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RESEARCH ARTICLE

ON *KV* INDICES AND THEIR POLYNOMIALS OF TWO FAMILIES OF DENDRIMERS

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ABSTRACT

Let $M_G(u)$ denote the product of the degrees of all vertices adjacent to a vertex u. We introduce the first and second KV indices, the first vertex KV index, the minus KV index and their polynomials of a molecular graph. In this paper, we compute the first and second KV indices, and their polynomials, and minus KV index and its polynomial of tetrathiafulvalene dendrimers and POPAM dendrimers.

Keywords: KV indices, minus KV index, dendrimer.
Mathematics Subject Classification: 05*C*05, 05*C*07, 05*C*12, 05*C*35.

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INTRODUCTION

Chemical Graph Theory is a branch of Mathematical Chemistry which has an important effect on the development of Chemical Sciences. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. In Organic Chemistry, topological indices have been found to be useful in chemical documentation, isomer discrimination, structure property relationships, structure activity relationships and pharmaceutical drug design. There has been considerable interest in the general problem of determining topological indices.

Let G be a finite, simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. Let $M_G(v)$ denote the product of degrees of all vertices adjacent to a vertex v. The edge connecting vertices u and v will be denoted by uv. For other definitions and notations, readers are referred to [1].

We introduce the first and second KV indices of a graph G as

$$KV_1(G) = \sum_{uv \in E(G)} \left[M_G(u) + M_G(v) \right] \tag{1}$$

and

$$KV_2(G) = \sum_{uv \in E(G)} M_G(u) M_G(v) \tag{2}$$

Recently, in [2] the first and second K Banhatti indices, in [3] the first and second Gourava indices, in [4] the first and second Revan indices, in [5] the first and second reverse indices, in [6] the first and second ve-degree indices were introduced and studied. Considering the KV indices, we propose the first and second KV polynomials of a graph G as

$$KV_1(G,x) = \sum_{uv \in E(G)} x^{M_G(u)+M_G(v)} \tag{3}$$

and

$$KV_2(G,x) = \sum_{uv \in E(G)} x^{M_G(u)M_G(v)} \tag{4}$$

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Recently, some polynomials were studied, for example, in [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18].

The first vertex KV index of a graph G is defined as

$$KV_{01}(G) = \sum_{u \in V(G)} M_G(u)^2. \tag{5}$$

Considering the first vertex KV index, we propose the first KV vertex polynomial of a graph G as

$$KV_{01}(G,x) = \sum_{u \in V(G)} x^{M_G(u)^2}. \tag{6}$$

The minus KV index of a graph G is defined as

$$KV_m(G) = \sum_{uv \in E(G)} \left| M_G(u) - M_G(v) \right|. \tag{7}$$

Considering the minus KV index, we define the minus KV polynomial of a graph G as

$$KV_m(G,x) = \sum_{uv \in E(G)} x^{\left| M_G(u) - M_G(v) \right|}. \tag{8}$$

In this paper, we consider the families of tetrathiafulvalene dendrimers and POPAM dendrimers, see [19]. In this paper, the first and second KV indices, and their polynomials, and the minus KV index and its polynomial of two families of dendrimers are computed.

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 0. The molecular graph of $TD_2[2]$ is shown in Figure 1.

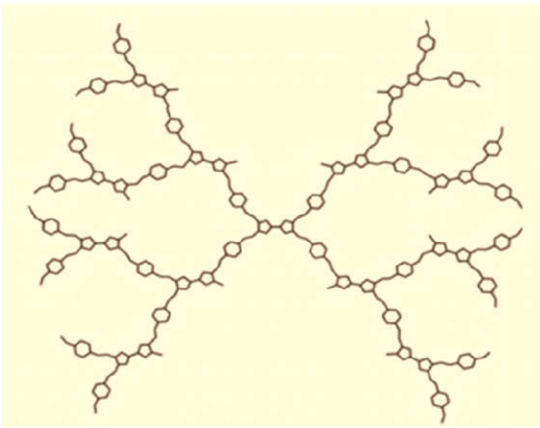

Figure 1. The molecular graph of $TD_2[2]$

Let G be the molecular graph of tetrathiafulvalene dendrimers $TD_2[n]$. By calculation, we obtain that G has $31 \times 2^{n+2} - 74$ vertices and $35 \times 2^{n+2} - 85$ edges. Also the edge partition of $TD_2[n]$ based on the degree product of neighbors of end vertices of each edge is obtained as given in Table 1.

Table 1. Edge partition of $TD_2[n]$

$M_G(u), M_G(v) \backslash uv\ E(G)$	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)	$2 \times 2^{n+2} - 5$

Theorem 1. The first and second KV indices of a tetrathiafulvalene dendrimer $TD_2[n]$ are given by

(a) $KV_1(TD_2[n]) = 542 \times 2^{n+2} - 1392.$

(b) $KV_2(TD_2[n]) = 2250 \times 2^{n+2} - 5904.$

Proof: Let G be the graph of a tetrathiafulvalene dendrimer $TD_2[n]$.

