

Research Article

Molecular Irregularity Indices of Nanostar, Fullerene, and Polymer Dendrimers

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Received 21 July 2019; Accepted 17 December 2019; Published 28 February 2020

Academic Editor: Juan L. G. Guirao

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Dendrimers are highly branched organic macromolecules with successive layers of branch units surrounding a central core. Some properties like toxicity, entropy, and heats of vaporization of these dendrimers can be forecasted using topological indices. The present article is devoted to study of irregularity indices of three well-known classes of dendrimers, namely, nanostar dendrimer $D[p]$, fullerene dendrimer $NS_4[p]$, and polymer dendrimer $NS_5[p]$, where p is the step size. We also see the relation of irregularity of these dendrimers on the step size graphically.

1. Introduction

Dendrimers are nanosized, gradually well-formed molecules with precise, homogeneous, and monodispersed structure consisting of tree-like arms or branches used as anticancer drug [1]. These molecules were formed initially in 1978, by D. Tomalia and coworkers in the early 1980s and at the same time independently by George. Dendrimers might be labeled as “cascade molecules,” but this term is not fixed as dendrimers [2–4]. Dendrimers are approximately monodisperse macromolecules consisting of symmetric branched units constructed around a small molecule or a linear polymer core [5–7]. Dendrimers are used in supermolecular chemistry, especially in hot-guest reactions and self-assembly processes. These are eminently defined artificial macromolecules, which are described by a combination of a high number of functional groups and a compact molecular structure [3]. These materials are fresh addition in a class of macromolecular nanoscale delivery devices [8]. In Figure 1, the main three general parts of a dendrimer are elaborated.

The formations of dendrimer molecules start with the central atom or group of atoms called core [5, 9–12]. There is a debate about the exact arrangement of dendrimers, whether they are fully enlarged with high density at the surface or whether the end-groups bend back into a closely

packed interior [5, 11, 12]. Dendrimers have several applications in different fields of medicines like anticancer drugs in biomedical fields, a transdermal drug delivery, and gene delivery and as a magnetic resonance imaging contrast agent and as a dendritic sensor [13–15].

The subject matter of the present article is degree-based irregularity indices of some dendrimers. We are interested in the study of irregularity determinants of some famous dendrimers, namely, nanostar dendrimer $D[p]$, fullerene dendrimer $NS_4[p]$, and polymer dendrimer $NS_5[p]$. It has been keenly observed that the geometry and pattern of chemical systems characterize its physical aspects [16–24].

2. Preliminaries and Notations

Let G be a simple connected graph with vertex V and edge set E , and d_u be the degree of vertices u . A topological invariant is an isomorphism of the graph that preserves the topology of the graph. A graph is said to be regular if every vertex of the graph has the same degree. A topological invariant is called an irregularity index if this index vanishes for a regular graph and is nonzero for a nonregular graph. Regular graphs have been extensively investigated, particularly in mathematics. Their applications in chemical graph theory came to be known after the discovery of nanotubes and fullerenes.

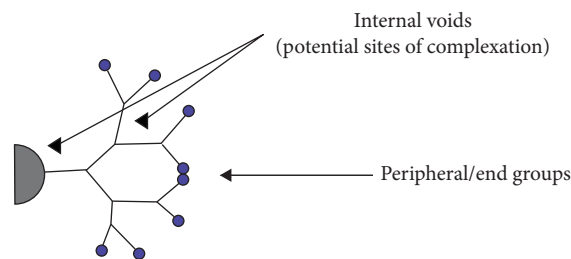


FIGURE 1: Three main parts of a dendrimer.

Paul Erdos emphasized this in the study of irregular graphs for the first time in history in [25]. In the Second Krakow Conference on Graph Theory, Erdos officially posed an open problem to “determine the extreme size of highly irregular graphs of given order” [26–28]. Since then, irregular graphs and the degree of irregularity have become one of the core open problems of graph theory. A graph in which each vertex has a different degree than the other vertices is known as a perfect graph. The authors of [27] demonstrated that there does not exist any perfect graph. The graphs lying in between are called quasiperfect graphs, in which all except two vertices have different degrees [29]. Irregularity of networks is discussed in [30]. Simplified ways of expressing the irregularities are irregularity indices. These irregularity indices have been studied recently in a novel way [31–33]. The first such irregularity index was introduced in [32]. Most of these indices used the concept of the imbalance of an edge defined as $\text{imball}_{uv} = |d_u - d_v|$ [33]. The Albertson index, $\text{AL}(G)$, was defined by Albertson in [32] as $\text{AL}(G) = \sum_{UV \in E} |d_u - d_v|$. In this index, the imbalance of edges is computed. The irregularity indices $\text{IRL}(G)$ and $\text{IRLU}(G)$ are introduced by Vukićević and Graovac [33] as $\text{IRL}(G) = \sum_{UV \in E} |\ln d_u - \ln d_v|$ and $\text{IRLU}(G) = \sum_{UV \in E} (|d_u - t d_v| / \min(d_u, d_v))$. Recently, Abdo et al. introduced the new term “total irregularity measure of a graph G ”, which is defined as $\text{IRR}_t(G) = 1/2 \sum_{UV \in E} |d_u - d_v|$ [34–36]. Recently, Gutman introduced the $\text{IRF}(G)$ irregularity index of the graph G , which is described as $\text{IRF}(G) = \sum_{UV \in E} (d_u - d_v)^2$ in [37]. The Randic index itself is directly related to an irregularity measure, which is described as $\text{IRA}(G) = \sum_{UV \in E} (d_u^{-1/2} - t d_v^{-1/2})^2$ in [38]. Further irregularity indices of similar nature can be traced in [37, 39] in detail. These indices are given as $\text{IRDIF}(G) = \sum_{UV \in E} |(d_u/d_v) - t (d_v/d_u)|$, $\text{IRLF}(G) = \sum_{UV \in E} (|d_u - d_v| / \sqrt{(d_u d_v)})$, $\text{LA}(G) = 2 \sum_{UV \in E} (|d_u - d_v| / (d_u + d_v))$, $\text{IRD1} = \sum_{UV \in E} \ln\{1 + |d_u - d_v|\}$, $\text{IRGA}(G) = \sum_{UV \in E} \ln(d_u + d_v / 2 \sqrt{(d_u d_v)})$, and $\text{IRB}(G) = \sum_{UV \in E} (d_u^{(1/2)} - d_v^{(1/2)})^2$. Recently, Zahid et al. computed the irregularity indices of a nanotube [40]. Gao et al. recently computed irregularity measures of some dendrimer structures in [41] and molecular structures in [42]. Hussain et al. discussed irregularity indices of some well-known benzenoid systems in [43] and some classes of nanostar dendrimers $\text{NS}_1[p]$, $\text{NS}_2[p]$, and $\text{NS}_3[p]$ in [44]. Liu et al. computed Zagreb and multiple Zagreb indices of

Eulerian graphs in [45] and number of spanning trees and normalized Laplacian of some network in [46].

