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Exploring Reverse Imbalance Irregularities in Nanomaterials: Applications in Nanotechnology

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Abstract: A topological index can be viewed as a conversion of a molecular structure to a real number and it is also known as a parameter to predict important values related to molecular structure. In general, irregularity indices are often used for quantitative analysis of non-regular graph of topological structure. In various applications and challenges in biomedical engineering and chemistry it is important to understand how irregular a molecular structure is? In this paper we determine the reverse irregularity indices of polypropylenimine octamin dendrimers $NS_1[k]$, $NS_2[k]$ and $NS_3[k]$.

Keywords: Nanometirials, Nanotechnology, Dendrimers, Topological Invariants.

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1. Introduction

Dendrimers are nano-sized molecules with radially symmetrical structures, with very good homogeneity and monodispersal arms [1]. Unusual properties like small size, high flexibility, cavities, well-defined three-dimensional structure, and globular shape are acknowledged in dendrimers. These are unusual candidates for the use of nano-technology and various biomedical purposes [2]. Dendrimers consist of a fundamental atom or the group of atoms which we call the core, branches of other atoms known as "dendrons" rise from this central structure through different chemical reactions. Compared to ordinary linear polymers, dendrimers have significantly enhanced physical and chemical properties. Today dendrimers are attracting huge number of people in the fields of material, nanoscience, chemistry, medicine and physics because of their broad range of brilliant applications [3,4]. Let the maximum degree among the vertices of graph G is denoted by $\Delta(G)$. The reverse vertex degree of a vertex v in G is defined in [5] as $c_v = \Delta(G) - d_u + 1$. Graphs can be used to study theoretical and computational aspects of dendrimers. Recently this approach has proved remarkable in relating properties of substances with involved structural parameters [6]. Topological indices are used here as major ingredients [7]. Some nanotubes, modified electrodes, chemical sensors, micro- and macro-capsule, and colored glasses can be designed using nanostar dendrimers. The structure of polymer molecules in a plane depends on the adjacency of their units. Figure 1 shows the spatial arrangements of $NS_1[1]$, $NS_1[2]$ polypropylenimine octaamin dendrimers in plane. The recursive nature of these dendrimers is evident from this figure. Graph theoretic models of these dendrimers can potentially be used in fractals.

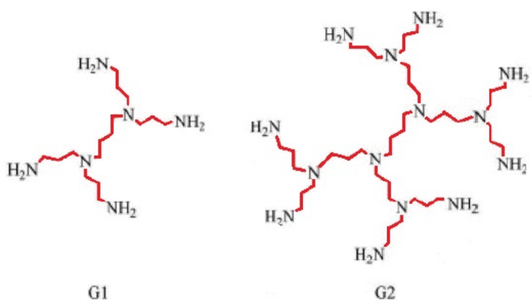

Figure 1. Molecular structure of $NS_1[k]$ dendrimer with $k = 1$ and $k = 2$.

In Figure 1, G_1 shows the structure of polypropylenimine octaamin dendrimers when $k = 1$, and G_2 represents the structure of $NS_2[k]$ when $k = 2$.
The next object will be polypropylenimine octaamin dendrimer $NS_2[k]$. Figure 2 is a graph theoretical representation for this dendrimer.

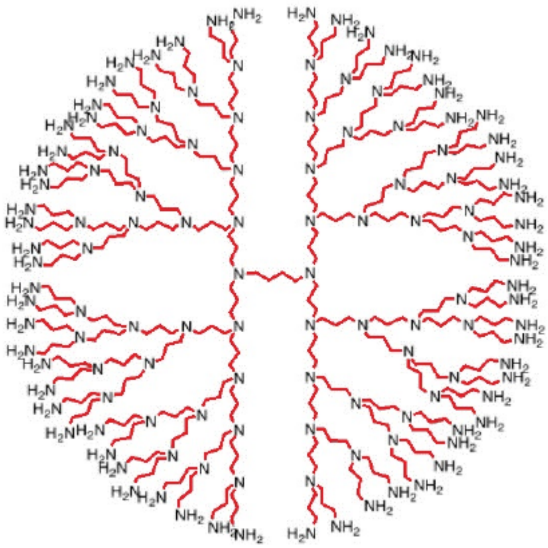

Figure 2. Molecular structure of $NS_2[k]$ dendrimers.

The third object of interest is the $NS_3[k]$, also known as polymer dendrimer. Figure 3 shows the molecular structure of this dendrimer.

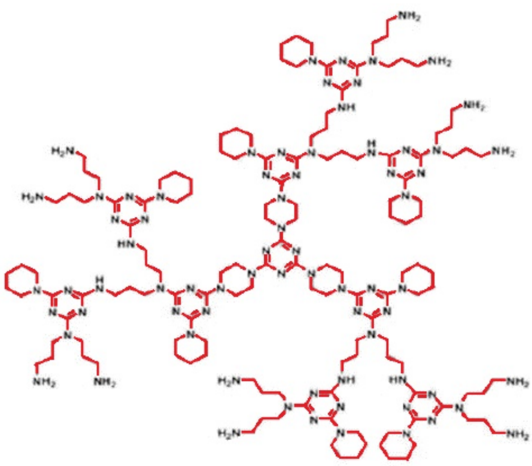

Figure 3. Molecular structure of $NS_3[k]$ dendrimers.

In the current article, we are interested in imbalance-based irregularity indices of the above discussed families of three dendrimers. We use techniques from combinatorics and graph theory to avoid the use of quantum mechanics, as has been done recently in most of the cases. Important tools which are used for this purpose are structural and functional polynomials. These tools use structural parameters as inputs and the outputs are the key information that is used to determine properties of the material under discussion. Certain properties of matters like standard enthalpy, toxicity, entropy as well as reactivity and biological mechanics are theoretically based on these tools. Estrada related the atom bond connectivity index with energies of the branched alkanes.

