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NEIGHBORHOOD NIRMALA INDEX AND IT'S EXPONENTIAL OF NANOCONES AND DENDRIMERS

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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 sum of the degrees of the pairs of adjacent vertices. In this paper, we introduce some new Nirmala indices: the second, third, fourth and neighborhood (or fifth) Nirmala indices of a graph. Furthermore, we compute the neighborhood Nirmala index and its exponential for certain important chemical structures such as nanocones and dendrimers.

KEYWORDS: *Nirmala index, neighborhood Nirmala index, nanocone, dendrimer.*
Mathematics Subject Classification: *05C05, 05C12, 05C90.*

1. INTRODUCTION
Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex u is the number of vertices adjacent to u and it is denoted by $d_G(u)$. Let $S_G(u)$ denote the sum of the degrees of all vertices adjacent to a vertex u. For undefined term and notation, we refer the book [1].

A molecular graph is a graph such that its vertices represent to the atoms and the edges to the bonds. Chemical Graph Theory is a branch of Mathematical Chemistry whose focus of interest is finding topological indices of a molecular graph which correlate well with chemical properties of the chemical molecules, see [2].

In [3], Kulli introduced the Nirmala index of a graph and defined it as

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

Recently, some Nirmala indices were studied, for example, in [4, 5, 6, 7].

Motivated by the previous research in Nirmala index and its applications, we now introduce the second, third and fourth Nirmala indices of the molecular graph as follows:

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

$$N_2(G) = \sum_{uv \in E(G)} \sqrt{n_u + n_v}$$

where the number n_u of vertices of G lying closer to the vertex u than to the vertex v for the edge uv of a graph G.

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

$$N_3(G) = \sum_{uv \in E(G)} \sqrt{m_u + m_v}$$

where the number m_u of edges of G lying closer to the vertex u than to the vertex v for the edge uv of a graph G.

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Impact Factor: 5.164
CODEN: IJESS7

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

$$N_4(G) = \sum_{uv \in E(G)} \sqrt{\varepsilon(u) + \varepsilon(v)}$$

where the number ε(u) is the eccentricity of vertex u.

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

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

Considering the neighborhood Nirmala index, we introduce the neighborhood Nirmala exponential of a graph G and defined it as

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

Recently, some neighborhood indices were studied, for example, in [8, 9, 10, 11, 12,13, 14, 15, 16, 17, 18, 19]. In this study, we compute the neighborhood Nirmala index, the neighborhood Nirmala exponential of some important nanostructures which appeared in nanoscience. For nanocones and dendrimers, see [20, 21].

2. RESULTS FOR NANOCONES $C_n[k]$

In this section, we consider nanocones $C_n[k]$. The molecular structure of $C_4[2]$ is shown in Figure 1.

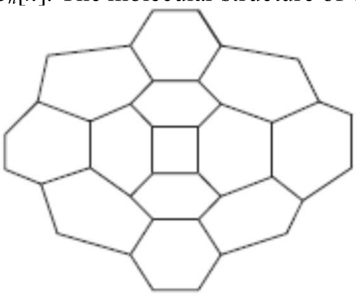

Figure 1. The molecular structure of $C_4[2]$

Let G be the molecular structure of $C_n[k]$. By calculation, G has $n(k+1)^2$ vertices and $\frac{n}{2}(k+1)(3k+2)$ edges. Also by calculation, we obtain that G has five types of edges based on $S_G(u)$ and $S_G(v)$ the degrees of end vertices of each edge as given in Table 1.

Table 1 . Edge partition of $C_n[k]$ based on $S_G(u)$, $S_G(v)$

$S_G(u), S_G(v) \setminus uv \in E(G)$	Number of edges
(5, 5)	n
(5, 7)	$2n$
(6, 7)	$2(k-1)n$
(7, 9)	nk
(9, 9)	$\frac{nk}{2}(3k-1)$

In the following theorem, we compute the neighborhood Nirmala index and its exponential of $C_n[k]$.