In the current article, we are interested in finding the degree of irregularity of the nanostar dendrimers $D[p]$, fullerene dendrimer $\text{NS}_4[p]$, and polymer dendrimer $\text{NS}_5[p]$. Figures 2–4 represent molecular graphs of these three systems. The main motivation comes from the fact that graphs of the irregularity indices show close and accurate results about properties like entropy, standard enthalpy, vaporization, and acentric factors of octane isomers [39]. The molecular pattern and topology of these three dendrimers are shown in these figures. Figure 2 represents the structure of $D[p]$ nanostar dendrimer. In Figures 3 and 4, structure of $\text{NS}_4[p]$ fullerene dendrimers and $\text{NS}_5[p]$ polymer dendrimer is shown, respectively.

3. Main Results

In this section, we present our main theoretical results.

Theorem 1. Let D_p be the nanostar dendrimer, then the irregularity indices of D_p are as follows:

- (1) $\text{IRDIF}(D[p]) = 5(5 \times 2^{p-1} - 4)$.
- (2) $\text{IRR}(D[p]) = 6(5 \times 2^{p-1} - 4)$.
- (3) $\text{IRL}(D[p]) = 2.432790649(5 \times 2^{p-1} - 4)$.
- (4) $\text{IRLU}(D[p]) = 3(5 \times 2^{p-1} - 4)$.
- (5) $\text{IRLF}(D[p]) = 2.449489743(5 \times 2^{p-1} - 4)$.
- (6) $\sigma(D[p]) = 6(5 \times 2^{p-1} - 4)$.
- (7) $\text{IRLA}(D[p]) = 2.4(5 \times 2^{p-1} - 4)$.
- (8) $\text{IRD1} = 4.158883083(5 \times 2^{p-1} - 4)$.
- (9) $\text{IRA}(D[p]) = 0.1010205144(5 \times 2^{p-1} - 4)$.
- (10) $\text{IRGA}(D[p]) = 0.1224659836(5 \times 2^{p-1} - 4)$.
- (11) $\text{IRB}(D[p]) = 0.6061230866(5 \times 2^{p-1} - 4)$.
- (12) $\text{IRR}_t(D[p]) = 3(5 \times 2^{p-1} - 4)$.

Proof. In order to prove the above theorem, we have to consider Figure 2 along with Table 1.

Now using Table 1 and the above definitions, we have

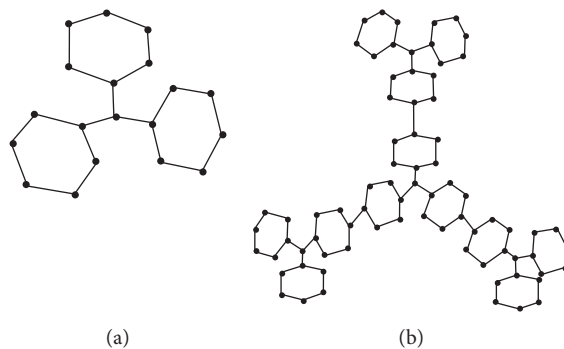


FIGURE 2: The nanostar dendrimer D_p for $p = 1$ shown in (a) and for $p = 2$ shown in (b).

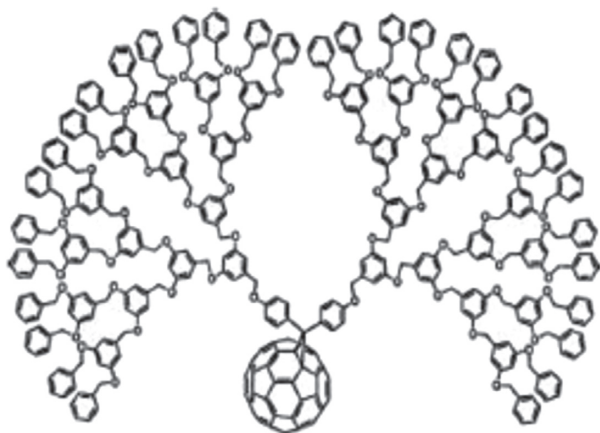


FIGURE 3: Fullerene dendrimer $NS_4[p]$.

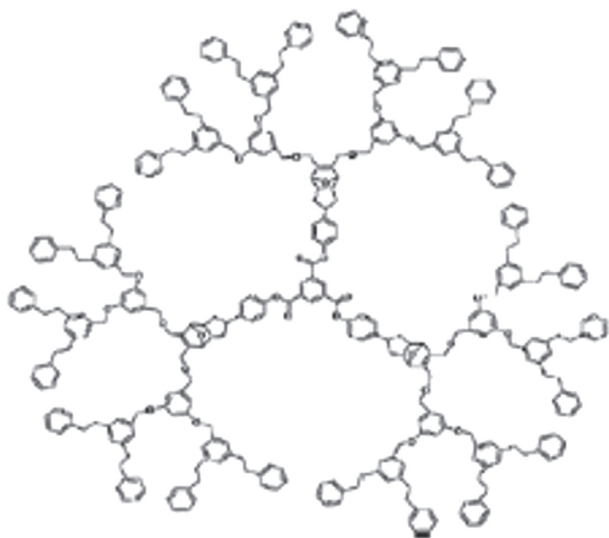


FIGURE 4: Polymer dendrimer $NS_5[p]$.

$$IRR(DIF(G)) = \sum_{UV \in E} \left| \frac{d_u}{d_v} - \frac{d_v}{d_u} \right|,$$

$$\begin{aligned} IRR(D_p, x, y) &= 12(2 \times 2^{p-1} - 1) \left| \frac{2}{2} - \frac{2}{2} \right| \\ &\quad + 6(5 \times 2^{p-1} - 4) \left| \frac{3}{2} - \frac{2}{3} \right| \\ &\quad + 6(12 \times 2^{p-1} - 9) \left| \frac{3}{3} - \frac{3}{3} \right| \\ &= 6(5 \times 2^{p-1} - 4) \left| \frac{3}{2} - \frac{2}{3} \right|, \end{aligned} \tag{1}$$

$$IRR(G) = \sum_{UV \in E} \text{imb}(e) \quad (\because \text{imb}(e) = |d_u - d_v|),$$

$$\begin{aligned} IRR(D_p, x, y) &= 12(2 \times 2^{p-1} - 1) |2 - 2| \\ &\quad + 6(5 \times 2^{p-1} - 4) |3 - 2| \\ &\quad + 6(12 \times 2^{p-1} - 9) |3 - 3| \\ &= 6(5 \times 2^{p-1} - 4) |3 - 2|, \end{aligned} \tag{2}$$

$$IRL(G) = \sum_{UV \in E} |\ln d_u - \ln d_v|,$$

$$\begin{aligned} IRL(D_p, x, y) &= (2 \times 2^{p-1} - 1) |\ln 2 - \ln 2| \\ &\quad + 6(5 \times 2^{p-1} - 4) |\ln 3 - \ln 2| \\ &\quad + 6(12 \times 2^{p-1} - 9) |\ln 3 - \ln 3| \\ &= 6(5 \times 2^{p-1} - 4) \left| \ln \frac{3}{2} \right|, \end{aligned} \tag{3}$$

TABLE 1: Edge partition of nanostar dendrimer D_p .