2. Preliminaries and Notations

In this part we lay out some basic material and notations which will be used throughout the article. All graphs will be connected. We fix the symbol G for a simple connected graph, $V(G)$ for the set of vertices of G, E for the set of edges, d_u and d_v are the degrees of vertices u and v, respectively. Topological index is an invariant of the graph that preserves the structural aspects of the graph. A degree based topological index is based on the end degrees of edges. A graph is said to be regular if every vertex of the graph has the same degree. A topological invariant is called irregularity index if the index vanishes for a regular graph and is non-zero for a non-regular graph. Regular graphs have been investigated a lot, particularly in mathematics. Their applications in chemical graph theory came to be known after the discovery of nanotubes and fullerenes. Paul Erdos emphasized the study of irregular graphs for the first time in history in [8]. At the Second Krakow Conference on Graph Theory (1994), Erdos officially posed an open problem about determination of the extreme size of highly irregular graphs of given order [9]. Since then, the irregular graphs and the degree of irregularity have become the basic open problem of graph theory. A graph in which each vertex has a different degree than other vertices is known as a perfect graph. Authors in [10], proved that no graph is perfect. The graphs lying in between are called quasi-perfect graphs in which each, except two vertices, have different degrees [1]. A simplified way of expressing the irregularity is the irregularity index. Irregularity indices have been studied recently in a novel way [12]. The first such irregularity index was introduced in [13]. Most of these indices used the concept of imbalance of an edge defined as $imball_{uv} = |d_u - d_v|$. The Albertson index, $AL(G)$, was defined by Alberston in [43] as $AL(G) = \sum_{uv \in E(G)} |c_u - c_v|$. In this index, the imbalance of edges is computed. The irregularity index $IRLU(G)$ is introduced by Vukicevic and Gasparov in [44] as $IRLU(G) = \sum_{uv \in E(G)} \frac{|c_u - c_v|}{min(c_u, c_v)}$. Recently, Abdo et al. introduced the new term "total irregularity measure of a graph G", which is defined in [14] as $IRR_t(G) = \frac{1}{2} \sum_{uv \in E} |c_u - c_v|$. Recently, Gutman et al. introduced the $\sigma(G)$ irregularity index of the graph G, which is described as $\sigma(G) = \sum_{uv \in E(G)} (c_u - c_v)^2$ in [5]. The Randic index itself is directly related to an irregularity measure, which is described as $IRA(G) = \sum_{uv \in E(G)} \left(c_u^{-\frac{1}{2}} - c_u^{-\frac{1}{2}} \right)^2$ in [16]. These indices are given as $IRDIF(G) = \sum_{uv \in E(G)} \left| \frac{c_u}{c_v} - \frac{c_u}{c_v} \right|$, $IRLF(G) = \sum_{uv \in E(G)} \frac{|c_u - c_v|}{\sqrt{(c_u . c_v)}}$, $IRLA(G) = 2 \sum_{uv \in E(G)} \frac{|c_v - c_u|}{c_v + c_u}$, $IRGA(G) = \sum_{uv \in E(G)} \ln \left(\frac{c_u + c_v}{2\sqrt{c_u . c_v}} \right)$ and
$IRB(G) = \sum_{uv \in E(G)} \left(c_u^{\frac{1}{2}} - c_v^{\frac{1}{2}} \right)^2$. Recently authors computed irregularity indices of a nanotube [17]. Recently Gao et al. computed irregularity measures of some dendrimer structures in [18]. Actually, the authors computed only four irregularity measures for some classes of dendrimers in [9]. These structures are used as long infinite chain macromolecules in chemistry and related areas. Hussain et al. computed these irregularity measures for some classes of benzenoid systems in [20].

In [21], V.R Kulli determined the first two reverse Zagreb indices, the first two reverse hyper Zagreb indices and their polynomials of rhombus silicate networks and Hussain, et al. computed imbalance based irregularity indices of polypropylenimine octamin dendrimers $NS_1[k]$, $NS_2[k]$ and $NS_3[k]$. Motivated by this work, we introduce some revrese irregularity indices in Table 1 and compute these indices for polypropylenimine octamin dendrimers $NS_1[k]$, $NS_2[k]$ and $NS_3[k]$.

Table 1. Reverse irregularity indices

$IRDIFC(G) = \sum_{uv\in E(G)} \left\lvert \frac{c_u}{c_v} - \frac{c_u}{c_v} \right\rvert$	$IRRC(G) = \sum_{uv\in E(G)} \lvert c_u - c_v \rvert$
$IRLUC(G) = \sum_{uv\in E(G)} \frac{\lvert c_u - c_v\rvert}{min(c_u, c_v)}$	$IRLFC(G) = \sum_{uv\in E(G)} \frac{\lvert c_u - c_v\rvert}{\sqrt{(c_u . c_v)}}$
$\sigma C(G) = \sum_{uv\in E(G)} (c_u - c_v)^2$	$IRLAC(G) = 2 \sum_{uv\in E(G)} \frac{\lvert c_v - c_u\rvert}{c_v + c_u}$
$IRAC(G) = \sum_{uv\in E(G)} \left(c_u^{-\frac{1}{2}} - c_u^{-\frac{1}{2}} \right)^2$	$IRGAC(G) = \sum_{uv\in E(G)} \ln\left(\frac{c_u + c_v}{2\sqrt{c_u . c_v}} \right)$
$IRBC(G) = \sum_{uv\in E(G)} \left(c_u^{\frac{1}{2}} - c_v^{\frac{1}{2}} \right)^2$	$IRR_tC(G) = \frac{1}{2} \sum_{uv\in E} \lvert c_u - c_v \rvert$

3. Main Results And Proofs

In this section, we represent our main results.

Theorem 1. *Let G be graph of $NS_1[k]$ dendrimer. Then reverse irregularity indices of $NS_1[k]$ dendrimer are,*

1. $IRDIFC(G) = \frac{100.2^k - 95}{3}$
2. $IRRC(G) = 24.2^k - 22$
3. $IRLUC(G) = 23.2^k - 22$
4. $IRLFC(G) = (2^{k+1})\frac{1}{\sqrt{6}} + 4(2^k - 1)\frac{2}{\sqrt{3}} + 14(2^k - 1)\frac{1}{\sqrt{2}}$
5. $\sigma C(G) = 32.2^k - 30$
6. $IRLAC(G) = \frac{212.2^k - 200}{15}$
7. $IRAC(G) = 2^k\left(\frac{5-2\sqrt{6}}{3}\right) + 4(2^k - 1)\left(\frac{4-2\sqrt{3}}{3}\right) + 14(2^k - 1)\left(\frac{3-2\sqrt{2}}{2}\right)$
8. $IRGAC(G) = (2^{k+1})\ln\frac{5}{2\sqrt{6}} + 4(2^k - 1)\ln\frac{2}{\sqrt{3}} + 14(2^k - 1)\ln\frac{3}{2\sqrt{2}}$
9. $IRBC(G) = (2^{k+1})\left(5 - 2\sqrt{6}\right) + 4(2^k - 1)\left(4 - 2\sqrt{3}\right) + 14(2^k - 1)\left(3 - 2\sqrt{2}\right)$
10. $IRR_tC(G) = 12.2^k - 11$

Proof. Let G be the graph of $NS_1[k]$ dendrimer. From Figure 1, we have:

Table 2. Edge partition of $NS_1[k]$.

