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Computation of Inverse Nirmala Indices of Certain Nanostructures

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Abstract: Recently, a novel invariant is considered, which is the Nirmala index defined as the sum of the square root of the degrees of the pairs of adjacent vertices. In this paper, we introduce the first and second inverse Nirmala indices of a graph and compute exact formulas for certain nanostructures.

Key Words: Topological index, inverse Nirmala indices, dendrimer.

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§1. 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 molocular 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].

In [15], Kulli introduced the Nirmala index of a graph G and it is defined as

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

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We now define the first and second inverse Nirmala indices of a graph G as

$$IN_1(G) = \sum_{uv\in E(G)} \left[\frac{1}{d_G(u)} + \frac{1}{d_G(v)}\right]^{\frac{1}{2}},$$

$$IN_2(G) = \sum_{uv\in E(G)} \left[\frac{1}{d_G(u)} + \frac{1}{d_G(v)}\right]^{-\frac{1}{2}}.$$

In this study, we compute the first and second inverse Nirmala indices for four families of dendrimers. For dendrimers, see [16].

§2. 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.

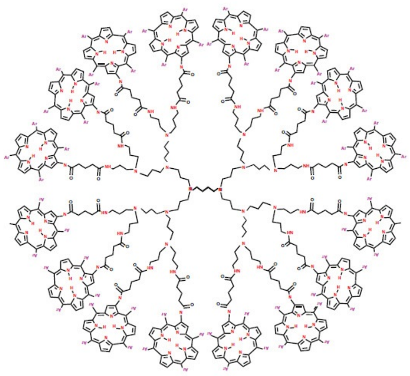

Figure 1. The molecular graph of D_nP_n

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 first and second inverse Nirmala indices of D_nP_n.

Theorem 2.1 *Let D_nP_n be the family of porphyrin dendrimers. Then*

$$IN_1(D_nP_n) = \left(\frac{4}{\sqrt{3}} + 12\sqrt{5} + 10 + 48\frac{\sqrt{5}}{\sqrt{6}} + 13\frac{\sqrt{2}}{\sqrt{3}} + \frac{4\sqrt{7}}{\sqrt{3}}\right)n - 5 - 6\frac{\sqrt{5}}{\sqrt{6}},$$

$$IN_2(D_nP_n) = \left(\sqrt{3} + \frac{48}{\sqrt{5}} + 10 + 48\frac{\sqrt{6}}{\sqrt{5}} + 13\frac{\sqrt{3}}{\sqrt{2}} + \frac{16\sqrt{3}}{\sqrt{7}}\right)n - 5 - 6\frac{\sqrt{6}}{\sqrt{5}}.$$

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

$$\begin{aligned} IN_1(D_nP_n) &= 2n\left[\frac{1}{1}+\frac{1}{3}\right]^{\frac{1}{2}} + 24n\left[\frac{1}{1}+\frac{1}{4}\right]^{\frac{1}{2}} + (10n-5)\left[\frac{1}{2}+\frac{1}{2}\right]^{\frac{1}{2}} \\ &+ (48n-6)\left[\frac{1}{2}+\frac{1}{3}\right]^{\frac{1}{2}} + 13n\left[\frac{1}{3}+\frac{1}{3}\right]^{\frac{1}{2}} + 8n\left[\frac{1}{3}+\frac{1}{4}\right]^{\frac{1}{2}} \\ &= \left(\frac{4}{\sqrt{3}} + 12\sqrt{5} + 10 + 48\frac{\sqrt{5}}{\sqrt{6}} + 13\frac{\sqrt{2}}{\sqrt{3}} + \frac{4\sqrt{7}}{\sqrt{3}}\right)n - 5 - 6\frac{\sqrt{5}}{\sqrt{6}}. \end{aligned}$$

