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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 Nirmla index.*

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

Mathematics Subject Classification: 05*C*05, 05*C*12, 05*C*35.

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

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

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

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

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

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

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.

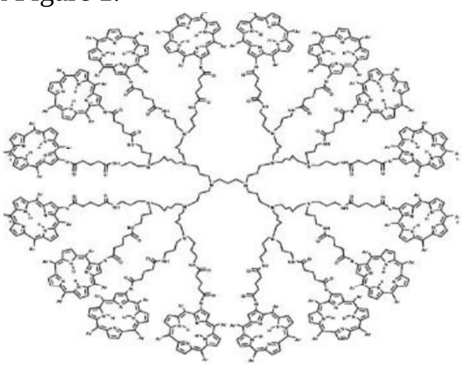

Figure 1. The molecular graph of D_nP_n

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.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(3, 3)	(3, 4)
Number of edges	$2n$	$24n$	$10n - 5$	$48n - 6$	$13n$	$8n$

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

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

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

(i)
$$\begin{aligned}N\left(D_nP_n\right) &= \sum_{uv\in E(G)}\left[d_G(u)+d_G(v)\right]^{\frac{1}{2}}\\
&=(1+3)^{\frac{1}{2}}2n+(1+4)^{\frac{1}{2}}24n+(2+2)^{\frac{1}{2}}(10n-5)+(2+3)^{\frac{1}{2}}(48n-6)\\
&\quad+(3+3)^{\frac{1}{2}}13n+(3+4)^{\frac{1}{2}}8n\\
&=\left(24+72\sqrt{5}+13\sqrt{6}+8\sqrt{7}\right)n-\left(10+6\sqrt{5}\right).\end{aligned}$$

(ii)
$$\begin{aligned}N\left(D_nP_n, x\right) &= \sum_{uv\in E(G)} x^{\left[d_G(u)+d_G(v)\right]^{\frac{1}{2}}}\\
&=2nx^{(1+3)^{\frac{1}{2}}}+24nx^{(1+4)^{\frac{1}{2}}}+(10n-5)x^{(2+2)^{\frac{1}{2}}}+(48n-6)x^{(2+3)^{\frac{1}{2}}}+13nx^{(3+3)^{\frac{1}{2}}}+8nx^{(3+4)^{\frac{1}{2}}}\\
&=(12n-5)x^2+(72n-6)x^{\sqrt{5}}+13nx^{\sqrt{6}}+8nx^{\sqrt{7}}.\end{aligned}$$

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.

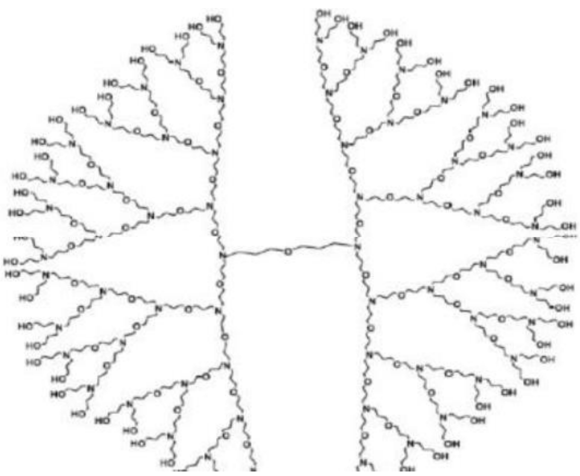

Figure 2. The molecular graph of *PETIM*

Let G be the molecular graph of *PETIM*. By calculation, we find that G has $24\times2^n - 23$ vertices and $24\times2^n - 24$ edges. In *PETIM*, there are three types of edges based on degrees of end vertices of each edge as given in Table 2.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(1, 2)	(2, 2)	(2, 3)
Number of edges	2×2^n	$16 \times 2^n - 18$	$6 \times 2^n - 6$

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 porpyl ether imine dendrimers. Then

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

(ii) $N(PETIM, x) = 2\times2^n x^{\sqrt{3}} + \left(16\times2^n - 18\right)x^2 + \left(6\times2^n - 6\right)x^{\sqrt{5}}$.

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

(i)
$$N(PETIM) = \sum_{uv\in E(G)} \left[d_G(u)+d_G(v)\right]^{\frac{1}{2}}$$
$$= (1+2)^{\frac{1}{2}} 2\times2^n + (2+2)^{\frac{1}{2}}\left(16\times2^n - 18\right) + (2+3)^{\frac{1}{2}}\left(6\times2^n - 6\right)$$
$$= \left(2\sqrt{3}+32+6\sqrt{5}\right)2^n - \left(36+6\sqrt{5}\right).$$

(ii)
$$N(PETIM, x) = \sum_{uv\in E(G)} x^{\left[d_G(u)+d_G(v)\right]^{\frac{1}{2}}}$$
$$= 2\times2^n x^{(1+2)^{\frac{1}{2}}} + \left(16\times2^n - 18\right)x^{(2+2)^{\frac{1}{2}}} + \left(6\times2^n - 6\right)x^{(2+3)^{\frac{1}{2}}}$$
$$= 2\times2^n x^{\sqrt{3}} + \left(16\times2^n - 18\right)x^2 + \left(6\times2^n - 6\right)x^{\sqrt{5}}.$$