(d_u, d_v)	Number of edges
(1,2)	$\lvert E_{12}(G)\rvert = 2^{k+1}$
(1,3)	$\lvert E_{13}(G)\rvert = 4(2^k - 1)$
(2,2)	$\lvert E_{22}(G)\rvert = 12.2^k - 11$
(2,3)	$\lvert E_{23}(G)\rvert = 14(2^k - 1)$

where $\lvert E_{d_u d_v}(G)\rvert$ shows number of edges corresponding to d_u and d_v of graph G. By using the definition $c_v = \Delta(G) - d_u + 1$, reverse edge partition is given in Table 3,

Table 3. Reverse edge partition of $NS_1[k]$.

(c_u, c_v)	Number of edges
(3,2)	$\lvert CE_{32}(G)\rvert = 2^{k+1}$
(3,1)	$\lvert CE_{31}(G)\rvert = 4(2^k - 1)$
(2,2)	$\lvert CE_{22}(G)\rvert = 12.2^k - 11$
(2,1)	$\lvert CE_{21}(G)\rvert = 14(2^k - 1)$

where $\lvert CE_{c_u c_v}(G)\rvert$ shows number of edges corresponding to c_u and c_v of graph G. With the help of the partition given in the Table 3, we can easily find the required results. We apply these information to calculate our indices. Since,

1.

$$
\begin{aligned}
IRDIFC(G) &= \sum_{uv\in E}\left|\frac{c_u}{c_v}-\frac{c_v}{c_u}\right| \\
&= 2^{k+1}\left|\frac{3}{2}-\frac{2}{3}\right| + 4(2^k-1)\left|\frac{3}{1}-\frac{1}{3}\right| + (12.2^k-11)\left|\frac{2}{2}-\frac{2}{2}\right| + 14(2^k-1)\left|\frac{2}{1}-\frac{1}{2}\right| \\
&= \frac{100.2^k-95}{3}
\end{aligned}
$$

2.

$$
\begin{aligned}
IRRC(G) &= \sum_{uv\in E}|c_u-c_v| \\
&= (2^{k+1})|3-2| + 4(2^k-1)|3-1| + (12.2^k-11)|2-2| + 14(2^k-1)|2-1| \\
&= 24.2^k-22
\end{aligned}
$$

3.

$$
\begin{aligned}
IRLUC(G) &= \sum_{uv\in E}\frac{|c_u-c_v|}{min(c_u,c_v)} \\
&= (2^{k+1})\frac{|3-2|}{2} + 4(2^k-1)\frac{|3-1|}{1} + (12.2^k-11)\frac{|2-2|}{2} + 14(2^k-1)\frac{|2-1|}{1} \\
&= 23.2^k-22
\end{aligned}
$$

4.

$$
\begin{aligned}
IRLFC(G) &= \sum_{uv\in E}\frac{|c_u-c_v|}{\sqrt{c_uc_v}} \\
&= (2^{k+1})\frac{|3-2|}{\sqrt{(3)(2)}} + (4(2^k-1)\frac{|3-1|}{\sqrt{(3)(1)}} + (12.2^k-11)\frac{|2-2|}{\sqrt{(2)(2)}} + 14(2^k-1)\frac{|2-1|}{\sqrt{(2)(1)}} \\
&= (2^{k+1})\frac{1}{\sqrt{6}} + 4(2^k-1)\frac{2}{\sqrt{3}} + 14(2^k-1)\frac{1}{\sqrt{2}}
\end{aligned}
$$

5.

$$
\begin{aligned}
\sigma C(G) &= \sum_{uv\in E(G)}(c_u-c_v)^2 \\
&= (2^{k+1})(3-2)^2 + 4(2^k-1)(3-1)^2 + (12.2^k-11)(2-2)^2 + 4(2^k-1)(2-1)^2 \\
&= 32.2^k-30
\end{aligned}
$$

6.

$$\begin{aligned}
IRLAC(G) &= 2\sum_{uv\in E}\frac{|c_u-c_v|}{c_u+c_v}\\
&= 2\left((2^{k+1})\frac{|3-2|}{3+2}+4(2^k-1)\frac{|3-1|}{3+1}+(12.2^k-11)\frac{|2-2|}{2+2}+14(2^k-1)\frac{|2-2|}{2+1}\right)\\
&= (2^{k+1})\left(\frac{2}{5}\right)+4(2^k-1)+14(2^k-1)\left(\frac{2}{3}\right)\\
&= \frac{212.2^k-200}{15}
\end{aligned}$$

7.

$$\begin{aligned}
IRAC(G) &= \sum_{uv\in E}|c_u^{-1/2}-c_v^{-1/2}|^2\\
&= (2^{k+1})\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{2}}\right)^2+4(2^k-1)\left(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{1}}\right)^2+(12.2^k-11)\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{2}}\right)^2\\
&\quad +14(2^k-1)\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{1}}\right)^2\\
&= (2^{k+1})\left(\frac{\sqrt{3}-\sqrt{2}}{\sqrt{6}}\right)^2+4(2^k-1)\left(\frac{1-\sqrt{3}}{\sqrt{3}}\right)^2+14(2^k-1)\left(\frac{1-\sqrt{2}}{\sqrt{2}}\right)^2\\
&= 2^k\left(\frac{5-2\sqrt{6}}{3}\right)+4(2^k-1)\left(\frac{4-2\sqrt{3}}{3}\right)+14(2^k-1)\left(\frac{3-2\sqrt{2}}{2}\right)
\end{aligned}$$

