Nirmala Index

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Abstract: In Chemical Graph Theory, several degree based topological indices were introduced and studied since 1972. In this paper, a novel invariant is considered, which is the Nirmala index defined as the sum of the square root of sum of the degrees of the pairs of adjacent vertices. We initiate a study of the Nirmala index.

Keywords: topological index, Nirmala index, Nirmala exponential, dendrimer.

Mathematics Subject Classification: 05C05, 05C12, 05C35.

I. Introduction

Let $G$ be a simple, finite, connected graph with the vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex $u$ is the number of vertices adjacent to $u$. The additional definitions and notations, the reader may refer to [1].

A molecular graph is a graph in which the vertices correspond to the atoms and the edges to the bonds of a molecule. A topological index is a numeric quantity from structural graph of a molecule. Several topological indices have been considered in Theoretical Chemistry, and have found some applications, especially in QSPR/QSAR study, see [2, 3, 4].

In Chemical Science, numerous vertex degree based topological indices or graph indices have been introduced and extensively studied in [4, 5].

The Sombor index was defined by Gutman in [6] as

$$SO(G) = \sum_{u \in V(G)} \sqrt{d_G(u)^2 + d_G(v)^2}.$$ 

Recently, some Sombor indices were studied in [7, 8, 9, 10, 11, 12, 13, 14].

Inspired by work on Sombor indices, we introduce the Nirmala index of a graph $G$ as follows:

The Nirmala index of a molecular graph $G$ is defined as

$$N(G) = \sum_{u \in V(G)} \sqrt{d_G(u) + d_G(v)}.$$ 

Considering the Nirmala index, we define the Nirmala exponential of a graph $G$ as

$$N(G, x) = \sum_{u \in V(G)} x^{d_G(u) + d_G(v)}.$$ 

In this study, we compute the Nirmala index, Nirmala exponential of four families of dendrimers. For dendrimers, see [15].

II. Results for Porphyrin Dendrimer $D_nP_n$

We consider the family of porphyrin dendrimers. This family of dendrimers is denoted by $D_nP_n$. The molecular graph of $D_nP_n$ is shown in Figure 1.

Figure 1. The molecular graph of $D_nP_n$
Let $G$ be the molecular graph of $D_nP_n$. By calculation, we find that $G$ has $96n - 10$ vertices and $105n - 11$ edges. In $D_nP_n$, there are six types of edges based on degrees of end vertices of each edge as given in Table 1.

<table>
<thead>
<tr>
<th>$d_G(u), d_G(v) \forall uv \in E(G)$</th>
<th>(1, 3)</th>
<th>(1, 4)</th>
<th>(2, 2)</th>
<th>(2, 3)</th>
<th>(3, 3)</th>
<th>(3, 4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of edges</td>
<td>$2n$</td>
<td>$24n$</td>
<td>$10n - 5$</td>
<td>$48n - 6$</td>
<td>$13n$</td>
<td>$8n$</td>
</tr>
</tbody>
</table>

**Table 1. Edge partition of $D_nP_n$**

In the following theorem, we compute the Nirmala index and its exponential of $D_nP_n$.

**Theorem 1.** Let $D_nP_n$ be the family of porphyrin dendrimers. Then

(i) $N(D_nP_n) = (24 + 72\sqrt{5} + 13\sqrt{6} + 8\sqrt{7})n - (10 + 6\sqrt{5})$.

(ii) $N(D_nP_n, x) = (12n - 5)x^2 + (72n - 6)x^5 + 13nx^6 + 8nx^7$.

**Proof:** From definitions and by using Table 1, we deduce

(i) $N(D_nP_n) = \sum_{uv \in E(G)} \left[ d_G(u) + d_G(v) \right]^2$

$= (1 + 3)^2 2n + (1 + 4)^2 24n + (2 + 2)^2 (10n - 5) + (2 + 3)^2 (48n - 6)$

$+ (3 + 3)^2 13n + (3 + 4)^2 8n$

$= (24 + 72\sqrt{5} + 13\sqrt{6} + 8\sqrt{7})n - (10 + 6\sqrt{5})$.