| Number of edges (d_u, d_v) | Number of indices |
|------------------------------|----------------------------|
| (2,2) | $12(2 \times 2^{p-1} - 1)$ |
| (2,3) | $6(5 \times 2^{p-1} - 4)$ |
| (3,3) | $6(12 \times 2^{p-1} - 9)$ |

$$\begin{aligned} \text{IRLU}(G) &= \sum_{UV \in E} \frac{|d_u - d_v|}{\min(d_u, d_v)}, \\ \text{IRLU}(D_p, x, y) &= (2 \times 2^{p-1} - 1) \frac{|2-2|}{2} \\ &\quad + 6(5 \times 2^{p-1} - 4) \frac{|3-2|}{2} \\ &\quad + 6(12 \times 2^{p-1} - 9) \frac{|3-3|}{3} \\ &= 6(5 \times 2^{p-1} - 4) \frac{|3-2|}{2}, \end{aligned} \quad (4)$$

$$\begin{aligned} \text{IRLF}(G) &= \sum_{UV \in E} \frac{|d_u - d_v|}{\sqrt{(d_u d_v)}}, \\ \text{IRLF}(D_p, x, y) &= (2 \times 2^{p-1} - 1) \frac{|2-2|}{\sqrt{4}} \\ &\quad + 6(5 \times 2^{p-1} - 4) \frac{|3-2|}{\sqrt{6}} \\ &\quad + 6(12 \times 2^{p-1} - 9) \frac{|3-3|}{\sqrt{9}} \\ &= 6(5 \times 2^{p-1} - 4) \frac{|3-2|}{\sqrt{6}}, \end{aligned} \quad (5)$$

$$\begin{aligned} \sigma(G) &= \sum_{UV \in E} (d_u - d_v)^2, \\ \sigma(D_p, x, y) &= (2 \times 2^{p-1} - 1)(2-2)^2 \\ &\quad + 6(5 \times 2^{p-1} - 4)(3-2)^2 \\ &\quad + 6(12 \times 2^{p-1} - 9)(3-3)^2 \left(\frac{\varepsilon}{2}\right) \\ &= 6(5 \times 2^{p-1} - 4)(3-2)^2, \end{aligned} \quad (6)$$

$$\begin{aligned} \text{IRLA}(G) &= 2 \sum_{UV \in E} \frac{|d_u - d_v|}{(d_u + d_v)}, \\ \text{IRLA}(D_p, x, y) &= 2 \left[(2 \times 2^{p-1} - 1) \frac{|2-2|}{4} \right. \\ &\quad + 6(5 \times 2^{p-1} - 4) \frac{|3-2|}{5} \\ &\quad \left. + 6(12 \times 2^{p-1} - 9) \frac{|3-3|}{6} \right] \\ &= 2 \left[6(5 \times 2^{p-1} - 4) \frac{|3-2|}{5} \right], \end{aligned} \quad (7)$$

$$\begin{aligned} \text{IRD1} &= \sum_{UV \in E} \ln\{1 + |d_u - d_v|\}, \\ \text{IRD1}(D_p, x, y) &= (2 \times 2^{p-1} - 1) \ln\{1 + |2-2|\} \\ &\quad + 6(5 \times 2^{p-1} - 4) \ln\{1 + |3-2|\} \\ &\quad + 6(12 \times 2^{p-1} - 9) \ln\{1 + |3-3|\} \\ &= 6(5 \times 2^{p-1} - 4) \ln 2, \end{aligned} \quad (8)$$

$$\begin{aligned} \text{IRA}(G) &= \sum_{UV \in E} (d_u^{(-1/2)} - d_v^{(-1/2)})^2, \\ \text{IRA}(D_p, x, y) &= (2 \times 2^{p-1} - 1) \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 \\ &\quad + 6(5 \times 2^{p-1} - 4) \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right)^2 \\ &\quad + 6(12 \times 2^{p-1} - 9) \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)^2 \\ &= 6(5 \times 2^{p-1} - 4) \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right)^2, \end{aligned} \quad (9)$$

$$\begin{aligned} \text{IRGA}(G) &= \sum_{UV \in E} \ln \frac{d_u + d_v}{2\sqrt{(d_u d_v)}}, \\ \text{IRGA}(D_p, x, y) &= (2 \times 2^{p-1} - 1) \ln \frac{|2+2|}{2\sqrt{4}} \\ &\quad + 6(5 \times 2^{p-1} - 4) \ln \frac{|3+2|}{2\sqrt{6}} \\ &\quad + 6(12 \times 2^{p-1} - 9) \ln \frac{|3+3|}{2\sqrt{9}} \\ &= 6(5 \times 2^{p-1} - 4) \ln \frac{|3+2|}{2\sqrt{6}}, \end{aligned} \quad (10)$$

$$\begin{aligned} \text{IRB}(G) &= \sum_{UV \in E} (d_u^{(1/2)} - d_v^{(1/2)})^2, \\ \text{IRB}(D_p, x, y) &= (2 \times 2^{p-1} - 1) (\sqrt{2} - \sqrt{2})^2 \\ &\quad + 6(5 \times 2^{p-1} - 4) (\sqrt{3} - \sqrt{2})^2 + \\ &\quad + 6(12 \times 2^{p-1} - 9) (\sqrt{3} - \sqrt{3})^2 \\ &= 6(5 \times 2^{p-1} - 4) (\sqrt{3} - \sqrt{2})^2, \end{aligned} \quad (11)$$

$$\begin{aligned} \text{IRR}_t(G) &= \frac{1}{2} \sum_{u, v \in V(G)} |d_u - d_v|, \\ \text{IRR}_t(D_p, x, y) &= \frac{1}{2} \left[12(2 \times 2^{p-1} - 1)|2-2| \right. \\ &\quad + 6(5 \times 2^{p-1} - 4)|3-2| \\ &\quad \left. + 6(12 \times 2^{p-1} - 9)|3-3| \right] \\ &= 3(5 \times 2^{p-1} - 4). \end{aligned} \quad (12)$$

Table 2 shows the values of these irregularity indices for some test values of parameter p . \square

Theorem 2. Let $NS_4[p]$ be the fullerene dendrimer, then the irregularity indices of $NS_4[p]$ are as follows:

- (1) $IRDIF(NS_4[p]) = 26.666.2^{p-1} + 2.66667.2^{p+1} - 0.6664.$
- (2) $IRR(NS_4[p]) = 32.2^{p-1} + 2.2^{p+1} - 2.$
- (3) $IRL(NS_4[p]) = 12.97488.2^{p-1} + 1.6986.2^{p+1} - 1.517628.$
- (4) $IRLU(NS_4[p]) = 16.2^{p-1} + 2.2^{p+1} - 2.$
- (5) $IRLF(NS_4[p]) = 13.063936.2^{p-1} + 1.1547.2^{p+1} - 1.533934.$
- (6) $\sigma(NS_4[p]) = 32.2^{p-1} + 4.2^{p+1} - 2.$
- (7) $IRLA(NS_4[p]) = 12.8.2^{p-1} + 2^{p+1} - 1.485714.$
- (8) $IRD1 = 22.180704.2^{p-1} + 1.098612.2^{p+1} - 1.386294.$
- (9) $IRA(NS_4[p]) = 0.538784.2^{p-1} + 0.17863322^{p+1} - 0.128713.$
- (10) $IRGA(NS_4[p]) = 57.242453.2^{p-1} + 1.242453.2^{p+1} + 0.473936.$
- (11) $IRB(NS_4[p]) = 3.232672.2^{p-1} + 0.535898.2^{p+1} - 0.377386.$
- (12) $IRR_t(NS_4[p]) = 16.2^{p-1} + 2^{p+1} - 1.$

Proof. In order to prove the above theorem, we have to consider Figure 3 and Table 3.