8.

$$\begin{aligned}
IRGAC(G) &= \sum_{uv\in E}\ln\frac{c_u+c_v}{(2)\sqrt{c_uc_v}}\\
&= (2^{k+1})\ln\frac{3+2}{2\sqrt{(3)(2)}}+4(2^k-1)\ln\frac{3+1}{2\sqrt{(3)(1)}}+(12.2^k-11)\ln\frac{2+2}{2\sqrt{(2)(2)}}\\
&\quad +14(2^k-1)\ln\frac{2+1}{2\sqrt{(2)(1)}}\\
&= (2^{k+1})\ln\frac{5}{2\sqrt{6}}+4(2^k-1)\ln\frac{2}{\sqrt{3}}+14(2^k-1)\ln\frac{3}{2\sqrt{2}}
\end{aligned}$$

9.

$$\begin{aligned}
IRBC(G) &= \sum_{uv\in E}|c_u^{1/2}-c_v^{1/2}|^2\\
&= (2^{k+1})(\sqrt{3}-\sqrt{2})^2+4(2^k-1)\left(\sqrt{3}-\sqrt{1}\right)^2+(12.2^k-11)\left(\sqrt{2}-\sqrt{2}\right)^2\\
&\quad +14(2^k-1)\left(\sqrt{2}-\sqrt{1}\right)^2\\
&= (2^{k+1})\left(5-2\sqrt{6}\right)+4(2^k-1)\left(4-2\sqrt{3}\right)+14(2^k-1)\left(3-2\sqrt{2}\right)
\end{aligned}$$

10.

$$\begin{aligned} IRR_tC(G) &= \frac{1}{2}\sum_{uv\in E}|c_u - c_v| \\ &= \frac{1}{2}\Big((2^{k+1})|3-2| + 4(2^k-1)|3-1| + (12.2^k-11)|2-2| + 14(2^k-1)|2-1|\Big) \\ &= 12.2^k - 11 \end{aligned}$$

□

The values of reverse irregularity indices of $NS_1[k]$ dendrimer for some growth stages k is shown in Table 4.

Table 4. Values for $NS_1[k]$ dendrimer.

Indices	k=1	k=2	k=3	k=4	k=5
IRDIFC(G)	35	101.6667	235	501.6667	1035
IRRC(G)	26	74	170	362	746
IRLUC(G)	24	70	162	346	714
IRLFC(G)	16.1512	46.8208	108.1600	230.8304	476.1951
σ C(G)	34	98	226	482	994
IRLAC(G)	14.9333	43.2000	99.7333	212.8000	438.9333
IRAC(G)	1.9828	5.8813	13.6781	29.2719	60.4593
IRGAC(G)	5.4823	12.3645	26.1288	53.6575	108.7149
IRBC(G)	4.9496	14.4450	33.4356	71.4168	147.3793
IRR_tC(G)	13	37	85	181	373

Theorem 2. *Let G be graph of $NS_2[k]$ dendrimer. Then reverse irregularity indices of $NS_2[k]$ dendrimer are,*

1. $IRDIFC(G) = \frac{32.2^k-27}{3}$
2. $IRRC(G) = 8.2^k - 6$
3. $IRLUC(G) = 8.2^k - 6$
4. $IRLFC(G) = (2^{k+1})\frac{1}{\sqrt{6}} + 6(2^k-1)\frac{1}{\sqrt{2}}$
5. $\sigma C(G) = 8.2^k - 6$
6. $IRLAC(G) = \frac{19.2^k-15}{5}$
7. $IRAC(G) = (2^{k+1})\left(\frac{\sqrt{3}-\sqrt{2}}{\sqrt{6}}\right)^2 + 6(2^k-1)\left(\frac{\sqrt{2}-1}{\sqrt{2}}\right)^2$
8. $IRGAC(G) = (2^{k+1})\ln\frac{5}{2\sqrt{6}} + 4(2^k-1)\ln\frac{2}{\sqrt{3}} + 14(2^k-1)\ln\frac{3}{2\sqrt{2}}$
9. $IRBC(G) = (2^{k+1})\left(10-4\sqrt{6}\right) + 6(2^k-1)\left(3-2\sqrt{2}\right)$
10. $IRR_tC(G) = 4.2^k - 3$

Proof. Let G be the graph of $NS_2[k]$ dendrimer. From Figure 2, we have:

Table 5. Edge partition of $NS_2[k]$.

(d_u, d_v)	Number of edges
(1,2)	$\|E_{12}(G)\| = 2^{k+1}$
(2,2)	$\|E_{22}(G)\| = 8.2^k - 5)$
(2,3)	$\|E_{23}(G)\| = 6(2^k - 1)$

where $|CE_{d_u d_v}(G)|$ shows number of edges corresponding to d_u and d_v of graph G. By using the definition $c_v = \Delta(G) - d_u + 1$, reverse edge partition is given in Table 6,

Table 6. Reverse edge partition of $NS_2[k]$.

(c_u, c_v)	Number of edges
(3,2)	$\lvert CE_{32}(G)\rvert = 2^{k+1}$
(2,2)	$\lvert CE_{22}(G)\rvert = 8.2^k - 5$
(2,1)	$\lvert CE_{21}(G)\rvert = 6(2^k - 1)$

where $|E_{c_u c_v}(G)|$ shows number of edges corresponding to c_u and c_v of graph G. With the help of the partition given in the Table 6, we can easily find the required results. We apply these information to calculate our indices. Since,

1.

$$\begin{aligned} IRDIFC(G) &= \sum_{uv\in E}\left|\frac{c_u}{c_v} - \frac{c_v}{c_u}\right| \\ &= 2^{k+1}\left|\frac{3}{2} - \frac{2}{3}\right| + (8.2^k - 5)\left|\frac{2}{2} - \frac{2}{2}\right| + 6(2^k - 1)\left|\frac{2}{1} - \frac{1}{2}\right| \\ &= \frac{32.2^k - 27}{3} \end{aligned}$$

2.

$$\begin{aligned} IRRC(G) &= \sum_{uv\in E}|c_u - c_v| \\ &= 2^{k+1}|3-2| + (8.2^k - 5)|2-2| + 6(2^k - 1)|2-1| \\ &= 8.2^k - 6 \end{aligned}$$

