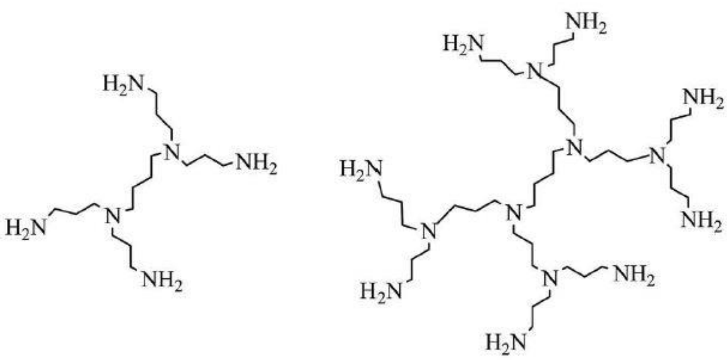

Fig. 1. Polypropylenimine octaamine dendrimer $(NS_1[n])$.

Proof. Applying the definition of (a,b) −Zagreb index, we get

$$Z_{a,b}(NS_1[n]) = \sum_{uv\in E(NS_1[n])} [d_{NS_1[n]}(u)^a d_{NS_1[n]}(v)^b + d_{NS_1[n]}(u)^b d_{NS_1[n]}(v)^a]$$

$$= \sum_{uv\in E_1(NS_1[n])} (1^a.2^b + 1^b.2^a) + \sum_{uv\in E_2(NS_1[n])} (1^a.3^b + 1^b.3^a) + \sum_{uv\in E_3(NS_1[n])} (2^a.2^b + 2^b.2^a) + \sum_{uv\in E_4(NS_1[n])} (2^a.3^b + 2^b.3^a)$$

$$= |E_1(NS_1[n])|(2^a + 2^b) + |E_2(NS_1[n])|(3^a + 3^b) + |E_3(NS_1[n])|(2^{a+b} + 2^{a+b}) + |E_4(NS_1[n])|(2^a.3^b + 2^b.3^a)$$

$$= 2^{n+1}.(2^a + 2^b) + 4(2^n - 1)(3^a + 3^b) + (12.2^n - 11).2.2^{a+b}$$

$$+(14.2^n - 14)(2^a.3^b + 2^b.3^a).$$

Hence, the theorem.

Corollary 2.1. From equation 1, we derived the following results,

(i) $M_1(NS_1[n]) = Z_{1,0}(NS_1[n]) = 10(14.2^n - 13)$,

(ii) $M_2(NS_1[n]) = \frac{1}{2}Z_{1,1}(NS_1[n]) = 4(37.2^n - 35)$,

(iii)

$F(NS_1[n]) = Z_{2,0}(NS_1[n]) = 5.2^{n+1} + 40(2^n - 1) + 8(12.2^n - 11) + 182(2^n - 1)$,

(iv) $ReZM(NS_1[n]) = Z_{2,1}(NS_1[n]) = 6.2^{n+1} + 48(2^n - 1) + 16(12.2^n - 11)$

$+420(2^n - 1)$,

(v) $M^a(NS_1[n]) = Z_{a-1,0}(NS_1[n]) = 2^{n+1}(20.2^{a-1} + 9.3^{a-1} + 3) - 36.2^{a-1}$

$-18.3^{a-1} - 4$,

(vi) $R_a(NS_1[n]) = \frac{1}{2}Z_{a,a}(NS_1[n]) = 2^n(2^{a+1} + 4.3^a + 12.4^a + 7.2^{a+1}.3^a)$
$-(4.3^a + 11.4^a + 7.2^{a+1}.3^a)$,

(vii)

$SDD(NS_1[n]) = Z_{1,-1}(NS_1[n]) = 5.2^n + \frac{40}{3}(2^n - 1) + 2(12.2^n - 11) + \frac{91}{3}(2^n - 1).$

Now, we consider the nanostar $NS_2[n]$ and obtained the (a,b)-Zagreb index of this nanostar. The figure of nanostar $NS_2[n]$ is shown in Fig. 2. The edge sets and all the vertex degree of this nanostar are shown as follows:

$E_1(\mathrm{NS_2[n]}) = \{e = uv \in E(\mathrm{NS_2[n]}): d_{\mathrm{NS_2[n]}}(u) = 1 \ and\ d_{\mathrm{NS_2[n]}}(v) = 2\}$

$E_2(\mathrm{NS_2[n]}) = \{e = uv \in E(\mathrm{NS_2[n]}): d_{\mathrm{NS_2[n]}}(u) = 2 \ and\ d_{\mathrm{NS_2[n]}}(v) = 2\}$

$E_3(\mathrm{NS_2[n]}) = \{e = uv \in E(\mathrm{NS_2[n]}): d_{\mathrm{NS_2[n]}}(u) = 2 \ and\ d_{\mathrm{NS_2[n]}}(v) = 3\}$

such that, $|E_1(\mathrm{NS_2[n]})| = 2^{n+1}, |E_2(\mathrm{NS_2[n]})| = 8.(2^n - 5),$

$|E_3(\mathrm{NS_2[n]})| = (6.2^n - 6).$

Theorem 2.2. For nanostar NS2[n], the (a; b)-Zagreb is given by

$$\mathrm{Z_{a,b}}(\mathrm{NS_2[n]}) = 2^{n+1}(2^a + 2^b) + (8.2^n - 5).2^{a+b+1}$$
$$+6(2^n - 1)(2^a.3^b + 2^b.3^a). \qquad (2)$$

Proof. Using the concept of (a,b)-Zagreb index, we get

$$Z_{a,b}(NS_2[n]) = \sum_{uv \in E(NS_2[n])} [d_{NS_2[n]}(u)^a d_{NS_2[n]}(v)^b + d_{NS_2[n]}(u)^b d_{NS_2[n]}(v)^a]$$

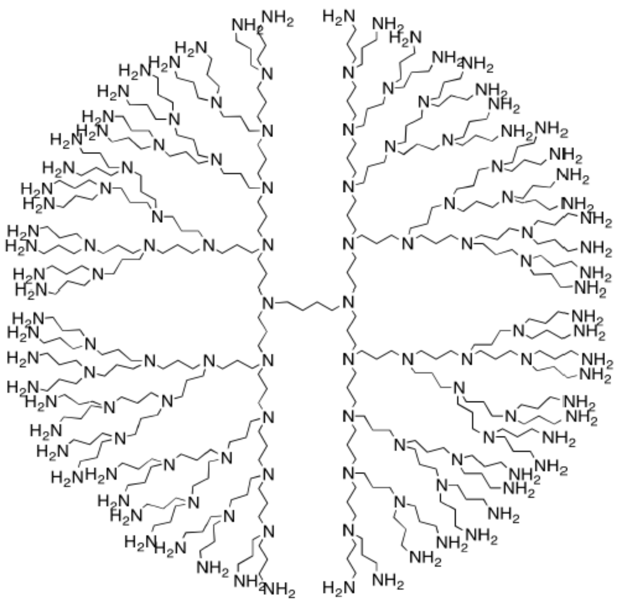

Fig. 2. Polypropylenimine octaamine dendrimer NS2[n]

$$= \sum_{uv \in E_1(NS_2[n])} \left(1^a.2^b + 1^b.2^a\right) + \sum_{uv \in E_2(NS_2[n])} \left(2^a.2^b + 2^b.2^a\right) + \sum_{uv \in E_3(NS_2[n])} \left(2^a.3^b + 2^b.3^a\right)$$

$$= |E_1(NS_2[n])|\left(2^a + 2^b\right) + |E_2(NS_2[n])|2.2^{a+b} + |E_3(NS_2[n])|\left(2^a.3^b + 2^b.3^a\right)$$

$$= 2^{n+1}.\left(2^a + 2^b\right) + \left(8.2^n - 5\right).2.2^{a+b} + 6(2^n - 1)\left(2^a.3^b + 2^b.3^a\right).$$

Which is the required theorem.

