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## Computing the F-index of nanostar dendrimers

Nilanjan De <sup>a,\*</sup>, Sk. Md. Abu Nayeem <sup>b</sup><sup>a</sup> Department of Basic Sciences and Humanities (Mathematics), Calcutta Institute of Engineering and Management, Kolkata, India<sup>b</sup> Department of Mathematics, Aliah University, New Town, Kolkata 700 156, India

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## ABSTRACT

Dendrimers are highly branched nanostructures and are considered a building block in nanotechnology with a variety of suitable applications. In this paper, a vertex degree-based topological index, namely, the F-index, which is defined as the sum of cubes of a graph's vertex degrees, is studied for certain dendrimers. In this study, we present exact expressions for the F-index and F-polynomial of six infinite classes of nanostar dendrimers.

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## 1. Introduction

Chemical graph theory is a branch of mathematical chemistry in which different tools from graph theory are used to model chemical phenomena mathematically. Molecules and molecular compounds are modelled as molecular graphs, in which the vertices correspond to the atoms and the edges correspond to the chemical bonds between the atoms. A topological index is a numeric value that is graph invariant and correlates the physico-chemical properties of a molecular graph. Topological indices are used for studying quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR) for predicting different properties of chemical compounds and their biological activities. In chemistry, biochemistry and nanotechnology, different topological indices are found to be useful in isomer discrimination, QSAR, QSPR and pharmaceutical drug design. There are several studies regarding different topological indices of special molecular graphs, a few of which we mention [6–13].

Among various topological indices, degree based topological indices are the most important and widely used. These have great application in chemical graph theory. Suppose  $G$  to be a simple connected (molecular) graph and  $V(G)$  and  $E(G)$ , respectively, denote the vertex set and edge set of  $G$ . Let, for any vertex,  $v \in V(G)$ ,  $d_G(v)$  denote its degree, and  $N(v)$  denote the set of vertices which are the neighbours of the vertex,  $v$ , so that  $|N(v)| = d_G(v)$ . The first and second Zagreb indices of a graph, denoted by  $M_1(G)$  and  $M_2(G)$  are among the oldest, most popular and extensively studied vertex-degree based topological indices, and are respectively defined as

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

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

These indices were introduced in a paper in 1972 [1] to study the structure-dependency of the total amount of  $\pi$ -electron energy in conjugated systems. Soon after that, it was found that the Zagreb indices provided a measure of the underlying molecules of carbon skeleton branching. For more information and recent results about Zagreb indices, see [27–31]. In the same paper, another topological index, defined as the sum of cubed degrees of the vertices of a graph, was also shown to relate  $\pi$ -electron energy. However, this index was

\* Corresponding author.

E-mail addresses: [de.nilanjan@rediffmail.com](mailto:de.nilanjan@rediffmail.com) (N. De), [nayeem.math@aliah.ac.in](mailto:nayeem.math@aliah.ac.in) (Sk.Md.A. Nayeem).

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never studied in detail then. Recently, Furtula and Gutman [2] have restudied this index to establish some basic properties and have also demonstrated that the predictive ability of this index is similar to that of the first Zagreb index with respect to entropy and acetic factors of the molecules and both first Zagreb index and this index yield correlation coefficients greater than 0.95. They named this index the “forgotten topological index” or “F-index”. Very recently, the present authors have studied this index for different graph operations [3] and also introduced its coindex version [4]. Abdo et al. investigated the extremal trees with respect to the F-index [5]. In symbolic notation, the F-index is given as follows:

$$F(G) = \sum_{v \in V(G)} d_G(v)^3 = \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2]. \tag{1}$$

Analogous to other topological polynomials, the F-polynomial of graph G is also defined as:

$$F(G, x) = \sum_{uv \in E(G)} x^{[d_G(u)^2 + d_G(v)^2]}. \tag{2}$$

Dendrimers are hyper-branched nanostructures that can be synthesized by divergent or convergent methods, and they are built up from branched units called monomers using a nanoscale fabrication process. Dendrimers have a very well-defined chemical structure with three major architectural components. These are the core, branches and end groups, where new branches are emitted from the core and are added in steps. Dendrimers are considered one of the most important, commercially available building blocks in nanotechnology. Dendrimers are used in the formation of nanotubes, nanolatex, chemical sensors, micro and macro capsules, coloured glass, modified electrodes, and photon funnels such as artificial antennas [21,26]. Because dendrimers are widely used in such different applied fields, the study of nanostar dendrimers has received a great deal of attention in both chemical and mathematical literature. Graovac et al. derived a fifth geometric–arithmetic index for nanostar dendrimers [14]. Further, one of the present authors presented first and second reformulated Zagreb indices of a class of nanostar dendrimers [15]. Madanshekar calculated the Randic index of some classes of nanostar dendrimers [16]. Additionally, Madanshekar et al. calculated different topological indices of some nanostar dendrimers [17,18]. Siddiqui et al. presented the Zagreb indices and Zagreb polynomials of different nanostar dendrimers [19]. For other different applications regarding dendrimers, we refer to [20–26]. Until now, the study of the F-index for special chemical- and nano-structures have been largely limited. Thus, we have been attracted to studying the mathematical properties of the F-index and its polynomial version of some nanostar dendrimers. In this paper, we consider six infinite classes of dendrimer nanostars, namely:  $NS_1[n]$ ,  $NS_2[n]$ ,  $NS_3[n]$ ,  $NS_4[n]$ ,  $NS_5[n]$  and  $D_n$ . Their structures are given in Figs. 1–6.