(a)By using equation (1) and Table 1, we derive

$$\begin{aligned} KV_1(TD_2[n]) &= \sum_{uv \in E(G)} \left[M_G(u) + M_G(v)\right] \\ &= (2+3)2^{n+2} + (3+6)(2^{n+2}-4) + (3+8)2^{n+2} + (6+6)(7 \times 2^{n+2} - 16) \\ &\quad + (6+8)(11 \times 2^{n+2} - 24) + (6+9)(2^{n+2}-4) + (6+12)(3 \times 2^{n+2} - 8) \\ &\quad + (9+12)(8 \times 2^{n+2} - 24) + (12+12)(2 \times 2^{n+2} - 5) \\ &= 542 \times 2^{n+2} - 1392. \end{aligned}$$

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

$$\begin{aligned} KV_2(TD_2[n]) &= \sum_{uv \in E(G)} M_G(u) M_G(v) \\ &= (2 \times 3)2^{n+2} + (3 \times 6)(2^{n+2}-4) + (3 \times 8)2^{n+2} + (6 \times 6)(7 \times 2^{n+2} - 16) \\ &\quad + (6 \times 8)(11 \times 2^{n+2} - 24) + (6 \times 9)(2^{n+2}-4) + (6 \times 12)(3 \times 2^{n+2} - 8) \\ &\quad + (9 \times 12)(8 \times 2^{n+2} - 24) + (12 \times 12)(2 \times 2^{n+2} - 5) \\ &= 2250 \times 2^{n+2} - 5904. \end{aligned}$$

Theorem 2. The first and second KV polynomials of a tetrathiafulvalene dendrimer $TD_2[n]$ are given by

(a) $$\begin{aligned} KV_1(TD_2[n], x) &= 2^{n+2}x^5 + (2^{n+2}-4)x^9 + 2^{n+2}x^{11} + (7 \times 2^{n+2} - 16)x^{12} \\ &\quad + (11 \times 2^{n+2} - 24)x^{14} + (2^{n+2}-4)x^{15} + (3 \times 2^{n+2} - 8)x^{18} \\ &\quad + (8 \times 2^{n+2} - 24)x^{21} + (2 \times 2^{n+2} - 5)x^{24}. \end{aligned}$$

(b) $$\begin{aligned} KV_2(TD_2[n], x) &= 2^{n+2}x^6 + (2^{n+2}-4)x^{18} + 2^{n+2}x^{24} + (7 \times 2^{n+2} - 16)x^{36} \\ &\quad + (11 \times 2^{n+2} - 24)x^{48} + (2^{n+2}-4)x^{54} + (3 \times 2^{n+2} - 8)x^{72} \\ &\quad + (8 \times 2^{n+2} - 24)x^{108} + (2 \times 2^{n+2} - 5)x^{144}. \end{aligned}$$

Proof: Let G be the graph of a tetrathiafulvalene dendrimer $TD_2[n]$.

(a)By using equation (3) and Table 1, we derive

$$\begin{aligned} KV_1(TD_2[n], x) &= \sum_{uv \in E(G)} x^{\left[M_G(u) + M_G(v)\right]} \\ &= 2^{n+2}x^5 + (2^{n+2}-4)x^9 + 2^{n+2}x^{11} + (7 \times 2^{n+2} - 16)x^{12} + (11 \times 2^{n+2} - 24)x^{14} \\ &\quad + (2^{n+2}-4)x^{15} + (3 \times 2^{n+2} - 8)x^{18} + (8 \times 2^{n+2} - 24)x^{21} + (2 \times 2^{n+2} - 5)x^{24} \end{aligned}$$

(b)By using equation (4) and Table 1, we derive

$$\begin{aligned} KV_2(TD_2[n], x) &= \sum_{uv \in E(G)} x^{M_G(u) M_G(v)} \\ &= 2^{n+2}x^6 + (2^{n+2}-4)x^{18} + 2^{n+2}x^{24} + (7 \times 2^{n+2} - 16)x^{36} + (11 \times 2^{n+2} - 24)x^{48} \\ &\quad + (2^{n+2}-4)x^{54} + (3 \times 2^{n+2} - 8)x^{72} + (8 \times 2^{n+2} - 24)x^{108} + (2 \times 2^{n+2} - 5)x^{144}. \end{aligned}$$

Theorem 3. The minus *KV* index and its polynomial of a tetrathiafulvalene dendrimer $TD_2[n]$ are given by

(a) $KV_m\left(TD_2[n]\right)=76\times 2^{n+2}-192.$

(b) $KV_m\left(TD_2[n],x\right)=\left(9\times 2^{n+2}-21\right)x^0+2^{n+2}x^1+\left(11\times 2^{n+2}-24\right)x^2$
$+\left(10\times 2^{n+2}-32\right)x^3+2^{n+2}x^5+\left(3\times 2^{n+2}-8\right)x^6.$

Proof: Let G be the graph of a tetrathiafulvalene dendrimer $TD_2[n]$.