Now using Table 3 and the above definitions, we have

$$IRDIF(G) = \sum_{UV \in E} \left| \frac{d_u}{d_v} - \frac{d_v}{d_u} \right|,$$

$$IRDIF(NS_4[p], x, y) = 32.2^{p-1} - 8 \left| \frac{3}{2} - \frac{2}{3} \right| + 2^{p+1} + 2 \left| \frac{2}{2} - \frac{2}{2} \right| + 2^{p+1} \left| \frac{3}{1} - \frac{1}{3} \right| + 86. \left| \frac{3}{3} - \frac{3}{3} \right| + 6 \left| \frac{4}{3} - \frac{3}{4} \right| + 3 \left| \frac{4}{4} - \frac{4}{4} \right|$$

$$= 32.2^{p-1} - 8 \left| \frac{3}{2} - \frac{2}{3} \right| + 2^{p+1} \left| \frac{3}{1} - \frac{1}{3} \right| + 6 \left| \frac{4}{3} - \frac{3}{4} \right|,$$

$$IRR(G) = \sum_{UV \in E} \text{imb}(e) \quad \therefore \text{imb}(e) = |d_u - d_v|,$$

$$IRR(NS_4[p], x, y) = 32.2^{p-1} - 8|3 - 2| + 2^{p+1} + 2|2 - 2| + 2^{p+1}|3 - 1| + 86.|3 - 3| + 6|4 - 3| + 3|4 - 4| = 32.2^{p-1} - 8 + 2.2^{p+1} + 6,$$
(14)

$$IRL(G) = \sum_{UV \in E} |\ln d_u - \ln d_v|,$$

$$IRL(NS_4[p], x, y) = 32.2^{p-1} - 8|\ln 3 - \ln 2| + 2^{p+1} + 2|\ln 2 - \ln 2| + 2^{p+1}|\ln 3 - \ln 1| + 86.|\ln 3 - \ln 3| + 6|\ln 4 - \ln 3| + 3|\ln 4 - \ln 4| = 32.2^{p-1} - 8 \ln \frac{3}{2} + 2^{p+1} \ln \frac{3}{1} + 6. \ln \frac{4}{3},$$
(15)

$$IRLU(G) = \sum_{UV \in E} \frac{|d_u - d_v|}{\min(d_u, d_v)},$$

$$IRLU(NS_4[p], x, y) = 32.2^{p-1} - 8 \frac{|3 - 2|}{2} + 2^{p+1} + 2 \frac{|2 - 2|}{2} + 2^{p+1} \frac{|3 - 1|}{1} + 86. \frac{|3 - 3|}{3} + 6. \frac{|4 - 3|}{3} + 3. \frac{|4 - 4|}{4} = \frac{32.2^{p-1} - 8}{2} + 2.2^{p+1} + 2,$$
(16)

$$IRLF(G) = \sum_{UV \in E} \frac{|d_u - d_v|}{\sqrt{(d_u d_v)}},$$

$$IRLF(NS_4[p], x, y) = 32.2^{p-1} - 8 \frac{|3 - 2|}{\sqrt{6}} + 2^{p+1} + 2 \frac{|2 - 2|}{\sqrt{4}} + 2^{p+1} \frac{|3 - 1|}{\sqrt{3}} + 86. \frac{|3 - 3|}{\sqrt{9}} + 6. \frac{|4 - 3|}{\sqrt{12}} + 3. \frac{|4 - 4|}{\sqrt{16}} = \frac{32.2^{p-1} - 8}{\sqrt{6}} + \frac{2.2^{p+1}}{\sqrt{3}} + \frac{6}{\sqrt{12}},$$
(17)

$$\sigma(G) = \sum_{UV \in E} (d_u - d_v)^2,$$

$$\sigma(NS_4[p], x, y) = 32.2^{p-1} - 8(3 - 2)^2 + 2^{p+1} + 2(2 - 2)^2 + 2^{p+1}(3 - 1)^2 + 86.(3 - 3)^2 + 6.(4 - 3)^2 + 3.(4 - 4)^2 = 32.2^{p-1} - 8 + 4.2^{p+1} + 6,$$
(18)

TABLE 2: Irregularity indices for nanostar dendrimer D_p .

| Irregularity indices | $p = 1$ | $p = 2$ | $p = 3$ | $p = 4$ | $p = 5$ |
|---|---------|---------|---------|----------|----------|
| $\text{IRDIF}(G) = \sum_{UV \in E} (d_u/d_v) - (d_v/d_u) $ | 5 | 30 | 80 | 180 | 380 |
| $\text{AL}(G) = \sum_{UV \in E} d_u - d_v $ | 6 | 36 | 96 | 216 | 456 |
| $\text{IRL}(G) = \sum_{UV \in E} \ln d_u - \ln d_v $ | 2.4328 | 14.5968 | 38.9246 | 87.5805 | 184.8921 |
| $\text{IRLU}(G) = \sum_{UV \in E} (d_u - d_v /\min(d_u, d_v))$ | 3 | 18 | 48 | 108 | 228 |
| $\text{IRLU}(G) = \sum_{UV \in E} (d_u - d_v /\sqrt{(d_u d_v)})$ | 2.4495 | 14.6969 | 39.1918 | 88.1816 | 186.1612 |
| $\text{IRF}(G) = \sum_{UV \in E} (d_u - d_v)^2$ | 6 | 36 | 96 | 216 | 456 |
| $\text{IRLA}(G) = 2 \sum_{UV \in E} (d_u - d_v /(d_u + d_v))$ | 2.4 | 14.4 | 38.4 | 86.4 | 182.4 |
| $\text{IRD1} = \sum_{UV \in E} \ln\{1 + d_v - d_u \}$ | 4.1589 | 24.9533 | 66.5422 | 149.7198 | 316.0751 |
| $\text{IRA}(G) = \sum_{UV \in E} (d_u^{(-1/2)} - d_v^{(-1/2)})^2$ | 0.10102 | 0.6061 | 1.6163 | 3.6367 | 7.6775 |
| $\text{IRGA}(G) = \sum_{UV \in E} \ln(d_u + d_v/2\sqrt{(d_u d_v)})$ | 0.1225 | 0.73479 | 1.9594 | 4.4087 | 9.3074 |
| $\text{IRB}(G) = \sum_{UV \in E} (d_u^{(1/2)} - d_v^{(1/2)})^2$ | 0.6061 | 3.6367 | 9.6979 | 21.8204 | 46.0653 |
| $\text{IRR}_t(G) = (1/2) \sum_{UV \in E} d_u - d_v $ | 3 | 18 | 48 | 108 | 228 |

