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Connectivity Neighborhood Dakshayani Indices of *POPAM* Dendrimers

V.R.Kulli

Department of Mathematics
Gulbarga University, Gulbarga 585 106, India
E-mail: vrkulli@gmail.com

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Abstract. In Chemical Graph Theory, connectivity indices are applied to measure the chemical characteristics of chemical compounds. In this study, we introduce the sum connectivity neighborhood Dakshayani index, product connectivity neighborhood Dakshayani index, atom bond connectivity neighborhood Dakshayani index, geometric arithmetic neighborhood Dakshayani index and arithmetic-geometric neighborhood Dakshayani index of a molecular graph. We compute these connectivity neighborhood Dakshayani indices of *POPAM* dendrimers.

Keywords: neighborhood Dakshayani indices, connectivity neighborhood Dakshayani indices, dendrimer.

AMS Mathematics Subject Classification (2019): 05*C*07, 05*C*35, 05*C*76

1. Introduction

Throughout this paper, we consider only finite, connected, undirected graphs without loops and multiple edges. The degree of a vertex, denoted by $d_G(v)$, is the number of vertices adjacent to v. The set of all vertices which adjacent to v is called open neighborhood of v and denoted by $N_G(v)$. The closed neighborhood of v is the set $N_G[v] = N_G(v)\cup\{v\}$. The set $N_G[v]$ is the set of closed neighborhood vertices of v. Let $D_G(v) = d_G(v) + \sum_{u\in N_G(v)} D_G(u)$ be the degree sum of closed neighborhood vertices of v. We refer [1] for undefined terminologies and notations from graph theory.

A molecular graph or a chemical graph is a graph such that the vertices correspond to the atoms and edges to the bonds. Chemical Graph Theory is a breach of Mathematical Chemistry whose focus of interest is to finding topological indices or graph indices of a molecular graph which correlate well with chemical properties of the chemical molecules. Numerous graph indices have been considered in Chemistry and have found some applications in QSPR/QSAR research see [2, 3]

In [4], Kulli introduced the first and second neighborhood Dakshayani indices of a graph, defined as

$$ND_1(G) = \sum_{uv\in E(G)} \left[D_G(u) + D_G(v)\right], \qquad ND_2(G) = \sum_{uv\in E(G)} D_G(u)D_G(v).$$

The first and second hyper neighborhood Dakshayani indices were proposed and studied by Kulli in [4], defined as

$$HND_1(G)=\sum_{uv\in E(G)}\left[D_G(u)+D_G(v)\right]^2, \qquad HND_2(G)=\sum_{uv\in E(v)}\left[D_G(u)D_G(v)\right]^2.$$

Motivated by the definitions of the connectivity indices, we now introduce the connectivity neighborhood indices as follows.

The sum and product connectivity neighborhood Dakshayani indices of a graph G are defined as

$$SND(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{D_G(u)+D_G(v)}}.$$

$$PND(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{D_G(u)D_G(v)}}.$$

The atom bond connectivity (ABC) neighborhood Dakshayani index of a graph G is defined as

$$ABCND(G)=\sum_{uv\in E(G)}\sqrt{\frac{D_G(u)+D_G(v)-2}{D_G(u)D_G(v)}}. \tag{1}$$

The geometric-arithmetic neighborhood Dakshayani index of a graph G is defined as

$$GAND(G)=\sum_{uv\in E(G)}\frac{2\sqrt{D_G(u)D_G(v)}}{D_G(u)+D_G(v)}. \tag{2}$$

The arithmetic-geometric neighborhood Dakshayani index of a graph G is defined as

$$AGND(G)=\sum_{uv\in E(G)}\frac{D_G(u)+D_G(v)}{2\sqrt{D_G(u)D_G(v)}}. \tag{3}$$

The reciprocal neighborhood Dakshayani index of a graph G is defined as

$$RND(G)=\sum_{uv\in E(G)}\sqrt{D_G(u)D_G(v)}.$$

The general first and second neighborhood Dakshayani indices of a graph G are defined as

$$ND_1^a(G)=\sum_{uv\in E(G)}\left[D_G(u)+D_G(v)\right]^a, \tag{4}$$

$$ND_2^a(G)=\sum_{uv\in E(G)}\left[D_G(u)D_G(v)\right]^a, \tag{5}$$

where a is a real number.

Recently, some now connectivity indices were introduced and studied such as sum connectivity index [5], sum connectivity Revan index [6], sum connectivity Gourava index [7], atom bond connectivity Kulli-Basava index [8], sum and product connectivity F-indices [9], multiplicative connectivity *KV* indices [10], sum connectivity leap index [11], connectivity *KV* indices [12]. Very recently some new variants of neighborhood Dakshayani indices were proposed and studied such as *F*-neighborhood Dakshayani index [13], square neighborhood Dakshayani index [14], multiplicative neighborhood indices [15].

In this paper, some neighborhood Dakshayani indices of *POPAM* dendrimers are determined.