ISSN: 2277-9655
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CODEN: IJESS7

Theorem 1. Let $C_n[k]$ be the family of nanocones. Then

(i) $NN(G) = \frac{9}{\sqrt{2}}nk^2 - \left(\frac{3}{\sqrt{2}} - 2\sqrt{13} - 4\right)nk + \left(\sqrt{10} + 4\sqrt{3} - 2\sqrt{13}\right)n.$

(ii) $NN(G,x) = nx^{\sqrt{10}} + 2nx^{2\sqrt{3}} + 2(k-1)nx^{\sqrt{13}} + nkx^4 + \frac{nk}{2}(3k-1)x^{3\sqrt{2}}.$

Proof: Let G be the molecular graph of $C_n[k]$. By using the definitions and Table 1, we deduce

(i) $$NN(G) = \sum_{uv \in E(G)} \sqrt{S_G(u) + S_G(v)}$$

$$= (5+5)^{\frac{1}{2}}n + (5+7)^{\frac{1}{2}}2n + (6+7)^{\frac{1}{2}}2(k-1)n + (7+9)^{\frac{1}{2}}nk + (9+9)^{\frac{1}{2}}\frac{nk}{2}(3k-1).$$

After simplification, we get the desired result.

(ii) $$NN(G,x) = \sum_{uv \in E(G)} x^{\sqrt{S_G(u)+S_G(v)}}$$

$$= nx^{(5+5)^{\frac{1}{2}}} + 2nx^{(5+7)^{\frac{1}{2}}} + 2(k-1)nx^{(6+7)^{\frac{1}{2}}} + nkx^{(7+9)^{\frac{1}{2}}} + \frac{nk}{2}(3k-1)x^{(9+9)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

3. RESULTS FOR $NS_2[n]$ DENDRIMERS

In this section, we focus on the class of $NS_2[n]$ dendrimers with $n \geq 1$. The graph of $NS_2[3]$ is shown in Figure 2.