TABLE 3: Edge partition of fullerene dendrimers.

| Number of edges (d_u, d_v) | Number of indices |
|------------------------------|------------------------|
| (2,3) | $32 \cdot 2^{p-1} - 8$ |
| (2,2) | $2^{p+1} + 2$ |
| (1,3) | 2^{p+1} |
| (3,3) | 86 |
| (3,4) | 6 |
| (4,4) | 3 |

$$\text{IRLA}(G) = 2 \sum_{UV \in E} \frac{|d_u - d_v|}{(d_u + d_v)},$$

$$\begin{aligned} \text{IRLA}(\text{NS}_3[p], x, y) &= 2 \left[32 \cdot 2^{p-1} - 8 \frac{|3-2|}{5} + 2^{p+1} \right. \\ &\quad + 2 \frac{|2-2|}{4} + 2^{p+1} \frac{|3-1|}{4} + 86 \cdot \frac{|3-3|}{6} \\ &\quad \left. + 6 \cdot \frac{|4-3|}{7} + 3 \cdot \frac{|4-4|}{8} \right] \\ &= 2 \left[\frac{32 \cdot 2^{p-1} - 8}{5} + \frac{2^{p+1}}{2} + \frac{6}{7} \right], \end{aligned} \quad (19)$$

$$\text{IRD1} = \sum_{UV \in E} \ln\{1 + |d_v - d_u|\},$$

$$\begin{aligned} \text{IRD1}(\text{NS}_4[n], x, y) &= 32 \cdot 2^{p-1} - 8 \ln\{1 + |3-2|\} \\ &\quad + 2^{p+1} + 2 \ln\{1 + |2-2|\} \\ &\quad + 2^{p+1} \ln\{1 + |3-1|\} \\ &\quad + 86 \ln\{1 + |3-3|\} \\ &\quad + 6 \ln\{1 + |4-3|\} \\ &\quad + 3 \ln\{1 + |4-4|\} \\ &= 32 \cdot 2^{p-1} - 8 \ln 2 \\ &\quad + 2^{p+1} \ln 3 + 6 \ln 2, \end{aligned} \quad (20)$$

$$\text{IRA}(G) = \sum_{UV \in E} (d_u^{(-1/2)} - d_v^{(-1/2)})^2,$$

$$\begin{aligned} \text{IRA}(\text{NS}_4[p], x, y) &= 32 \cdot 2^{p-1} - 8 \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right)^2 + 2^{p+1} \\ &\quad + 2 \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 + 2^{p+1} \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{1}} \right)^2 \\ &\quad + 86 \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)^2 + 6 \left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{3}} \right)^2 \\ &\quad + 3 \left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{4}} \right)^2 \\ &= 32 \cdot 2^{p-1} - 8 \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right)^2 \\ &\quad + 2^{p+1} \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{1}} \right)^2 + 6 \left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{3}} \right)^2, \end{aligned} \quad (21)$$

$$\text{IRGA}(G) = \sum_{UV \in E} \ln \frac{d_u + d_v}{2\sqrt{(d_u d_v)}},$$

$$\begin{aligned} \text{IRGA}(\text{NS}_4[p], x, y) &= 32 \cdot 2^{p-1} - 8 \ln \frac{|3+2|}{2\sqrt{6}} + 2^{p+1} \\ &\quad + 2 \ln \frac{|2+2|}{2\sqrt{4}} + 2^{p+1} \ln \frac{|3+1|}{2\sqrt{3}} \\ &\quad + 86 \ln \frac{|3+3|}{2\sqrt{9}} + 6 \ln \frac{|4+3|}{2\sqrt{12}} \\ &\quad + 3 \ln \frac{|4+4|}{2\sqrt{16}} \\ &= 32 \cdot 2^{p-1} - 8 \ln \frac{5}{2\sqrt{6}} \\ &\quad + 2^{p+1} \ln \frac{4}{2\sqrt{3}} + 6 \ln \frac{7}{2\sqrt{12}}, \end{aligned} \quad (22)$$

$$\begin{aligned}
\text{IRB}(G) &= \sum_{UV \in E} (d_u^{(1/2)} - d_v^{(1/2)})^2, \\
\text{IRB}(NS_4[p], x, y) &= 32.2^{p-1} - 8(\sqrt{3} - \sqrt{2})^2 + 2^{p+1} \\
&\quad + 2(\sqrt{2} - \sqrt{2})^2 + 2^{p+1}(\sqrt{3} - \sqrt{1})^2 \\
&\quad + 86(\sqrt{3} - \sqrt{3})^2 + 6(\sqrt{4} - \sqrt{3})^2 \\
&\quad + 3(\sqrt{4} - \sqrt{4})^2 \\
&= 32.2^{p-1} - 8(\sqrt{3} - \sqrt{2})^2 \\
&\quad + 2^{p+1}(\sqrt{3} - \sqrt{1})^2 + 6(\sqrt{4} - \sqrt{3})^2,
\end{aligned} \tag{23}$$

$$\begin{aligned}
\text{IRR}_t(G) &= \frac{1}{2} \sum_{UV \in E} |d_u - d_v|, \\
\text{IRR}_t(NS_4[p], x, y) &= \frac{1}{2} [32.2^{p-1} - 8|3 - 2| + 2^{p+1} \\
&\quad + 2|2 - 2| + 2^{p+1}|3 - 1| \\
&\quad + 86|3 - 3| + 6|4 - 3| + 3|4 - 4|] \\
&= \frac{1}{2} [32.2^{p-1} - 8 + 2.2^{p+1} + 6].
\end{aligned} \tag{24}$$

Table 4 demonstrates the values of these irregularity indices of fullerene dendrimers for some test values of parameter p . \square

Theorem 3. Let $NS_5[p]$ be the polymer dendrimer, then the irregularity indices of $NS_5[p]$ are as follows:

- (1) $\text{IRDIF}(NS_5[p]) = 4.999998.2^{p+3} + 8.2^{p+1} + 3.$
- (2) $\text{IRR}(NS_5[p]) = 6.2^{p+3} + 6.2^{p+1}.$
- (3) $\text{IRL}(NS_5[p]) = 2.43279.2^{p+3} + 3.295836.2^{p+1} + 0.8630546.$
- (4) $\text{IRLU}(NS_5[p]) = 3.2^{p+3} + 6.2^{p+1} + 3.$
- (5) $\text{IRLF}(NS_5[p]) = 4.242641.2^{p+3} + 2.44949.2^{p+1} - 1.793151.$
- (6) $\sigma(NS_5[p]) = 6.2^{p+3} + 12.2^{p+1} + 6.$
- (7) $\text{IRLA}(NS_5[p]) = 2.4.2^{p+3} + 3.2^{p+1} + 0.6.$
- (8) $\text{IRD1} = 4.158882.2^{p+3} + 3.295836.2^{p+1} - 0.863046.$
- (9) $\text{IRA}(NS_5[p]) = 0.101022.2^{p+3} + 0.535899.2^{p+1} + 0.434877.$
- (10) $\text{IRGA}(NS_5[p]) = 10.87302.2^{p+3} + 3.727359.2^{p+1} - 7.145661.$
- (11) $\text{IRB}(NS_5[p]) = 0.606126.2^{p+3} + 1.607694.2^{p+1} + 1.001568.$
- (12) $\text{IRR}_t(NS_5[p]) = 3.2^{p+3} + 3.2^{p+1}.$

Proof. In order to prove the above theorem, we have to consider Figure 4 and Table 5.

