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General Fifth M-Zagreb Indices and Fifth M-Zagreb Polynomials of PAMAM Dendrimers

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Abstract. A molecular graph or a chemical graph is a simple graph related to the structure of a chemical compound. In this paper, we introduce the general fifth M-Zagreb indices and fifth M_3-Zagreb index and their polynomials of a molecular graph. Also we compute the general fifth *M*-Zagreb indices and fifth M_3-Zagreb index of PAMAM dendrimer graphs. Finally, we compute the fifth M_3-Zagreb polynomial of PAMAM dendrimer graphs.

Keywords: general fifth M_1-Zagreb index, general fifth M_2-Zagreb index, fifth M_3-Zagreb index, PAMAM dendrimer.

AMS Mathematics Subject Classification (2010): 05C69, 05C07, 05C35

1. Introduction

All graphs considered here are finite, undirected without isolated vertices, loops and multiple edges. For all further notation and terminology we refer the reader to [1].

A molecular graph is simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edge to the bonds between atoms.

Let $S_G(u)$ denote the sum of the degrees of all vertices adjacent to a vertex u. We introduce the general fifth *M*-Zagreb indices of a molecular graph *G* as

$$M_1^aG_5(G)=\sum_{uv\in E(G)}\left[S_G(u)+S_G(v)\right]^a, \qquad M_2^aG_5(G)=\sum_{uv\in E(G)}\left[S_G(u)S_G(v)\right]^a. \tag{1}$$

In [2], Graovac et al. defined fifth *M* -Zagreb indices as

$$M_1G_5(G)=\sum_{uv\in E(G)}\left[S_G(u)+S_G(v)\right], \qquad M_2G_5(G)=\sum_{uv\in E(G)}S_G(u)S_G(v).$$

We introduce the fifth hyper-M-Zagreb indices as

$$HM_1G_5(G)=\sum_{uv\in E(G)}\left[S_G(u)+S_G(v)\right]^2, \quad HM_2G_5(G)=\sum_{uv\in E(G)}\left[S_G(u)S_G(v)\right]^2.$$

We define a new version of third Zagreb index or fifth M_3-Zagreb index as

$$M_3G_5(G)=\sum_{uv\in E(G)}\left|S_G(u)-S_G(v)\right|. \tag{2}$$

Corresponding the above indices, we define the Zagreb polynomials as follows:

The general fifth M_1-Zagreb polynomial and the general fifth M_2-Zagreb polynomial of a molecular graph G are defined as

$$M_1^aG_5(G,x)=\sum_{uv\in E(G)}x^{[S_G(u)+S_G(v)]^a}, \qquad M_2^aG_5(G,x)=\sum_{uv\in E(G)}x^{[S_G(u)S_G(v)]^a}. \tag{3}$$

The fifth M_1-Zagreb polynomial and fifth M_2-Zagreb polynomial of a molecular graph G are defined as

$$M_1G_5(G,x)=\sum_{uv\in E(G)}x^{S_G(u)+S_G(v)}, \qquad M_2G_5(G,x)=\sum_{uv\in E(G)}x^{S_G(u)S_G(v)}.$$

The fifth hyper- M_1-Zagreb polynomial and fifth hyper- M_2-Zagreb polynomial of a molecular graph G are defined as

$$HM_1G_5(G,x)=\sum_{uv\in E(G)}x^{[S_G(u)+S_G(v)]^2}, \qquad HM_2G_5(G,x)=\sum_{uv\in E(G)}x^{[S_G(u)S_G(v)]^2}.$$

Recently, some polynomials were studied, for example, in [3,4] and also some topological indices were studied, for example, in [5,6,7,8,9,10,11].

2. PAMAM Dendrimer

We consider the PAMAM dendrimers with n growth stages, denoted by $PD_1[n]$ for every $n \geq 0$, see Figure 1 [12].

