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On Hyper *KV* and Square *KV* Indices and their Polynomials of Certain Families of Dendrimers

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ABSTRACT

We introduce the first and second hyper *KV* indices of a molecular graph. Considering these hyper *KV* indices, we propose the first and second hyper *KV* polynomials of a graph. Furthermore we introduce the square *KV* index of a graph. Considering the square *KV* index, we define the square *KV* polynomial of a graph. In this paper, we compute the first and second hyper- *KV* indices, square *KV* index and their polynomials of two families of dendrimers.

Mathematics Subject Classification : 05*C*05, 05*C*07, 05*C*35.

Keywords: hyper *KV* indices, square *KV* index, dendrimer.

1. INTRODUCTION

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 a vertex v. Let $M_G(v)$ denote the product of the degrees of all vertices adjacent to a vertex v. The edge connecting the vertices u and v will be denoted by uv. We refer to[1] for undefined term and notation.

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. In Chemical Sciences, 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.

The first and second KV indices[2] of a graph G are respectively defined as

$$KV_1(G) = \sum_{uv \in E(G)} \left[M_G(u) + M_G(v) \right], \quad KV_2(G) = \sum_{uv \in E(G)} M_G(u) M_G(v).$$

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

$$HKV_1(G)=\sum_{uv\in E(G)}\left[M_G(u)+M_G(v)\right]^2, \quad (1)$$

$$HKV_2(G)=\sum_{uv\in E(G)}\left[M_G(u)M_G(v)\right]^2. \quad (2)$$

Recently, in[3] the first and second hyper Banhatti indices, in[4] the first and second hyper-Gourava indices, in[5] the first and second hyper Revan indices, in[6] the first and second reverse hyper-Zagreb indices were introduced and studied.

Considering the first and second hyper-*KV* indices, we introduce the first and second hyper -*KV* polynomials as

$$HKV_1(G,x)=\sum_{uv\in E(G)}x^{\left[M_G(u)+M_G(v)\right]^2}, \quad (3)$$

$$HKV_2(G,x)=\sum_{uv\in E(G)}x^{\left[M_G(u)M_G(v)\right]^2}. \quad (4)$$

The square *ve* degree index[3] of a graph *G* is defined as

$$Q_{ve}(G)=\sum_{uv\in E(G)}\left[d_{ve}(u)-d_{ve}(v)\right]^2.$$

Motivated by the definition of the square *ve*-degree index, we now define the square *KV* index of a molecular graph as follows:

The square *KV* index of a graph *G* is defined as

$$SqKV(G)=\sum_{uv\in E(G)}\left[M_G(u)-M_G(v)\right]^2. \quad (5)$$

Considering the square *KV* index, we propose the square *KV* polynomial as

$$SqKV(G,x)=\sum_{uv\in E(G)}x^{\left[M_G(u)-M_G(v)\right]^2}. \quad (6)$$

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

We consider two families of dendrimers such as tetrathiafulvalene dendrimers and POPAM dendrimers see[18]. In this paper, the first and second hyper *KV indices, square KV index* and their polynomials of tetrathiafulvalene and POPAM dendrimers are determined.

2. TETRATHIAFULVALENE DENDRIMERS

We now 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 graph of $TD_2{}^2$ is presented in Figure1.

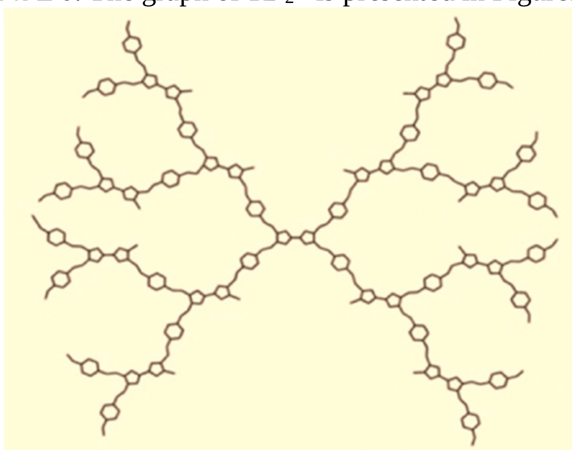

Figure 1. The graph of $TD_2[2]$

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

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

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

a) $HKV_1(TD_2[n]) = 9270 \times 2^{n+2} - 24288$.

b) $HKV_2(TD_2[n]) = 188604 \times 2^{n+2} - 503712$.