Now, using Table 5 and the above definitions, we have

$$\begin{aligned}
\text{IRDIF}(G) &= \sum_{UV \in E} \left| \frac{d_u}{d_v} - \frac{d_v}{d_u} \right|, \\
\text{IRDIF}(NS_5[p], x, y) &= 6(2^{p+3} - 1) \left| \frac{3}{2} - \frac{2}{3} \right| + 6(2^{p+1}) \left| \frac{2}{2} - \frac{2}{2} \right| \\
&\quad + (24) \left| \frac{3}{3} - \frac{3}{3} \right| + 3(2^{p+1} + 1) \left| \frac{3}{1} - \frac{1}{3} \right| \\
&= 6(2^{p+3} - 1) \left| \frac{3}{2} - \frac{2}{3} \right| \\
&\quad + 3(2^{p+1} + 1) \left| \frac{3}{1} - \frac{1}{3} \right|,
\end{aligned} \tag{25}$$

$$\begin{aligned}
\text{IRR}(G) &= \sum_{UV \in E} \text{imb}(e) \quad \therefore \text{imb}(e) \\
\text{IRR}(NS_5[p], x, y) &= 6(2^{p+3} - 1)|3 - 2| \\
&\quad + 6(2^{p+1})|2 - 2| + (24)|3 - 3| \\
&\quad + 3(2^{p+1} + 1)|3 - 1| \\
&= 6(2^{p+3} - 1) + 6(2^{p+1} + 1),
\end{aligned} \tag{26}$$

$$\begin{aligned}
\text{IRL}(G) &= \sum_{UV \in E} |\ln d_u - \ln d_v|, \\
\text{IRL}(NS_5[p], x, y) &= 6(2^{p+3} - 1)|\ln 3 - \ln 2| \\
&\quad + 6(2^{p+1})|\ln 2 - \ln 2| + (24)|\ln 3 - \ln 3| \\
&\quad + 3(2^{p+1} + 1)|\ln 3 - \ln 1| \\
&= 6(2^{p+3} - 1)\ln \frac{3}{2} + 3(2^{p+1} + 1)\ln \frac{3}{1},
\end{aligned} \tag{27}$$

$$\begin{aligned}
\text{IRLU}(G) &= \sum_{UV \in E} \frac{|d_u - d_v|}{\min(d_u, d_v)}, \\
\text{IRLU}(NS_5[p], x, y) &= 6(2^{p+3} - 1) \frac{|3 - 2|}{2} \\
&\quad + 6(2^{p+1}) \frac{|2 - 2|}{2} + 24 \frac{|3 - 3|}{3} \\
&\quad + 3(2^{p+1} + 1) \frac{|3 - 1|}{1} \\
&= 3(2^{p+3} - 1) + 6(2^{p+1} + 1),
\end{aligned} \tag{28}$$

$$\begin{aligned}
\text{IRLF}(G) &= \sum_{UV \in E} \frac{|d_u - d_v|}{\sqrt{(d_u d_v)}}, \\
\text{IRLF}(NS_5[p], x, y) &= 6(2^{p+3} - 1) \frac{|3 - 2|}{\sqrt{6}} \\
&\quad + 6(2^{p+1}) \frac{|2 - 2|}{\sqrt{4}} + 24 \frac{|3 - 3|}{\sqrt{9}} \\
&\quad + 3(2^{p+1} + 1) \frac{|3 - 1|}{\sqrt{3}} \\
&= \frac{6(2^{p+3} - 1)}{\sqrt{2}} + \frac{6(2^{p+1} + 1)}{\sqrt{6}},
\end{aligned} \tag{29}$$

TABLE 4: Irregularity indices for fullerene dendrimer $NS_4[p]$.

| Irregularity indices | $p = 1$ | $p = 2$ | $p = 3$ | $p = 4$ | $p = 5$ |
|--|-----------|-----------|-----------|-----------|-----------|
| $IRDIF(G) = \sum_{UV \in E} (d_u/d_v) - t(d_v/d_u) $ | 36.66628 | 73.99896 | 148.66432 | 297.99504 | 596.65648 |
| $AL(G) = \sum_{UV \in E} d_u - d_v $ | 38 | 78 | 158 | 318 | 638 |
| $IRL(G) = \sum_{UV \in E} \ln d_u - \ln d_v $ | 18.251652 | 38.0209 | 77.5594 | 156.636 | 314.7908 |
| $IRLU(G) = \sum_{UV \in E} d_u - d_v /\min(d_u, d_v)$ | 22 | 46 | 94 | 190 | 382 |
| $IRLU(G) = \sum_{UV \in E} (d_u - d_v /\sqrt{(d_u d_v)})$ | 16.148802 | 33.83153 | 69.197010 | 139.92795 | 281.38984 |
| $IRF(G) = \sum_{UV \in E} (d_u - d_v)^2$ | 46 | 94 | 190 | 382 | 766 |
| $IRLA(G) = 2 \sum_{UV \in E} (d_u - d_v /(d_u + d_v))$ | 15.31428 | 32.11428 | 65.714286 | 132.91428 | 267.31428 |
| $IRD1 = \sum_{UV \in E} \ln\{1 + d_u - d_v \}$ | 25.18885 | 51.7640 | 104.9143 | 211.2149 | 423.8161 |
| $IRA(G) = \sum_{UV \in E} (d_u^{(-1/2)} - d_v^{(-1/2)})^2$ | 1.1246038 | 2.3779206 | 4.8845542 | 9.8978214 | 19.924355 |
| $IRGA(G) = \sum_{UV \in E} \ln(d_u + t d_v)/2\sqrt{(d_u d_v)}$ | 58.958842 | 117.44374 | 234.4135 | 468.3531 | 936.2324 |
| $IRB(G) = \sum_{UV \in E} (d_u^{(1/2)} - d_v^{(1/2)})^2$ | 4.99887 | 10.375142 | 21.127670 | 42.6327 | 85.642838 |
| $IRR_t(G) = (1/2) \sum_{UV \in E} d_u - d_v $ | 19 | 39 | 79 | 159 | 319 |

TABLE 5: Edge partition of polymer dendrimer $NS_5[p]$.

