ON CONNECTIVITY KV INDICES OF CERTAIN FAMILIES OF DENDRIMERS

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(Received On: 17-12-18; Revised & Accepted On: 04-02-19)

ABSTRACT

In Chemical Graph Theory, the connectivity indices are applied to measure the chemical characteristics of chemical compounds. In this paper, we propose the product connectivity KV, sum connectivity KV indices of a molecular graph. Also, we compute these connectivity KV indices for certain dendrimers of chemical importance like tetrathiafulvalene dendrimers and POPAM dendrimers.

MSC: 05C05, 05C07, 05C12, 05C35.

Keywords: product connectivity KV index, sum connectivity KV index, dendrimer.

1. INTRODUCTION

A topological index for a graph is used to determine some property of the graph of molecular by a single number. Many topological indices have been considered in Mathematical Chemistry.

Throughout this paper, we consider only finite, connected, undirected graphs without multiple edges and loops. The degree of a vertex v, denoted by $d_G(v)$, is the number of edges incident to a vertex v. Let $M_G(v) = \prod_{i \in G} d_G(u)$,

where N(v) is the set of all adjacent vertices of v. We refer [1] for undefined terminologies and notations from graph theory.

Recently, Kulli introduced the first and second
$$KV$$
 indices, defined as [2]
$$KV_{1}(G) = \sum_{uv \in E(G)} \left[M_{G}(u) + M_{G}(v) \right], \qquad KV_{2}(G) = \sum_{uv \in E(G)} M_{G}(u) M_{G}(v).$$

Very recently, some novel variants of KV indices were introduced and studied such as hyper KV indices [3], multiplicative KV indices [4], square KV index [3].

We propose some connectivity KV indices of a graph as follows:

The product connectivity KV index of a graph G is defined as

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

The sum connectivity KV index of G is defined as

$$SKV(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{M_G(u) + M_G(v)}}.$$
(2)

In recent years, some new connectivity indices have been introduced and studied such as sum connectivity Gourava index [5], sum connectivity index [6], geometric-arithmetic reverse and sum connectivity reverse indices [7], sum connectivity Revan index [8]. Also some connectivity indices were studied, for example, in [9, 10, 11, 12, 13].

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In this paper, some connectivity KV indices for tetrathiafulvalene dendrimers and POPAM dendrimers are determined. For denrimers see [14].

2. TETRATHIAFULVALENE DENDRIMERS

We consider the family of tetrathiapulvalene dendrimers. This family of dendrimers is denoted by $TD_2[n]$, where n is the steps of growth in this type of dendrimers. The graph of $TD_2[2]$ is presented in Figure 1.

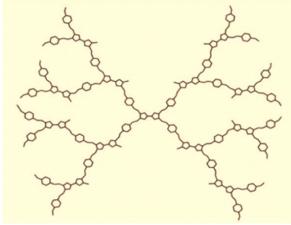


Figure-1; Graph of $TD_2[2]$

Let $G = TD_2[n]$. By calculation, we have $|V(G)| = 31 \times 2^{n+2} - 24$, $|E(G)| = 32 \times 2^{n+2} - 85$. The edge partition of G based on the degree product of neighbors of end vertices of each edge is given in Table 1

$M_G(u), M_G(v) \setminus uv \in E(G)$	Number of edges
(2,3)	2^{n+2}
(3,6)	$2^{n+2}-4$
(3,8)	2^{n+2}
(6,6)	$7 \times 2^{n+2} - 16$
(6,8)	$11 \times 2^{n+2} - 24$
(6,9)	$2^{n+2}-4$
(6, 12)	$3 \times 2^{n+2} - 8$
(9,12)	$8 \times 2^{n+2} - 24$
(12, 12)	$2 \times 2^{n+2} - 5$

Table-1: Edge partition of $TD_2[n]$

In the following theorem, we compute the product connectivity KV index of $TD_2[n]$.