3.

$$\begin{aligned} IRLUC(G) &= \sum_{uv\in E}\frac{|c_u - c_v|}{min(c_u, c_v)} \\ &= (2^{k+1})\frac{|3-2|}{2} + (8.2^k - 5)\frac{|2-2|}{2} + 6(2^k - 1)\frac{|2-1|}{1} \\ &= 8.2^k - 6 \end{aligned}$$

4.

$$\begin{aligned} IRLFC(G) &= \sum_{uv\in E}\frac{|c_u - c_v|}{\sqrt{c_u c_v}} \\ &= (2^{k+1})\frac{|3-2|}{\sqrt{(3)(2)}} + (8.2^k - 6)\frac{|2-2|}{\sqrt{(2)(2)}} + 6(2^k - 1)\frac{|2-1|}{\sqrt{(2)(1)}} \\ &= (2^{k+1})\frac{1}{\sqrt{6}} + 6(2^k - 1)\frac{1}{\sqrt{2}} \end{aligned}$$

5.

$$\begin{aligned} \sigma C(G) &= \sum_{uv\in E(G)}(c_u - c_v)^2 \\ &= (2^{k+1})(3-2)^2 + (8.2^k - 5)(2-2)^2 + 6(2^k - 1)(2-1)^2 \\ &= 8.2^k - 6 \end{aligned}$$

6.

$$
\begin{aligned}
IRLAC(G) &= 2\sum_{uv\in E}\frac{|c_u-c_v|}{c_u+c_v}\\
&= 2\left((2^{k+1})\frac{|3-2|}{3+2}+(8.2^k-5)\frac{|2-2|}{2+2}+6(2^k-1)\frac{|2-1|}{2+2}\right)\\
&= \frac{19.2^k-15}{5}
\end{aligned}
$$

7.

$$
\begin{aligned}
IRAC(G) &= \sum_{uv\in E}|c_u^{-1/2}-c_v^{-1/2}|^2\\
&= (2^{k+1})\left(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{2}}\right)^2+(8.2^k-5)\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{2}}\right)^2+6(2^k-1)\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{1}}\right)^2\\
&= (2^{k+1})\left(\frac{\sqrt{3}-\sqrt{2}}{\sqrt{6}}\right)^2+6(2^k-1)\left(\frac{\sqrt{2}-1}{\sqrt{2}}\right)^2
\end{aligned}
$$

8.

$$
\begin{aligned}
IRGAC(G) &= \sum_{uv\in E}\ln\frac{c_u+c_v}{(2)\sqrt{c_uc_v}}\\
&= (2^{k+1})\ln\frac{3+2}{2\sqrt{(3)(2)}}+4(2^k-1)\ln\frac{3+1}{2\sqrt{(3)(1)}}+(12.2^k-11)\ln\frac{2+2}{2\sqrt{(2)(2)}}\\
&\quad+14(2^k-1)\ln\frac{2+1}{2\sqrt{(2)(1)}}\\
&= (2^{k+1})\ln\frac{5}{2\sqrt{6}}+4(2^k-1)\ln\frac{2}{\sqrt{3}}+14(2^k-1)\ln\frac{3}{2\sqrt{2}}
\end{aligned}
$$

9.

$$
\begin{aligned}
IRBC(G) &= \sum_{uv\in E}|c_u^{1/2}-c_v^{1/2}|^2\\
&= (2^{k+1})(\sqrt{3}-\sqrt{2})^2+(8.2^k-6)\left(\sqrt{2}-\sqrt{2}\right)^2+6(2^k-1)\left(\sqrt{2}-\sqrt{1}\right)^2\\
&= (2^{k+1})\left(10-4\sqrt{6}\right)+6(2^k-1)\left(3-2\sqrt{2}\right)
\end{aligned}
$$

10.

$$
\begin{aligned}
IRR_tC(G) &= \frac{1}{2}\sum_{uv\in E}|c_u-c_v|\\
&= \frac{1}{2}\left((2^{k+1})|3-2|+(8.2^k-6)|2-2|+6(2^k-1)|2-1|\right)\\
&= 4.2^k-3
\end{aligned}
$$

□

The values of reverse irregularity indices of $NS_2[k]$ dendrimer for some growth stages k is shown in Table 7.

Table 7. Values for $NS_2[k]$ dendrimer.

Indices	k=1	k=2	k=3	k=4	k=5
IRDIFC(G)	12.3333	33.6667	76.3333	161.6667	323.3333
IRRC(G)	10	26	58	122	250
IRLUC(G)	10	26	58	122	250
IRLFC(G)	5.8756	15.9939	36.2305	76.7036	157.6498
σ C(G)	10	26	58	122	250
IRLAC(G)	4.6	12.2	27.4	57.8	8.6
IRAC(G)	0.5821	1.6788	3.8724	8.2596	17.0338
IRGAC(G)	0.4350	1.2233	2.8	5.9534	12.2601
IRBC(G)	1.4335	3.8965	8.8224	18.6742	38.3779
IRR_tC(G)	5	13	29	66	125

Theorem 3. *Let G be graph of $NS_3[k]$ dendrimer. Then reverse irregularity indices of $NS_3[k]$ dendrimer are,*

1. $IRDIFC(G) = 52.2^k - 27$
2. $IRRC(G) = 36.2^k - 18$
3. $IRLUC(G) = \frac{69.2^k - 36}{2}$
4. $IRLFC(G) = (3.2^k)\frac{1}{\sqrt{6}} + (33.2^k - 18)\frac{1}{\sqrt{2}}$
5. $\sigma C(G) = 36.2^k - 18$
6. $IRLAC(G) = \frac{116.2^k - 60}{5}$
7. $IRAC(G) = 2^k\left(\frac{5-2\sqrt{3}}{2}\right) + (33.2^k - 18)\left(\frac{3-2\sqrt{2}}{2}\right)$
8. $IRGAC(G) = (3.2^k)\ln\frac{5}{2\sqrt{6}} + (33.2^k - 18)\ln\frac{3}{2\sqrt{2}}$
9. $IRBC(G) = (3.2^k)\left(5 - 2\sqrt{6}\right) + (33.2^k - 18)\left(3 - 2\sqrt{2}\right)$
10. $IRR_tC(G) = 18.2^k - 9$

Proof. Let G be the graph of $NS_3[k]$ dendrimer. From Figure 3, we have:

Table 8. Edge partition of $NS_3[k]$.