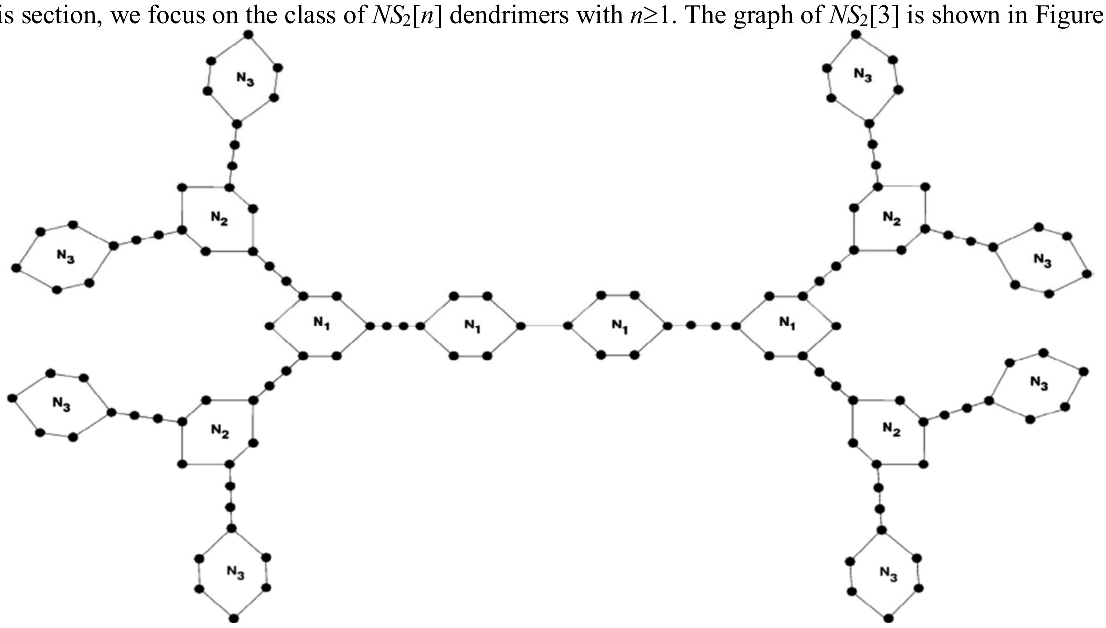

Figure 2 . The graph of $NS_2[3]$

Let G be the graph of $NS_2[n]$. By calculation, G has $16 \times 2^n - 4$ vertices and $18 \times 2^n - 5$ edges. Also by calculation, we obtain that G has seven types of edges based on $S_G(u)$, $S_G(v)$ the degrees of end vertices of each edge as given in Table 2.

ISSN: 2277-9655
Impact Factor: 5.164
CODEN: IJESS7

Table 2. Edge partition of $NS_2[n]$ based on $S_G(u)$ and $S_G(v)$

$S_G(u), S_G(v) \setminus uv \in E(G)$	(4, 4)	(5, 4)	(5, 5)	(5, 6)	(7, 7)	(5, 7)	(6, 6)
Number of edges	2×2^n	2×2^n	$2\times2^n+2$	6×2^n	1	4	$6\times2^n-12$

In the following theorem, we compute the neighborhood Nirmala index and its exponential of $NS_2[n]$.

Theorem 2. Let $NS_2[n]$ be the family of dendrimers. Then

(i) $NN(G) = \left(4\sqrt{2}+6+2\sqrt{10}+6\sqrt{11}+12\sqrt{3}\right)2^n + 2\sqrt{10}+\sqrt{14}-40\sqrt{3}.$

(ii) $NN(G,x) = 2\times2^n x^{2\sqrt{2}} + 2\times2^n x^3 + (2\times2^n+2)x^{\sqrt{10}} + 6\times2^n x^{\sqrt{11}} + x^{\sqrt{14}} + (6\times2^n-8)x^{2\sqrt{3}}.$

Proof: Let G be the molecular graph of $NS_2[n]$. By using the definitions and Table 2, we deduce

(i) $$NN(G) = \sum_{uv\in E(G)} \sqrt{S_G(u)+S_G(v)}$$

$$= (4+4)^{\frac{1}{2}}\,2\times2^n + (5+4)^{\frac{1}{2}}\,2\times2^n + (5+5)^{\frac{1}{2}}(2\times2^n+2) + (5+6)^{\frac{1}{2}}\,6\times2^n + (7+7)^{\frac{1}{2}}$$

$$+(5+7)^{\frac{1}{2}}\,4 + (6+6)^{\frac{1}{2}}(6\times2^n-12).$$

After simplification, we obtain the desired result.

(ii) $$NN(G,x) = \sum_{uv\in E(G)} x^{\sqrt{S_G(u)+S_G(v)}}$$

$$= 2\times2^n x^{(4+4)^{\frac{1}{2}}} + 2\times2^n x^{(5+4)^{\frac{1}{2}}} + (2\times2^n+2)x^{(5+5)^{\frac{1}{2}}} + 6\times2^n x^{(5+6)^{\frac{1}{2}}} + x^{(7+7)^{\frac{1}{2}}} + 4x^{(5+7)^{\frac{1}{2}}} + (6\times2^n-12)x^{(6+6)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

4. RESULTS FOR $NS_3[n]$ DENDRIMERS

In this section, we focus on another type of dendrimers $NS_3[n]$ with $n\geq1$. The molecular structure of $NS_3[2]$ is presented in Figure 3.

Let G be the molecular graph of $NS_3[n]$. By calculation, we obtain that G has $18\times2^n - 12$ vertices and $21\times2^n - 15$ edges. Also by calculation, we get that G has five types of edges based on $S_G(u)$ and $S_G(v)$ the degrees of end vertices of each edge as given in Table 3.