and

$$\begin{aligned} IN_2(D_nP_n) &= 2n\left[\frac{1}{1}+\frac{1}{3}\right]^{-\frac{1}{2}} + 24n\left[\frac{1}{1}+\frac{1}{4}\right]^{-\frac{1}{2}} + (10n-5)\left[\frac{1}{2}+\frac{1}{2}\right]^{-\frac{1}{2}} \\ &+ (48n-6)\left[\frac{1}{2}+\frac{1}{3}\right]^{-\frac{1}{2}} + 13n\left[\frac{1}{3}+\frac{1}{3}\right]^{-\frac{1}{2}} + 8n\left[\frac{1}{3}+\frac{1}{4}\right]^{-\frac{1}{2}} \\ &= \left(\sqrt{3} + \frac{48}{\sqrt{5}} + 10 + 48\frac{\sqrt{6}}{\sqrt{5}} + 13\frac{\sqrt{3}}{\sqrt{2}} + \frac{16\sqrt{3}}{\sqrt{7}}\right)n - 5 - 6\frac{\sqrt{6}}{\sqrt{5}}. \end{aligned}$$ □

§3. 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.

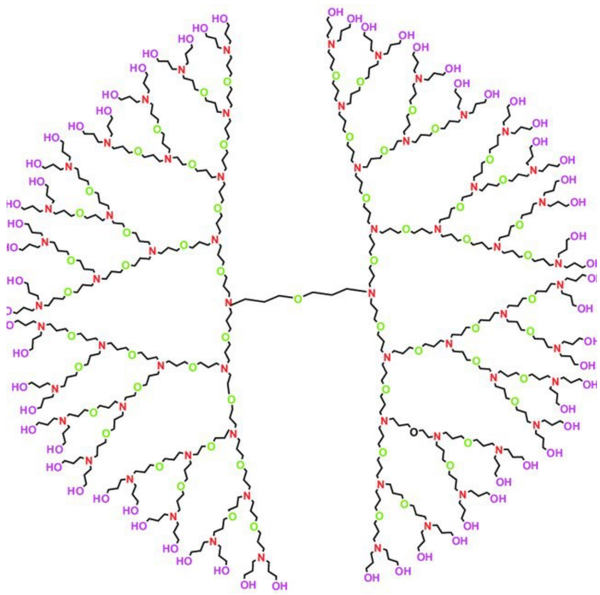

Figure 2. The molecular graph of $PETIM$

Let G be the molecular graph of $PETIM$. By calculation, we find that G has $24 \times 2^n - 23$

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.

$d_G(u), d_G(v) \setminus uv \in E(G)$	$(1,2)$	$(2,2)$	$(2,3)$
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 first and second inverse Nirmala indices of $PETIM$.

Theorem 3.1 *Let $PETIM$ be the family of propyl ether imine dendrimers. Then*

$$IN_1(PETIM) = (\sqrt{6} + 16 + \sqrt{30})2^n - (18 + \sqrt{30}),$$
$$IN_2(PETIM) = \left(\frac{2\sqrt{2}}{\sqrt{3}} + 16 + \frac{6\sqrt{6}}{\sqrt{5}}\right)2^n - \left(18 + \frac{6\sqrt{6}}{\sqrt{5}}\right).$$

Proof From definitions and by using Table 2, we derive

$$IN_1(PETIM) = (2 \times 2^n)\left[\frac{1}{1} + \frac{1}{2}\right]^{\frac{1}{2}} + (16 \times 2^n - 18)\left[\frac{1}{2} + \frac{1}{2}\right]^{\frac{1}{2}} + (6 \times 2^n - 6)\left[\frac{1}{2} + \frac{1}{3}\right]^{\frac{1}{2}}$$
$$= (\sqrt{6} + 16 + \sqrt{30})2^n - (18 + \sqrt{30}),$$
$$IN_2(PETIM) = (2 \times 2^n)\left[\frac{1}{1} + \frac{1}{2}\right]^{-\frac{1}{2}} + (16 \times 2^n - 18)\left[\frac{1}{2} + \frac{1}{2}\right]^{-\frac{1}{2}} + (6 \times 2^n - 6)\left[\frac{1}{2} + \frac{1}{3}\right]^{-\frac{1}{2}}$$
$$= \left(\frac{2\sqrt{2}}{\sqrt{3}} + 16 + \frac{6\sqrt{6}}{\sqrt{5}}\right)2^n - \left(18 + \frac{6\sqrt{6}}{\sqrt{5}}\right). \qquad \square$$

§4. Results for Poly Ethylene Amide 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.