2. Results for *POPAM* Dendrimers

In this section, we focus on the graph of *POPAM* dendrimer. This family of dendrimers is symbolized by $POD_2[n]$, where n is the steps of growth in *POPAM* dendrimers. A graph of $POD_2[2]$ is shown in Figure 1.

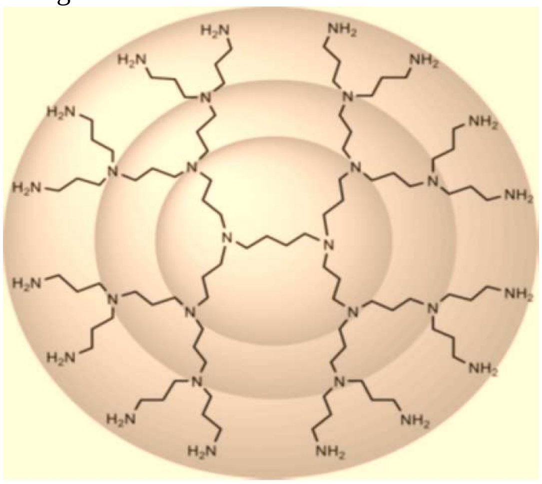

Figure 1: Graph of $POD_2[2]$

Let G be a graph of a $POD_2[n]$ dendrimer. By calculation G has $2^{n+5} - 10$ vertices and $2^{n+5} - 11$ edges. The edge partition of G based on the degree gum of closed neighborhood end vertices of each edge is obtained as given in Table 1.

Table 1: Edge partition of $POD_2[n]$

$D_G(u), D_G(v) \setminus uv \in E(G)$	(3, 5)	(5, 6)	(6, 6)	(6, 7)	(7, 9)
Number of edges	2^{n+2}	2^{n+2}	1	$3\times2^{n+2} - 6$	$3\times2^{n+2} - 6$

Theorem 1. The general first neighborhood Dakshayani index of a *POPAM* dendrimer $POD_2[n]$ is

$$ND_2^a\left[POD_2(n)\right] = \left(8^a + 11^a + 3\times13^a + 3\times16^a\right)2^{n+2} + \left(12^a - 6\times13^a - 6\times16^a\right) \quad (6)$$

Proof: Let G be a graph of *POPAM* dendrimer $POD_2[n]$. By using equation (4) and Table 1, we obtain

$$ND_1^a\left(POD_2[n]\right) = \sum_{uv\in E(G)} \left[D_G(u) + D_G(v)\right]^a$$

$$= (3+5)^a\, 2^{n+2} + (5+6)^a\, 2^{n+2} + (6+6)^a + (6+7)^a\left(3\times2^{n+2} - 6\right) + (7+9)^a\left(3\times2^{n+2} - 6\right)$$

$$= \left(8^a + 11^a + 3\times13^a + 3\times16^a\right)2^{n+2} + \left(12^a - 6\times13^a - 6\times16^a\right).$$

We obtain the following results by using Theorem 1.

Corollary 1.1. If $POD_2[n]$ is graph of *POPAM* dendrimer, then

i) $ND_1(POD_2[n]) = 106 \times 2^{n+2} - 162.$

ii) $HND_1(POD_2[n]) = 1460 \times 2^{n+2} - 2406.$

iii) $SND(POD_2[n]) = \left(\frac{1}{\sqrt{8}} + \frac{1}{\sqrt{11}} + \frac{3}{\sqrt{13}} + \frac{3}{4}\right)2^{n+2} + \left(\frac{1}{\sqrt{12}} - \frac{6}{\sqrt{13}} - \frac{6}{4}\right)$

Proof: Put a = 1, 2, – ½ in equation (6), we get the required results.

Theorem 2. The general second neighborhood Dakshayani index of *POPAM* dendrimer $POD_2[n]$ is

$$ND_2^a\left[POD_2(n)\right] = \left(15^a + 30^a + 3\times 42^a + 3\times 63^a\right)2^{n+2} + \left(36^a - 6\times 42^a - 6\times 63^a\right) \quad (7)$$

Proof: Let G be a graph of *POPAM* dendrimer $POD_2[n]$. By using equation (5) and Table 1, we deduce

$$ND_1^a(POD_2[n]) = \sum_{uv\in E(G)} \left[D_G(u)D_G(v)\right]^a$$

$$= (3\times 5)^a\, 2^{n+2} + (5\times 6)^a\, 2^{n+2} + (6\times 6)^a + (6\times 7)^a\left(3\times 2^{n+2} - 6\right) + (7\times 9)^a\left(3\times 2^{n+2} - 6\right)$$

$$= \left(15^a + 30^a + 3\times 42^a + 3\times 63^a\right)2^{n+2} + \left(36^a - 6\times 42^a - 6\times 63^a\right).$$