Table 3. Edge partition of $NS_3[n]$ based on $S_G(u)$ and $S_G(v)$

$S_G(u), S_G(v) \setminus uv \in E(G)$	(4, 4)	(5, 4)	(5, 7)	(6, 7)	(7, 7)
Number of edges	3×2^n	3×2^n	3×2^n	$9\times2^n-12$	$3\times2^n-3$

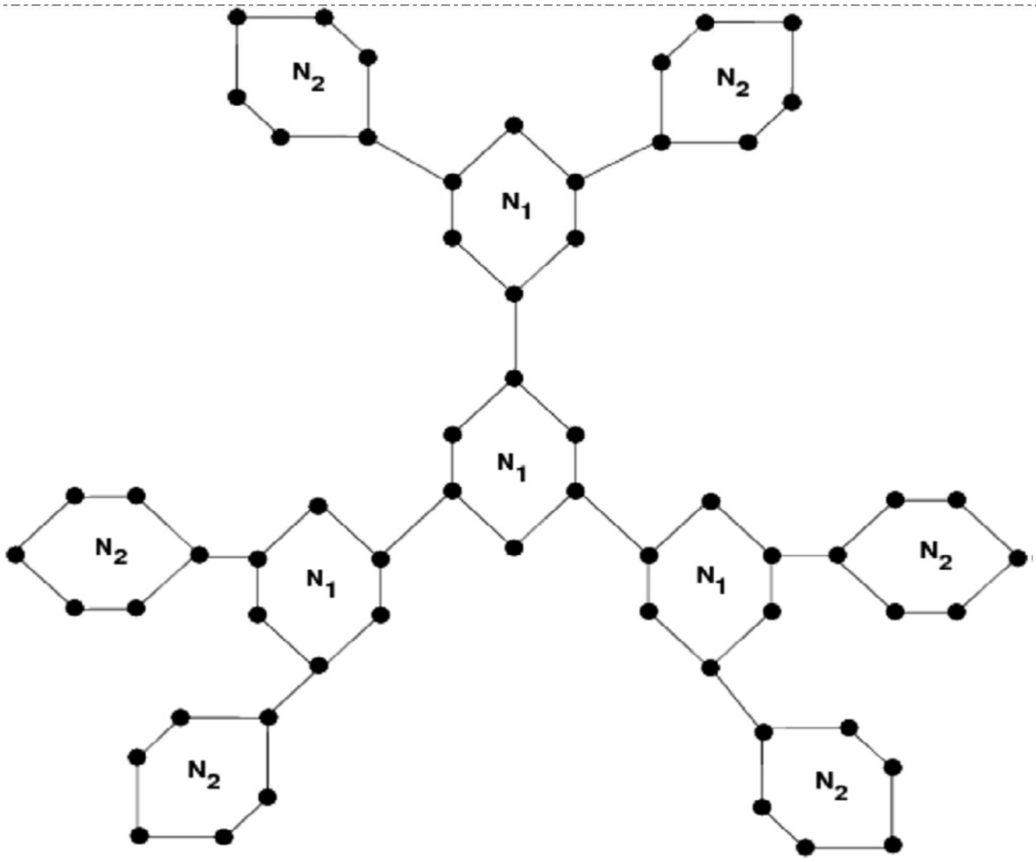

Figure 3. The structure of NS3[2]

In the following theorem, we compute the neighborhood Nirmala index and its exponential of $NS_3[n]$.

Theorem 3. Let $NS_3[n]$ be the family of dendrimers. Then

(i) $NN(G)=\left(6\sqrt{2}+9+6\sqrt{3}+9\sqrt{13}+3\sqrt{14}\right)2^n-12\sqrt{13}-3\sqrt{14}.$

(ii) $NN(G,x)=3\times 2^n x^{2\sqrt{2}}+3\times 2^n x^3+3\times 2^n x^{2\sqrt{3}}+(9\times 2^n-12)x^{\sqrt{13}}+(3\times 2^n-3)x^{\sqrt{14}}.$

Proof: Let G be the molecular graph of $NS_3[n]$. By using definitions and Table 3, we deduce

(i) $$NN(G)=\sum_{uv\in E(G)}\sqrt{S_G(u)+S_G(v)}$$

$$=(4+4)^{\frac{1}{2}}3\times 2^n+(4+5)^{\frac{1}{2}}3\times 2^n+(5+7)^{\frac{1}{2}}3\times 2^n+(6+7)^{\frac{1}{2}}(9\times 2^n-12)+(7+7)^{\frac{1}{2}}(3\times 2^n-3).$$

After simplification, we obtain the desired result.