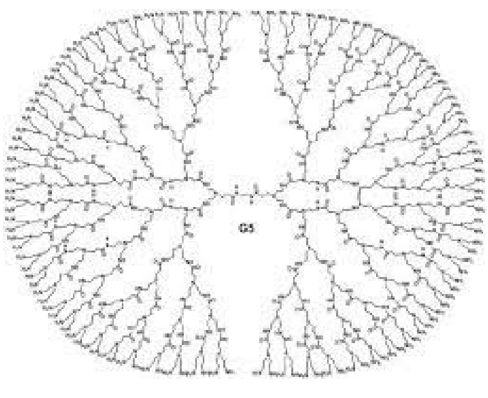

Figure 3. The molecular graph of $PETAA$

Let G be the molecular graph of $PETAA$. By calculation, we find that G has $44 \times 2^n - 18$ vertices and $44 \times 2^n - 19$ edges. In $PETAA$, there are four 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 compute the first and second inverse Nirmala indices of $PETAA$.

Theorem 4.1 *Let* $PETAA$ *be the family of poly ethylene amide amine dendrimers. Then*

$$\begin{aligned} IN_1(PETAA) &= \left(\frac{4\sqrt{3}}{\sqrt{2}} + \frac{8}{\sqrt{3}} + 16 + \frac{20\sqrt{5}}{\sqrt{6}}\right)2^n - \left(\frac{4}{\sqrt{3}} + 8 + \frac{9\sqrt{5}}{\sqrt{6}}\right), \\ IN_2(PETAA) &= \left(\frac{4\sqrt{2}}{\sqrt{3}} + 2\sqrt{3} + 16 + \frac{20\sqrt{6}}{\sqrt{5}}\right)2^n - \left(\sqrt{3} + 8 + \frac{9\sqrt{6}}{\sqrt{5}}\right). \end{aligned}$$

Proof By using definitions and Table 3, we obtain

$$\begin{aligned} IN_1(PETAA) = {} & (4 \times 2^n)\left[\frac{1}{1} + \frac{1}{2}\right]^{\frac{1}{2}} + (4 \times 2^n - 2)\left[\frac{1}{1} + \frac{1}{3}\right]^{\frac{1}{2}} + (16 \times 2^n - 8)\left[\frac{1}{2} + \frac{1}{2}\right]^{\frac{1}{2}} \\ & + (20 \times 2^n - 9)\left[\frac{1}{2} + \frac{1}{3}\right]^{\frac{1}{2}} \\ = {} & \left(\frac{4\sqrt{3}}{\sqrt{2}} + \frac{8}{\sqrt{3}} + 16 + \frac{20\sqrt{5}}{\sqrt{6}}\right)2^n - \left(\frac{4}{\sqrt{3}} + 8 + \frac{9\sqrt{5}}{\sqrt{6}}\right). \end{aligned}$$

and

$$\begin{aligned} IN_2(PETAA) = {} & (4 \times 2^n)\left[\frac{1}{1} + \frac{1}{2}\right]^{-\frac{1}{2}} + (4 \times 2^n - 2)\left[\frac{1}{1} + \frac{1}{3}\right]^{-\frac{1}{2}} + (16 \times 2^n - 8)\left[\frac{1}{2} + \frac{1}{2}\right]^{-\frac{1}{2}} \\ & + (20 \times 2^n - 9)\left[\frac{1}{2} + \frac{1}{3}\right]^{-\frac{1}{2}} \\ = {} & \left(\frac{4\sqrt{2}}{\sqrt{3}} + 2\sqrt{3} + 16 + \frac{20\sqrt{6}}{\sqrt{5}}\right)2^n - \left(\sqrt{3} + 8 + \frac{9\sqrt{6}}{\sqrt{5}}\right). \qquad \square \end{aligned}$$

§5. 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.

