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Authors:
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Article

Imbalance-Based Irregularity Molecular Descriptors of Nanostar Dendrimers

Zafar Hussain 1, Mubeen Munir 2,†, Shazia Rafique 3, Tayyab Hussnain 3, Haseeb Ahmad 2, Young Chel Kwun 4,* and Shin Min Kang 5,6

1 Department of Mathematics and Statistics, The University of Lahore, Lahore 54500, Pakistan
2 Department of Mathematics, Division of Science and Technology, University of Education, Lahore 54000, Pakistan
3 Center for Excellence in Molecular Biology, Punjab University Lahore, Lahore 53700, Pakistan
4 Department of Mathematics, Dong-A University, Busan 49315, Korea
5 Department of Mathematics, Gyeongsang National University, Jinju 52828, Korea
6 Center for General Education, China Medical University, Taichung 40402, Taiwan

* Correspondence: yckwun@dau.ac.kr

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Abstract: Dendrimers are branched organic macromolecules with successive layers of branch units surrounding a central core. The molecular topology and the irregularity of their structure plays a central role in determining structural properties like enthalpy and entropy. Irregularity indices which are based on the imbalance of edges are determined for the molecular graphs associated with some general classes of dendrimers. We also provide graphical analysis of these indices for the above said classes of dendrimers.

Keywords: nanostar dendrimer; irregularity measure; complexity of structure; \( NS_1[p] \); \( NS_2[p] \); \( NS_3[p] \)

1. Introduction

Algebra, topology, geometry and combinatorics are the main branches of mathematics which are employed to study the symmetries and irregularities of the structures of different substances. Dendrimers have consistently attracted the attention of both chemists as well as pure mathematicians because of the complexities of the underlying molecular graphs. Dendrimers are highly branched, star-shaped macromolecules with nanometer-scale dimensions. Dendrimers are constituted by main parts: A central core, an internal part called ‘branch’, and an exterior surface with functional surface groups. The varied combination of these components yields products of different shapes and sizes with shielded interior cores that are ideal candidates for applications in both biological and materials sciences. Some recent applications include drug delivery, gene transfection, catalysis, energy harvesting, photo activity, molecular weight and size determination, rheology modification, and nanoscale science and technology [1–3].

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 [4–7]. Topological indices are used here as major ingredients [7–14]. 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. For detailed insight, see [1–3,14–18] and references therein. Figure 1 shows the spatial arrangements of \( NS_1[1] \), \( NS_1[2] \) polypropyleneimine 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.
In Figure 1, $G_1$ shows the structure of polypropylenimine octaamin dendrimers $N_S^1[p]$ when $p = 1$, and $G_2$ represents the structure of $N_S^1[p]$ when $p = 2$.

The next object will be polypropylenimine octaamin dendrimer $N_S^2[p]$. Figure 2 is a graph theoretical representation for this dendrimer.

The third object of interest is the $N_S^3[p]$, also known as polymer dendrimer. Figure 3 shows the molecular structure of this dendrimer.
The above three families have been used a lot recently for their theoretical properties. De et al. in [14], computed the F-index of nanostar dendrimers; Siddiqui et al. computed the Zagreb indices for different nanostar dendrimers in [15], and Madanshekaf computed the Randić index for some different classes of nanostar dendrimers in [16,17]. Munir, et al. computed M-polynomial and related indices of these nanostar dendrimers in [18], titania nanotubes in [19], polyhez nanotubes in [20] and circulant graphs in [21].

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, see [7–14]. 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 [4–6]. Estrada related the atom bond connectivity index with energies of the branched alkanes in [9]. Some applications of indices in pharmacy are given in [10] and in Quantitative structure activity analysis in [11].

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, $V$ for the set of vertices of $G$, $E$ for the set of edges, $du$ and $dv$ 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 [22]. 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 [23]. 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 [24], 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 [25].

A simplified way of expressing the irregularity is the irregularity index. Irregularity indices have been studied recently in a novel way [26,27]. The first such irregularity index was introduced in [28]. Most of these indices used the concept of imbalance of an edge defined as $imbal_{uv} = |d_u - d_v|$. [25–27]. The Albertson index, $AL(G)$, was defined by Alberston in [29] as $AL(G) = \sum_{uv \in E} |d_u - d_v|$. Recently, Gutman et al. introduced the $\sigma$-index $\sigma(G) = \sum_{uv \in E} d_u d_v$. Further details are given in [34] in detail. These indices are directly related to an irregularity measure, which is described as $IRA(G) = \sum_{uv \in E} \left( d_u^2 - d_v^2 \right)$. In this part, we give our main theoretical results.

3. Main Results

In this part, we give our main theoretical results.

**Theorem 1.** Let $NS_1[p]$ be the polypropyleneimine octaamin dendrimers, then the irregularity indices of $NS_1[p]$ are:

1. $\text{IRDIF}(NS_1[p]) = 1.5 \left( 2^{p+1} \right) + 22.3372p - 22.334$
2. $\text{IRR}(NS_1[p]) = 2^{p+1} + 22(2^p) - 22$
3. $\text{IRL}(NS_1[p]) = 0.69314718 \left( 2^{p+1} \right) + 10.070961 (2^p) - 10.070961$
4. $\text{IRLU}(NS_1[p]) = 2^{p+1} + 15(2^p) - 15$
5. $\text{IRLF}(NS_1[p]) = 0.7071068 \left( 2^{p+1} \right) + 10.334278(2^p) - 10.334278$
6. $\text{RI}(NS_1[p]) = 2^{p+1} + 30(2^p) - 30$
7. $\text{IRLA}(NS_1[p]) = 0.6667(2^p) + 9.6(2^p) - 9.6$
8. $\text{IRD1} = 0.69314 \left( 2^{p+1} \right) + 14.098(2^p) - 14.098$
9. $\text{IRA}(NS_1[p]) = 0.085786432 \left( 2^{p+1} \right) + 0.950245633(2^p) - 0.950245633$
10. $\text{IRGA}(NS_1[p]) = 0.06036(2^{p+1}) + 0.8610954(2^p) - 0.8610954$
11. $\text{IRB}(NS_1[p]) = 0.171528753 \left( 2^{p+1} \right) + 3.557593539(2^p) - 3.557593539$
12. $\text{IRR}_t(NS_1[p]) = 12(2^p) - 11$