(ii) $$NN(G,x)=\sum_{uv\in E(G)}x^{\sqrt{S_G(u)+S_G(v)}}$$

$$=3\times 2^n x^{(4+4)^{\frac{1}{2}}}+3\times 2^n x^{(4+5)^{\frac{1}{2}}}+3\times 2^n x^{(5+7)^{\frac{1}{2}}}+(9\times 2^n-12)x^{(6+7)^{\frac{1}{2}}}+(3\times 2^n-3)x^{(7+7)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

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5. RESULYS FOR PAMAM DENDRIMER $PD_1[n]$

We consider the PAMAM dendrimers with n growth stages, denoted by $PD_1[n]$ for every $n \geq 0$, see Figure 4.

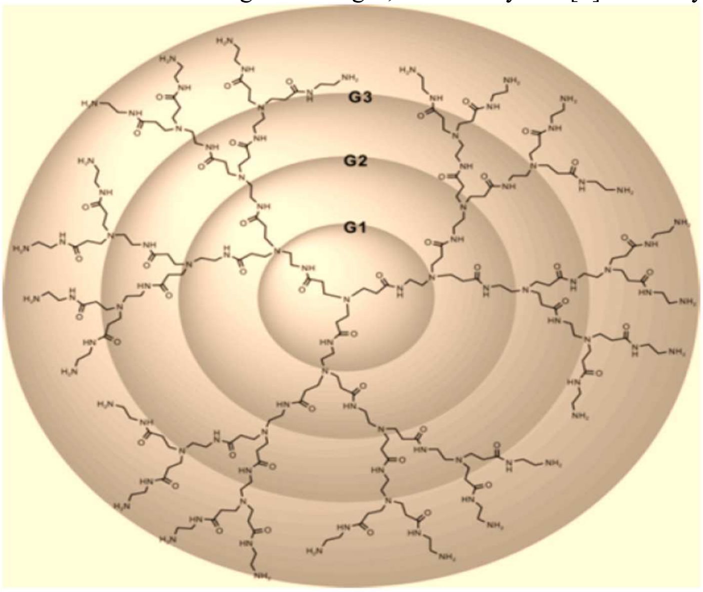

Figure 4. PAMAM dendrimer $PD_1[n]$

Let G be the graph of PAMAM dendrimer $PD_1[n]$. By calculation, we see that G has $12\times2^{n+2} - 23$ vertices and $12\times2^{n+2} - 24$ edges. Also the edge partition of the form (2,3), (3,4), (3,5), (4,5), (5,5), (5,6) for PAMAM dendrimer $PD_1[n]$ based on the degree sum of neighbors of end vertices of each edge is obtained, as given in Table 4.

Table 4. Edge partition of $PD_1[n]$ based on $S_G(u)$ and $S_G(v)$

$S_G(u)\ S_G(v) \backslash\ uv \in E(G)$	(2, 3)	(3,4)	(3, 5)	(4, 5)	(5, 5)	(5, 6)
Number of edges	3×2^n	3×2^n	$6\times2^n - 3$	$9\times2^n - 6$	$18\times2^n - 9$	$9\times2^n - 6$

In the following theorem, we compute the neighborhood Nirmala index and its exponential of $PD_1[n]$.