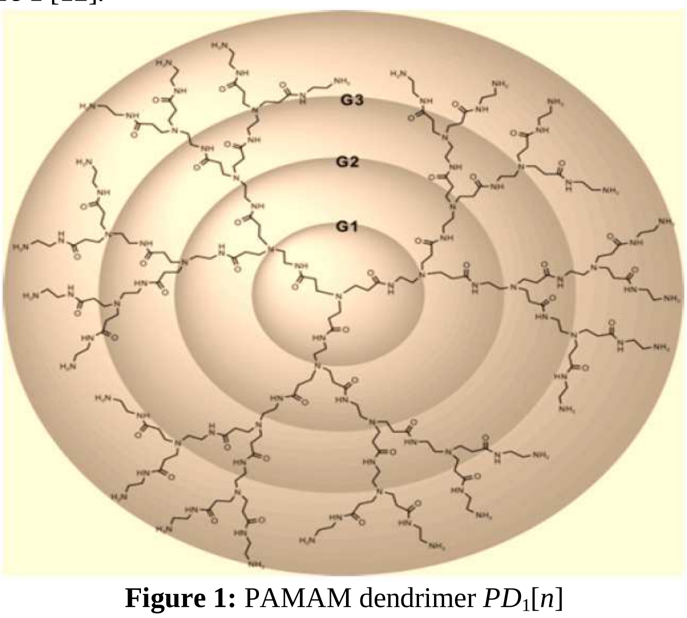

Figure 1: PAMAM dendrimer $PD_1[n]$

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 1.

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

Table 1: Edge partition of $PD_1[n]$

Theorem 1. The general fifth M_1-Zagreb index of a PAMAM dendrimer is

$$M_1^aG_5(PD_1[n]) = 3\times2^n(5^a+7^a)+(6\times2^n-3)8^a+(9\times2^n-6)9^a+(18\times2^n-9)10^a+(9\times2^n-6)11^a$$

Proof: From equation (1) and Table 1, we have

$$M_1^aG_5(PD_1[n]) = \sum_{uv\in E(G)}\left[S_G(u)+S_G(v)\right]^a$$

$$=3\times2^n5^a+3\times2^n7^a+(6\times2^n-3)8^a+(9\times2^n-6)9^a+(18\times2^n-9)10^a+(9\times2^n-6)11^a$$

Corollary 1.1. The fifth M_1-Zagreb index of a PAMAM dendrimer is

$$M_1G_5(PD_1[n]) = M_1^1G_5(PD_1[n]) = 444\times2^n-234.$$

Corollary 1.2. The fifth M_1-Zagreb index of a PAMAM dendrimer is

$$HM_1G_5(PD_1[n] = M_1^2G_5(PD_1[n] = 4224\times2^n-2304.$$

Theorem 2. The general fifth M_2-Zagreb index of a PAMAM dendrimer is

$$M_2^aG_5(PD_1[n]) = 3\times2^n(6^a+12^a)+(6\times2^n-3)15^a+(9\times2^n-6)20^a+(18\times2^n-9)25^a+(9\times2^n-6)30^a.$$

Proof: From equation (1) and Table 1, we have

$$M_2^aG_5(PD_1[n]) = \sum_{uv\in E(G)}\left[S_G(u)S_G(v)\right]^a$$

$$=3\times2^n6^a+3\times2^n12^a+(6\times2^n-3)15^a+(9\times2^n-6)20^a+(18\times2^n-9)25^a+(9\times2^n-6)20^a$$

Corollary 2.1. The fifth M_2-Zagreb index of a PAMAM dendrimer is

$$M_2G_5(PD_1[n]) = M_2^1G_5(PD_1[n]) = 1044\times2^n-570.$$

Corollary 2.2. The fifth M_2-Zagreb index of a PAMAM dendrimer is

$$HM_2G_5(PD_1[n]) = M_2^2G_5(PD_1[n]) = 24840\times2^{\mathrm{n}}-14100.$$

Theorem 3. The fifth M_3-Zagreb index of a PAMAM dendrimer is

$$M_3G_5(PD_1[n]) = 48\times2^n-24.$$

Proof: From equation (2) and Table 1, we have

$$M_3G_5(PD_1[n]) = \sum_{uv\in E(G)}\left|S_G(u)-S_G(v)\right|$$

$$=3\times2^n+3\times2^n+(6\times2^n-3)4+(9\times2^n-6)+(18\times2^n-9)0+(9\times2^n-6)$$