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

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

$$HKV_1(TD_2[n]) = \sum_{uv \in E(G)} \left[M_G(u) + M_G(v)\right]^2.$$
$$= (2+3)^2 2^{n+2} + (3+6)^2 (2^{n+2} - 4) + (2+8)^2 2^{n+2} + (6+6)^2 (7 \times 2^{n+2} - 16)$$
$$+ (6+8)^2 (11 \times 2^{n+2} - 24) + (6+9)^2 (2^{n+2} - 4) + (6 \times 12)^2 (3 \times 2^{n+2} - 8)$$
$$+ (9+12)^2 (8 \times 2^{n+2} - 24) + (12+12)^2 (2 \times 2^{n+2} - 5)$$
$$= 9270 \times 2^{n+2} - 24288.$$

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

$$HKV_2(TD_2[n]) = \sum_{uv \in E(G)} \left[M_G(u) M_G(v)\right]^2.$$
$$= (2 \times 3)^2 2^{n+2} + (3 \times 6)^2 (2^{n+2} - 4) + (3 \times 8)^2 2^{n+2} + (6 \times 6)^2 (7 \times 2^{n+2} - 8)$$
$$+ (6 \times 8)^2 (11 \times 2^{n+2} - 24) + (6 \times 9)^2 (2^{n+2} - 4) + (6 \times 12)^2 (3 \times 2^{n+2} - 8)$$
$$+ (9 \times 12)^2 (8 \times 2^{n+2} - 24) + (12 \times 12)^2 (2 \times 2^{n+2} - 5)$$
$$= 188604 \times 2^{n+2} - 503712.$$

Theorem 2. The first and second hyper *KV* polynomial of a tetrathiafulvalene demdrimer $TD_2[n]$ are given by

(a)
$$HKV_1(TD_2[n], x) = 2^{n+2} x^{25} + (2^{n+2} - 4) x^{81} + 2^{n+2} x^{121} + (7 \times 2^{n+2} - 16) x^{144}$$
$$+ (11 \times 2^{n+2} - 24) x^{196} + (2^{n+2} - 4) x^{225} + (3 \times 2^{n+2} - 8) x^{324}$$
$$+ (8 \times 2^{n+2} - 24) x^{441} + (2 \times 2^{n+2} - 5) x^{576}.$$

(b)
$$HKV_2(TD_2[n], x) = 2^{n+2} x^{36} + (2^{n+2} - 4) x^{324} + 2^{n+2} x^{576} + (7 \times 2^{n+2} - 16) x^{1296}$$
$$+ (11 \times 2^{n+2} - 24) x^{2304} + (2^{n+2} - 4) x^{2916} + (3 \times 2^{n+2} - 8) x^{5184}$$
$$+ (8 \times 2^{n+2} - 24) x^{11664} + (2 \times 2^{n+2} - 5) x^{20736}.$$

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

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

$$HKV_1(TD_2[n], x) = \sum_{uv \in E(G)} x^{\left[M_G(u) + M_G(v)\right]^2}$$
$$= 2^{n+2} x^{5^2} + (2^{n+2} - 4) x^{9^2} + 2^{n+2} x^{11^2} + (7 \times 2^{n+2} - 16) x^{12^2}$$
$$+ (11 \times 2^{n+2} - 24) x^{12^2} + (2^{n+2} - 4) x^{15^2} + (3 \times 2^{n+2} - 8) x^{18^2}$$
$$+ (8 \times 2^{n+2} - 24) x^{21^2} + (2 \times 2^{n+2} - 5) x^{24^2}.$$

By simple calculation, we get the desired result.

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

$$HKV_2\left(TD_2[n],x\right)=\sum_{uv\in E(G)} x^{\left[M_G(u)M_G(v)\right]^2}$$
$$=2^{n+2}x^{6^2}+\left(2^{n+2}-4\right)x^{18^2}+2^{n+2}x^{24^2}+\left(7\times 2^{n+2}-16\right)x^{36^2}$$
$$+\left(11\times 2^{n+2}-24\right)x^{48^2}+\left(2^{n+2}-4\right)x^{54^2}+\left(3\times 2^{n+2}-8\right)x^{72^2}$$
$$+\left(8\times 2^{n+2}-24\right)x^{108^2}+\left(2\times 2^{n+2}-5\right)x^{144^2}.$$

By simple calculation, we get the desired result.