## 2. F-index and polynomials of nanostar dendrimers

Let the number of edges of G connecting vertices of degrees i and j be denoted by  $e_{ij}$  such that  $e_{ij} = e_{ji}$ . As dendrimer are hyper-branched molecules, for the sake of computation, let us denote the number of edges connecting vertices of degrees i and j in each branch of the dendrimer by  $e'_{ij}$ .

Let us consider the first type of nanostar dendrimer, denoted by  $NS_1[n]$ , where n is the number of growth steps (See Fig. 1). For this type of dendrimer, there are four similar branches and three extra edges. Therefore, in this case, we have:  $e_{12} = 4e'_{12}$ ,  $e_{22} = 4e'_{22} + 1$ ,  $e_{13} = 4e'_{13}$  and  $e_{23} = 4e'_{23} + 2$ . Additionally, from direct calculation, we get:  $e'_{12} = 2^{n-1}$ ,  $e'_{22} = 3n - 3$ ,  $e'_{13} = 2^n - 1$  and  $e'_{23} = 3(2^n - 1) + (2^{n-1} - 1)$ . Therefore, we have:  $e_{12} = 2.2^n$ ,

$e_{22} = 12.2^n - 11$ ,  $e_{13} = 4.2^n - 4$ , and  $e_{12} = 14.2^n - 14$ . Now, we compute the F-index and polynomial of this type of dendrimer through the following theorem.

**Theorem 1.** Let  $NS_1[n]$  be the nanostar dendrimer. Then

$$F(NS_1[n]) = 5.2^{n+1} + 40(2^n - 1) + 8(12.2^n - 11) + 13(14.2^n - 14), \text{ and}$$

$$F(NS_1[n], x) = 2^{n+1}x^5 + 4(2^n - 1)x^{10} + (12.2^n - 11)x^8 + (14.2^n - 14)x^{13}.$$

*Proof.* The edge set of  $NS_1[n]$  is divided into four edge classes, based on the degrees of the end vertices. Thus, we write:  $E(NS_1[n]) = \bigcup_{i=1}^4 E_i(NS_1[n])$ , where

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

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

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

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

so that,  $|E_1(NS_1[n])| = 2^{n+1}$ ,  $|E_2(NS_1[n])| = 4(2^n - 1)$ ,  $|E_3(NS_1[n])| = 12.2^n - 11$  and  $|E_4(NS_1[n])| = 14.2^n - 14$ . So, from (1) the F-index of  $NS_1[n]$  is given by:

$$\begin{aligned} F(NS_1[n]) &= \sum_{uv \in E_1(NS_1[n])} [d(u)^2 + d(v)^2] + \sum_{uv \in E_2(NS_1[n])} [d(u)^2 + d(v)^2] \\ &+ \sum_{uv \in E_3(NS_1[n])} [d(u)^2 + d(v)^2] + \sum_{uv \in E_4(NS_1[n])} [d(u)^2 + d(v)^2] \\ &= 5|E_1(NS_1[n])| + 10|E_2(NS_1[n])| + 8|E_3(NS_1[n])| \\ &+ 13|E_4(NS_1[n])| \\ &= 5.2^{n+1} + 40(2^n - 1) + 8(12.2^n - 11) + 13(14.2^n - 14). \end{aligned}$$

Similarly, from (2), the F-polynomial of nanostar dendrimer  $NS_1[n]$  is calculated as:

$$\begin{aligned} F(NS_1[n], x) &= \sum_{uv \in E_1(NS_1[n])} x^{[d(u)^2 + d(v)^2]} + \sum_{uv \in E_2(NS_1[n])} x^{[d(u)^2 + d(v)^2]} \\ &+ \sum_{uv \in E_3(NS_1[n])} x^{[d(u)^2 + d(v)^2]} + \sum_{uv \in E_4(NS_1[n])} x^{[d(u)^2 + d(v)^2]} \\ &= \sum_{uv \in E_1(NS_1[n])} x^5 + \sum_{uv \in E_2(NS_1[n])} x^{10} + \sum_{uv \in E_3(NS_1[n])} x^8 \\ &+ \sum_{uv \in E_4(NS_1[n])} x^{13} \\ &= |E_1(NS_1[n])|x^5 + |E_2(NS_1[n])|x^{10} + |E_3(NS_1[n])|x^8 \\ &+ |E_4(NS_1[n])|x^{13} \\ &= 2^{n+1}x^5 + 4(2^n - 1)x^{10} + (12.2^n - 11)x^8 \\ &+ (14.2^n - 14)x^{13}. \end{aligned}$$

Next, we consider a second class of nanostar dendrimer denoted as  $NS_2[n]$ , where n is the steps of growth (See Fig. 2). This graph has four similar branches and five extra edges. Therefore, we have  $e_{12} = 4e'_{12}$ ,  $e_{22} = 4e'_{22} + 3$  and  $e_{23} = 4e'_{23} + 2$ . Additionally, from direct calculation, we obtain  $e'_{12} = 2^{n-1}$ ,  $e'_{22} = 2(2^n - 1)$  and  $e'_{23} = 3.2^n - 2$ . Thus,  $e_{12} = 2.2^{n+1}$ ,  $e_{22} = 8.2^n - 5$  and  $e_{23} = 6.2^n - 6$ .