**Proof.** In order to prove the above theorem we have to consider Figure 1.

We can see that the edges $NS_1[p]$ admit the following partition in Table 1. □
Table 1. Edge partition of $NS_1[p]$ polypropylenimine octaamin dendrimers.

<table>
<thead>
<tr>
<th>Edge Type $(d_u, d_v)$</th>
<th>Number of Edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1,2)</td>
<td>$2^{p+1}$</td>
</tr>
<tr>
<td>(1,3)</td>
<td>$4(2^p - 1)$</td>
</tr>
<tr>
<td>(2,2)</td>
<td>$[12 \times 2^p - 11]$</td>
</tr>
<tr>
<td>(2,3)</td>
<td>$14(2^p - 1)$</td>
</tr>
</tbody>
</table>

Now, using above Table 1 and definitions we have:

1. \[ IRDIF(G) = \sum_{U \subseteq E} \left| \frac{dx}{dx} - \frac{dy}{dy} \right| \]
   \[ IRDIF(NS_1[p], x, y) = 2^{p+1}\left| \frac{2}{4} - \frac{1}{2} \right| + 4(2^p - 1)\left| \frac{3}{4} - \frac{1}{2} \right| + [12 \times 2^p - 11]\left| \frac{2}{3} - \frac{2}{2} \right| + 14(2^p - 1)\left| \frac{2}{3} - \frac{2}{2} \right| \]
   \[ = 2^{p+1}\left| \frac{1}{4} - \frac{1}{2} \right| + 4(2^p - 1)\left| \frac{3}{4} - \frac{1}{2} \right| + 14(2^p - 1)\left| \frac{3}{4} - \frac{1}{2} \right|. \]

2. \[ IR(G) = \sum_{U \subseteq E} \text{imb}(e) \]
   \[ IRR(NS_1[p], x, y) = 2^{p+1}|2 - 1| + 4(2^p - 1)|3 - 1| + [12 \times 2^p - 11]|2 - 2| + 14(2^p - 1) \]
   \[ = 2^{p+1} + 4(2^p - 1)|2| + 14(2^p - 1). \]

3. \[ IRL(G) = \sum_{U \subseteq E} |\text{in}(u) - \text{in}(v)| \]
   \[ IRL(NS_1[p], x, y) = 2^{p+1}|ln2 - ln1| + 4(2^p - 1)|ln3 - ln1| + [12 \times 2^p - 11]|ln2 - ln2| + 14(2^p - 1)|ln3 - ln2| \]
   \[ = 2^{p+1}|ln2| + 4(2^p - 1)|ln3| + 14(2^p - 1)|ln\frac{1}{2}|. \]

4. \[ IRLU(G) = \sum_{U \subseteq E} \frac{|d_u - d_v|}{\min(d_u, d_v)} \]
   \[ IRLU(NS_1[p], x, y) = 2^{p+1}\left| \frac{2p-1}{V^2} \right| + 4(2^p - 1)\left| \frac{3p-1}{V^3} \right| + [12 \times 2^p - 11]\left| \frac{2p-2}{V^4} \right| + 14(2^p - 1)\left| \frac{2p-2}{V^4} \right| \]
   \[ = 2^{p+1} + 8(2^p - 1) + 7(2^p - 1). \]

5. \[ IRLF(G) = \sum_{U \subseteq E} \frac{|d_u - d_v|}{(d_u + d_v)^2} \]
   \[ IRLF(NS_1[p], x, y) = 2^{p+1}\left| \frac{2p-1}{V^2} \right| + 4(2^p - 1)\left| \frac{3p-1}{V^3} \right| + [12 \times 2^p - 11]\left| \frac{2p-2}{V^4} \right| + 14(2^p - 1)\left| \frac{2p-2}{V^4} \right| \]
   \[ = \frac{2^{p+1}}{V^2} + \frac{8(2^p - 1)}{V^3} + \frac{14(2^p - 1)}{V^6}. \]

6. \[ \sigma(G) = \sum_{U \subseteq E} (d_u - d_v)^2 \]
   \[ \sigma(NS_1[p], x, y) = 2^{p+1}(2 - 1)^2 + 4(2^p - 1)(3 - 1)^2 + [12 \times 2^p - 11](2 - 2)^2 + 14(2^p - 1)(3 - 2)^2 \]
   \[ = 2^{p+1} + 16(2^p - 1) + 14(2^p - 1). \]

7. \[ IRLA(G) = 2 \sum_{U \subseteq E} \frac{|d_u - d_v|}{(d_u + d_v)} \]
   \[ IRLA(NS_1[p], x, y) = 2\left[ 2^{p+1}\left| \frac{2p-1}{(2+1)} \right| + 4(2^p - 1)\left| \frac{3p-1}{(3+1)} \right| + [12 \times 2^p - 11]\left| \frac{2p-2}{(2+2)} \right| + 14(2^p - 1)\left| \frac{2p-2}{(3+2)} \right| \right] \]
   \[ = 2\left[ 2^{p+1}\left| \frac{2p-1}{(2+1)} \right| + 4(2^p - 1)\left| \frac{3p-1}{(3+1)} \right| + 14(2^p - 1)\left| \frac{3p-2}{(3+2)} \right| \right]. \]