(ii) $N(D_nP_n, x) = \sum_{uv \in E(G)} x^{(d_G(u) + d_G(v))^2}$

$= 2nx^{(1+3)^2} + 24nx^{(1+4)^2} + (10n - 5)x^{(2+2)^2} + (48n - 6)x^{(2+3)^2} + 13nx^{(3+3)^2} + 8nx^{(3+4)^2}$

$= (12n - 5)x^2 + (72n - 6)x^5 + 13nx^6 + 8nx^7$.

**III. Results for Propyl Ether Imine Dendrimer PETIM**

We consider the family of propyl ether imine dendrimers. This family of dendrimers is denoted by PETIM. The molecular graph of PETIM is depicted in Figure 2.
Let $G$ be the molecular graph of $PETIM$. By calculation, we find that $G$ has $24 \times 2^n - 23$ vertices and $24 \times 2^n - 24$ edges. In $PETIM$, there are three types of edges based on degrees of end vertices of each edge as given in Table 2.

<table>
<thead>
<tr>
<th>$d_G(u), d_G(v) \setminus uv \in E(G)$</th>
<th>(1, 2)</th>
<th>(2, 2)</th>
<th>(2, 3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of edges</td>
<td>$2 \times 2^n$</td>
<td>$16 \times 2^n - 18$</td>
<td>$6 \times 2^n - 6$</td>
</tr>
</tbody>
</table>

Table 2. Edge partition of $PETIM$

In the following theorem, we compute the Nirmala index and its exponential of $PETIM$.

**Theorem 2.** Let $PETIM$ be the family of polypropyl ether imine dendrimers. Then

(i) $N(PETIM) = (2\sqrt{3} + 32 + 6\sqrt{5}) 2^n - (36 + 6\sqrt{5})$.

(ii) $N(PETIM, x) = 2 \times 2^n x^{\frac{1}{2}} + (16 \times 2^n - 18) x^2 + (6 \times 2^n - 6) x^{\frac{3}{2}}$.

**Proof:** From definitions and by using Table 2, we derive

(i) $N(PETIM) = \sum_{uv \in E(G)} \left[ d_G(u) + d_G(v) \right]^{\frac{1}{2}}$

$$= (1 + 2) \frac{1}{2} 2 \times 2^n + (2 + 2)^{\frac{1}{2}} (16 \times 2^n - 18) + (2 + 3)^{\frac{1}{2}} (6 \times 2^n - 6)$$

$$= (2\sqrt{3} + 32 + 6\sqrt{5}) 2^n - (36 + 6\sqrt{5}) .$$

(ii) $N(PETIM, x) = \sum_{uv \in E(G)} x^{[d_G(u) + d_G(v)]^{\frac{1}{2}}}$

$$= 2 \times 2^n x^{(1+2)^{\frac{1}{2}}} + (16 \times 2^n - 18) x^{(2+2)^{\frac{1}{2}}} + (6 \times 2^n - 6) x^{(2+3)^{\frac{1}{2}}};$$

$$= 2 \times 2^n x^{\frac{1}{2}} + (16 \times 2^n - 18) x^2 + (6 \times 2^n - 6) x^{\frac{3}{2}} .$$

**IV. Results for Poly Ethylene Amide Amine Dendrimer PETAA**

We consider the family of polyethylene amide amine dendrimers. This family of dendrimers is denoted by $PETAA$. The molecular graph of $PETAA$ is presented in Figure 3.

![Figure 3. The molecular graph of PETAA](image_url)
In the following theorem, we determine the Nirmala index and its exponential of $PET_{AA}$.

**Theorem 3.** Let $PET_{AA}$ be the family of poly ethylene amide amine dendrimers. Then

(i) $N(PET_{AA}) = (4\sqrt{3} + 40 + 20\sqrt{5})2^n - (16 + 9\sqrt{5})$.

(ii) $N(PET_{AA}, x) = 4 \times 2^n x^{45} + (20 \times 2^n - 10) x^2 + (20 \times 2^n - 9) x^{65}$.