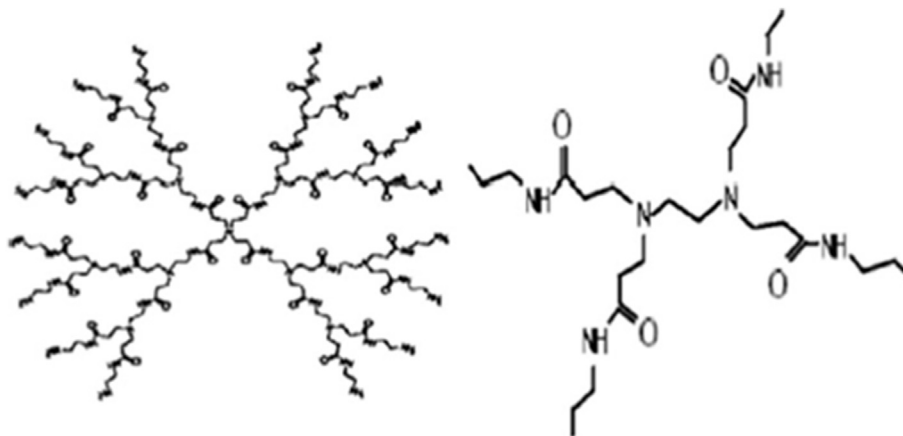


Fig. 1. Polypropylenimine octaamine dendrimer (NS<sub>1</sub>[n]).

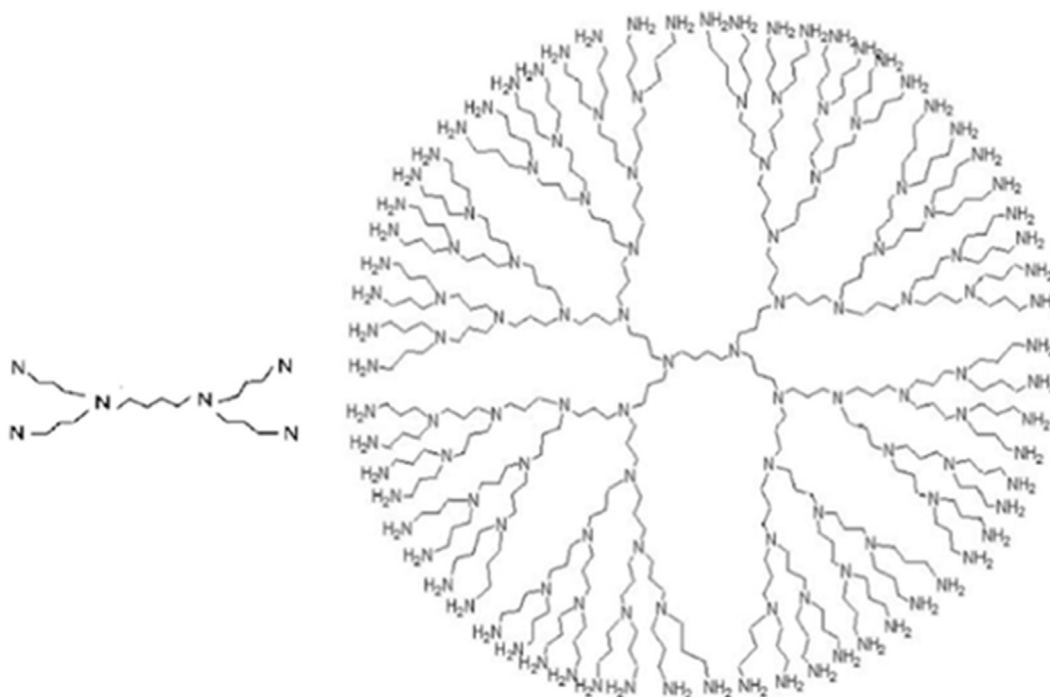


Fig. 2. Polypropylenimine octaamine dendrimer (NS<sub>2</sub>[n]).

Now in the following theorem we compute the F-index and polynomial of this type of dendrimer.

**Theorem 2.** Let NS<sub>2</sub>[n] be the nanostar dendrimer. Then,

$$F(NS_2[n]) = 5.2^{n+1} + 8(8.2^n - 5) + 13(6.2^n - 6) \text{ and } F(NS_2[n], x) = 2^{n+1}x^5 + (8.2^n - 5)x^8 + (6.2^n - 6)x^{13}.$$

*Proof.* Let the edge set of NS<sub>2</sub>[n] be divided into three classes based on the degree of the end vertices as follows:

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

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

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

Thus,  $|E_1(NS_2[n])| = 2^{n+1}$ ,  $|E_2(NS_2[n])| = 8.2^n - 5$  and  $|E_3(NS_2[n])| = 6.2^n - 6$ . So from (1), the F-index of NS<sub>2</sub>[n] is given by:

$$\begin{aligned} F(NS_2[n]) &= \sum_{uv \in E_1(NS_2[n])} [d(u)^2 + d(v)^2] + \sum_{uv \in E_2(NS_2[n])} [d(u)^2 + d(v)^2] \\ &+ \sum_{uv \in E_3(NS_2[n])} [d(u)^2 + d(v)^2] \\ &= 5|E_1(NS_2[n])| + 8|E_2(NS_2[n])| + 13|E_3(NS_2[n])| \\ &= 5.2^{n+1} + 8(8.2^n - 5) + 13(6.2^n - 6). \end{aligned}$$