8. \[ IRD1 = \sum_{U \subseteq E} \ln(1 + |d_u - d_v|) \]
   \[ IRD1(NS_1[p], x, y) = 2^{p+1}\ln(1 + |2 - 1|) + 4(2^p - 1)\ln(1 + |3 - 1|) + [12 \times 2^p - 11]\ln(1 + |2 - 2|) + 14(2^p - 1)\ln(1 + |3 - 2|) \]
   \[ = 2^{p+1}\ln(1 + |2 - 1|) + 4(2^p - 1)\ln(1 + |3 - 1|) + 14(2^p - 1)\ln(1 + |3 - 2|). \]
9. \( IRA(G) = \sum_{UV \in E} \left( \frac{1}{d_u} - \frac{1}{d_v} \right)^2 \)

\[
IRA(NS_1[p], x, y) = 2^{p+1} \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 + 4(2^p - 1) \left( \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)^2 + 14(2^p - 1) \left( \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{5}} \right)^2
\]

10. We have \( IRGA(G) = \sum_{UV \in E} \ln \frac{d_u + d_v}{x \sqrt{d_ud_v}} \)

\[
IRGA(NS_1[p], x, y) = 2^{p+1} \left[ \ln \left( \frac{2^{p+1}}{2\sqrt{3}} \right) + 4(2^p - 1) \ln \left( \frac{2^{p+1}}{2\sqrt{3}} \right) + 14(2^p - 1) \ln \left( \frac{2^{p+1}}{2\sqrt{3}} \right) \right]
\]

11. \( IRB(G) = \sum_{UV \in E} \left( \frac{1}{d_u} - \frac{1}{d_v} \right)^2 \)

\[
IRB(NS_1[p], x, y) = 2^{p+1} \left[ \ln \left( \frac{2^{p+1}}{2\sqrt{3}} \right) + 4(2^p - 1) \ln \left( \frac{2^{p+1}}{2\sqrt{3}} \right) + 14(2^p - 1) \ln \left( \frac{2^{p+1}}{2\sqrt{3}} \right) \right]
\]

12. \( IRR_i(G) = \frac{1}{2} \sum_{UV \in E} |d_u - d_v| \)

\[
IRR_i(NS_1[p], x, y) = \frac{1}{2} \left[ 2^{p+1} \left| 2 - 1 \right| + 4(2^p - 1) \left| 3 - 1 \right| + 12(2^p - 11) \left| 2 - 2 \right| + 14(2^p - 1) \left| 2 - 1 \right| \right]
\]

The following Table 2 shows the values of these irregularity indices for some test values of parameter \( p \).

<table>
<thead>
<tr>
<th>Irregularity Indices</th>
<th>( p = 1 )</th>
<th>( p = 2 )</th>
<th>( p = 3 )</th>
<th>( p = 4 )</th>
<th>( p = 5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>IRDIFF(G) = ( \sum_{UV \in E}</td>
<td>d_u - d_v</td>
<td>)</td>
<td>28.340</td>
<td>79.014</td>
<td>180.335</td>
</tr>
<tr>
<td>ALI(G) = ( \sum_{UV \in E}</td>
<td>d_u - d_v</td>
<td>)</td>
<td>26</td>
<td>74</td>
<td>170</td>
</tr>
<tr>
<td>IRLI(G) = ( \sum_{UV \in E} \frac{</td>
<td>d_u - d_v</td>
<td>}{\min(d_u, d_v)} )</td>
<td>19</td>
<td>53</td>
<td>121</td>
</tr>
<tr>
<td>IRLU(G) = ( \sum_{UV \in E} \frac{\min(d_u, d_v)}{</td>
<td>d_u - d_v</td>
<td>} )</td>
<td>13.1627</td>
<td>36.6596</td>
<td>83.6536</td>
</tr>
<tr>
<td>IRF(G) = ( \sum_{UV \in E} (d_u - d_v)^2 )</td>
<td>34</td>
<td>98</td>
<td>226</td>
<td>482</td>
<td>994</td>
</tr>
<tr>
<td>IRLA(G) = ( 2 \sum_{UV \in E} \frac{</td>
<td>d_u - d_v</td>
<td>}{\min(d_u, d_v)} )</td>
<td>12.268</td>
<td>34.136</td>
<td>77.872</td>
</tr>
<tr>
<td>IRD1 = ( \sum_{UV \in E} \ln(1 +</td>
<td>d_u - d_v</td>
<td>) )</td>
<td>16.870</td>
<td>47.839</td>
<td>109.776</td>
</tr>
<tr>
<td>IRA(G) = ( \sum_{UV \in E} (d_u^2 - d_v^2)^2 )</td>
<td>1.2934</td>
<td>3.5370</td>
<td>8.0243</td>
<td>16.9988</td>
<td>34.9479</td>
</tr>
<tr>
<td>IRGA(G) = ( \sum_{UV \in E} \ln \frac{d_u + d_v}{x \sqrt{d_ud_v}} )</td>
<td>1.1025</td>
<td>3.0661</td>
<td>6.9934</td>
<td>14.8480</td>
<td>30.5571</td>
</tr>
<tr>
<td>IRB(G) = ( \sum_{UV \in E} \left( \frac{1}{d_u} - \frac{1}{d_v} \right)^2 )</td>
<td>4.2437</td>
<td>12.0450</td>
<td>27.6476</td>
<td>58.8528</td>
<td>121.2632</td>
</tr>
<tr>
<td>IRR_i(G) = ( \frac{1}{2} \sum_{UV \in E}</td>
<td>d_u - d_v</td>
<td>)</td>
<td>13</td>
<td>37</td>
<td>85</td>
</tr>
</tbody>
</table>