Theorem 1: The product connectivity KV index of tetrathiafulvalene dendrimers is given by

$$PKV\left(TD_{2}\left[n\right]\right) = \left(\frac{11}{6\sqrt{6}} + \frac{5}{6\sqrt{2}} + \frac{49}{12\sqrt{3}} + \frac{4}{3}\right)2^{n+2} - \left(\frac{8}{3\sqrt{2}} + \frac{10}{\sqrt{3}} + \frac{4}{3\sqrt{6}} + \frac{37}{12}\right).$$

Proof: By using equation (1) and Table 1, we deduce

$$PKV(TD_{2}[n]) = \sum_{uv \in E(G)} \frac{1}{\sqrt{M_{G}(u)M_{G}(v)}}$$

$$= \left(\frac{1}{\sqrt{2 \times 3}}\right) 2^{n+2} + \left(\frac{1}{\sqrt{3 \times 6}}\right) (2^{n+2} - 4) + \left(\frac{1}{\sqrt{3 \times 8}}\right) (2^{n+2}) + \left(\frac{1}{\sqrt{6 \times 6}}\right) (7 \times 2^{n+2} - 16)$$

$$+ \left(\frac{1}{\sqrt{6 \times 8}}\right) (11 \times 2^{n+2} - 24) + \left(\frac{1}{\sqrt{6 \times 9}}\right) (2^{n+2} - 4) + \left(\frac{1}{\sqrt{6 \times 12}}\right) (3 \times 2^{n+2} - 8)$$

$$+ \left(\frac{1}{\sqrt{9 \times 12}}\right) (8 \times 2^{n+2} - 24) + \left(\frac{1}{\sqrt{12 \times 12}}\right) (2 \times 2^{n+2} - 5)$$

$$= \left(\frac{11}{6\sqrt{6}} + \frac{5}{6\sqrt{2}} + \frac{49}{12\sqrt{3}} + \frac{4}{3}\right) 2^{n+2} - \left(\frac{8}{3\sqrt{2}} + \frac{10}{\sqrt{3}} + \frac{4}{3\sqrt{6}} + \frac{37}{12}\right).$$

In the following theorem, we compute the sum connectivity KV index of $TD_2[n]$.

Theorem 2: The sum connectivity KV index of tetrathiafulvalene dendrimers is given by

$$SKV\left(TD_{2}[n]\right) = \left(\frac{1}{\sqrt{5}} + \frac{1}{3} + \frac{1}{\sqrt{11}} + \frac{7}{\sqrt{12}} + \frac{11}{\sqrt{14}} + \frac{1}{\sqrt{15}} + \frac{1}{\sqrt{2}} + \frac{8}{\sqrt{21}} + \frac{1}{\sqrt{6}}\right) 2^{n+2}$$
$$-\left(\frac{4}{3} + \frac{8}{\sqrt{3}} + \frac{24}{\sqrt{14}} + \frac{8}{\sqrt{18}} + \frac{24}{\sqrt{21}} + \frac{5}{\sqrt{24}}\right).$$

Proof: By using equation (2) and Table 1, we deduce

$$SKV (TD_{2}[n]) = \sum_{uv \in E(G)} \frac{1}{\sqrt{M_{G}(u) + M_{G}(v)}}$$

$$= \left(\frac{1}{\sqrt{2+3}}\right) 2^{n+2} + \left(\frac{1}{\sqrt{3+6}}\right) (2^{n+2} - 4) + \left(\frac{1}{\sqrt{3+8}}\right) (2^{n+2}) + \left(\frac{1}{\sqrt{6+6}}\right) (7 \times 2^{n+2} - 16)$$

$$+ \left(\frac{1}{\sqrt{6\times8}}\right) (11 \times 2^{n+2} - 24) + \left(\frac{1}{\sqrt{6\times9}}\right) (2^{n+2} - 4) + \left(\frac{1}{\sqrt{6\times12}}\right) (3 \times 2^{n+2} - 8)$$

$$+ \left(\frac{1}{\sqrt{9+12}}\right) (8 \times 2^{n+2} - 24) + \left(\frac{1}{\sqrt{12+12}}\right) (2 \times 2^{n+2} - 5)$$

$$= \left(\frac{1}{\sqrt{5}} + \frac{1}{3} + \frac{1}{\sqrt{11}} + \frac{7}{\sqrt{12}} + \frac{11}{\sqrt{14}} + \frac{1}{\sqrt{15}} + \frac{1}{\sqrt{2}} + \frac{8}{\sqrt{21}} + \frac{1}{\sqrt{6}}\right) 2^{n+2}$$

$$- \left(\frac{4}{3} + \frac{8}{\sqrt{3}} + \frac{24}{\sqrt{14}} + \frac{8}{\sqrt{18}} + \frac{24}{\sqrt{21}} + \frac{5}{\sqrt{24}}\right).$$

3. POPAM DENDRIMERS

We consider the family of POPAM dendrimers which is symbolized by $POD_2[n]$. The graph of $POD_2[2]$ is depicted in Figure 2.