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

a) $SqKV\left(TD_2[n]\right)=268\times 2^{n+2}-672$

b) $SqKV\left(TD_2[n],x\right)=\left(9\times 2^{n+2}-21\right)x^0+2^{n+2}x^1+\left(11\times 2^{n+2}-21\right)x^4$
$+\left(10\times 2^{n+2}-32\right)x^9+2^{n+2}x^{25}+\left(3\times 2^{n+2}-8\right)x^{36}.$

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

(a) By using equation (5) and Table 1, we derive

$$SqKV\left(TD_2[n]\right)=\sum_{uv\in E(G)}\left[M_G(u)-M_G(v)\right]^2$$
$$=(2-3)^2 2^{n+2}+(2-6)^2\left(2^{n+2}-4\right)+(3-8)^2 2^{n+2}+(6-6)^2\left(7\times 2^{n+2}-16\right)$$
$$+(6-8)^2\left(11\times 2^{n+2}-24\right)+(6-9)^2\left(2^{n+2}-4\right)+(6-12)^2\left(3\times 2^{n+2}-8\right)$$
$$+(9-12)\left(8\times 2^{n+2}-24\right)+(12-12)\left(2\times 2^{n+2}-5\right).$$
$$=268\times 2^{n+2}-672.$$

(b) By using equation (6) and Table 1, we derive

$$SqKV\left(TD_2[n],x\right)=\sum_{uv\in E(G)} x^{\left[M_G(u)-M_G(v)\right]^2}$$
$$=2^{n+2}x^1\left(2^{n+2}-4\right)x^9+2^{n+2}x^{25}\left(7\times 2^{n+2}-16\right)x^0+\left(11\times 2^{n+2}-24\right)x^4$$
$$+\left(2^{n+2}-4\right)x^9+\left(3\times 2^{n+2}-8\right)x^{36}+\left(8\times 2^{n+2}-24\right)x^9+\left(2\times 2^{n+2}-5\right)x^0$$
$$=\left(9\times 2^{n+2}-12\right)x^0+2^{n+2}x^1\left(11\times 2^{n+2}-24\right)x^4+\left(10\times 2^{n+2}-32\right)x^9$$
$$+2^{n+2}x^{25}+\left(3\times 2^{n+2}-8\right)x^{36}.$$

3. POPAM DENDRIMERS

We now focus on the graph of POPAM dendrimers. This family of dendrimers is symbolized by $POD_2[n]$, where n is the steps of growth in this type of dendrimers. The graph of $POD_2[2]$ is depicted in Figure 2.

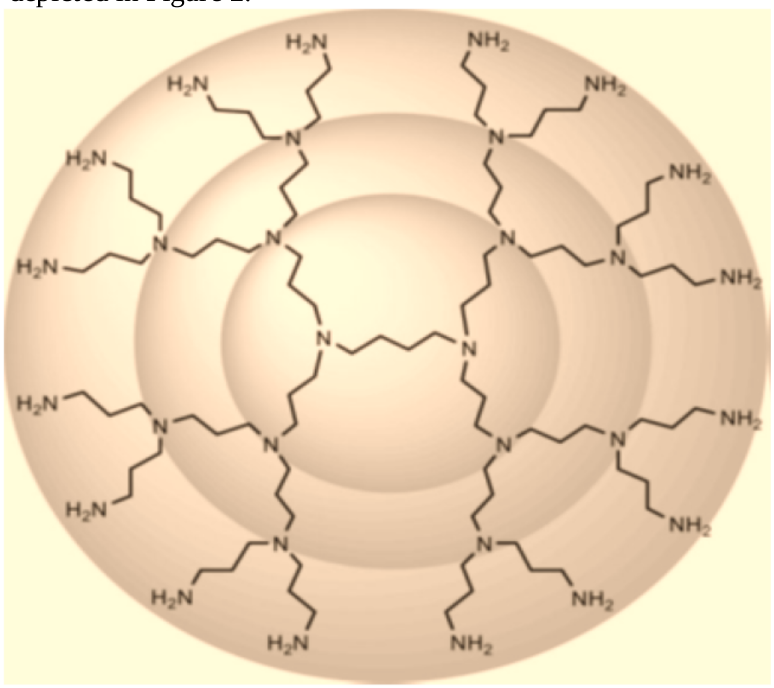

Figure 2. The graph of $POD_2[2]$

Let G be the graph of a POPAM dendrimer $POD_2[n]$. By calculation, we obtain that G has $2^{n+5} - 10$ vertices and $2^{n+5} - 11$ edges. Also by calculation, 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 $POD_2[n]$