Theorem 2. Let \( NS_2[p] \) be the nanostar polypropyleneimine octaamin dendrimers, then the irregularity indices of \( NS_2[p] \) are:

1. \( IRDIFF(NS_2[p]) = 1.5(2^{p-1}) + 5(2^p) - 5 \)
2. \( IRR(NS_2[p]) = 2^{p+1} + 6(2^p) - 6 \)
3. \( IRL(NS_2[p]) = 0.6931471(2^{p+1}) + 2.4328(2^p) - 2.4328 \)
4. \( \text{IRLU}(NS_2[p]) = 2^{p+1} + 3(2^p) - 3 \)
5. \( \text{IRLF}(NS_2[p]) = 0.707106(2^{p+1}) + 2.4494897(2^p) - 2.4494897 \)
6. \( \sigma(NS_2[p]) = 2^{p+1} + 6(2^p) - 6 \)
7. \( \text{IRLA}(NS_2[p]) = 0.6667(2^{p+1}) + 2.4(2^p) - 2.4 \)
8. \( \text{IRD1} = 0.6931471806(2^{p+1}) + 4.15888302(2^p) - 4.15888302 \)
9. \( \text{IRA}(NS_2[p]) = 0.08578644(2^{p+1}) + 0.1010205144(2^p) - 0.1010205144 \)
10. \( \text{IRGA}(NS_2[p]) = 0.0588915178(2^{p+1}) + 0.1224659836(2^p) - 0.1224659836 \)
11. \( \text{IRB}(NS_2[p]) = 0.171578(2^{p+1}) + 0.606123086(2^p) - 0.606123086 \)
12. \( \text{IRR}(NS_2[p]) = 4(2^p) - 3 \)

**Proof.** In order to prove the above theorem, we have to consider Figure 2. We can see that the edges of \( NS_2[p] \) admit the following partition in Table 3. □

<table>
<thead>
<tr>
<th>Edge Type ( (d_u,d_v) )</th>
<th>Number of Edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1,2)</td>
<td>( 2^{p+1} )</td>
</tr>
<tr>
<td>(2,2)</td>
<td>( 8 \times 2^p - 5 )</td>
</tr>
<tr>
<td>(2,3)</td>
<td>( 6(2^p - 1) )</td>
</tr>
</tbody>
</table>

Table 3. Edge partition of nanostar polypropyleneimine octaamin dendrimers.

We can see that the edges of \( NS_2[p] \) admit the following partition in Table 3. Now using above Table 3 and the above definitions, we have:

1. \( \text{IRDIF}(G) = \sum_{UVE \in E} |d_U - d_V| \)
   \[
   \text{IRDIF}(NS_2[p], x, y) = 2^{p+1}|2 - 1| + |8 \times 2^p - 5| |2 - 2| + 6(2^p - 1)|2 - 3| = 2^{p+1} + 6(2^p - 1). \]

2. \( \text{IRR}(G) = \sum_{UVE \in E} \text{imb}(e) \cdot \text{imb}(e) = |d_u - d_v| \)
   \[
   \text{IRR}(NS_2[p], x, y) = 2^{p+1}|2 - 1| + |8 \times 2^p - 5| |2 - 2| + 6(2^p - 1)|3 - 2| = 2^{p+1} + 6(2^p - 1). \]

3. \( \text{IRL}(G) = \sum_{UVE \in E} |\ln d_u - \ln d_v| \)
   \[
   \text{IRL}(NS_2[p], x, y) = 2^{p+1} |\ln 2 - \ln 1| + |8 \times 2^p - 5| |\ln 2 - \ln 2| + 6(2^p - 1)|\ln 3 - \ln 2| = 2^{p+1} + 6(2^p - 1). \]

4. \( \text{IRLU}(G) = \sum_{UVE \in E} \frac{|d_u - d_v|}{\min(d_u,d_v)} \)
   \[
   \text{IRLU}(NS_2[p], x, y) = 2^{p+1} |\frac{2 - 1}{2} + |8 \times 2^p - 5| \frac{2 - 2}{2} + 6(2^p - 1) \frac{2 - 2}{2}| = 2^{p+1} + 3(2^p - 1). \]

5. \( \text{IRLF}(G) = \sum_{UVE \in E} \frac{|d_u - d_v|}{\sqrt{(d_u,d_v)}} \)
   \[
   \text{IRLF}(NS_2[p], x, y) = 2^{p+1} \frac{|2 - 1|}{\sqrt{2}} + |8 \times 2^p - 5| \frac{2 - 2}{\sqrt{2}} + 6(2^p - 1) \frac{2 - 2}{\sqrt{2}} = 2^{p+1} + 6(2^p - 1). \]
6. $\sigma(G) = \sum_{UV \in E} (du - dv)^2$

$\sigma(NS_2[p], x, y) = 2^{p+1}(2-1)^2 + [8 \times 2^p - 5](2-2)^2 + 6(2^p - 1)(3-2)^2$