(a)By using equation (7) and Table 1, we derive

$$\begin{aligned}KV_m\left(TD_2[n]\right)&=\sum_{uv\in E(G)}\left|M_G(u)-M_G(v)\right|\\&=1\times 2^{n+2}+3\times\left(2^{n+2}-4\right)+5\times 2^{n+2}+0\times\left(7\times 2^{n+2}-16\right)+2\times\left(11\times 2^{n+2}-24\right)\\&\quad+3\times(2^{n+2}-4)+6\times\left(3\times 2^{n+2}-8\right)+3\times\left(8\times 2^{n+2}-24\right)+0\times\left(2\times 2^{n+2}-5\right)\\&=76\times 2^{n+2}-192.\end{aligned}$$

(b)By using equation (8) and Table 1, we derive

$$\begin{aligned}KV_m\left(TD_2[n],x\right)&=\sum_{uv\in E(G)}x^{\left|M_G(u)-M_G(v)\right|}\\&=2^{n+2}x^1+\left(2^{n+2}-4\right)x^3+2^{n+2}x^5+\left(7\times 2^{n+2}-16\right)x^0+\left(11\times 2^{n+2}-24\right)x^2\\&\quad+\left(2^{n+2}-4\right)x^3+\left(3\times 2^{n+2}-8\right)x^6+\left(8\times 2^{n+2}-24\right)x^3+\left(2\times 2^{n+2}-5\right)x^0\\&=\left(9\times 2^{n+2}-21\right)x^0+2^{n+2}x^1+\left(11\times 2^{n+2}-24\right)x^2\\&\quad+\left(10\times 2^{n+2}-32\right)x^3+2^{n+2}x^5+\left(3\times 2^{n+2}-8\right)x^6.\end{aligned}$$

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 presented in Figure 2.

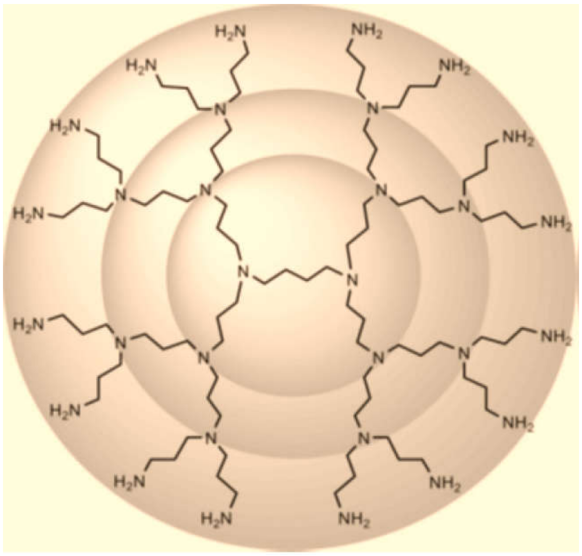

Figure 2. The graph of POPAM dendrimer $POD_2[2]$

Let G be the molecular graph of POPAM dendrimers $POD_2[n]$. By calculation, we obtain that G has $2^{n+5}-10$ and $2^{n+5}-11$ edges. The edge partition of $POD_2[n]$ based on the degree product of neighbors of end vertices of each edge is obtained as given in Table 2.

Table 2. Edge partition of $POD_2[n]$

$M_G(u)$, $M_G(v)\backslash uv$ $E(G)$	(2, 2)	(2, 4)	(4, 4)	(4, 6)	(6, 8)
Number of edges	2^{n+2}	2^{n+2}	1	$3\times2^n-6$	$3\times2^n-6$

In the following theorem, we compute the values of $KV_1(POD_2[n])$ and $KV_2(POD_2[n])$.

Theorem 4. The first and second KV indices of a POPAM dendrimer $TD_2[n]$ are given by

(a) $KV_1\left(POD_2[n]\right) = 82 \times 2^{n+2} - 136.$

(b) $KV_2\left(POD_2[n]\right) = 230 \times 2^{n+2} - 416.$

Proof: Let G be the graph of a POPAM dendrimer $POD_2[n]$.