Corollary 2.2. We derived the following results by using equation 2,

(i) $M_1(NS_2[n]) = Z_{1,0}(NS_2[n]) = 68.2^n - 50,$

(ii) $M_2(NS_2[n]) = \frac{1}{2}Z_{1,1}(NS_2[n]) = 72.2^n - 56,$

(iii) $F(NS_2[n]) = Z_{2,0}(NS_2[n]) = 5.2^{n+1} + 8(8.2^n - 5) + 78(2^n - 1),$

(iv) $ReZM(NS_2[n]) = Z_{2,1}(NS_2[n]) = 6.2^{n+1} + 16(8.2^n - 5) + 180(2^n - 1),$

(v)

$M^a(NS_2[n]) = Z_{a-1,0}(NS_2[n]) = 2^{n+1}(12.2^{a-1} + 3.3^{a-1} + 1) - 2(8.2^{a-1} + 3.3^{a-1})$

,

(vi) $R_a(NS_2[n]) = \frac{1}{2} Z_{a,a}(NS_2[n]) = 2^n(2^{a+1} + 8.4^a + 2^{a+1}.3^{a+1})$
$-(5.4^a + 2^{a+1}.3^{a+1}),$

(vii) $SDD(NS_2[n]) = Z_{1,-1}(NS_2[n]) = 5.2^n + 2(8.2^n - 5) + 13(2^n - 1).$

Here, we consider the nanostar $NS_3[n]$ and derived the (a,b)-Zagreb index for this nanostar. The figure of $NS_3[n]$ is shown in Fig. 3. The edge sets and the degree of vertices of $NS_3[n]$ are shown as follows:

$E_1(\mathrm{NS_3[n]}) = \{e = uv \in E(\mathrm{NS_3[n]}): d_{\mathrm{NS_3[n]}}(u) = 2 \text{ and } d_{\mathrm{NS_3[n]}}(v) = 3\}$

$E_2(\mathrm{NS_3[n]}) = \{e = uv \in E(\mathrm{NS_3[n]}): d_{\mathrm{NS_3[n]}}(u) = 2 \text{ and } d_{\mathrm{NS_3[n]}}(v) = 2\}$

$E_3(\mathrm{NS_3[n]}) = \{e = uv \in E(\mathrm{NS_3[n]}): d_{\mathrm{NS_3[n]}}(u) = 3 \text{ and } d_{\mathrm{NS_3[n]}}(v) = 3\}$

$E_4(\mathrm{NS_3[n]}) = \{e = uv \in E(\mathrm{NS_3[n]}): d_{\mathrm{NS_3[n]}}(u) = 1 \text{ and } d_{\mathrm{NS_3[n]}}(v) = 2\}$

note that, $|E_1(\mathrm{NS_3[n]})| = 66.(2^{n-1} - 1) + 48$, $|E_2(\mathrm{NS_3[n]})| = 54.2^{n-1} - 24$, $|E_3(\mathrm{NS_3[n]})| = 3.2^{n+1}$, $|E_4(\mathrm{NS_3[n]})| = 3.2^n$.

Theorem 2.3. The (a; b)-Zagreb index of $NS_3[n]$ is given by

$$\mathrm{Z_{a,b}(NS_3[n])} = \{66(2^{n-1} - 1) + 48\}(2^a.3^b + 2^b.3^a) + (54.2^{n-1} - 24)2^{a+b+1} + 2^{n+2}.3^{a+b+1} + 3.2^n(2^a + 2^b). \quad (3)$$

Proof. From definition of (a,b)-Zagreb index, we get

$$Z_{a,b}(NS_3[n]) = \sum_{uv \in E(NS_3[n])} [d_{NS_3[n]}(u)^a d_{NS_3[n]}(v)^b + d_{NS_3[n]}(u)^b d_{NS_3[n]}(v)^a]$$

$$= \sum_{uv\in E_1(NS_3[n])} (2^a.3^b + 2^b.3^a) + \sum_{uv\in E_2(NS_3[n])} (2^a.2^b + 2^b.2^a)$$
$$+ \sum_{uv\in E_3(NS_3[n])} (3^a.3^b + 3^b.3^a) + \sum_{uv\in E_4(NS_3[n])} (1^a.2^b + 1^b.2^a)$$