$= 2^{p+1}(2-1)^2 + 6(2^p - 1)(3-2)^2.$

7. $IRL(G) = 2 \sum_{UV \in E} \frac{|du - dv|}{d_u + d_v}$

$IRL(NS_2[p], x, y) = 2 \left( 2^{p+1} \left[ \frac{2-1}{2+1} + [8 \times 2^p - 5] \frac{2-2}{2+2} + 6(2^p - 1) \frac{3-2}{3+2} \right] \right)$

$= 2 \left[ 2^{p+1} + 6(2^p - 1) \right].$

8. $IRD_1 = \sum_{UV \in E} \ln(1 + |du - dv|)$

$IRD_1(NS_2[p], x, y) = 2^{p+1} \ln(1 + |2| + [8 \times 2^p - 5] \ln(1 + |2|) + 6(2^p - 1) \ln(1 + |3| - 2))$

$= 2^{p+1} \ln 2 + 6(2^p - 1) \ln 2.$

9. $IRA(G) = \sum_{UV \in E} \left( d_u^2 - d_v^2 \right)^2$

$IRA(NS_2[p], x, y) = 2^{p+1} \left[ \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{6}} \right]^2 + [8 \times 2^p - 5] \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{6}} \right)^2 + 6(2^p - 1) \left( \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}} \right)^2$

$= 2^{p+1} \left[ \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{6}} \right]^2 + 6(2^p - 1) \left( \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}} \right)^2.$

10. $IRGA(G) = \sum_{UV \in E} \ln \frac{d_u + d_v}{2 \sqrt{(du + dv)}}$

$IRGA(NS_2[p], x, y) = 2^{p+1} \ln \left[ \frac{2+1}{2 \sqrt{2}} + [8 \times 2^p - 5] \ln \left( \frac{2+2}{2 \sqrt{6}} \right) + 6(2^p - 1) \ln \left( \frac{3+2}{2 \sqrt{6}} \right) \right]

= 2^{p+1} \ln \frac{5}{2 \sqrt{6}} + 6(2^p - 1) \ln \frac{5}{2 \sqrt{6}}.$

11. $IRB(G) = \sum_{UV \in E} \left( d_u^2 - d_v^2 \right)^2$

$IRB(NS_2[p], x, y) = 2^{p+1} \left[ \sqrt{2} - \sqrt{1} \right]^2 + [8 \times 2^p - 5] \left( \sqrt{2} - \sqrt{2} \right)^2 + 6(2^p - 1) \left( \sqrt{3} - \sqrt{2} \right)^2$

$= 2^{p+1} \left[ \sqrt{2} - \sqrt{1} \right]^2 + 14(2^p - 1) \left( \sqrt{3} - \sqrt{2} \right)^2.$

12. $IRR_t(G) = \frac{1}{2} \sum_{UV \in E} |du - dv|$.

$IRR_t(NS_2[p], x, y) = \frac{1}{2} \left[ 2^{p+1}|2-1| + |8 \times 2^p - 5||2-2| + 6(2^p - 1)|3-2| \right]

= \frac{1}{2} \left[ 2^{p+1} + 6(2^p - 1) \right].$

Table 4 represents some calculated values of irregularity indices of $NS_2[p]$ for some test values of $p$. 
Table 4. Irregularity indices for NS$_2[p]$ polypropylenimine octaamin dendrimers.

<table>
<thead>
<tr>
<th>Irregularity indices</th>
<th>$p = 1$</th>
<th>$p = 2$</th>
<th>$p = 3$</th>
<th>$p = 4$</th>
<th>$p = 5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>IRDIFF(G) = $\sum_{u \in V} \frac{d_u}{d_u} - d_v$</td>
<td>11</td>
<td>27</td>
<td>59</td>
<td>123</td>
<td>251</td>
</tr>
<tr>
<td>AL(G) = $\sum_{u \in V}</td>
<td>d_u - d_v</td>
<td>$</td>
<td>10</td>
<td>26</td>
<td>58</td>
</tr>
<tr>
<td>IRL(G) = $\sum_{u \in V}</td>
<td>d_u - d_v</td>
<td>$</td>
<td>5.2054</td>
<td>12.844</td>
<td>28.1199</td>
</tr>
<tr>
<td>ILLU(G) = $\sum_{u \in V} \frac{</td>
<td>d_u - d_v</td>
<td>}{\min(d_u, d_v)}$</td>
<td>7</td>
<td>17</td>
<td>37</td>
</tr>
<tr>
<td>IRLF(G) = $\sum_{u \in V} \frac{</td>
<td>d_u - d_v</td>
<td>}{\sqrt{d_u d_v}}$</td>
<td>5.2779</td>
<td>13.0053</td>
<td>28.4601</td>
</tr>
<tr>
<td>IRF(G) = $\sum_{u \in V} (d_u - d_v)^2$</td>
<td>10</td>
<td>26</td>
<td>58</td>
<td>122</td>
<td>250</td>
</tr>
<tr>
<td>IRFA(G) = $\sum_{u \in V}</td>
<td>d_u - d_v</td>
<td>$</td>
<td>5.0668</td>
<td>12.5336</td>
<td>27.4672</td>
</tr>
<tr>
<td>IRF1 = $\sum_{u \in V}</td>
<td>\ln(1 +</td>
<td>d_u - d_v</td>
<td>)$</td>
<td>6.9315</td>
<td>18.0218</td>
</tr>
<tr>
<td>IRA(G) = IRF(G) = $\sum_{u \in V} \left(\frac{d_u^2}{d_u} - d_v^2\right)^2$</td>
<td>0.4442</td>
<td>0.9894</td>
<td>2.0797</td>
<td>4.2605</td>
<td>8.62197</td>
</tr>
<tr>
<td>IRGA(G) = IRF(G) = $\sum_{u \in V} \ln\left(\frac{d_u + d_v}{2\sqrt{d_u d_v}}\right)$</td>
<td>0.3580</td>
<td>0.8385</td>
<td>1.7995</td>
<td>3.7215</td>
<td>7.5655</td>
</tr>
<tr>
<td>IRB(G) = $\sum_{u \in V} \left(\frac{d_u^2}{d_v} - d_v^2\right)^2$</td>
<td>1.2924</td>
<td>3.1909</td>
<td>6.9881</td>
<td>14.5823</td>
<td>29.7708</td>
</tr>
<tr>
<td>IRR(G) = $\frac{1}{2} \sum_{u \in V}</td>
<td>d_u - d_v</td>
<td>$</td>
<td>5</td>
<td>13</td>
<td>29</td>
</tr>
</tbody>
</table>