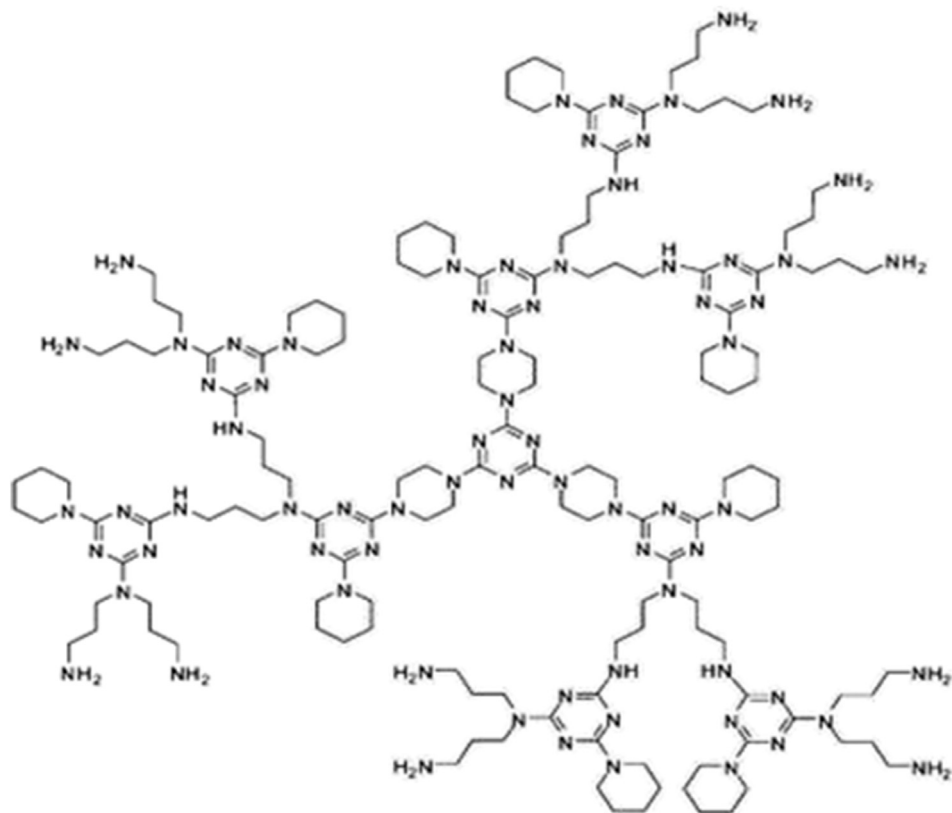


Fig. 3. Polymer dendrimer ( $NS_3[n]$ ).

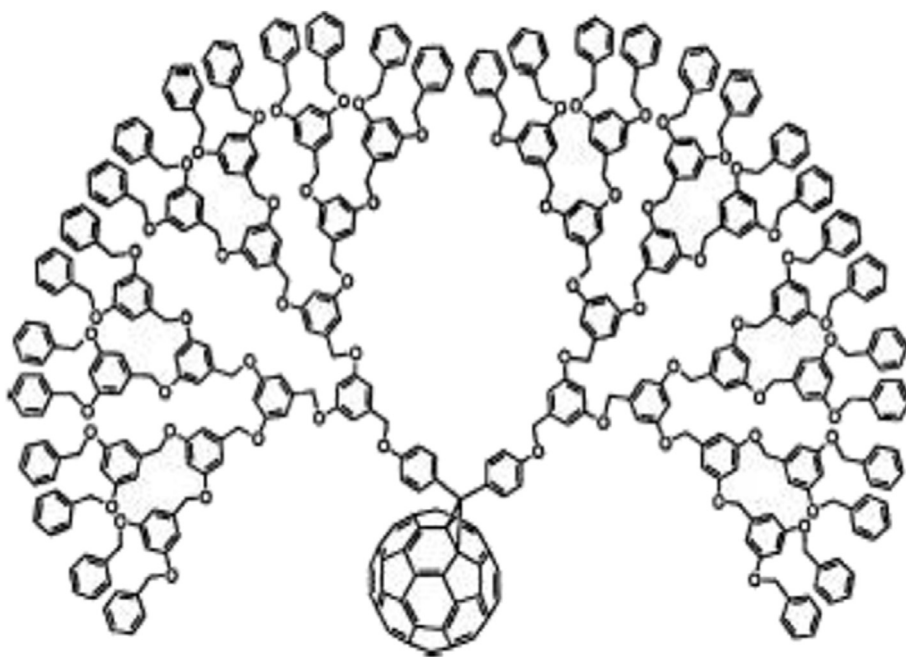


Fig. 4. Fullerene dendrimer ( $NS_4[n]$ ).