$$= |E_1(NS_3[n])|(2^a.3^b + 2^b.3^a) + |E_2(NS_3[n])|(2^a.2^b + 2^b.2^a)$$

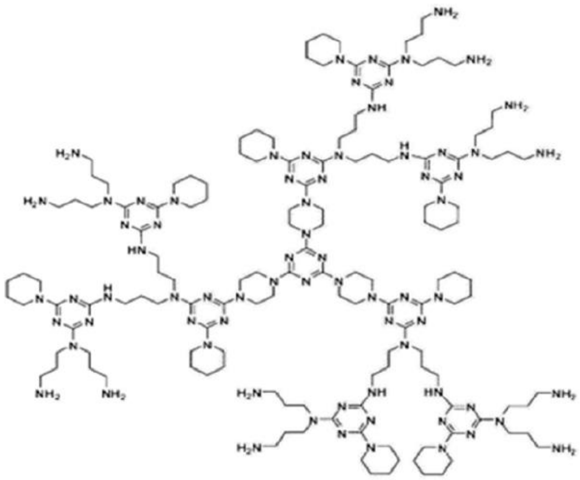

Fig. 3. Polymer dendrimer NS3[n].

$$+|E_3(NS_3[n])|(3^a.3^b + 3^b.3^a) + |E_4(NS_3[n])|(1^a.2^b + 1^b.2^a)$$
$$= \{66(2^{n-1} - 1) + 48\}(2^a.3^b + 2^b.3^a) + (54.2^{n-1} - 24)2.2^{a+b}$$
$$+3.2^{n+1}.(2.3^{a+b}) + 3.2^n(2^a + 2^b).$$

Hence, the theorem.

Corollary 2.3. From equation 3, we derived the following results:

(i) $M_1(NS_3[n]) = Z_{1,0}(NS_3[n]) = 5\{66(2^{n-1} - 1) + 48\}+4$
$(54.2^{n-1} - 24) + 9.2^{n+2} + 9.2^n$,

(ii) $M_2(NS_3[n]) = \frac{1}{2}Z_{1,1}(NS_3[n]) = 6\{66(2^{n-1} - 1) + 48\}+4(54.2^{n-1} - 24)$
$+27.2^{n+2} + 6.2^n$,

(iii) $F(NS_3[n]) = Z_{2,0}(NS_3[n]) = 13\{66(2^{n-1} - 1) + 48\}$+8$(54.2^{n-1} - 24)$

$+27.2^{n+2} + 15.2^{n}$,

(iii) $ReZM(NS_3[n]) = Z_{2,1}(NS_3[n]) = 30\{66(2^{n-1} - 1) + 48\}$+16

$(54.2^{n-1} - 24)$

$+81.2^{n+2} + 18.2^{n}$,

(v) $M^{a}(NS_3[n]) = Z_{a-1,0}(NS_3[n]) = \{66(2^{n-1} - 1) + 48\}(2^{a-1} + 3^{a-1})$

$+2^{a}(54.2^{n-1} - 24) + 2^{n+2}.3^{a} + 3.2^{n+a+1}$,

(vi) $R_a(NS_3[n]) = \frac{1}{2}Z_{a,a}(NS_3[n]) = \{66(2^{n-1} - 1) + 48\}2^{a+1}.3^{a}$

$+2^{2a+1}(54.2^{n-1} - 24) + 2^{n+2}.3^{2a+1} + 3.2^{n+a+1}$,

(vii)

$SDD(NS_3[n]) = Z_{1,-1}(NS_3[n]) = 13\{11(2^{n-1} - 1) + 8\} + 2.(54.2^{n-1} - 24)$

$+3.2^{n+2} + 15.2^{n-1}$.

Similarly, we obtained (a,b)-Zagreb index of nanostar $NS_4[n]$. The edge sets and degree of vertices of nanostar $NS_4[n]$ are given by

$E_1(NS_4[n]) = \{e = uv \in E(NS_4[n]) : d_{NS_4[n]}(u) = 2 \ and \ d_{NS_4[n]}(v) = 3\}$

$E_2(NS_4[n]) = \{e = uv \in E(NS_4[n]) : d_{NS_4[n]}(u) = 2 \ and \ d_{NS_4[n]}(v) = 2\}$