Our next aim is to determine the irregularity indices of polymer dendrimers.

**Theorem 3.** Let NS$_3[p]$ be polymer dendrimer then the irregularity indices of NS$_3[p]$ are:

1. $IRDIFF(NS_3[p]) = 4.5(2^p) + 54.999978(2^{p-1}) - 14.999994$
2. $IRR(NS_3[p]) = 3(2^p) + 66(2^{p-1}) - 18$
3. $IRL(NS_3[p]) = 2.079441(2^p) + 26.76069(2^{p-1}) - 7.29837$
4. $IRLU(NS_3[p]) = 3(2^p) + 33(2^{p-1}) - 9$
5. $IRLF(NS_3[p]) = 2.12132(2^p) + 26.944384(2^{p-1}) - 7.348468$
6. $\alpha(NS_3[p]) = 3(2^p) + 66(2^{p-1}) - 18$
7. $IRLA(NS_3[p]) = 2(2^p) + 26.4(2^{p-1}) - 7.2$
8. $IRD1 = 2.079441(2^p) + 45.747702(2^{p-1}) - 12.476646$
9. $IRA(NS_3[p]) = 1.5(2^p) + 1.111242(2^{p-1}) - 0.303066$
10. $IRGA(NS_3[p]) = 0.176673(2^p) + 1.347126(2^{p-1}) - 0.367398$
11. $IRB(NS_3[p]) = 0.514719(2^p) + 6.667386(2^{p-1}) - 1.8378$
12. $IRR\_I(NS_3[p]) = 1.5(2^p) + 33(2^{p-1}) - 9$

**Proof.** In order to prove the above theorem we have to consider Figure 3. \[\square\]

We can see that the edges of NS$_3[p]$ admit the following partition in Table 5.

**Table 5.** Edge partition of polymer dendrimer.

<table>
<thead>
<tr>
<th>Edges Type ((d_u,d_v))</th>
<th>Number of Edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1,2)</td>
<td>3.2$^p$</td>
</tr>
<tr>
<td>(2,2)</td>
<td>54(2^{p-1}) - 24</td>
</tr>
<tr>
<td>(2,3)</td>
<td>66(2^{p-1}) - 1 + 48</td>
</tr>
<tr>
<td>(3,3)</td>
<td>3.2^{p+1}</td>
</tr>
</tbody>
</table>

Now using above Table 5 and the above definitions we have:
1. \( \text{IRDIF}(G) = \sum_{UV \in E} | \frac{d_u}{d_U} - \frac{d_v}{d_V} | \)

\[
\text{IRDIF}(\text{NS}_3[p], x, y) = 3.2\left[\frac{2}{3} - \frac{1}{2}\right] + 54(2^{p-1}) - 24\left[\frac{2}{3} - \frac{2}{3}\right] + 66(2^{p-1} - 1) + 48\left[\frac{3}{2} - \frac{3}{3}\right] + 3.2^{p+1}\left[\frac{3}{3} - \frac{3}{3}\right].
\]

2. \( \text{IRR}(G) = \sum_{UV \in E} \text{imb}(e) \cdot \text{imb}(e) = |d_u - d_v| \)

\[
\text{IRR}(\text{NS}_3[p], x, y) = 3.2p|2 - 1| + 54(2^{p-1}) - 24|2 - 2| + 66(2^{p-1} - 1) + 48|3 - 2| + 3.2^{p+1}|3 - 3| = 3.2p + 66(2^{p-1} - 1) + 48.
\]

3. \( \text{IRL}(G) = \sum_{UV \in E} |\text{imb}(e)| \)

\[
\text{IRL}(\text{NS}_3[p], x, y) = 3.2p|\text{ln}2 - \text{ln}1| + 54(2^{p-1}) - 24|\text{ln}2 - \text{ln}2| + 66(2^{p-1} - 1) + 48|\text{ln}3 - \text{ln}2| + 3.2^{p+1}|\text{ln}3 - \text{ln}3| = 3.2p|\text{ln}2 - \text{ln}1| + 66(2^{p-1} - 1) + 48|\text{ln}3 - \text{ln}2|.
\]

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

\[
\text{IRLU}(\text{NS}_3[p], x, y) = 3.2p\left[\frac{2}{3} - \frac{1}{2}\right] + 54(2^{p-1}) - 24\left[\frac{2}{3} - \frac{2}{4}\right] + 66(2^{p-1} - 1) + 48\left[\frac{3}{2} - \frac{2}{6}\right] + 3.2^{p+1}\left[\frac{3}{3} - \frac{3}{9}\right]
= 3.2p + 66(2^{p-1} - 1) + 48.
\]