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

$$\begin{aligned} KV_1\left(POD_2[n]\right) &= \sum_{uv \in E(G)} \left[M_G(u) + M_G(v)\right] \\ &= (2+2)2^{n+2} + (2+4)2^{n+2} + (4+4) + (4+6)\left(3 \times 2^{n+2} - 6\right) + (6+8)\left(3 \times 2^{n+2} - 6\right) \\ &= 82 \times 2^{n+2} - 136. \end{aligned}$$

(b)By using equation (2) and Table 2, we deduce

$$\begin{aligned} KV_2\left(TD_2[n]\right) &= \sum_{uv \in E(G)} M_G(u) M_G(v) \\ &= (2 \times 2)2^{n+2} + (2 \times 4)2^{n+2} + (4 \times 4) + (4 \times 6)\left(3 \times 2^{n+2} - 6\right) + (6 \times 8)\left(3 \times 2^{n+2} - 6\right) \\ &= 230 \times 2^{n+2} - 416. \end{aligned}$$

In the following theorem, we compute the values of $KV_1(POD_2[n], x)$ and $KV_2(POD_2[n], x)$.

Theorem 5. The first and second KV polynomials of a POPAM dendrimer $TD_2[n]$ are given by

(a) $KV_1\left(POD_2[n], x\right) = 2^{n+2}x^4 + 2^{n+2}x^6 + x^8 + \left(3 \times 2^{n+2} - 6\right)x^{10} + \left(3 \times 2^{n+2} - 6\right)x^{14}$

(b) $KV_2\left(POD_2[n], x\right) = 2^{n+2}x^4 + 2^{n+2}x^8 + x^{16} + \left(3 \times 2^{n+2} - 6\right)x^{24} + \left(3 \times 2^{n+2} - 6\right)x^{48}$

Proof: Let G be the graph of a POPAM dendrimer $POD_2[n]$.

(a)By using equation (3) and Table 2, we derive

$$\begin{aligned} KV_1\left(POD_2[n], x\right) &= \sum_{uv \in E(G)} x^{\left[M_G(u) + M_G(v)\right]} \\ &= 2^{n+2}x^{2+2} + 2^{n+2}x^{2+4} + x^{4+4} + \left(3 \times 2^{n+2} - 6\right)x^{4+6} + \left(3 \times 2^{n+2} - 6\right)x^{6+8} \\ &= 2^{n+2}x^4 + 2^{n+2}x^6 + x^8 + \left(3 \times 2^{n+2} - 6\right)x^{10} + \left(3 \times 2^{n+2} - 6\right)x^{14}. \end{aligned}$$

(b)By using equation (4) and Table 2, we derive

$$\begin{aligned} KV_2\left(POD_2[n], x\right) &= \sum_{uv \in E(G)} x^{M_G(u) M_G(v)} \\ &= 2^{n+2}x^{2\times2} + 2^{n+2}x^{2\times4} + x^{4\times4} + \left(3 \times 2^{n+2} - 6\right)x^{4\times6} + \left(3 \times 2^{n+2} - 6\right)x^{6\times8} \\ &= 2^{n+2}x^4 + 2^{n+2}x^8 + x^{16} + \left(3 \times 2^{n+2} - 6\right)x^{24} + \left(3 \times 2^{n+2} - 6\right)x^{48}. \end{aligned}$$

We now compute the values of $KV_1(POD_2[n])$ and $KV_2(POD_2[n], x)$.

Theorem 6. The minus KV index and its polynomial of a POPAM dendrimer $POD_2[n]$ are given by

(a) $KV_m\left(POD_2[n]\right) = 14 \times 2^{n+2} - 24.$

(b) $KV_m\left(POD_2[n], x\right) = \left(7 \times 2^{n+2} - 12\right)x^2 + \left(2^{n+2} + 1\right)x^0.$

Proof: Let G be the graph of a POPAM dendrimer $POD_2[n]$.

(a)By using equation (7) and Table 2, we derive

$$
\begin{aligned}
KV_m\left(POD_2[n]\right) &= \sum_{uv\in E(G)} \left|M_G(u)-M_G(v)\right| \\
&= 0\times 2^{n+2} + 2\times 2^{n+2} + 0\times 1 + 2\left(3\times 2^{n+2}-6\right) + 2\left(3\times 2^{n+2}-6\right) \\
&= 14\times 2^{n+2} - 24.
\end{aligned}
$$

(b)By using equation (8) and Table 2, we obtain

$$
\begin{aligned}
KV_m\left(POD_2[n],x\right) &= \sum_{uv\in E(G)} x^{\left|M_G(u)-M_G(v)\right|} \\
&= 2^{n+2}x^0 + 2^{n+2}x^2 + x^0 + \left(3\times 2^{n+2}-6\right)x^2 + \left(3\times 2^{n+2}-6\right)x^2 \\
&= \left(7\times 2^{n+2}-12\right)x^2 + \left(2^{n+2}+1\right)x^0.
\end{aligned}
$$

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