**Proof:** By using definitions and Table 3, we obtain

(i) $N(PET_{AA}) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v)\right]^{\frac{1}{2}}$

\[= (1 + 2)^\frac{1}{2} 4 \times 2^n + (1 + 3)^\frac{1}{2} (4 \times 2^n - 2) + (2 + 2)^\frac{1}{2} (16 \times 2^n - 8) + (2 + 3)^\frac{1}{2} (20 \times 2^n - 9)\]

\[= (4\sqrt{3} + 40 + 20\sqrt{5})2^n - (16 + 9\sqrt{5}).\]

(ii) $N(PET_{AA}, x) = \sum_{uv \in E(G)} x^{\left[d_G(u) + d_G(v)\right]}$

\[= 4 \times 2^n x^{(1+2)^\frac{1}{2}} + (4 \times 2^n - 2) x^{(1+3)^\frac{1}{2}} + (16 \times 2^n - 8) x^{(2+2)^\frac{1}{2}} + (20 \times 2^n - 9) x^{(2+3)^\frac{1}{2}}\]

\[= 4 \times 2^n x^{45} + (20 \times 2^n - 10) x^2 + (20 \times 2^n - 9) x^{65}.

**V. Results for Zinc Prophyrin Dendrimer $DPZ_n$**

We consider the family of zinc prophyrin dendrimers. This family of dendrimers is denoted by $DPZ_n$, where $n$ is the steps of growth in this type of dendrimers. The molecular graph of $DPZ_n$ is shown in Figure 4.

![Figure 4](image)

**Table 3. Edge partition of $PET_{AA}$**

<table>
<thead>
<tr>
<th>$d_G(u), d_G(v) \setminus uv \in E(G)$</th>
<th>(1, 2)</th>
<th>(1, 3)</th>
<th>(2, 2)</th>
<th>(2, 3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of edges</td>
<td>$4 \times 2^n$</td>
<td>$4 \times 2^n - 2$</td>
<td>$16 \times 2^n - 8$</td>
<td>$20 \times 2^n - 9$</td>
</tr>
</tbody>
</table>

**Table 4. Edge partition of $DPZ_n$**

<table>
<thead>
<tr>
<th>$d_G(u), d_G(v) \setminus uv \in E(G)$</th>
<th>(2, 2)</th>
<th>(2, 3)</th>
<th>(3, 3)</th>
<th>(3, 4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of edges</td>
<td>$16 \times 2^n - 4$</td>
<td>$40 \times 2^n - 16$</td>
<td>$8 \times 2^n + 12$</td>
<td>$4$</td>
</tr>
</tbody>
</table>
In the following theorem, we determine the Nirmala index and its exponential of $DPZ_n$.

**Theorem 4.** Let $DPZ_n$ be the family of zinc prophyrin dendrimers. Then

(i) $N(DPZ_n) = (32 + 40\sqrt{5} + 8\sqrt{6})2^n - (8 + 16\sqrt{5} - 12\sqrt{6} + 4\sqrt{7})$.

(ii) $N(DPZ_n, x) = (16 \times 2^n - 4)x^2 + (40 \times 2^n - 16)x^\sqrt{5} + (8 \times 2^n + 12)x^\sqrt{6} + 4x^\sqrt{7}$.

**Proof:** From definitions and by using Table 4, we deduce

(i) $N(DPZ_n) = \sum_{uv \in E(G)} \left[ d_G(u) + d_G(v) \right]^{-\frac{1}{2}}$

$= (2 + 2)^{\frac{1}{2}} (16 \times 2^n - 4) + (2 + 3)^{\frac{1}{2}} (40 \times 2^n - 16) + (3 + 3)^{\frac{1}{2}} (8 \times 2^n + 12) + (3 + 4)^{\frac{1}{2}} 4$

$= (32 + 40\sqrt{5} + 8\sqrt{6})2^n - (8 + 16\sqrt{5} - 12\sqrt{6} + 4\sqrt{7})$.

(ii) $N(DPZ_n, x) = \sum_{uv \in E(G)} x^{d_G(u) + d_G(v)}$

$= (16 \times 2^n - 4)x^{2 + 2} + (40 \times 2^n - 16)x^{2 + 3} + (8 \times 2^n + 12)x^{3 + 3} + 4x^{3 + 4}$

$= (16 \times 2^n - 4)x^2 + (40 \times 2^n - 16)x^\sqrt{5} + (8 \times 2^n + 12)x^\sqrt{6} + 4x^\sqrt{7}$.

**CONCLUSION**

In this study, a novel invariant is considered which is the Nirmala index. Also we have defined the Nirmala exponential of a molecular graph. Furthermore, the Nirmala index and its corresponding exponential for certain dendrimers are computed.

**REFERENCES**