$E_3(NS_4[n]) = \{e = uv \in E(NS_4[n]) : d_{NS_4[n]}(u) = 1 \ and \ d_{NS_4[n]}(v) = 3\}$

$E_4(NS_4[n]) = \{e = uv \in E(NS_4[n]) : d_{NS_4[n]}(u) = 3 \ and \ d_{NS_4[n]}(v) = 3\}$

$E_5(NS_4[n]) = \{e = uv \in E(NS_4[n]) : d_{NS_4[n]}(u) = 3 \ and \ d_{NS_4[n]}(v) = 4\}$

$E_6(NS_4[n]) = \{e = uv \in E(NS_4[n]) : d_{NS_4[n]}(u) = 4 \ and \ d_{NS_4[n]}(v) = 4\}$

note that, $|E_1(NS_4[n])| = 32.2^{n-1} - 8$, $|E_2(NS_4[n])| = 2^{n+1} + 2$, $|E_3(NS_4[n])| = 2^{n+1}$, $|E_4(NS_4[n])| = 86$, $|E_4(NS_4[n])| = 6$, $|E_4(NS_4[n])| = 3$. The figure of $NS_4[n]$ is shown in Fig. 4.

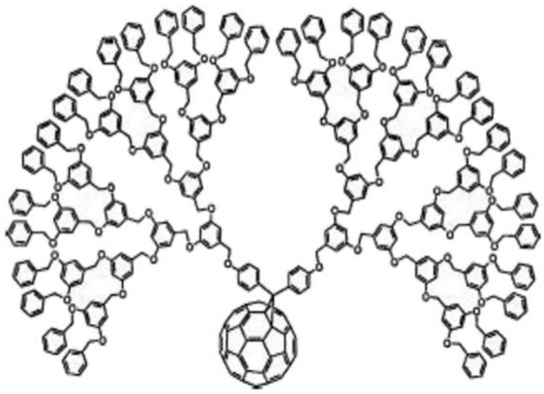

Fig. 4. Fullerene dendrimer NS4[n].

Theorem 2.4. For $NS_4[n]$, the (a; b)-Zagreb index

$$Z_{a,b}(NS_4[n]) = (32.2^{n-1} - 8)(2^a.3^b + 2^b.3^a) + (2^{n+1} + 2).2^{a+b+1}$$
$$+2^{n+1}.(3^a + 3^b) + 172.3^{a+b} + 6(3^a.4^b + 3^b.4^a) + 6.4^{a+b}. \quad (4)$$

Proof. Using the concept of (a,b)-Zagreb index, we get

$$Z_{a,b}(NS_4[n]) = \sum_{uv\in E(NS_4[n])} [d_{NS_4[n]]}(u)^a d_{NS_4[n]}(v)^b + d_{NS_4[n]}(u)^b d_{NS_4[n]}(v)^a]$$

$$= \sum_{uv\in E_1(NS_4[n])} (2^a.3^b + 2^b.3^a) + \sum_{uv\in E_2(NS_4[n])} (2^a.2^b + 2^b.2^a)$$
$$+ \sum_{uv\in E_3(NS_4[n])} (1^a.3^b + 1^b.3^a) + \sum_{uv\in E_4(NS_4[n])} (3^a.3^b + 3^b.3^a)$$
$$+ \sum_{uv\in E_4(NS_4[n])} (3^a.4^b + 3^b.4^a) + \sum_{uv\in E_4(NS_4[n])} (4^a.4^b + 4^b.4^a)$$

$$= |E_1(NS_4[n])|(2^a.3^b + 2^b.3^a) + |E_2(NS_4[n])|(2^a.2^b + 2^b.2^a)$$
$$+|E_3(NS_4[n])|(1^a.3^b + 1^b.3^a) + |E_4(NS_4[n])|(3^a.3^b + 3^b.3^a)$$
$$+|E_5(NS_4[n])|(3^a.4^b + 3^b.4^a) + |E_6(NS_4[n])|(4^a.4^b + 4^b.4^a)$$

$$= (32.2^{n-1} - 8)(2^a.3^b + 2^b.3^a) + (2^{n+1} + 2).2.2^{a+b}$$

$$+2^{n+1}.(3^a+3^b)+86.2.3^{a+b}+6(3^a.4^b+3^b.4^a)+3.2.4^{a+b}.$$

Which is the desired result.