Theorem 4. Let $PD_1[n]$ be the family of PAMAM dendrimers. Then

(i) $NN(G) = \left(3\sqrt{5} + 3\sqrt{7} + 12\sqrt{2} + 27 + 18\sqrt{10} + 9\sqrt{11}\right)2^n - (6\sqrt{2} + 18 + 9\sqrt{10} + 6\sqrt{11}).$

(ii) $NN(G,x) = 3\times2^n x^{\sqrt{5}} + 3\times2^n x^{\sqrt{7}} + (6\times2^n - 3)x^{2\sqrt{2}} + (9\times2^n - 6)x^3 + (18\times2^n - 9)x^{\sqrt{10}} + (9\times2^n - 6)x^{\sqrt{11}}.$

Proof: Let G be the molecular graph of $PD_1[n]$. By using the definitions and Table 4, we deduce

(i) $$NN(G) = \sum_{uv \in E(G)} \sqrt{S_G(u) + S_G(v)}$$

$$= (2+3)^{\frac{1}{2}} 3\times2^n + (3+4)^{\frac{1}{2}} 3\times2^n + (3+5)^{\frac{1}{2}} (6\times2^n - 3) + (4+5)^{\frac{1}{2}} (9\times2^n - 6)$$

$$+ (5+5)^{\frac{1}{2}} (18\times2^n - 9) + (5+6)^{\frac{1}{2}} (9\times2^n - 6).$$

After simplification, we obtain the desired result.

ISSN: 2277-9655
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(ii) $NN(G,x)=\sum_{uv\in E(G)} x^{\sqrt{S_G(u)+S_G(v)}}$

$$=3\times 2^n x^{(2+3)^{\frac{1}{2}}}+3\times 2^n x^{(3+4)^{\frac{1}{2}}}+(6\times 2^n-3)x^{(3+5)^{\frac{1}{2}}}+(9\times 2^n-6)x^{(4+5)^{\frac{1}{2}}}+(18\times 2^n-9)x^{(5+5)^{\frac{1}{2}}}+(9\times 2^n-6)x^{(5+6)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

6. RESULTS FOR TETRATHIAFULVALENE DENDRIMERS $TD_2[n]$

In this section, we focus on the molecular graph of a tetrathiafulvalene dendrimer. This family of tetrathiafulvalene dendrimers is denoted by $TD_2[n]$, where n is the steps of growth in this type of dendrimers for $n\geq 0$. The molecular graph of $TD_2[2]$ is shown in Figure 5.

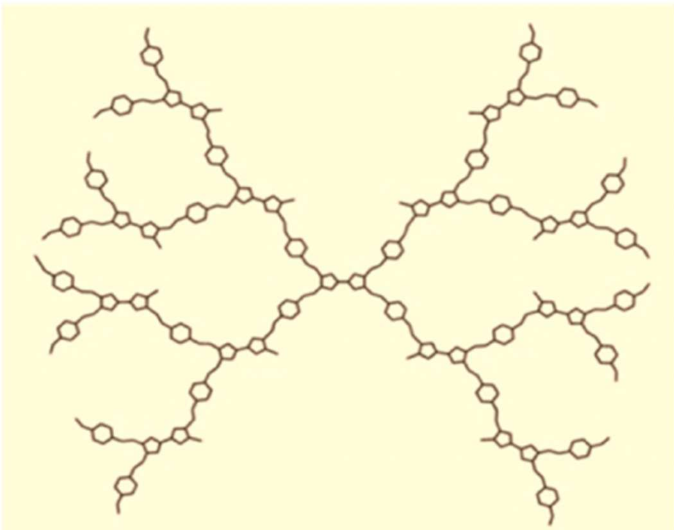

Figure 5. The molecular graph of $TD_2[2]$

Let G be the molecular graph of tetrathiafulvalene dendrimers $TD_2[n]$. By algebraic method, we obtain that $|V(G)|=31\times 2^{n+2}-74$ and $|E(G)|=35\times 2^{n+2}-85$. Also the edge partition of $TD_2[n]$ based on the degree sum of neighbors of end vertices of each edge is obtained as given in Table 5.