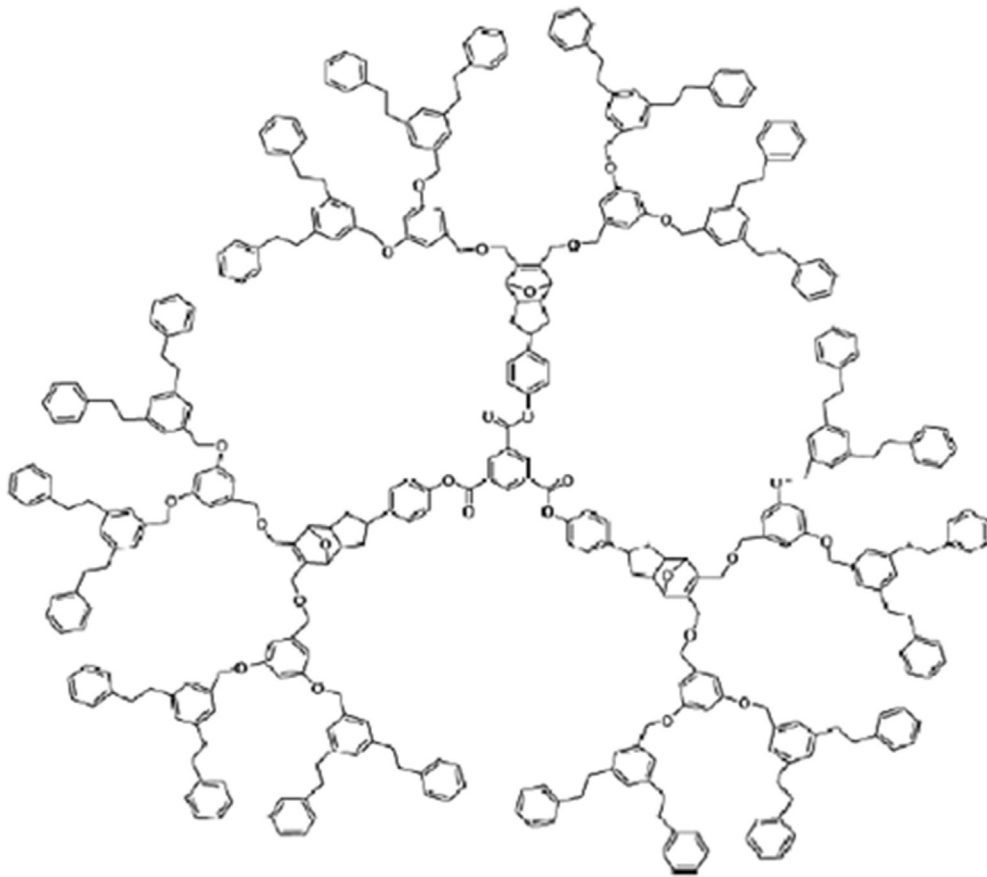


Fig. 5. The polymer dendrimer ( $NS_5[n]$ ).

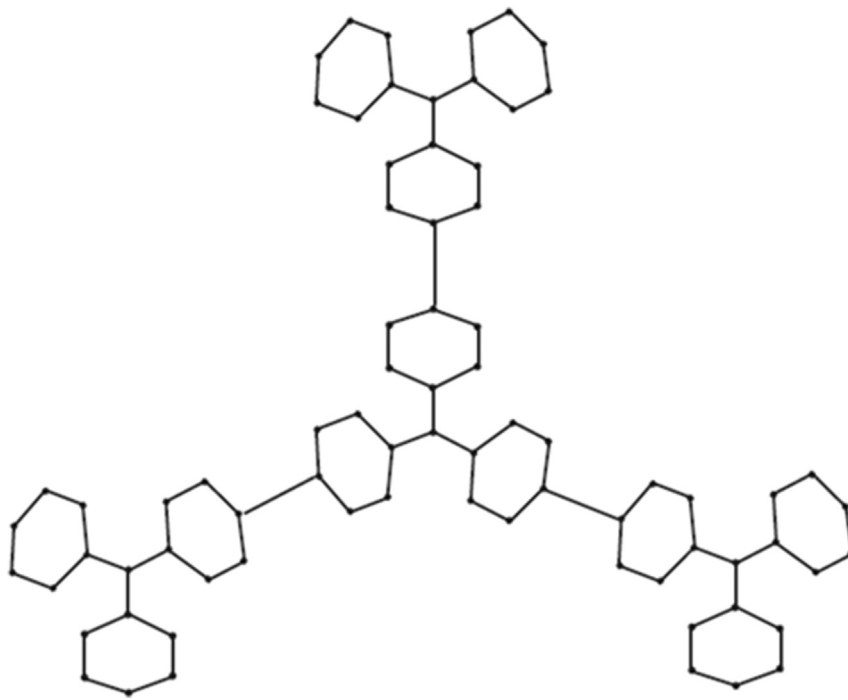


Fig. 6. The nanostar dendrimer  $D_n(n=2)$ .

Using (2), the F-polynomial of  $NS_2[n]$  is calculated as follows:

$$\begin{aligned} F(NS_2[n], x) &= \sum_{uv \in E_1(NS_2[n])} x^{[d(u)^2+d(v)^2]} + \sum_{uv \in E_2(NS_2[n])} x^{[d(u)^2+d(v)^2]} \\ &\quad + \sum_{uv \in E_3(NS_2[n])} x^{[d(u)^2+d(v)^2]} \\ &= \sum_{uv \in E_1(NS_2[n])} x^5 + \sum_{uv \in E_2(NS_2[n])} x^8 + \sum_{uv \in E_3(NS_2[n])} x^{13} \\ &= |E_1(NS_2[n])|x^5 + |E_2(NS_2[n])|x^8 + |E_3(NS_2[n])|x^{13} \\ &= 2^{n+1}x^5 + (8 \cdot 2^n - 5)x^8 + (6 \cdot 2^n - 6)x^{13}. \end{aligned}$$

We now consider the class of nanostar dendrimer  $NS_3[n]$ , where  $n$  is the steps of growth (See Fig. 3). By direct calculation, we can show that:  $e_{23} = 66(2^{n-1} - 1) + 48$ ,  $e_{22} = 54 \cdot 2^{n-1} - 24$ ,  $e_{33} = 3 \cdot 2^{n+1}$  and  $e_{12} = 3 \cdot 2^n$ . In the following, we compute the F-index and polynomial of this type of dendrimer.