(d_u, d_v)	Number of edges
(1,2)	$\lvert E_{12}(G)\rvert = 3.2^k$
(2,2)	$\lvert E_{22}(G)\rvert = 27.2^k - 24$
(2,3)	$\lvert E_{23}(G)\rvert = 33.2^k - 18$
(3,3)	$\lvert E_{33}(G)\rvert = 6.2^k$

where $|E_{d_u d_v}(G)|$ shows number of edges corresponding to d_u and d_v of graph G. By using the definition $c_v = \Delta(G) - d_u + 1$, reverse edge partition is given in Table 9,

Table 9. Reverse edge partition of $NS_3[k]$.

(c_u, c_v)	Number of edges
(3,2)	$\lvert CE_{32}(G)\rvert = 3.2^k$
(2,2)	$\lvert CE_{22}(G)\rvert = 27.2^k - 24$
(2,1)	$\lvert CE_{21}(G)\rvert = 33.2^k - 18$
(1,1)	$\lvert CE_{11}(G)\rvert = 6.2^k$

where $|CE_{c_u c_v}(G)|$ shows number of edges corresponding to c_u and c_v of graph G With the help of the partition given in the Table 9, we can easily find the required results. We apply these information to calculate our indices. Since,

1.

$$
\begin{aligned}
IRDIFC(G) &= \sum_{uv\in E}\left|\frac{c_u}{c_v}-\frac{c_v}{c_u}\right| \\
&= (3.2^k)\left|\frac{3}{2}-\frac{2}{3}\right| + (27.2^k-24)\left|\frac{2}{2}-\frac{2}{2}\right| + (33.2^k-18)\left|\frac{2}{1}-\frac{2}{1}\right| + (6.2^k)\left|\frac{1}{1}-\frac{1}{1}\right| \\
&= 52.2^k-27
\end{aligned}
$$

2.

$$
\begin{aligned}
IRRC(G) &= \sum_{uv\in E}|c_u-c_v| \\
&= (3.2^k)|3-2| + (27.2^k-1)|2-2| + (33.2^k-18)|2-1|(+6.2^k)|1-1| \\
&= 36.2^k-18
\end{aligned}
$$

3.

$$
\begin{aligned}
IRLUC(G) &= \sum_{uv\in E}\frac{|c_u-c_v|}{min(c_u,c_v)} \\
&= (3.2^k)\frac{|3-2|}{2} + (27.2^k-24)\frac{|2-2|}{2} + (33.2^k-18)\frac{|2-1|}{1} + (6.2^k)\frac{|1-1|}{1} \\
&= \frac{69.2^k-36}{2}
\end{aligned}
$$

4.

$$
\begin{aligned}
IRLFC(G) &= \sum_{uv\in E}\frac{|c_u-c_v|}{\sqrt{c_uc_v}} \\
&= (3.2^k)\frac{|3-2|}{\sqrt{(3)(2)}} + (27.2^k-24)\frac{|2-2|}{\sqrt{(2)(2)}} + (33.2^k-18)\frac{|2-1|}{\sqrt{(2)(1)}} + (6.2^k)\frac{|1-1|}{\sqrt{(2)(1)}} \\
&= (3.2^k)\frac{1}{\sqrt{6}} + (33.2^k-18)\frac{1}{\sqrt{2}}
\end{aligned}
$$

5.

$$
\begin{aligned}
\sigma C(G) &= \sum_{uv\in E(G)}(c_u-c_v)^2 \\
&= (3.2^k)(3-2)^2 + (27.2^k-24)(2-2)^2 + (33.2^k-18)(2-1)^2 + 4(2^k-1)(1-1)^2 \\
&= 36.2^k-18
\end{aligned}
$$

6.

$$
\begin{aligned}
IRLAC(G) &= 2\sum_{uv\in E}\frac{|c_u-c_v|}{c_u+c_v} \\
&= 2\left(3.2^k\frac{|3-2|}{3+2} + (27.2^k-24)\frac{|2-2|}{2+2} + (33.2^k-18)\frac{|2-1|}{2+1} + (6.2^k)\frac{|1-1|}{1+1}\right) \\
&= \frac{116.2^k-60}{5}
\end{aligned}
$$

7.

$$
\begin{aligned}
IRAC(G) &= \sum_{uv\in E} |c_u^{-1/2} - c_v^{-1/2}|^2 \\
&= (3.2^k)\left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}}\right)^2 + (27.2^k - 24)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}}\right)^2 + (33.2^k - 18)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{1}}\right)^2 \\
&\quad +(6.2^k)\left(\frac{1}{\sqrt{1}} - \frac{1}{\sqrt{1}}\right)^2 \\
&= (3.2^k)\left(\frac{\sqrt{2}-\sqrt{3}}{\sqrt{6}}\right)^2 + (33.2^k - 18)\left(\frac{1-\sqrt{2}}{\sqrt{2}}\right)^2 \\
&= 2^k\left(\frac{5-2\sqrt{3}}{2}\right) + (33.2^k - 18)\left(\frac{3-2\sqrt{2}}{2}\right)
\end{aligned}
$$

8.

$$
\begin{aligned}
IRGAC(G) &= \sum_{uv\in E} \ln \frac{c_u + c_v}{2\sqrt{c_u c_v}} \\
&= (3.2^k)\ln\frac{3+2}{2\sqrt{(3)(2)}} + (27.2^k - 24)\ln\frac{2+2}{2\sqrt{(3)(1)}} + (33.2^k - 18)\ln\frac{2+1}{2\sqrt{(2)(1)}} \\
&\quad +(6.2^k)\ln\frac{1+1}{2\sqrt{(1)(1)}} \\
&= (3.2^k)\ln\frac{5}{2\sqrt{6}} + (33.2^k - 18)\ln\frac{3}{2\sqrt{2}}
\end{aligned}
$$

9.