Table 5. Edge partition of $TD_2[n]$ based on $S_G(u)$ and $S_G(v)$

$S_G(u), S_G(v)\backslash uv\in E(G)$	Number of edges
(2, 4)	2^{n+2}
(3, 6)	$2^{n+2}-4$
(4, 6)	2^{n+2}
(5, 5)	$7\times 2^{n+2}-16$
(5, 6)	$11\times 2^{n+2}-24$
(5, 7)	$3\times 2^{n+2}-8$
(6, 6)	$2^{n+2}-4$
(6, 7)	$8\times 2^{n+2}-24$
(7, 7)	$2\times 2^{n+2}-5$

In the following theorem, we compute the neighborhood Nirmala index and its exponential of $TD_2[n]$.

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Impact Factor: 5.164
CODEN: IJESS7

Theorem 5. Let $TD_2[n]$ be the family of dendrimers. Then

(i) $NN(G) = \left(\sqrt{6} + 3 + 8\sqrt{10} + 11\sqrt{11} + 8\sqrt{3} + 8\sqrt{13} + 2\sqrt{14}\right)2^{n+2}$
$-(12 + 16\sqrt{10} + 24\sqrt{11} + 24\sqrt{3} + 24\sqrt{13} + 5\sqrt{14}).$

(ii) $NN(G,x) = 2^{n+2}x^{\sqrt{6}} + (2^{n+2} - 4)x^3 + (8\times 2^{n+2} - 16)x^{\sqrt{10}} + (11\times 2^{n+2} - 24)x^{\sqrt{11}}$
$+(4\times 2^{n+2} - 12)x^{2\sqrt{3}} + (8\times 2^{n+2} - 24)x^{\sqrt{13}} + (2\times 2^{n+2} - 5)x^{\sqrt{14}}.$

Proof: Let G be the molecular graph of $TD_2[n]$. By using the definitions and Table 1, we deduce

(i) $$NN(G) = \sum_{uv\in E(G)} \sqrt{S_G(u) + S_G(v)}$$

$$= (2+4)^{\frac{1}{2}} 2^{n+2} + (3+6)^{\frac{1}{2}} (2^{n+2} - 4) + (4+6)^{\frac{1}{2}} 2^{n+2} + (5+5)^{\frac{1}{2}} (7\times 2^{n+2} - 1) + (5+6)^{\frac{1}{2}} (11\times 2^{n+2} - 24)$$

$$+(5+7)^{\frac{1}{2}} (3\times 2^{n+2} - 8) + (6+6)^{\frac{1}{2}} (2^{n+2} - 4) + (6+7)^{\frac{1}{2}} (8\times 2^{n+2} - 24) + (7+7)^{\frac{1}{2}} (2\times 2^{n+2} - 5).$$

After simplification, we obtain the desired result.

(ii) $$NN(G,x) = \sum_{uv\in E(G)} x^{\sqrt{S_G(u)+S_G(v)}}$$

$$= 2^{n+2}x^{(2+4)^{\frac{1}{2}}} + (2^{n+2} - 4)x^{(3+6)^{\frac{1}{2}}} + 2^{n+2}x^{(4+6)^{\frac{1}{2}}} + (7\times 2^{n+2} - 16)x^{(5+5)^{\frac{1}{2}}} + (11\times 2^{n+2} - 24)x^{(5+6)^{\frac{1}{2}}}$$

$$+(3\times 2^{n+2} - 8)x^{(5+7)^{\frac{1}{2}}} + (2^{n+2} - 4)x^{(6+6)^{\frac{1}{2}}} + (8\times 2^{n+2} - 24)x^{(6+7)^{\frac{1}{2}}} + (2\times 2^{n+2} - 5)x^{(7+7)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

7. RESULTS FOR POPAM DENDRIMERS $POD_2[n]$

In this section, we focus on the molecular graph of POPAM dendrimers. This family of dendrimers is denoted by $POD_2[n]$, where n is the steps of growth in this type of dendrimers. The molecular graph of $POD_2[2]$ is shown in Figure 6.