5. \( \text{IRLF}(G) = \sum_{UV \in E} \frac{|d_u - d_v|}{\sqrt{d_u d_v}} \)

\[
\text{IRLF}(\text{NS}_3[p], x, y) = 3.2p\left[\frac{2}{3} - \frac{1}{2}\right] + 54(2^{p-1}) - 24\left[\frac{2}{3} - \frac{2}{4}\right] + 66(2^{p-1} - 1) + 48\left[\frac{3}{2} - \frac{2}{6}\right] + 3.2^{p+1}\left[\frac{3}{3} - \frac{3}{9}\right]
= 3.2p\left[\frac{1}{2} + 66(2^{p-1} - 1) + 48\right].
\]

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

\[
\sigma(\text{NS}_3[p], x, y) = 3.2p(2 - 1)^2 + 54(2^{p-1}) - 24(2 - 2)^2 + 66(2^{p-1} - 1) + 48(3 - 2)^2 + 3.2^{p+1}(3 - 3)^2
= 3.2p + 66(2^{p-1} - 1) + 48.
\]

7. \( \text{IRLA}(G) = 2 \sum_{UV \in E} \frac{|d_u - d_v|}{d_u d_v} \)

\[
\text{IRLA}(\text{NS}_3[p], x, y) = 2\left[3.2p\left[\frac{2}{3} - \frac{1}{2}\right] + 54(2^{p-1}) - 24\left[\frac{2}{3} - \frac{2}{4}\right] + 66(2^{p-1} - 1) + 48\left[\frac{3}{2} - \frac{2}{6}\right] + 3.2^{p+1}\left[\frac{3}{3} - \frac{3}{9}\right]\right]
= 2\left[3.2p\left[\frac{1}{2} + 66(2^{p-1} - 1) + 48\right]\right].
\]

8. \( \text{IRD1} = \sum_{UV \in E} \ln(1 + |d_u - d_v|) \)

\[
\text{IRD1}(\text{NS}_3[n], x, y) = 3.2p\ln(1 + |2 - 1|) + 54(2^{p-1}) - 24\ln(1 + |2 - 2|) + 66(2^{p-1} - 1) + 48\ln(1 + |3 - 2|) + 3.2^{p+1}\ln(1 + |3 - 3|)
= 3.2p\ln2 + (66(2^{p-1} - 1) + 48)\ln2
\]

9. \( \text{IRA}(G) = \sum_{UV \in E} (d_u^2 - d_v^2)^2 \)

\[
\text{IRA}(\text{NS}_3[p], x, y) = 3.2p\left(\frac{1}{2} - \frac{1}{3}\right)^2 + 54(2^{p-1}) - 24\left(\frac{1}{2} - \frac{1}{3}\right)^2 + 66(2^{p-1} - 1) + 48\left(\frac{1}{3} - \frac{1}{3}\right)^2 + 3.2^{p+1}\left(\frac{1}{3} - \frac{1}{3}\right)^2
= 3.2p\left(\frac{1}{2} + 66(2^{p-1} - 1) + 48\right). 
\]
10. \( \text{IRGA}(G) = \sum_{UV \in E} \ln \frac{d_u + d_v}{\sqrt{(d_u d_v)}} \)

\[
\begin{align*}
\text{IRGA}(\text{NS}_3[p], x, y) & = 3.2p^2 \ln \left( \frac{p^2 + 1}{\sqrt{p^2}} \right) + 54(2p - 1) - 24(\sqrt{p^2} - \sqrt{3})^2 + 66(2p^2 - 1) + 48\ln \left( \frac{p^2 + 1}{\sqrt{p}} \right) + 3.2p^2 \ln \left( \frac{3^2 + 3}{\sqrt{6}} \right) \\
& = 3.2p^2 \ln \left( \frac{18}{\sqrt{2}} + (66(2p - 1) + 48) \ln \frac{3}{\sqrt{6}} \right).
\end{align*}
\]

11. \( \text{IRB}(G) = \sum_{UV \in E} \left( \frac{d_u^2 - d_v^2}{2} \right) \)

\[
\begin{align*}
\text{IRB}(\text{NS}_3[p], x, y) & = 3.2p^2 \ln \left( \sqrt{p^2} - \sqrt{3} \right)^2 + 54(2p - 1) - 24(\sqrt{p^2} - \sqrt{3})^2 + 66(2p^2 - 1) + 48(\sqrt{3} - \sqrt{5})^2 + 3.2p^2(\sqrt{3} - \sqrt{5})^2 \\
& = 3.2p^2 \ln \left( \sqrt{3} - \sqrt{5} \right)^2 + (66(2p - 1) + 48)(\sqrt{3} - \sqrt{5})^2.
\end{align*}
\]

12. \( \text{IRR}_t(G) = \frac{1}{2} \sum_{UV \in E} |d_u - d_v| \)

\[
\begin{align*}
\text{IRR}_t(\text{NS}_3[p], x, y) & = \frac{1}{2} \left[ 3.2p^2 \left( 2 - 1 \right) + 54(2p - 1) - 24(2 - 2) + 66(2p^2 - 1) + 48(3 - 2) + 3.2p^2(3 - 3) \right] \\
& = \frac{1}{2} \left[ 3.2p^2 + (66(2p^2 - 1) + 48) \right].
\end{align*}
\]

The following Table 6 represents some calculated values of irregularity indices of \( \text{NS}_3[p] \) for some test values of \( p \).