$$
\begin{aligned}
IRBC(G) &= \sum_{uv\in E}\left(c_u^{1/2} - c_v^{1/2}\right)^2 \\
&= (3.2^k)\left(\sqrt{3}-\sqrt{2}\right)^2 + (27.2^k - 24)\left(\sqrt{2}-\sqrt{2}\right)^2 + (33.2^k - 18)\left(\sqrt{2}-\sqrt{1}\right)^2 \\
&\quad +(6.2^k)\left(\sqrt{1}-\sqrt{1}\right)^2 \\
&= (3.2^k)\left(5-2\sqrt{6}\right) + (33.2^k - 18)\left(3-2\sqrt{2}\right)
\end{aligned}
$$

$$
\begin{aligned}
IRR_tC(G) &= \frac{1}{2}\sum_{uv\in E}|c_u - c_v| \\
&= \frac{1}{2}\Big((3.2^k)|3-2| + (27.2^k - 24)|2-2| + (33.2^k - 18)|2-1|\Big) \\
&= 18.2^k - 9
\end{aligned}
$$

□

The values of reverse irregularity indices of $NS_3[k]$ dendrimer for some growth stages k is shown in Table 10.

Table 10. Values for $NS_3[k]$ dendrimer.

Indices	k=1	k=2	k=3	k=4	k=5
IRDIFC(G)	7	181	389	805	1637
IRRC(G)	54	126	270	558	1134
IRLUC(G)	51	120	258	534	1086
IRLFC(G)	36.3906	85.5092	183.7462	380.2204	773.1687
σ C(G)	54	126	270	558	1134
IRLAC(G)	34.4	80.4	173.6	359.2	730.4
IRAC(G)	2.1599	5.0919	10.9558	22.6837	46.1395
IRGAC(G)	2.9493	6.6586	14.9772	31.0144	63.0889
IRBC(G)	8.8416	20.7716	44.1314	92.3512	187.7906
IRR_tC(G)	27	63	135	279	567

4. Graphical Comparison

In this part we discuss behavior of ten reverse irregularity indices. That indices are given above in Table 1. In our graph dependent variable reverse irregularity index is along Y-axis and independent variable growth stage number k is along X-axis. Value of reverse irregularity index depends upon the single parameter k that is growth stage number of dendrimer structure. We plot $NS_1[k]$, $NS_2[k]$ and $NS_3[k]$ on a single graph for every irregularity index. Red color shows the behavior of $NS_1[k]$ dendrimer, green color shows the behavior of $NS_2[k]$ dendrimer structure and blue color depicts the behavior of $NS_3[k]$ dendrimer structure. By using the values of Table[4,7,10], we plot the graphs for all the reverse irregularity indices in Figures [4-12] and analyze their behavior.

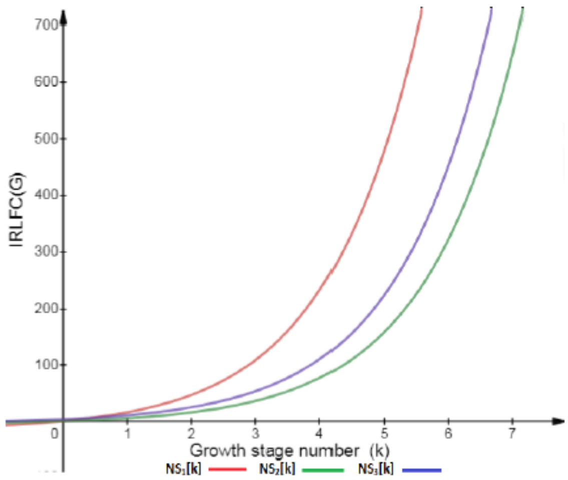

Figure 4. graph of IRLFC(G)

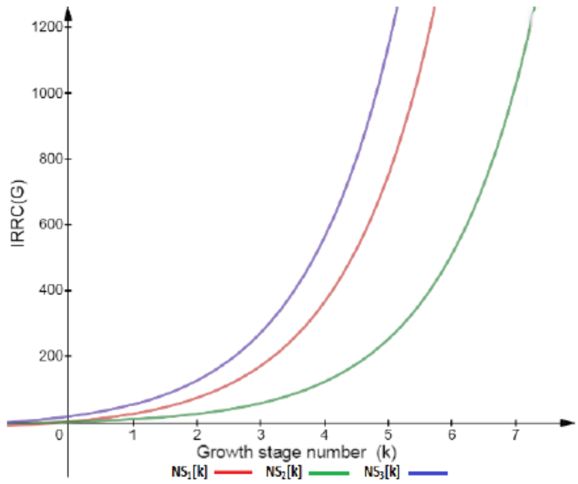

Figure 5. Graph of IRRC(G)

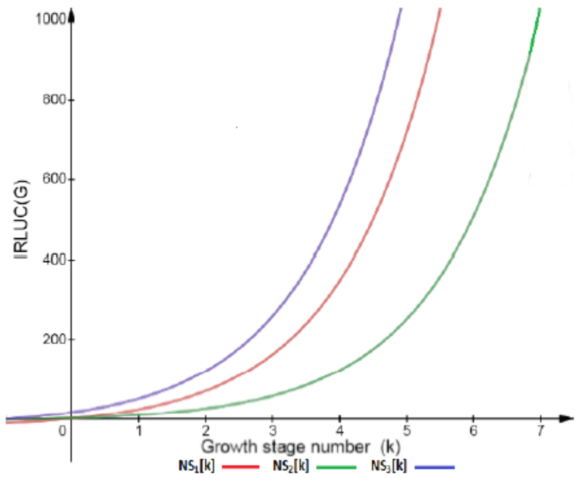

Figure 6. Graph of IRLUC(G)

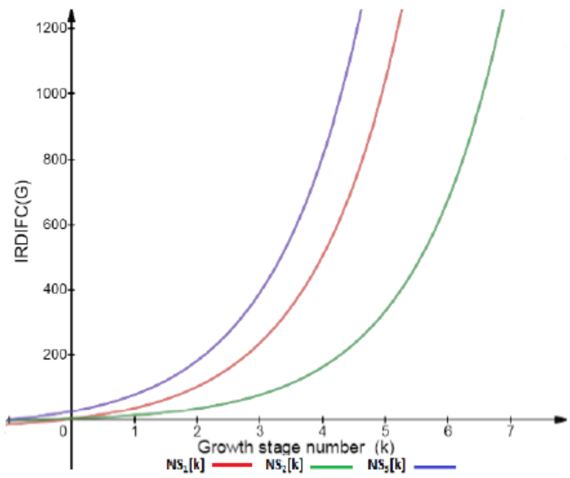

Figure 7. Graph of IRDIF(G)