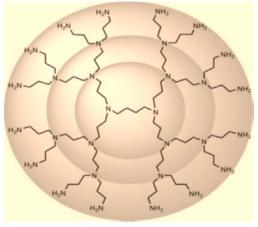


Figure-2: Graph of $POD_2[2]$

Let $G = POD_2[n]$. By calculation, we obtain $|V(G)| = 2^{n+5} - 10$ and $|E(G)| = 2^{n+5} - 11$. The edge partition of $POD_2[n]$ based on the degree product of neighbors of end vertices of each edge in given in Table 2.

$M_G(u), M_G(v) \setminus uv \in E(G)$	(2,2)	(2, 4)	(4, 4)	(4, 6)	(6, 8)
Number of edges	2^{n+2}	2^{n+2}	1	$3 \times 2^{n+2} - 6$	$3 \times 2^{n+2} - 6$

Table-2: Edge partition of $POD_2[n]$

In the following theorem, we compute the product connectivity KV index of $POD_2[n]$.

Theorem 3: The product connectivity KV index of POPAM dendrimers is given by

$$PKV\left(POD_{2}[n]\right) = \left(\frac{1}{2} + \frac{1}{2\sqrt{2}} + \frac{3}{2\sqrt{6}} + \frac{3}{4\sqrt{3}}\right)2^{n+2} - \left(\frac{1}{4} - \frac{6}{\sqrt{6}} - \frac{3}{2\sqrt{3}}\right).$$

Proof: By using equation (1) and Table 2, we derive

$$PKV(POD_{2}[n]) = \sum_{uv \in E(G)} \frac{1}{\sqrt{M_{G}(u)M_{G}(v)}}$$

$$= \left(\frac{1}{\sqrt{2 \times 2}}\right) 2^{n+2} + \left(\frac{1}{\sqrt{2 \times 4}}\right) 2^{n+2} + \left(\frac{1}{\sqrt{4 \times 4}}\right) + \left(\frac{1}{\sqrt{4 \times 6}}\right) (3 \times 2^{n+2} - 6) + \left(\frac{1}{\sqrt{6 \times 8}}\right) (3 \times 2^{n+2} - 6)$$

$$= \left(\frac{1}{2} + \frac{1}{2\sqrt{2}} + \frac{3}{2\sqrt{6}} + \frac{3}{4\sqrt{3}}\right) 2^{n+2} - \left(\frac{1}{4} + \frac{6}{\sqrt{6}} - \frac{3}{2\sqrt{3}}\right).$$

In the following theorem, we compute the sum connectivity KV index of $POD_2[n]$.

Theorem 4: The sum connectivity KV Index of POPAM denderimers is given by

$$SKV\left(POD_{2}[n]\right) = \left(\frac{1}{2} + \frac{1}{\sqrt{6}} + \frac{3}{\sqrt{10}} + \frac{3}{\sqrt{14}}\right)2^{n+2} - \left(\frac{1}{\sqrt{8}} - \frac{6}{\sqrt{10}} - \frac{6}{\sqrt{14}}\right).$$

Proof: From equation (2) and Table 2, we derive

$$SKV (POD_{2}[n]) = \sum_{uv \in E(G)} \frac{1}{\sqrt{M_{G}(u) + M_{G}(v)}}$$

$$= \left(\frac{1}{\sqrt{2+2}}\right) 2^{n+2} + \left(\frac{1}{\sqrt{2+4}}\right) 2^{n+2} + \left(\frac{1}{\sqrt{4+4}}\right) + \left(\frac{1}{\sqrt{4\times6}}\right) (3\times2^{n+2} - 6) + \left(\frac{1}{\sqrt{6+8}}\right) (3\times2^{n+2} - 6)$$

$$= \left(\frac{1}{2} + \frac{1}{\sqrt{6}} + \frac{3}{\sqrt{10}} + \frac{3}{\sqrt{14}}\right) 2^{n+2} + \left(\frac{1}{\sqrt{8}} - \frac{6}{\sqrt{10}} - \frac{6}{\sqrt{14}}\right).$$

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Source of support: Nil, Conflict of interest: None Declared.

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