<table>
<thead>
<tr>
<th>Irregularity Indices</th>
<th>( p = 1 )</th>
<th>( p = 2 )</th>
<th>( p = 3 )</th>
<th>( p = 4 )</th>
<th>( p = 5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{IRDIF}(G) )</td>
<td>48.9999</td>
<td>112.9999</td>
<td>240.9999</td>
<td>496.9998</td>
<td>1008.99</td>
</tr>
<tr>
<td>( \text{AL}(G) )</td>
<td>54</td>
<td>126</td>
<td>270</td>
<td>558</td>
<td>1134</td>
</tr>
<tr>
<td>( \text{IRL}(G) )</td>
<td>23.6212</td>
<td>54.541</td>
<td>116.379</td>
<td>240.058</td>
<td>487.414</td>
</tr>
<tr>
<td>( \text{IRLU}(G) )</td>
<td>30</td>
<td>69</td>
<td>147</td>
<td>303</td>
<td>615</td>
</tr>
<tr>
<td>( \text{IRLH}(G) )</td>
<td>23.8385</td>
<td>55.025</td>
<td>117.399</td>
<td>242.147</td>
<td>491.644</td>
</tr>
<tr>
<td>( \text{IRF}(G) )</td>
<td>54</td>
<td>126</td>
<td>270</td>
<td>558</td>
<td>1134</td>
</tr>
<tr>
<td>( \text{IRLA}(G) )</td>
<td>23.2</td>
<td>53.6</td>
<td>114.4</td>
<td>236</td>
<td>479.2</td>
</tr>
<tr>
<td>( \text{IRD1}(G) )</td>
<td>37.4299</td>
<td>87.3365</td>
<td>187.1496</td>
<td>386.7760</td>
<td>786.0286</td>
</tr>
<tr>
<td>( \text{IRA}(G) )</td>
<td>3.8082</td>
<td>7.9194</td>
<td>16.1419</td>
<td>32.5868</td>
<td>65.4768</td>
</tr>
<tr>
<td>( \text{IRG}(G) )</td>
<td>1.3331</td>
<td>3.0335</td>
<td>6.4345</td>
<td>13.236</td>
<td>26.84015</td>
</tr>
<tr>
<td>( \text{IRB}(G) )</td>
<td>5.8590</td>
<td>13.5558</td>
<td>28.9495</td>
<td>59.7368</td>
<td>121.3113</td>
</tr>
<tr>
<td>( \text{IRR}_t(G) )</td>
<td>27</td>
<td>63</td>
<td>135</td>
<td>279</td>
<td>567</td>
</tr>
</tbody>
</table>

4. Graphical Analysis, Discussions and Conclusions

In this part we give our comparative analysis of some of the irregularity indices of the above discussed dendrimers and the dependences of the irregularity indices on the parameter of the structures. Figures 4–7 contain three graphs of irregularity indices. The horizontal axis is used for step size \( p \) and the vertical axis shows the value of irregularity index. In the graphs, the red color shows the irregularity of \( \text{NS}_1[p] \), the blue color shows the irregularity of \( \text{NS}_2[p] \) and the green color shows the irregularity of the \( \text{NS}_3[p] \). In each graph, three different colored curves are depicted which shows the behavior of the irregularity indices with increase in \( p \).
From above graph it seems obvious that irregularities have a slight increase with an increase in the step size $p$ for the range $p \leq 12$. But after $p \geq 14$, these irregularity indices drastically increase with increase in $p$. So $NS_3[p]$ is the most irregular and asymmetric structure as far as most of the irregularity indices are concerned. Nanostar dendrimers are relatively less irregular, and $NS_1[p]$ are the most regular dendrimers. This trend is not restricted to only irregularity index $IRDIF$. Most of the irregularity indices behave pretty similarly as shown in the following figures. All other figures show the trends which can easily be understood in the Figures 5–7.

Figure 4. Graph of $IRDIF(G)$.

Figure 5. Graph of $IRLU(G)$. 

![Graph of $IRDIF(G)$](image1)

![Graph of $IRLU(G)$](image2)
All above graphs (Figures 4–7) indicate that \( N_S_3[p] \) is highly asymmetric as far as all irregularity indices are concerned, whereas \( N_S_1[p] \) is less asymmetric, and \( N_S_2[p] \) is the most regular structure with respect to all indices. In \( IR_B \), \( N_S_1[p] \) and \( N_S_3[p] \) show the same irregularity behavior. These facts typically relate geometry and topology of the structure of these dendrimers and can be used in modelling purposes.

From above graph it seems obvious that irregularities have a slight increase with an increase in the step size \( p \) for the range \( p \leq 12 \). But after \( p \geq 14 \), these irregularity indices drastically increase with increase in \( p \). So \( NS_3[p] \) is the most irregular and asymmetric structure as far as most of the irregularity indices are concerned. Nanostar dendrimers are relatively less irregular, and \( NS_1[p] \) are the most regular dendrimers. This trend is not restricted to only irregularity index \( IR_{DIF} \). Most of the irregularity indices behave pretty similarly as shown in the following figures. All other figures show the trends which can easily be understood in the Figures 5–7.
All above graphs (Figures 4–7) indicate that $\text{NS}_3[p]$ is highly asymmetric as far as all irregularity indices are concerned, whereas $\text{NS}_1[p]$ is less asymmetric, and $\text{NS}_2[p]$ is the most regular structure with respect to all indices. In IRB, $\text{NS}_1[p]$ and $\text{NS}_3[p]$ show the same irregularity behavior. These facts typically relate geometry and topology of the structure of these dendrimers and can be used in modelling purposes.

We foresee that our results could play an important role in determining properties of these dendrimers such as enthalpy, toxicity, resistance and entropy. Similar research has been done in [29], where authors discussed some properties of alkane isomers.

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