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

Theorem 4. The first and second hyper *KV* indices of POPAM dendrimer $POD_2[n]$ are given by

a) $HKV_1(POD_2[n]) = 940 \times 2^{n+2} - 1712.$

b) $HKV_2(POD_2[n]) = 8720 \times 2^{n+2} - 17024.$

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

(a) By using equation (1) and Table 2 we obtain

$$HKV_1\left(POD_2[n]\right)=\sum_{uv\in E(G)}\left[M_G(u)+M_G(v)\right]^2$$

$= (2+2)^2\, 2^{n+2} + (2+4)^2\, 2^{n+2} + (4+4)^2 + (4+6)^2\,(3\times2^{n+2} - 6)+(6+8)^2(3\times2^{n+2} - 6)$

By calculation, we get the desired result.

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

$$HKV_2\left(POD_2[n]\right)=\sum_{uv\in E(G)}\left[M_G(u)M_G(v)\right]^2$$

$= (2\times2)^2\, 2^{n+2} + (2\times4)^2\, 2^{n+2} + (4\times4)^2 + (4\times6)^2\,(3\times2^{n+2} - 6)+(6\times8)^2(3\times2^{n+2} - 6)$

By calculation, we get the desired result.

Theorem 5. The first and second hyper *KV* polynomials of a POPAM dendrimer $POD_2[n]$ are

a) $HKV_1(POD_2[n]) = 2^{n+2}\, x^{16} + 2^{n+2}\, x^{36} + x^{64} + (3\times2^{n+2} - 6)\, x^{100} + (3\times2^{n+2} - 6)\, x^{196}$.

b) $HKV_2(POD_2[n]) = 2^{n+2}\, x^{16} + 2^{n+2}\, x^{64} + x^{256} + (3\times2^{n+2} - 6)x^{576} + (3\times2^{n+2} - 6)\, x^{2304}$.

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

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

$$HKV_1\left(POD_2[n],x\right)=\sum_{uv\in E(G)}x^{\left[M_G(u)+M_G(v)\right]^2}$$

$$=2^{n+2}x^{(2+2)^2}+2^{n+2}x^{(2+4)^2}+x^{(4+2)^2}+\left(3\times2^{n+2}-6\right)x^{(4+6)^2}+\left(3\times2^{n+2}-6\right)x^{(6+8)^2}$$

By calculation, we get the desired result.

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

$$HKV_2\left(POD_2[n],x\right)=\sum_{uv\in E(G)}x^{\left[M_G(u)M_G(v)\right]^2}$$

$$=2^{n+2}x^{(2\times2)^2}+2^{n+2}x^{(2\times4)^2}+x^{(4\times4)^2}+\left(3\times2^{n+2}-6\right)x^{(4\times6)^2}+3\times2^{n+2}x^{(6\times8)^2}$$

By calculation, we get the desired result.

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

a) $SqKV(POD_2[n]) = 28 \times 2^{n+2} - 48$.

b) $SqKV(POD_2[n], x) = (1+2^{n+2})x^0 + (7\times2^{n+2} - 12)x^4$.

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

(a) By using equation (5) and Table 2, we obtain

$$SqKV_1\left(POD_2[n]\right)=\sum_{uv\in E(G)}x^{\left[M_G(u)-M_G(v)\right]^2}$$

$=(2-2)^2\,2^{n+2}+(2-4)^2\,2^{n+2}+(4-4)^2+(4-6)^2\left(3\times2^{n+2}-6\right)+(6-8)^2\left(3\times2^{n+2}-6\right)$ By calculation, we get the desired result.

(b) By using equation (6) and Table 2, we obtain

$$SqKV\left(POD_2[n],x\right)=\sum_{uv\in E(G)} x^{\left[M_G(u)M_G(v)\right]^2}$$

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

By calculation, we get the desired result.

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