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

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

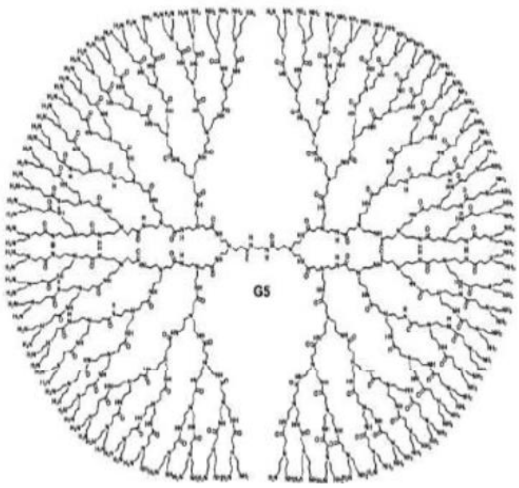

Figure 3. The molecular graph of *PETAA*

Let G be the molecular graph of *PETAA*. By calculation, we find that G has $44\times2^n - 18$ vertices and $44\times2^n - 19$ edges. In *PETAA*, there are three types of edges based on degrees of end vertices of each edge as given in Table 3.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(1, 2)	(1, 3)	(2, 2)	(2, 3)
Number of edges	4×2^n	$4 \times 2^n - 2$	$16 \times 2^n - 8$	$20 \times 2^n - 9$

Table 3. Edge partition of *PETAA*

In the following theorem, we determine the Nirmala index and its exponential of *PETAA*.

Theorem 3. Let *PETAA* be the family of poly ethylene amide amine dendrimers. Then

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

(ii) $N(PETAA, x) = 4\times 2^n x^{\sqrt{3}} + \left(20\times 2^n - 10\right)x^2 + \left(20\times 2^n - 9\right)x^{\sqrt{5}}.$

Proof: By using definitions and Table 3, we obtain

(i)
$$N(PETAA) = \sum_{uv\in E(G)} \left[d_G(u)+d_G(v)\right]^{\frac{1}{2}}$$
$$= (1+2)^{\frac{1}{2}} 4\times 2^n + (1+3)^{\frac{1}{2}}\left(4\times 2^n - 2\right) + (2+2)^{\frac{1}{2}}\left(16\times 2^n - 8\right) + (2+3)^{\frac{1}{2}}\left(20\times 2^n - 9\right)$$
$$= \left(4\sqrt{3}+40+20\sqrt{5}\right)2^n - \left(16+9\sqrt{5}\right).$$

(ii)
$$N(PETAA, x) = \sum_{uv\in E(G)} x^{\left[d_G(u)+d_G(v)\right]^{\frac{1}{2}}}$$
$$= 4\times 2^n x^{(1+2)^{\frac{1}{2}}} + \left(4\times 2^n - 2\right)x^{(1+3)^{\frac{1}{2}}} + \left(16\times 2^n - 8\right)x^{(2+2)^{\frac{1}{2}}} + \left(20\times 2^n - 9\right)x^{(2+3)^{\frac{1}{2}}}$$
$$= 4\times 2^n x^{\sqrt{3}} + \left(20\times 2^n - 10\right)x^2 + \left(20\times 2^n - 9\right)x^{\sqrt{5}}.$$

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.

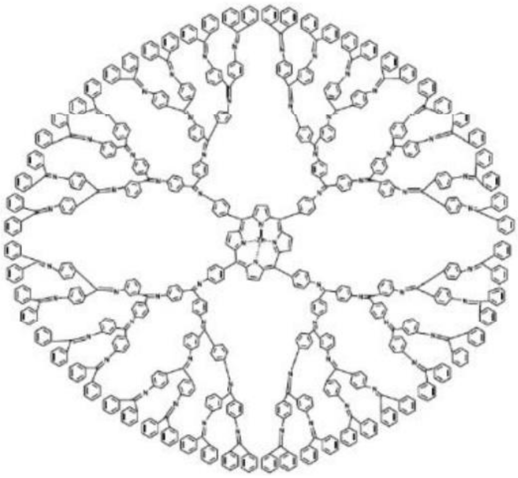

Figure 4. The molecular graph of DPZ_n

Let *G* be the molecular graph of DPZ_n. By calculation, we obtain that *G* has $56\times 2^n - 7$ vertices $64\times 2^n - 4$ edges. In DPZ_n, there are four types of edges based on degrees of end vertices of each edge as given in Table 4.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(2, 2)	(2, 3)	(3, 3)	(3, 4)
Number of edges	$16\times 2^n - 4$	$40\times 2^n - 16$	$8\times 2^n + 12$	4

Table 4. Edge partition of DPZ_n

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

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

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

(i)
$$N\left(DPZ_n\right)=\sum_{uv\in E(G)}\left[d_G(u)+d_G(v)\right]^{\frac{1}{2}}$$
$$=(2+2)^{\frac{1}{2}}\left(16\times 2^n-4\right)+(2+3)^{\frac{1}{2}}\left(40\times 2^n-16\right)+(3+3)^{\frac{1}{2}}\left(8\times 2^n+12\right)+(3+4)^{\frac{1}{2}}4$$
$$=\left(32+40\sqrt{5}+8\sqrt{6}\right)2^n-\left(8+16\sqrt{5}-12\sqrt{6}+4\sqrt{7}\right).$$

(ii)
$$N\left(DPZ_n,x\right)=\sum_{uv\in E(G)}x^{\left[d_G(u)+d_G(v)\right]^{\frac{1}{2}}}$$
$$=\left(16\times 2^n-4\right)^{(2+2)^{\frac{1}{2}}}+\left(40\times 2^n-16\right)x^{(2+3)^{\frac{1}{2}}}+\left(8\times 2^n+12\right)x^{(3+3)^{\frac{1}{2}}}+4x^{(3+4)^{\frac{1}{2}}}.$$
$$=\left(16\times 2^n-4\right)x^2+\left(40\times 2^n-16\right)x^{\sqrt{5}}+\left(8\times 2^n+12\right)x^{\sqrt{6}}+4x^{\sqrt{7}}.$$

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.

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