**Theorem 3.** Let  $NS_3[n]$  be the nanostar dendrimer. Then,

$$\begin{aligned} F(NS_3[n]) &= 13(66(2^{n-1} + 1) + 48) + 8(54 \cdot 2^{n-1} - 24) \\ &\quad + 18 \cdot 3 \cdot 2^{n+1} + 5 \cdot 3 \cdot 2^n \text{ and} \\ F(NS_3[n], x) &= (66(2^{n-1} + 1) + 48)x^{13} + (54 \cdot 2^{n-1} - 24)x^8 \\ &\quad + 3 \cdot 2^{n+1}x^{18} + 3 \cdot 2^n x^5. \end{aligned}$$

*Proof.* Let the edge set of  $NS_3[n]$  be divided into three classes based on the degree of the end vertices as follows:

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

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

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

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

Hence,  $|E_1(NS_3[n])| = 66(2^{n-1} + 1)48$ ,  $|E_2(NS_3[n])| = 54 \cdot 2^{n-1} - 24$ ,  $|E_3(NS_3[n])| = 3 \cdot 2^{n+1}$  and  $|E_4(NS_3[n])| = 3 \cdot 2^n$ . In the following, from (1), we calculate the F-index of nanostar dendrimer  $NS_3[n]$ .

$$\begin{aligned} F(NS_3[n]) &= \sum_{uv \in E_1(NS_3[n])} [d(u)^2+d(v)^2] + \sum_{uv \in E_2(NS_3[n])} [d(u)^2+d(v)^2] \\ &\quad + \sum_{uv \in E_3(NS_3[n])} [d(u)^2+d(v)^2] + \sum_{uv \in E_4(NS_3[n])} [d(u)^2+d(v)^2] \\ &= 13|E_1(NS_3[n])| + 8|E_2(NS_3[n])| + 18|E_3(NS_3[n])| \\ &\quad + 5|E_4(NS_3[n])| \\ &= 13(66(2^{n-1} + 1) + 48) + 8(54 \cdot 2^{n-1} - 24) + 18 \cdot 3 \cdot 2^{n+1} \\ &\quad + 5 \cdot 3 \cdot 2^n \end{aligned}$$

Again, from (2) we obtain the F-polynomial as

$$\begin{aligned} F(NS_3[n], x) &= \sum_{uv \in E_1(NS_3[n])} x^{[d(u)^2+d(v)^2]} + \sum_{uv \in E_2(NS_3[n])} x^{[d(u)^2+d(v)^2]} \\ &\quad + \sum_{uv \in E_3(NS_3[n])} x^{[d(u)^2+d(v)^2]} + \sum_{uv \in E_4(NS_3[n])} x^{[d(u)^2+d(v)^2]} \\ &= \sum_{uv \in E_1(NS_3[n])} x^{13} + \sum_{uv \in E_2(NS_3[n])} x^8 + \sum_{uv \in E_3(NS_3[n])} x^{18} \\ &\quad + \sum_{uv \in E_4(NS_3[n])} x^5 = |E_1(NS_3[n])|x^{13} + |E_2(NS_3[n])|x^8 \\ &\quad + |E_3(NS_3[n])|x^{18} + |E_4(NS_3[n])|x^5 \\ &= (66(2^{n-1} + 1) + 48)x^{13} + (54 \cdot 2^{n-1} - 24)x^8 \\ &\quad + 3 \cdot 2^{n+1}x^{18} + 3 \cdot 2^n x^5. \end{aligned}$$

Now, consider another class of dendrimer, denoted by  $NS_4[n]$ , where  $n$  is the number of steps of growth (see Fig. 4). The molecular graph of  $NS_4[n]$  has two similar branches. Therefore, from a similar calculation, we obtain  $e_{33} = 86$ ,  $e_{34} = 6$ ,  $e_{44} = 3$ ,  $e_{23} = 32 \cdot 2^{n-1} - 8$  and  $e_{22} = 2^{n+1} + 2$ . Now we calculate the F-index and polynomial of this type of dendrimer.

**Theorem 4.** Let  $NS_4[n]$  be the nanostar dendrimer. Then

$$\begin{aligned} F(NS_4[n]) &= 13(32 \cdot 2^{n-1} - 8) + 8(2^{n+1} + 2) + 10 \cdot 2^{n+1} + 18 \cdot 86 \\ &\quad + 25 \cdot 6 + 32 \cdot 3 \text{ and } F(NS_4[n], x) \\ &= (32 \cdot 2^{n-1} - 8)x^{13} + (2^{n+1} + 2)x^8 + 2^{n+1}x^{10} \\ &\quad + 86x^{18} + 6x^{25} + 3x^{32} \end{aligned}$$

*Proof.* Let the edge set of  $NS_4[n]$  be divided into three classes based on the degree of the end vertices as follows:

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

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

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

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

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

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

So,  $|E_1(NS_4[n])| = 32 \cdot 2^{n-1} - 8$ ,  $|E_2(NS_4[n])| = 2^{n+1} + 2$ ,  $|E_3(NS_4[n])| = 2^{n+1}$ ,  $|E_4(NS_4[n])| = 86$ ,  $|E_5(NS_4[n])| = 6$  and  $|E_6(NS_4[n])| = 3$ . So, from (1), the F-index is given as:

$$\begin{aligned}
 F(NS_4[n]) &= \sum_{uv \in E_1(NS_4[n])} [d(u)^2 + d(v)^2] + \sum_{uv \in E_2(NS_4[n])} [d(u)^2 \\
 &+ d(v)^2] + \sum_{uv \in E_3(NS_4[n])} [d(u)^2 + d(v)^2] \\
 &+ \sum_{uv \in E_4(NS_4[n])} [d(u)^2 + d(v)^2] + \sum_{uv \in E_5(NS_4[n])} [d(u)^2 \\
 &+ d(v)^2] + \sum_{uv \in E_6(NS_4[n])} [d(u)^2 + d(v)^2] \\
 &= 13|E_1(NS_4[n])| + 8|E_2(NS_4[n])| + 10|E_3(NS_4[n])| \\
 &+ 18|E_4(NS_4[n])| + 25|E_5(NS_4[n])| + 32|E_6(NS_4[n])| \\
 &= 13(32 \cdot 2^{n-1} - 8) + 8(2^{n+1} + 2) + 10 \cdot 2^{n+1} + 18 \cdot 86 \\
 &+ 25 \cdot 6 + 32 \cdot 3.
 \end{aligned}$$

In the following, we calculate the F-polynomial of  $NS_4[n]$  using (2).

$$\begin{aligned}
 F(NS_4[n], x) &= \sum_{uv \in E_1(NS_4[n])} x^{[d(u)^2+d(v)^2]} + \sum_{uv \in E_2(NS_4[n])} x^{[d(u)^2+d(v)^2]} \\
 &+ \sum_{uv \in E_3(NS_4[n])} x^{[d(u)^2+d(v)^2]} + \sum_{uv \in E_4(NS_4[n])} x^{[d(u)^2+d(v)^2]} \\
 &+ \sum_{uv \in E_5(NS_4[n])} x^{[d(u)^2+d(v)^2]} + \sum_{uv \in E_6(NS_4[n])} x^{[d(u)^2+d(v)^2]} \\
 &= \sum_{uv \in E_1(NS_4[n])} x^{13} + \sum_{uv \in E_2(NS_4[n])} x^8 + \sum_{uv \in E_3(NS_4[n])} x^{10} \\
 &+ \sum_{uv \in E_4(NS_4[n])} x^{18} + \sum_{uv \in E_5(NS_4[n])} x^{25} + \sum_{uv \in E_6(NS_4[n])} x^{32} \\
 &= |E_1(NS_4[n])|x^{13} + |E_2(NS_4[n])|x^8 + |E_3(NS_4[n])|x^{10} \\
 &+ |E_4(NS_4[n])|x^{18} + |E_5(NS_4[n])|x^{25} + |E_6(NS_4[n])|x^{32} \\
 &= (32 \cdot 2^{n-1} - 8)x^{13} + (2^{n+1} + 2)x^8 + 2^{n+1}x^{10} + 86x^{18} \\
 &+ 6x^{25} + 3x^{32}.
 \end{aligned}$$

Next, we consider the molecular graph of the class of dendrimer  $NS_5[n]$ , where  $n$  denotes the steps of growth (See Fig. 5). This dendrimer has three similar branches. So it is obvious that  $e_{23} = 3e'_{23} + 48$ ,  $e_{22} = 3e'_{23} + 12$  and  $e_{13} = 3e'_{13} + 3$ . Also from direct calculation, we have  $e'_{23} = 9(2^{n+1} - 2) - 2^{n+1}$ ,  $e'_{22} = 2^{n+1} - 2$  and  $e'_{13} = 2^{n+1}$ . Hence, we obtain  $e_{23} = 6(2^{n+3} - 1)$ ,  $e_{22} = 6(2^n + 1)$ ,  $e_{13} = 3(2^{n+1} + 1)$  and  $e_{33} = 24$ . Now, in the following theorem, we compute the F-index and polynomial of this type of dendrimer.

**Theorem 5.** Let  $NS_5[n]$  be the nanostar dendrimer. Then

$$\begin{aligned}
 F(NS_5[n]) &= 13.6(2^{n+3} - 1) + 8.6(2^n + 1) + 18.24 \\
 &+ 10.3(2^{n+1} + 1) \text{ and} \\
 F(NS_5[n], x) &= 6(2^{n+3} - 1)x^{13} + 6(2^n + 1)x^8 + 24x^{18} \\
 &+ 3(2^{n+1} + 1)x^{10}.
 \end{aligned}$$

*Proof.* Let the edge set of  $NS_5[n]$  be divided into three classes based on the degree of the end vertices as follows:

$$\begin{aligned}
 E_1(NS_5[n]) &= \{e = uv \in E(NS_5[n]) : d(u) = 2 \text{ and } d(v) = 3\} \\
 E_2(NS_5[n]) &= \{e = uv \in E(NS_5[n]) : d(u) = 2 \text{ and } d(v) = 2\} \\
 E_3(NS_5[n]) &= \{e = uv \in E(NS_5[n]) : d(u) = 3 \text{ and } d(v) = 3\} \\
 E_4(NS_5[n]) &= \{e = uv \in E(NS_5[n]) : d(u) = 1 \text{ and } d(v) = 3\}.
 \end{aligned}$$