Corollary 2.4. Using equation 4, we derived the following results:

(i) $M_1(NS_4[n]) = Z_{1,0}(NS_4[n]) = 6.2^{n+4} + 808,$

(ii) $M_2(NS_4[n]) = \frac{1}{2}Z_{1,1}(NS_4[n]) = 96.2^n + 3.2^{n+1} + 2^{n+3} + 1241,$

(iii)

$F(NS_4[n]) = Z_{2,0}(NS_4[n]) = 13(32.2^{n-1} - 8) + 8(2^{n+1} + 2) + 10.2^{n+1} + 1794,$

(iv)

$ReZM(NS_4[n]) = Z_{2,1}(NS_4[n]) = 30(32.2^{n-1} - 8) + 32(2^n + 1) + 12.2^{n+1} + 5532,$

(v) $M^a(NS_4[n]) = Z_{a-1,0}(NS_4[n]) = 16.2^n(2^{a-1} + 3^{a-1}) + 2^{n+2}.2^{a-1}$

$+2^{n+1}(3^{a-1} + 1) + 88.3^a + 12.4^{a-1} + 2^{a+1} - 40,$

(vi)

$R_a(NS_4[n]) = \frac{1}{2}Z_{a,a}(NS_4[n]) = 32.2^{n-1}.2^a.3^a - 8.2^a.3^a + 4^a.2^{n+1} + 2.4^a$

$$+2.2^n.3^a + 43.3^{2a+1} + 6.3^a.4^a + 3.16^a,$$

(vii)

$SDD(NS_4[n]) = Z_{1,-1}(NS_4[n]) = \frac{13}{6}(32.2^{n-1} - 8) + 4(2^n + 1) + \frac{10}{3}.2^{n+1} + \frac{381}{2}.$

Finally, we consider $NS_5[n]$ and obtained (a,b)-Zagreb index of this nanostar. The figure of $NS_5[n]$ is given in Fig. 5. The edge sets and degree of all the vertex of $NS_5[n]$ are as follows:

$E_1(NS_5[n]) = \{e = uv \in E(NS_5[n]) : d_{NS_5[n]}(u) = 2 \text{ and } d_{NS_5[n]}(v) = 3\}$
$E_2(NS_5[n]) = \{e = uv \in E(NS_5[n]) : d_{NS_5[n]}(u) = 2 \text{ and } d_{NS_5[n]}(v) = 2\}$

$E_3(NS_5[n]) = \{e = uv \in E(NS_5[n]) : d_{NS_5[n]}(u) = 3 \text{ and } d_{NS_5[n]}(v) = 3\}$

$E_4(NS_5[n]) = \{e = uv \in E(NS_5[n]) : d_{NS_5[n]}(u) = 1 \; and \; d_{NS_5[n]}(v) = 3\}$
such that, $|E_1(NS_5[n]) = 6.(2^{n+3} - 1)$, $|E_2(NS_5[n]) = 6.(2^n + 1)$,
$|E_3(NS_5[n]) = 24$, $|E_4(NS_5[n]) = 3.(2^{n+1} + 1)$.

Theorem 2.5. The (a; b)-Zagreb index of $NS_5[n]$ is given by

$$Z_{a,b}(NS_5[n]) = 6.\left(2^{n+3} - 1\right)\left(2^a.3^b + 2^b.3^a\right) + 6.(2^n + 1).2^{a+b+1} + 48.3^{a+b}$$
$$+3.(2^{n+1} + 1)\left(3^a + 3^b\right). \quad (5)$$

Proof. From definition of (a,b)-Zagreb index, we get

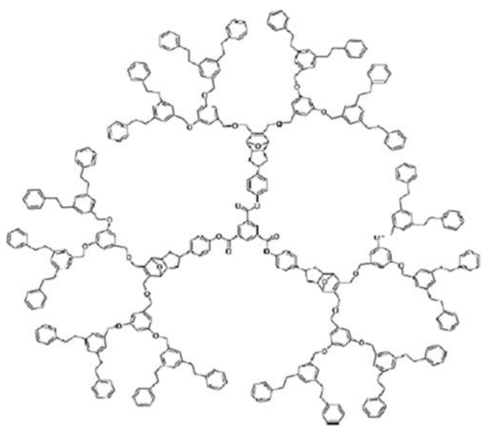

Fig. 5. The polymer dendrimer NS5[n].