Corollary 2.1. Let $POD_2[n]$ be a graph of *POPAM* dendrimer. Then

i) $ND_2(POD_2[n]) = 360 \times 2^{n+2} - 594.$

ii) $HND_2(POD_2[n]) = 18324 \times 2^{n+2} - 33102.$

iii) $PND(POD_2[n]) = \left(\frac{1}{\sqrt{15}} + \frac{1}{\sqrt{30}} + \frac{3}{\sqrt{42}} + \frac{3}{\sqrt{63}}\right)2^{n+2} + \left(\frac{1}{6} - \frac{6}{\sqrt{42}} - \frac{6}{\sqrt{63}}\right).$

iv) $RND(POD_2[n]) = \left(\sqrt{15} + \sqrt{30} + 3\times\sqrt{42} + 3\times\sqrt{63}\right)2^{n+2} + \left(6 - 6\times\sqrt{42} - 3\times\sqrt{63}\right).$

Proof: Put a = 1, 2, – ½, ½ in equation (7), we obtain the desired results.

Theorem 3. The atom bond connectivity neighborhood Dakshayani index of $POD_2[n]$ is

$$ABCND(POD_2[n]) = \left(\sqrt{\frac{2}{5}} + \sqrt{\frac{3}{10}} + 3\sqrt{\frac{11}{42}} + \sqrt{2}\right)2^{n+2} + \left(\sqrt{\frac{5}{18}} - 6\sqrt{\frac{11}{42}} - 2\sqrt{2}\right)$$

Proof: Let $G = POD_2[n]$. By using equation (1) and Table 1, we have

$$ABCND(POD_2[n]) = \sum_{uv\in E(G)} \sqrt{\frac{D_G(u) + D_G(v) - 2}{D_G(u)D_G(v)}}$$

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

$$+ \left(\sqrt{\frac{6+7-2}{6\times 7}}\right)\left(3\times 2^{n+2} - 6\right) + \left(\sqrt{\frac{7+9-2}{7\times 9}}\right)\left(3\times 2^{n+2} - 6\right)$$

$$=\left(\sqrt{\frac{2}{5}}+\sqrt{\frac{3}{10}}+3\sqrt{\frac{11}{42}}+\sqrt{2}\right)2^{n+2}+\left(\sqrt{\frac{5}{18}}-6\sqrt{\frac{11}{42}}-2\sqrt{2}\right).$$

Theorem 4. The geometric-arithmetic neighborhood Dakshayani index of $POD_2[n]$ is

$$GAND\left(POD_2[n]\right)=\left(\frac{\sqrt{15}}{4}+\frac{2\sqrt{30}}{11}+\frac{6\sqrt{42}}{13}+\frac{9\sqrt{7}}{8}\right)2^{n+2}+\left(1-\frac{12\sqrt{42}}{13}-\frac{18\sqrt{7}}{8}\right)$$

Proof: Let $G = POD_2[n]$. From equation (2) and by using Table 1, we obtain

$$GAND\left(POD_2[n]\right)=\sum_{uv\in E(G)}\frac{2\sqrt{D_G(u)D_G(v)}}{D_G(u)+D_G(v)}$$

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

$$+\left(\frac{2\sqrt{6\times 7}}{6+7}\right)\left(3\times 2^{n+2}-6\right)+\left(\frac{2\sqrt{7\times 9}}{7+9}\right)\left(3\times 2^{n+2}-6\right)$$

$$=\left(\frac{\sqrt{15}}{4}+\frac{2\sqrt{30}}{11}+\frac{6\sqrt{42}}{13}+\frac{9\sqrt{7}}{8}\right)2^{n+2}+\left(1-\frac{12\sqrt{42}}{13}-\frac{18\sqrt{7}}{8}\right).$$

Theorem 5. The arithmetic-geometric neighborhood Dakshayani index of $POD_2[n]$ is

$$AGND\left(POD_2[n]\right)=\left(\frac{4}{\sqrt{15}}+\frac{11}{2\sqrt{30}}+\frac{39}{2\sqrt{42}}+\frac{8}{\sqrt{7}}\right)2^{n+2}+\left(1-\frac{39}{\sqrt{42}}-\frac{16}{\sqrt{7}}\right)$$

Proof: Let $G = POD_2[n]$. By using equation (3) and Table 1, we deduce

$$AGND\left(POD_2[n]\right)=\sum_{uv\in E(G)}\frac{D_G(u)+D_G(v)}{2\sqrt{D_G(u)D_G(v)}}$$

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

$$+\left(\frac{6+7}{2\sqrt{6\times 7}}\right)\left(3\times 2^{n+2}-6\right)+\left(\frac{7+9}{2\sqrt{7\times 9}}\right)\left(3\times 2^{n+2}-6\right)$$

$$=\left(\frac{4}{\sqrt{15}}+\frac{11}{2\sqrt{30}}+\frac{39}{2\sqrt{42}}+\frac{8}{\sqrt{7}}\right)2^{n+2}+\left(1-\frac{39}{\sqrt{42}}-\frac{16}{\sqrt{7}}\right).$$

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