Banhatti Nirmala and Modified Banhatti Nirmala Indices of Certain Dendrimers

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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 Banhatti Nirmala index of a graph. We initiate a study of the Banhatti Nirmala index.**

***Index Terms*—dendrimer, modified Banhatti Nirmala index, Banhatti Nirmala index.**

I. INTRODUCTION

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 [1, 2, 3].

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

The Nirmala index [5] of a molecular graph G is defined as

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

Recently, some Nirmala indices were studied in [6, 7, 8, 9 10].

Motivated by Nirmala index, we introduce the Banhatti Nirmala index of a graph G as follows:

The Banhatti Nirmala index of a graph G is defined as

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

We define the modified Banhatti Nirmala index of a graph G as

$$^{m}BN(G)=\sum_{uv\in E(G)}\frac{d_G(u)d_G(v)}{\sqrt{d_G(u)+d_G(v)}}.$$

In this study, we compute the Banhatti Nirmala and modified Banhatti Nirmala indices of four families of dendrimers.

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.

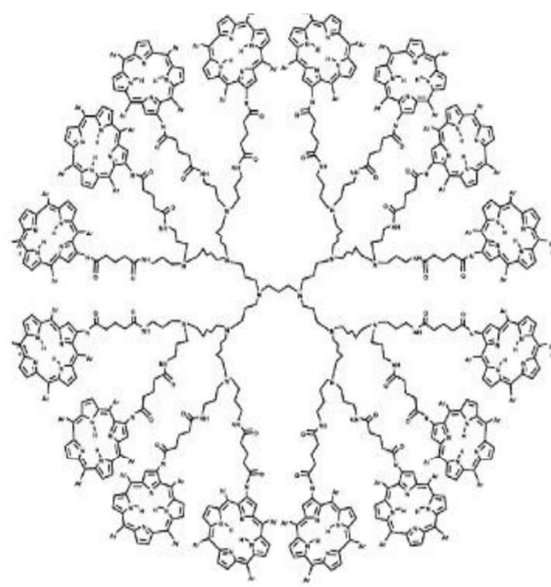

Figure 1. The molecular graph of D_nP_n

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.

dG(u), dG(v)\ uv □ E(G)	Number of edges
(1, 3)	2n
(1, 4)	24n
(2, 2)	10n − 5
(2, 3)	48n − 6

Table 1. Edge partition of D_nP_n

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

$$BN(G)=\left(\frac{19}{3}+14\sqrt{5}+\frac{13\sqrt{6}}{9}+\frac{2\sqrt{7}}{3}\right)n-\frac{5}{2}-\sqrt{5}.$$

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

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

$$=2n\frac{\sqrt{1+3}}{1\times 3}+24n\frac{\sqrt{1+4}}{1\times 4}$$

$$+(10n-5)\frac{\sqrt{2+2}}{2\times 2}+(48n-6)\frac{\sqrt{2+3}}{2\times 3}$$

$$+13n\frac{\sqrt{3+3}}{3\times 3}+8n\frac{\sqrt{3+4}}{3\times 4}$$

$$=\left(\frac{19}{3}+14\sqrt{5}+\frac{13\sqrt{6}}{9}+\frac{2\sqrt{7}}{3}\right)n-\frac{5}{2}-\sqrt{5}.$$

Theorem 2. Let D_nP_n be the family of porphyrin dendrimers. Then

$$^{m}BN(G)=\left(23+\frac{144}{\sqrt{5}}+\frac{117}{\sqrt{6}}+\frac{96}{\sqrt{7}}\right)n-10-\frac{36}{\sqrt{5}}.$$

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

$$^{m}BN(G)=\sum_{uv\in E(G)}\frac{d_G(u)d_G(v)}{\sqrt{d_G(u)+d_G(v)}}$$

$$=2n\frac{1\times 3}{\sqrt{1+3}}+24n\frac{1\times 4}{\sqrt{1+4}}$$

$$+(10n-5)\frac{2\times 2}{\sqrt{2+2}}+(48n-6)\frac{2\times 3}{\sqrt{2+3}}$$

$$=\left(23+\frac{144}{\sqrt{5}}+\frac{117}{\sqrt{6}}+\frac{96}{\sqrt{7}}\right)n-10-\frac{36}{\sqrt{5}}.$$

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.