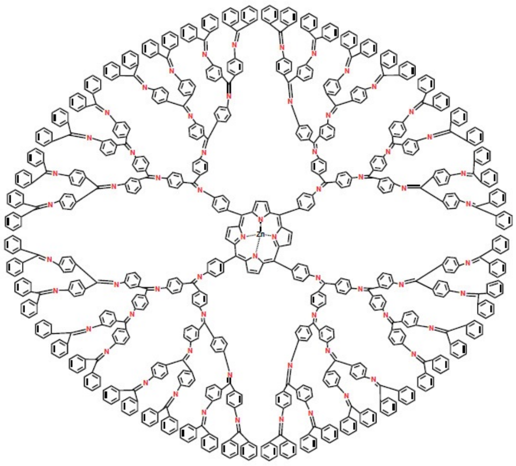

Figure 4. The molecular graph of DPZ_n

Let G be the molecular graph of DPZ_n. By calculation, we obtain that G has $56 \times 2^n - 7$ vertices and $64 \times 2^n - 4$ 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 5.1 *Let DPZ_n be the family of zinc prophyrin dendrimers. Then*

$$IN_1(DPZ_n) = \left(16 + \frac{40\sqrt{5}}{\sqrt{6}} + \frac{8\sqrt{2}}{\sqrt{3}}\right)2^n - \left(4 + \frac{16\sqrt{5}}{\sqrt{6}} + \frac{12\sqrt{2}}{\sqrt{3}} - \frac{2\sqrt{7}}{\sqrt{3}}\right),$$
$$IN_2(DPZ_n) = \left(16 + \frac{40\sqrt{6}}{\sqrt{5}} + \frac{8\sqrt{3}}{\sqrt{2}}\right)2^n - \left(4 + \frac{16\sqrt{6}}{\sqrt{5}} - \frac{12\sqrt{3}}{\sqrt{2}} - \frac{8\sqrt{3}}{\sqrt{7}}\right).$$

Proof From definitions and by using Table 4, we deduce

$$IN_1(DPZ_n) = (16 \times 2^n - 4)\left[\frac{1}{2} + \frac{1}{2}\right]^{\frac{1}{2}} + (40 \times 2^n - 16)\left[\frac{1}{2} + \frac{1}{3}\right]^{\frac{1}{3}}$$
$$+ (8 \times 2^n + 12)\left[\frac{1}{3} + \frac{1}{3}\right]^{\frac{1}{2}} + 4\left[\frac{1}{3} + \frac{1}{4}\right]^{\frac{1}{2}}$$
$$= \left(16 + \frac{40\sqrt{5}}{\sqrt{6}} + \frac{8\sqrt{2}}{\sqrt{3}}\right)2^n - \left(4 + \frac{16\sqrt{5}}{\sqrt{6}} + \frac{12\sqrt{2}}{\sqrt{3}} - \frac{2\sqrt{7}}{\sqrt{3}}\right).$$

and

$$\begin{aligned}IN_2(DPZ_n) &= (16\times 2^n-4)\left[\frac{1}{2}+\frac{1}{2}\right]^{-\frac{1}{2}}+(40\times 2^n-16)\left[\frac{1}{2}+\frac{1}{3}\right]^{-\frac{1}{3}}\\ &+(8\times 2^n+12)\left[\frac{1}{3}+\frac{1}{3}\right]^{-\frac{1}{2}}+4\left[\frac{1}{3}+\frac{1}{4}\right]^{-\frac{1}{2}}\\ &=\left(16+\frac{40\sqrt{6}}{\sqrt{5}}+\frac{8\sqrt{3}}{\sqrt{2}}\right)2^n-\left(4+\frac{16\sqrt{6}}{\sqrt{5}}-\frac{12\sqrt{3}}{\sqrt{2}}-\frac{8\sqrt{3}}{\sqrt{7}}\right).\end{aligned}$$ □

§6. Conclusion

In this study, we have defined the first and second inverse Nirmala indices of a molecular graph. Furthermore, the first and second inverse Nirmala indices for certain dendrimers are computed.

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