| Number of edges (d_u, d_v) | Number of indices |
|------------------------------|-------------------|
| (2,3) | $6(2^{p+3} - 1)$ |
| (2,2) | $6(2^{p+1})$ |
| (3,3) | 24 |
| (1,3) | $3(2^{p+1} + 1)$ |

$$\begin{aligned} \sigma(G) &= \sum_{UV \in E} (d_u - d_v)^2, \\ \sigma(NS_5[p], x, y) &= 6(2^{p+3} - 1)(3 - 2)^2 \\ &\quad + 6(2^{p+1})(2 - 2)^2 + 24 \cdot (3 - 3)^2 \quad (30) \\ &\quad + 3(2^{p+1} + 1)(3 - 1)^2 \\ &= 6(2^{p+3} - 1) + 12(2^{p+1} + 1), \end{aligned}$$

$$\begin{aligned} IRLA(G) &= 2 \sum_{UV \in E} \frac{|d_u - d_v|}{(d_u + d_v)}, \\ IRLA(NS_5[p], x, y) &= 2 \left[6(2^{p+3} - 1) \frac{|3 - 2|}{(3 + 2)} \right. \\ &\quad + 6(2^{p+1}) \frac{|2 - 2|}{(2 + 2)} + 24 \cdot \frac{|3 - 3|}{(3 + 3)} \\ &\quad \left. + 3(2^{p+1} + 1) \frac{|3 - 1|}{(3 + 1)} \right] \\ &= 2 \left[\frac{6(2^{p+3} - 1)}{5} + \frac{6(2^{p+1} + 1)}{4} \right], \quad (31) \end{aligned}$$

$$\begin{aligned} IRD1 &= \sum_{UV \in E} \ln\{1 + |d_u - d_v|\}, \\ IRD1(NS_5[p], x, y) &= 6(2^{p+3} - 1) \ln\{1 + |3 - 2|\} \\ &\quad + 6(2^{p+1}) \ln\{1 + |2 - 2|\} \\ &\quad + 24 \cdot \ln\{1 + |3 - 3|\} \quad (32) \\ &\quad + 3(2^{p+1} + 1) \ln\{1 + |3 - 1|\} \\ &= 6(2^{p+3} - 1) \ln 2 \\ &\quad + 3(2^{p+1} + 1) \ln 3, \end{aligned}$$

$$\begin{aligned} IRA(G) &= \sum_{UV \in E} (d_u^{(-1/2)} - d_v^{(-1/2)})^2, \\ IRA(NS_5[p], x, y) &= 6(2^{p+3} - 1) \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right)^2 \\ &\quad + 6(2^{p+1}) \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 \\ &\quad + 24 \cdot \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)^2 \\ &\quad + 3(2^{p+1} + 1) \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{1}} \right)^2 \\ &= 6(2^{p+3} - 1) \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right)^2 \\ &\quad + 3(2^{p+1} + 1) \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{1}} \right)^2, \quad (33) \end{aligned}$$

$$\begin{aligned} IRGA(G) &= \sum_{UV \in E} \ln \frac{d_u + d_v}{2\sqrt{(d_u d_v)}}, \\ IRGA(NS_5[p], x, y) &= 6(2^{p+3} - 1) \ln \frac{|3 + 2|}{2\sqrt{6}} \\ &\quad + 6(2^{p+1}) \ln \frac{|2 + 2|}{2\sqrt{4}} \\ &\quad + 24 \cdot \ln \frac{|3 + 3|}{2\sqrt{9}} \quad (34) \\ &\quad + 3(2^{p+1} + 1) \ln \frac{|3 + 1|}{2\sqrt{3}} \\ &= 6(2^{p+3} - 1) \ln \frac{5}{2\sqrt{6}} \\ &\quad + 3(2^{p+1} + 1) \ln \frac{4}{2\sqrt{3}}, \end{aligned}$$

TABLE 6: Irregularity indices for polymer dendrimer $NS_5[p]$.

| Irregularity indices | $p = 1$ | $p = 2$ | $p = 3$ | $p = 4$ | $p = 5$ |
|---|-----------|----------|----------|-----------|----------|
| $IRDIF(G) = \sum_{UV \in E} (d_u/d_v) - t(d_v/d_u) $ | 114.9999 | 226.999 | 450.99 | 898.999 | 1794.99 |
| $AL(G) = \sum_{UV \in E} d_u - d_v $ | 120 | 240 | 480 | 960 | 1920 |
| $IRL(G) = \sum_{UV \in E} \ln d_u - \ln d_v $ | 52.97103 | 105.0790 | 209.2949 | 417.7269 | 834.5907 |
| $IRLU(G) = \sum_{UV \in E} (d_u - td_v /\min(d_u, d_v))$ | 75 | 147 | 291 | 579 | 1155 |
| $IRLU(G) = \sum_{UV \in E} (d_u - td_v /\sqrt{(d_u d_v)})$ | 75.8870 | 153.567 | 308.9277 | 619.648 | 1241.090 |
| $IRF(G) = \sum_{UV \in E} (d_u - d_v)^2$ | 150 | 294 | 582 | 1158 | 2310 |
| $IRLA(G) = 2 \sum_{UV \in E} (d_u - td_v /(d_u + d_v))$ | 51 | 101.4 | 202.2 | 403.8 | 807 |
| $IRD1 = \sum_{UV \in E} \ln\{1 + d_u - d_v \}$ | 78.8624 | 158.5878 | 318.038 | 636.9406 | 1274.744 |
| $IRA(G) = \sum_{UV \in E} (d_u^{(-1/2)} - d_v^{(-1/2)})^2$ | 4.19482 | 7.95477 | 15.47466 | 30.514461 | 60.59404 |
| $IRGA(G) = \sum_{UV \in E} (\ln d_u + d_v/2\sqrt{(d_u d_v)})$ | 181.73209 | 370.6098 | 748.3653 | 1503.876 | 3014.898 |
| $IRB(G) = \sum_{UV \in E} (d_u^{(1/2)} - d_v^{(1/2)})^2$ | 17.1303 | 33.2591 | 65.5167 | 130.0319 | 259.062 |
| $IRR_t(G) = (1/2) \sum_{UV \in E} d_u - d_v $ | 60 | 120 | 240 | 480 | 960 |

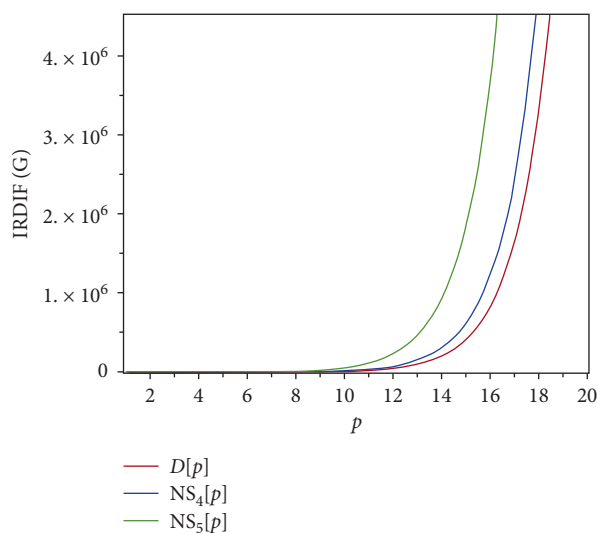


FIGURE 5: Graphs of irregularity index IRDIF.