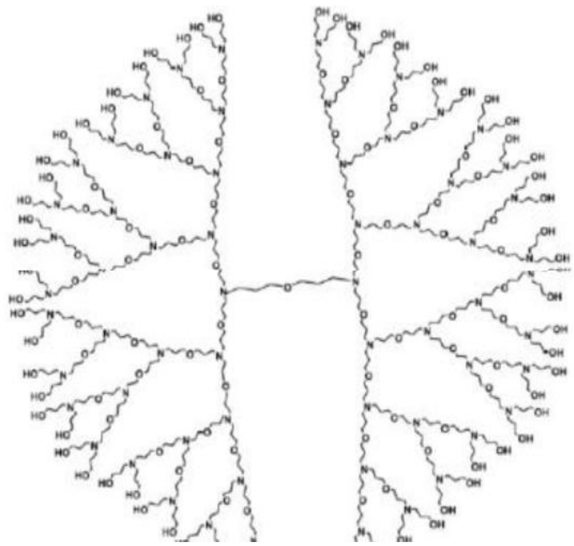

Figure 2. The molecular graph of PETIM

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

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

Table 2. Edge partition of PETIM

Theorem 3. Let PETIM be the family of propyl ether imine dendrimers. Then

$$BN(G)=\left(\sqrt{3}+8+\sqrt{5}\right)2^n-9-\sqrt{5}.$$

Proof: From definition and by using Table 2, we deduce

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

$$=2\times 2^n\frac{\sqrt{1+2}}{1\times 2}+\left(16\times 2^n-18\right)\frac{\sqrt{2+2}}{2\times 2}$$

$$+\left(6\times 2^n-6\right)\frac{\sqrt{2+3}}{2\times 3}$$
$$=\left(\sqrt{3}+8+\sqrt{5}\right)2^n-9-\sqrt{5}.$$

Theorem 4. Let PETIM be the family of propyl ether imine dendrimers. Then

$$^{m}BN(G)=\left(\frac{4}{\sqrt{3}}+32+\frac{36}{\sqrt{5}}\right)2^n-36-\frac{36}{\sqrt{5}}.$$

Proof: From definition and by using Table 2, we deduce

$$^{m}BN(G)=\sum_{uv\in E(G)}\frac{d_G(u)d_G(v)}{\sqrt{d_G(u)+d_G(v)}}$$
$$=2\times 2^n\frac{1\times 2}{\sqrt{1+2}}+\left(16\times 2^n-18\right)\frac{2\times 2}{\sqrt{2+2}}$$
$$+\left(6\times 2^n-6\right)\frac{2\times 3}{\sqrt{2+3}}$$
$$=\left(\frac{4}{\sqrt{3}}+32+\frac{36}{\sqrt{5}}\right)2^n-36-\frac{36}{\sqrt{5}}.$$

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.

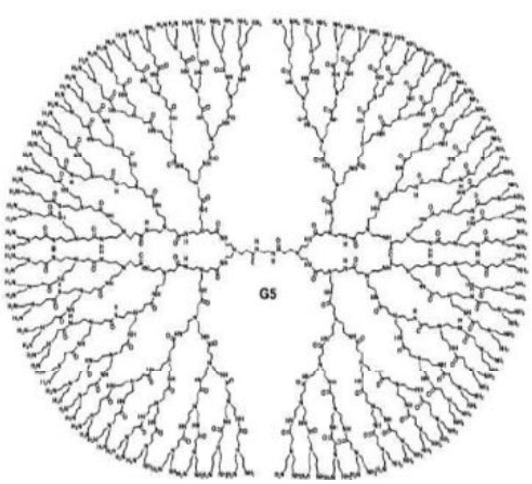

Figure 3. The molecular graph of PETAA

Let G be the molecular graph of PETAA. By calculation, we find that G has $44\times 2^n - 18$ vertices and $44\times 2^n - 19$ edges. In PETAA, there are three types of edges based on degrees of end vertices of each edge as given in Table 3.