$$Z_{a,b}(NS_5[n]) = \sum_{uv \in E(NS_5[n])} [d_{NS_5[n]}(u)^a d_{NS_5[n]}(v)^b + d_{NS_5[n]}(u)^b d_{NS_5[n]}(v)^a]$$

$$= \sum_{uv \in E_1(NS_5[n])} \left(2^a.3^b + 2^b.3^a\right) + \sum_{uv \in E_2(NS_5[n])} \left(2^a.2^b + 2^b.2^a\right)$$
$$+ \sum_{uv \in E_3(NS_5[n])} \left(3^a.3^b + 3^b.3^a\right) + \sum_{uv \in E_4(NS_5[n])} \left(1^a.3^b + 1^b.3^a\right)$$

$$= |E_1(NS_5[n])|\left(2^a.3^b + 2^b.3^a\right) + |E_2(NS_5[n])|\left(2^a.2^b + 2^b.2^a\right)$$
$$+ |E_3(NS_5[n])|\left(3^{a+b} + 3^{a+b}\right) + |E_4(NS_5[n])|\left(1^a.3^b + 1^b.3^a\right)$$

$$= 6.(2^{n+3} - 1)(2^a.3^b + 2^b.3^a) + 6.(2^n + 1).2.2^{a+b} + 24.2.3^{a+b}$$

$$+3.(2^{n+1} + 1)(3^a + 3^b).$$

Hence, the theorem.

Corollary 2.5. From equation 5, we obtained the following results,

(i)$M_1(NS_5[n]) = Z_{1,0}(NS_5[n]) = 15.2^{n+4} + 12.2^{n+1} + 6.2^{n+2} + 150,$

(ii)$M_2(NS_5[n]) = \frac{1}{2}Z_{1,1}(NS_5[n]) = 36.2^{n+4} + 24.2^{n+1} + 9.2^{n+2} + 426,$

(iii)

$F(NS_5[n]) = Z_{2,0}(NS_5[n]) = 78(2^{n+3} - 1) + 48(2^n + 1) + 30(2^{n+1} + 1) + 432,$

(iv)$ReZM(NS_5[n]) = Z_{2,1}(NS_5[n]) = 180(2^{n+3} - 1) + 96(2^n + 1)$

$+36(2^{n+1} + 1) + 1296,$

(v) $M^a(NS_5[n]) = Z_{a-1,0}(NS_5[n]) = 6(2^{a-1} + 3^{a-1}).2^{n+3} + 12.2^{a-1}.2^n$

$+3(3^{a-1} + 1).2^{n+1} - 6(2^{a-1} + 3^{a-1})$

$+ 6.2^a$

$+48.3^{a-1} + 3(3^{a-1} + 1),$

(vi)

$R_a(NS_5[n]) = \frac{1}{2}Z_{a,a}(NS_5[n]) = 6.2^a.3^a.2^{n+3} + 6.4^a.2^n + 3^{a+1}.2^{n+1} - 6.2^a.3^a$

$+6.4^a + +24.9^a + 3^{a+1},$

(vii)

$SDD(NS_5[n]) = Z_{1,-1}(NS_5[n]) = 13(2^{n+3} - 1) + 12(2^n + 1) + 10(2^{n+1} + 1) + 48.$

3. Conclusions

In some recent study it is found that, topological indices have their significance in predicting physical and chemical properties of molecular graphs theoretically. The above studied topological index is a generalised form of different other topological indices such as first and second Zagreb index, F-index, redefined Zagreb index, general first Zagreb index,

General Randic' index, Symmetric division deg index, and so on. In this paper, we found this (a; b)-Zagreb index of some nanostar dendrimers and hence consider some particular values of a and b. This (a; b)-Zagreb index has not much studied up to now, so the results for other chemical and nano structures, such as graphen, carbon graphite, crystal cubic carbon structure can be obtained in further study.

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