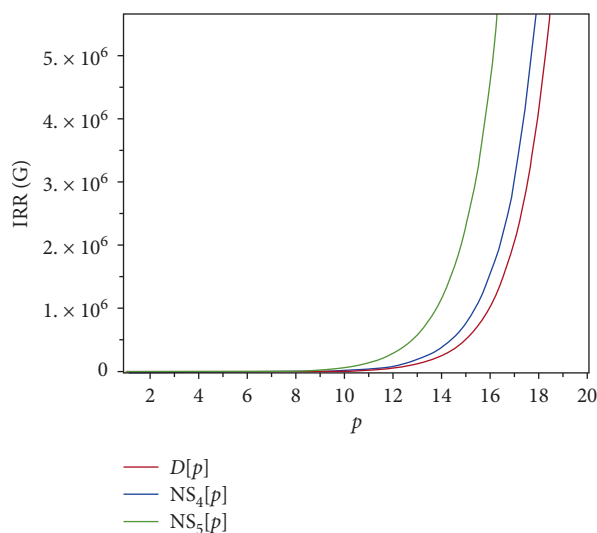


FIGURE 6: Curves of irregularity index IRR.

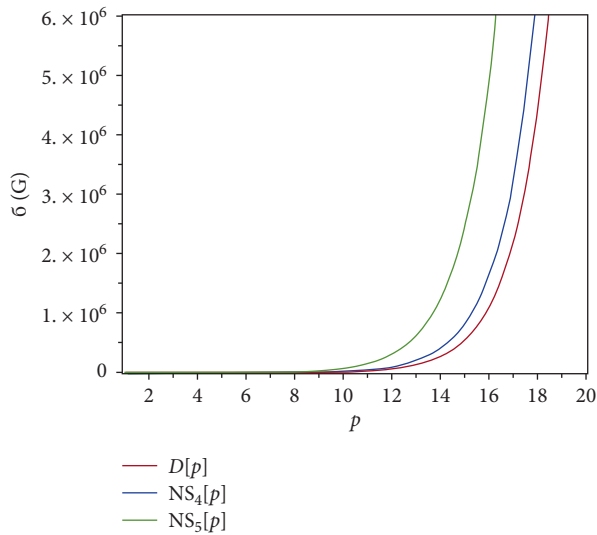
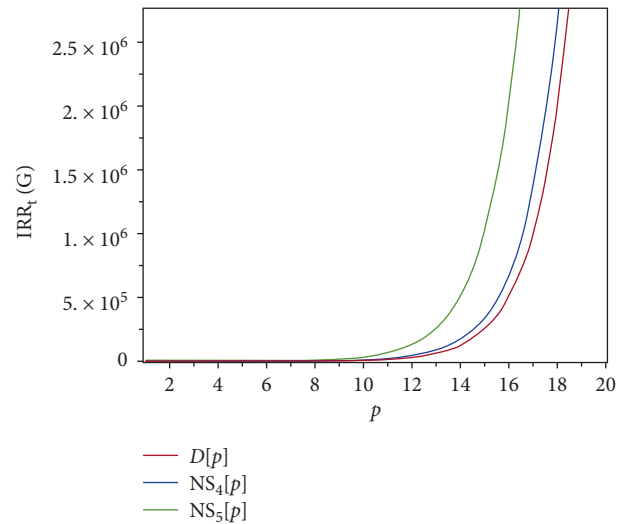
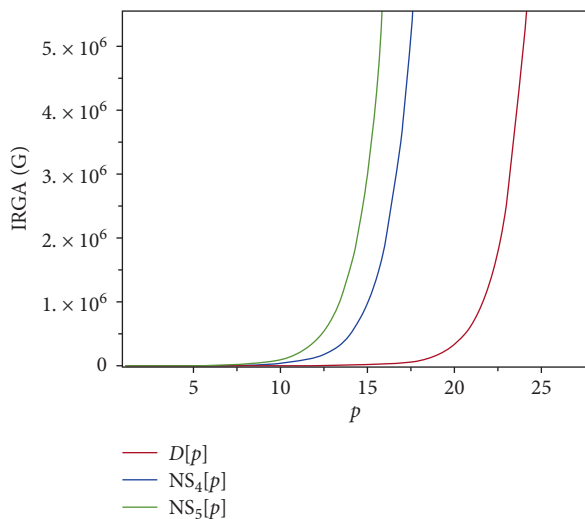
FIGURE 7: Curves of irregularity index σ .FIGURE 9: Curves of irregularity index IRR_t .

FIGURE 8: Curves of irregularity index IRGA.

$$\begin{aligned}
 IRB(G) &= \sum_{UV \in E} (d_u^{(1/2)} - d_v^{(1/2)})^2, \\
 IRB(NS_5[p], x, y) &= 6(2^{p+3} - 1)(\sqrt{3} - \sqrt{2})^2 \\
 &\quad + 6(2^{p+1})(\sqrt{2} - \sqrt{2})^2 \\
 &\quad + 24(\sqrt{3} - \sqrt{3})^2 \\
 &\quad + 3(2^{p+1} + 1)(\sqrt{3} - \sqrt{1})^2 \\
 &= 6(2^{p+3} - 1)(\sqrt{3} - \sqrt{2})^2 \\
 &\quad + 3(2^{p+1} + 1)(\sqrt{3} - \sqrt{1})^2,
 \end{aligned} \tag{35}$$

$$\begin{aligned}
 IRR_t(G) &= \frac{1}{2} \sum_{UV \in E} |d_u - d_v|, \\
 IRR_t(NS_5[p], x, y) &= \frac{1}{2} [6(2^{p+3} - 1)|3 - 2| \\
 &\quad + 6(2^{p+1})|2 - 2| + 24|3 - 3| \\
 &\quad + 3(2^{p+1} + 1)|3 - 1|] \\
 &= \frac{1}{2} [6(2^{p+3} - 1) + 6(2^{p+1} + 1)].
 \end{aligned} \tag{36}$$

Table 6 depicts the values of these irregularity indices for some test values of parameter p . \square

4. Graphical Analysis, Discussions, and Conclusions

In the present section, we give the graphical analysis of the irregularity measures of the above three classes of dendrimer structures. We summarize our findings in terms of graphs of irregularity indices against the step size p from 1 to 30.

Figure 5 presents three different curves for the values of irregularity index IRDIF against the step size p . It can be demonstrated that irregularity of all three dendrimers tends to increase with increase in step size. It is noticeable that for $p > 16$, IRDIF rises sharply showing that irregularity is nonuniform.

In Figure 6, curves of irregularity index IRR have been drawn against step size p and behavior of this index is similar to IRDIF.

All irregularity indices show the similar pattern for three dendrimers, as indicated in Figures 7–9.

From the above discussion, it can be concluded that $NS_5[p]$ is relatively more irregular than $NS_4[p]$ and $D[p]$ is

most regular in these three dendrimers. The dependence of irregularity of structures on step size could be a potential information carrier for modelling nanoscale drugs and devices.

Data Availability

No such data are associated with this article.

Conflicts of Interest

The authors declare no conflicts of interest.

Authors' Contributions

M. M. gave the idea, and H. A., Q. X., and Z. W. wrote the article.

Acknowledgments

This research was supported by the Natural Science Fund of Anhui Wenda University of Information Engineering (Grant no. XZR2019A10) and Quality Engineering Fund of Anhui Education Department (Project code: 2018jyxm1318).

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