So that:  $|E_1(NS_5[n])| = 6(2^{n+3} - 1)$ ,  $|E_2(NS_5[n])| = 6(2^n + 1)$ ,  $|E_3(NS_5[n])| = 24$  and  $|E_4(NS_5[n])| = 3(2^{n+1} + 1)$ . From (1), the F-index of  $NS_5[n]$  is given by:

$$\begin{aligned}
 F(NS_5[n]) &= \sum_{uv \in E_1(NS_5[n])} [d(u)^2 + d(v)^2] + \sum_{uv \in E_2(NS_5[n])} [d(u)^2 + d(v)^2] \\
 &+ \sum_{uv \in E_3(NS_5[n])} [d(u)^2 + d(v)^2] + \sum_{uv \in E_4(NS_5[n])} [d(u)^2 + d(v)^2] \\
 &= 13|E_1(NS_5[n])| + 8|E_2(NS_5[n])| + 18|E_3(NS_5[n])| \\
 &+ 10|E_4(NS_5[n])| \\
 &= 13.6(2^{n+3} - 1) + 8.6(2^n + 1) + 18.24 + 10.3(2^{n+1} + 1).
 \end{aligned}$$

From (2), the F-polynomial of  $NS_5[n]$  is given by:

$$\begin{aligned}
 F(NS_5[n], x) &= \sum_{uv \in E_1(NS_5[n])} x^{[d(u)^2+d(v)^2]} + \sum_{uv \in E_2(NS_5[n])} x^{[d(u)^2+d(v)^2]} \\
 &+ \sum_{uv \in E_3(NS_5[n])} x^{[d(u)^2+d(v)^2]} + \sum_{uv \in E_4(NS_5[n])} x^{[d(u)^2+d(v)^2]} \\
 &= \sum_{uv \in E_1(NS_5[n])} x^{13} + \sum_{uv \in E_2(NS_5[n])} x^8 + \sum_{uv \in E_3(NS_5[n])} x^{18} \\
 &+ \sum_{uv \in E_4(NS_5[n])} x^{10} \\
 &= |E_1(NS_5[n])|x^{13} + |E_2(NS_5[n])|x^8 + |E_3(NS_5[n])|x^{18} \\
 &+ |E_4(NS_5[n])|x^{10} \\
 &= 6(2^{n+3} - 1)x^{13} + 6(2^n + 1)x^8 + 24x^{18} \\
 &+ 3(2^{n+1} + 1)x^{10}.
 \end{aligned}$$

Finally, we consider another class of dendrimer, denoted as  $D_n$  (See Fig. 6). The total number of vertices and edges of  $D_n$  are calculated as  $(57 \cdot 2^{n-1} - 38)$  and  $(33 \cdot 2^n - 45)$ , respectively. In the following theorem we calculate the F-index and polynomial of  $D_n$ .

**Theorem 6.** Let  $D_n$  be the nanostar dendrimer. Then

$$\begin{aligned}
 F(D_n) &= 8(24 \times 2^{n-1} - 12) + 13(30 \times 2^{n-1} - 24) + 18(12 \\
 &\times 2^{n-1} - 9) \text{ and } F(D_n, x) \\
 &= (24 \times 2^{n-1} - 12)x^8 + (30 \times 2^{n-1} - 24)x^{13} + (12 \times 2^{n-1} \\
 &- 9)x^{18}.
 \end{aligned}$$

*Proof.* Let the edge set of  $D_n$  be divided into three classes based on the degree of the end vertices as follows:

$$E_1(D_n) = \{e = uv \in E(D_n) : d(u) = 2 \text{ and } d(v) = 2\}$$

$$E_2(D_n) = \{e = uv \in E(D_n) : d(u) = 2 \text{ and } d(v) = 3\}$$

$$E_3(D_n) = \{e = uv \in E(D_n) : d(u) = 3 \text{ and } d(v) = 3\}.$$

Thus,  $|E_1(D_n)| = 24 \cdot 2^{n-1} - 12$ ,  $|E_2(D_n)| = 30 \cdot 2^{n-1} - 24$  and  $|E_3(D_n)| = 12 \cdot 2^{n-1} - 9$ . So using (1), the F-index of  $D_n$  is calculated as follows:

$$\begin{aligned} F(D_n) &= \sum_{uv \in E_1(D_n)} [d(u)^2 + d(v)^2] + \sum_{uv \in E_2(D_n)} [d(u)^2 + d(v)^2] \\ &\quad + \sum_{uv \in E_3(D_n)} [d(u)^2 + d(v)^2] \\ &= 8|E_1(D_n)| + 13|E_2(D_n)| + 18|E_3(D_n)| \\ &= 8(24 \times 2^{n-1} - 12) + 13(30 \times 2^{n-1} - 24) + 18(12 \\ &\quad \times 2^{n-1} - 9). \end{aligned}$$

Again, from (2), the F-polynomial is given by:

$$\begin{aligned} F(D_n, x) &= \sum_{uv \in E_1(D_n)} x^{[d(u)^2 + d(v)^2]} + \sum_{uv \in E_2(D_n)} x^{[d(u)^2 + d(v)^2]} \\ &\quad + \sum_{uv \in E_3(D_n)} x^{[d(u)^2 + d(v)^2]} \\ &= \sum_{uv \in E_1(D_n)} x^8 + \sum_{uv \in E_2(D_n)} x^{13} + \sum_{uv \in E_3(D_n)} x^{18} \\ &= |E_1(D_n)|x^8 + |E_2(D_n)|x^{13} + |E_3(D_n)|x^{18} \\ &= (24 \times 2^{n-1} - 12)x^8 + (30 \times 2^{n-1} - 24)x^{13} + (12 \\ &\quad \times 2^{n-1} - 9)x^{18}. \end{aligned}$$

### 3. Conclusions

In this paper, we considered six different classes of nanostar dendrimers. We found the F-index and its corresponding polynomial version of these nanostar dendrimers. The results obtained in our study have prospects for application in the chemical, biological and pharmaceutical sciences.

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