$= 48\times 2^n - 24.$

Theorem 4. The general fifth M_1-Zagreb polynomial of a PAMAM dendrimer is
$M_1^aG_5(PD_1[n],x) = 3\times 2^n x^{5^a} + 3\times 2^n x^{7^a} + (6\times 2^n - 3)x^{8^a} + (9\times 2^n - 6)x^{9^a} + (18\times 2^n - 9)x^{10^a} + (9\times 2^n - 6)x^{11^a}.$

Proof: From equation (3) and Table 1, we have

$$M_1^aG_5(PD_1[n],x) = \sum_{uv\in E(G)} x^{[S_G(u)+S_G(v)]^a}$$

$$= 3\times 2^n x^{5^a} + 3\times 2^n x^{7^a} + (6\times 2^n - 3)x^{8^a} + (9\times 2^n - 6)x^{9^a} + (18\times 2^n - 9)x^{10^a} + (9\times 2^n - 6)x^{11^a}.$$

Corollary 4.1. The fifth M_1-Zagreb polynomial of a PAMAM dendrimer is

$$M_1G_5(PD_1[n],x) = 3\times 2^n x^5 + 3\times 2^n x^7 + (6\times 2^n - 3)x^8 + (9\times 2^n - 6)x^9 + (18\times 2^n - 9)x^{10} + (9\times 2^n - 6)x^{11}$$

Corollary 4.2. The fifth M_1-Zagreb polynomial of a PAMAM dendrimer is

$$HM_1G_5(PD_1[n],x) = 3\times 2^n x^{25} + 3\times 2^n x^{49} + (6\times 2^n - 3)x^{64} + (9\times 2^n - 6)x^{81} + (18\times 2^n - 9)x^{100} + (9\times 2^n - 6)x^{121}$$

Theorem 5. The general fifth M_2-Zagreb polynomial of a PAMAM dendrimer is

$$M_2^aG_5(PD_1[n],x) = 3\times 2^n x^{6^a} + 3\times 2^n x^{12^a} + (6\times 2^n - 3)x^{15^a}. + (9\times 2^n - 6)x^{20^a} + (18\times 2^n - 9)x^{25^a} + (9\times 2^n - 6)x^{30^a}$$

Proof: From equation (3) and Table 1, we have

$$M_2^aG_5(PD_1[n],x) = \sum_{uv\in E(G)} x^{[S_G(u)S_G(v)]^a}$$

$$= 3\times 2^n x^{6^a} + 3\times 2^n x^{12^a} + (6\times 2^n - 3)x^{15^a} + (9\times 2^n - 6)x^{20^a} + (18\times 2^n - 9)x^{25^a} + (9\times 2^n - 6)x^{30^a}.$$

Corollary 5.1. The fifth M_2 –Zagreb polynomial of a PAMAM dendrimer is

$$M_2G_5(PD_1[n],x) = 3\times 2^n x^6 + 3\times 2^n x^{12} + (6\times 2^n - 3)x^{15} + (9\times 2^n - 6)x^{20} + (18\times 2^n - 9)x^{25} + (9\times 2^n - 6)x^{30}.$$

Corollary 5.2. The fifth hyper- M_2 –Zagreb polynomial of a PAMAM dendrimer is

$$HM_2G_5(PD_1[n],x) = 3\times 2^n x^{36} + 3\times 2^n x^{144} + (6\times 2^n - 3)x^{225} + (9\times 2^n - 6)x^{400} + (18\times 2^n - 9)x^{625} + (9\times 2^n - 6)x^{900}.$$

Theorem 6. The fifth M_3-Zagreb polynomial of a PAMAM dendrimer is

$$M_3G_5\left(PD_1[n],x\right)=\left(6\times 2^n-3\right)x^2+\left(24\times 2^n-12\right)x+\left(18\times 2^n-9\right).$$

Proof: From Table 1, we have

$$M_3G_5\left(PD_1[n],x\right)=\sum_{uv\in E(G)} x^{\left|S_G(u)-S_G(v)\right|}$$

$$=3\times 2^n x+3\times 2^n x+\left(6\times 2^n-3\right)x^2+\left(9\times 2^n-6\right)x$$

$$+\left(18\times 2^n-9\right)x^0+\left(9\times 2^n-6\right)x$$

$$=\left(6\times 2^n-3\right)x^2+\left(24\times 2^n-12\right)x+\left(18\times 2^n-9\right).$$

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