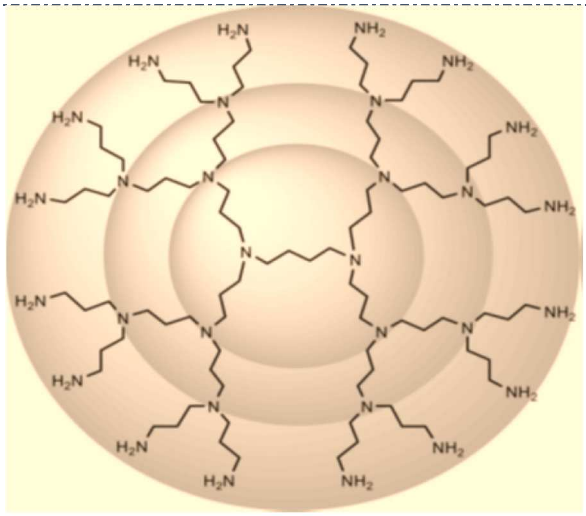

Figure 6. The molecular graph of $POD_2[n]$

Let G be the molecular graph of POPAM dendrimers $POD_2[n]$. By algebraic method, we obtain that $|V(POD_2[n])|= 2^{n+5} - 10$ and $|E(POD_2[n])|= 2^{n+5} - 11$. The edge partition of $POD_2[n]$ based on the degree sum of neighbors of end vertices of each edge is obtained as given in Table 6.

Table 6. Edge partition of $POD_2[n]$ based on $S_G(u)$ and $S_G(v)$

$S_G(u), S_G(v)\backslash uv\in E(G)$	(2, 3)	(3, 4)	(4, 4)	(4, 5)	(5, 6)
Number of edges	2^{n+2}	2^{n+2}	1	$3\times2^n - 6$	$3\times2^n - 6$

In the next theorem, we compute the neighborhood Nirmala index and its exponential of $POD_2[n]$.

Theorem 6. Let $POD_2[n]$ be the family of dendrimers. Then

(i) $NN(G) = \left(\sqrt{5}+\sqrt{7}+9+3\sqrt{11}\right)2^{n+2} + 2\sqrt{2} - 18 - 6\sqrt{11}.$

(ii) $NN(G,x) = 2^{n+2}x^{\sqrt{5}} + 2^{n+2}x^{\sqrt{7}} + x^{2\sqrt{2}} + (3\times2^{n+2}-6)x^3 + (3\times2^{n+2}-6)x^{\sqrt{11}}.$

Proof: Let G be the molecular graph of $POD_2[n]$. By using definitions and Table 6, we deduce

(i) $$NN(G) = \sum_{uv\in E(G)} \sqrt{S_G(u)+S_G(v)}$$

$$= (2+3)^{\frac{1}{2}}2^{n+2} + (3+4)^{\frac{1}{2}}2^{n+2} + (4+4)^{\frac{1}{2}} + (4+5)^{\frac{1}{2}}(3\times2^{n+2}-6) + (5+6)^{\frac{1}{2}}(3\times2^{n+2}-6).$$

After simplification, we obtain the desired result.

(ii) $$NN(G,x) = \sum_{uv\in E(G)} x^{\sqrt{S_G(u)+S_G(v)}}$$

$$= 2^{n+2}x^{(2+3)^{\frac{1}{2}}} + 2^{n+2}x^{(3+4)^{\frac{1}{2}}} + x^{(4+4)^{\frac{1}{2}}} + (3\times2^{n+2}-6)x^{(4+5)^{\frac{1}{2}}} + (3\times2^{n+2}-6)x^{(5+6)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

8. CONCLUSION

In this study, we have introduced some new Nirmala indices: the second, third, fourth and neighborhood Nirmala indices of a graph. We have computed the neighborhood Nirmala index and its exponential for nanocones and dendrimers.

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