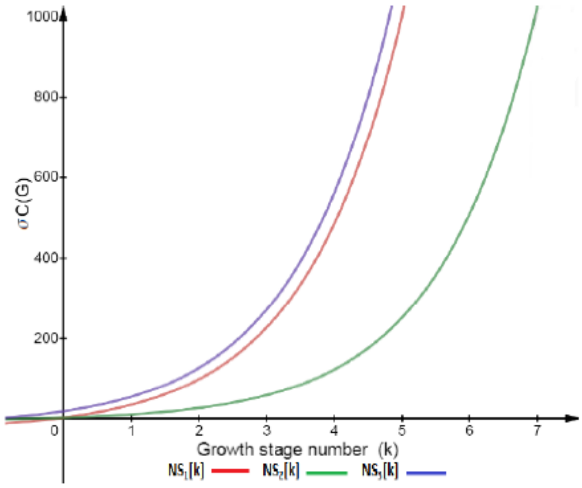

Figure 8. Graph of $\sigma C(G)$

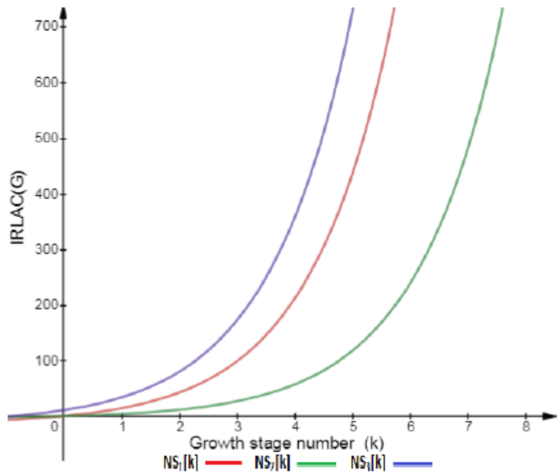

Figure 9. Graph of IRLAC(G)

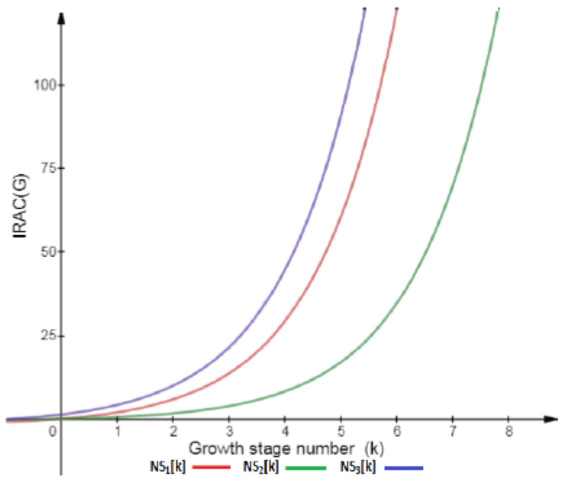

Figure 10. Graph of IRAC(G)

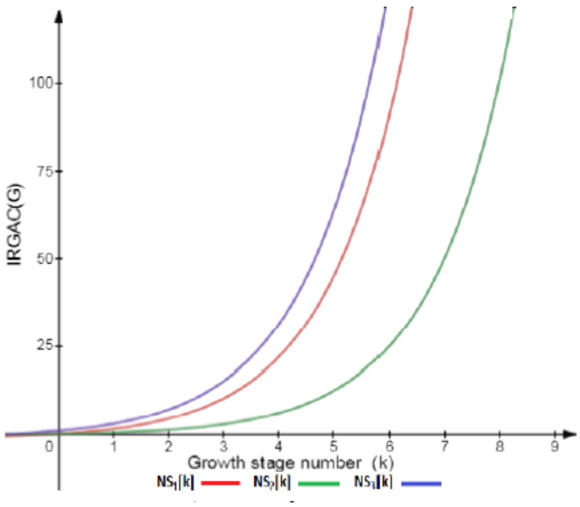

Figure 11. Graph of IRBC(G)

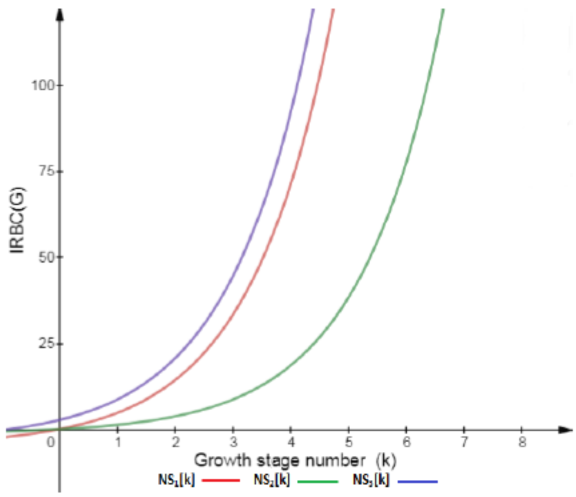

Figure 12. Graph of $IRR_tC(G)$

From above graph it seems obvious that irregularities have a slight increase with an increase in growth stage k. Comparison of reverse irregularity index $IRLFC(G)$ of all three demdrimers is illustrated in Figure 4. $NS_3[k]$ shows the greatest value and $NS_2[k]$ shows the lowest value and $NS_3[k]$ has greater value than $NS_2[k]$. All other reverse irregularity indices given in Table 1 shows the similar behavior in Figures [5-12] with $NS_1[k]$ shows the greatest value and $NS_2[k]$ shows the lowest value and $NS_1[k]$ has greater value than $NS_2[k]$.

5. Conclusion

In this work, we compute ten reverse irregularity indices of polypropylenimine octamin dendrimers $NS_1[k]$, $NS_2[k]$ and $NS_3[k]$ and give their comparative graphical analysis. We expect that our results could play an important role in predicting properties of these dendrimers such as enthalpy, toxicity, resistance and entropy.

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