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

Table 3. Edge partition of PETAA

Theorem 5. Let PETAA be the family of poly ethylene amide amine dendrimers. Then

$$BN(G)=\left(2\sqrt{3}+14\right)2^n-\frac{16}{3}-\frac{3\sqrt{5}}{2}.$$

Proof: From definition and by using Table 3, we deduce

$$BN(G)=\sum_{uv\in E(G)}\frac{\sqrt{d_G(u)+d_G(v)}}{d_G(u)d_G(v)}$$
$$=4\times 2^n\frac{\sqrt{1+2}}{1\times 2}+\left(4\times 2^n-2\right)\frac{\sqrt{1+3}}{1\times 3}$$
$$+\left(16\times 2^n-8\right)\frac{\sqrt{2+2}}{2\times 2}+\left(20\times 2^n-9\right)\frac{\sqrt{2+3}}{2\times 3}$$
$$=\left(2\sqrt{3}+14\right)2^n-\frac{16}{3}-\frac{3\sqrt{5}}{2}.$$

Theorem 6. Let PETAA be the family of poly ethylene amide amine dendrimers. Then

$$^{m}BN(G)=\left(\frac{8\sqrt{5}}{\sqrt{3}}+38+\frac{20}{\sqrt{5}}\right)2^n-19-\frac{54}{\sqrt{5}}.$$

Proof: From definition and by using Table 3, we deduce

$$^{m}BN(G)=\sum_{uv\in E(G)}\frac{d_G(u)d_G(v)}{\sqrt{d_G(u)+d_G(v)}}$$

$$= 4\times 2^n \frac{1\times 2}{\sqrt{1+2}} + (4\times 2^n - 2)\frac{1\times 3}{\sqrt{1+3}}$$

$$+(16\times 2^n - 8)\frac{2\times 2}{\sqrt{2+2}} + (20\times 2^n - 9)\frac{2\times 3}{\sqrt{2+3}}$$

$$= \left(\frac{8\sqrt{5}}{\sqrt{3}} + 38 + \frac{20}{\sqrt{5}}\right)2^n - 19 - \frac{54}{\sqrt{5}}.$$

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.

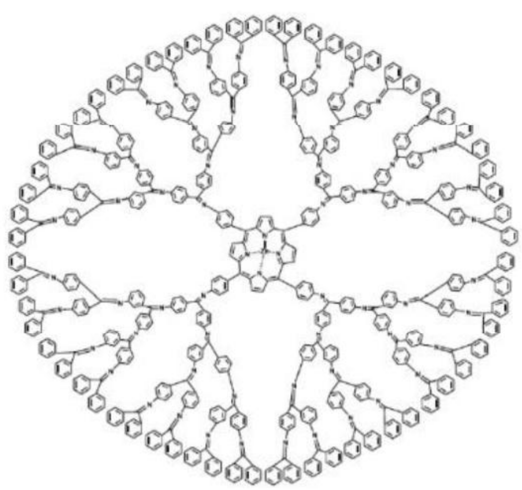

Figure 4. The molecular graph of DPZ_n

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.

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

Table 4. Edge partition of DPZ_n

Theorem 7. Let DPZ_n be the family of zinc prophyrin dendrimers. Then

$$BN(G) = \left(\frac{80}{9} + \frac{20\sqrt{5}}{3}\right)2^n - 2 - \frac{8\sqrt{5}}{3} + \frac{4\sqrt{6}}{3} + \frac{\sqrt{7}}{3}.$$

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

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

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

$$+(8\times 2^n + 12)\frac{\sqrt{3+3}}{3\times 3} + 4\frac{\sqrt{3+4}}{3\times 4}$$

$$= \left(\frac{80}{9} + \frac{20\sqrt{5}}{3}\right)2^n - 2 - \frac{8\sqrt{5}}{3} + \frac{4\sqrt{6}}{3} + \frac{\sqrt{7}}{3}.$$

Theorem 8. Let DPZ_n be the family of zinc prophyrin dendrimers. Then

$${}^{m}BN(G) = \left(32 + \frac{240}{\sqrt{5}} + \frac{72}{\sqrt{6}}\right)2^n - 8 - \frac{96}{\sqrt{5}} + \frac{108}{\sqrt{6}} + \frac{48}{\sqrt{7}}.$$

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

$${}^{m}BN(G) = \sum_{uv\in E(G)} \frac{d_G(u)d_G(v)}{\sqrt{d_G(u)+d_G(v)}}$$

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

$$+(8\times 2^n + 12)\frac{3\times 3}{\sqrt{3+3}} + 4\frac{3\times 4}{\sqrt{3+4}}$$

$$= \left(32 + \frac{240}{\sqrt{5}} + \frac{72}{\sqrt{6}}\right)2^n - 8 - \frac{96}{\sqrt{5}} + \frac{108}{\sqrt{6}} + \frac{48}{\sqrt{7}}.$$

VI. CONCLUSION

In this study, the Banhatti Nirmala and modified Banhatti Nirmala indices of four families of dendrimers are determined.

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