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GENERAL ZAGREB POLYNOMIALS AND *F*-POLYNOMIAL OF CERTAIN NANOSTRUCTURES

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ABSTRACT

We introduce the general first and second Zagreb polynomails of a molecular graph. In this paper, we compute the general first and second Zagreb polynomails of certain nanostructures. Also we determine the first and second Zagreb polynomials, the first and second hyper-Zagreb polynomials and F-polynomial of these nanostructures.

Keywords: *zagreb polynomial, hyper-zagreb polynomials, F-polynomial, nanostructure.*

Mathematics Subject Classification: *05C05, 05C12, 05C90.*

1. INTRODUCTION

We consider only finite, connected, undirected graphs without loops and multiple edges. Let G be a 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. For other undefined notations and terminology, we refer to [1].

In [2], Fath-Tabar defined the first and second Zagreb polynomials of a graph G. They are defined as

$$M_1(G,x)=\sum_{uv\in E(G)} x^{d_G(u)+d_G(v)}, \qquad M_2(G,x)=\sum_{uv\in E(G)} x^{d_G(u)d_G(v)}.$$

Recently in [3] Chal*uv*araju *et al.* defined the first and second hyper-Zagreb polynomials of a graph G. They are defined as

$$HM_1(G,x)=\sum_{uv\in E(G)} x^{\left[d_G(u)+d_G(v)\right]^2}, \qquad HM_2(G,x)=\sum_{uv\in E(G)} x^{\left[d_G(u)d_G(v)\right]^2}.$$

Motivated by these definitions, we define the general first and second Zagreb polynomials of a graph as follows:

The general first and second Zagreb polynomials of a graph G are defined as

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

In [4], Furtula *et al.* defined F-index or forgotten topological index of a graph G and it is defined as

$$F(G)=\sum_{uv\in E(G)}\left[d_G(u)^2+d_G(v)^2\right].$$

The F-polynomial [5] of a graph G is defined as

$$F(G,x)=\sum_{uv\in E(G)} x^{d_G(u)^2+d_G(v)^2}$$

In this paper, the general first and second Zagreb polynomials, F-polynomial of some nanostructures are determined. For more information about nanostructures see [6, 7, 8, 9].

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2. LINEAR [n] TETRACENE

The molecular graph of a linear [n]-tetracene is shown in Figure 1.

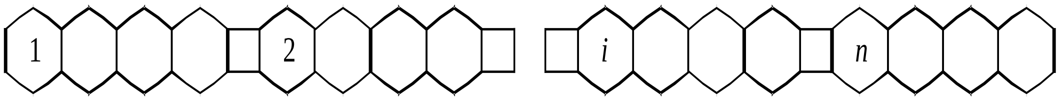

Figure-1: The molecular graph of a linear [n]-tetracene.

By algebraic method, we get that a linear [n]-tetracene has $18n$ vertices and $23n - 2$ edges. Let T be the graph of a linear [n]-tetracene. We have three partitions of the edge set $E(T)$ as follows:

$E_4 = \{uv \in E(T) \ / \ d_T(u) = d_T(v) = 2\}$, $|E_4| = 6$,
$E_5 = \{uv \in E(T) \ / \ d_T(u) = 2, d_T(v) = 3\}$, $|E_5| = 16n - 4$,
$E_6 = \{uv \in E(T) \ / \ d_T(u) = d_T(v) = 3\}$, $|E_6| = 7n - 4$,

Theorem 1: The general first Zagreb polynomial of a linear [n]-tetracene graph T is

$$M_1^a(T,x) = 6x^{4^a} + (16n-4)x^{5^a} + (7n-4)x^{6^a}.$$

Proof: For the general first Zagreb polynomial of a linear [n]-tetracene graph T, we have

$$\begin{aligned} M_1^a(T,x) &= \sum_{uv\in E(T)} x^{[d_T(u)+d_T(v)]^a} \\ &= \sum_{E_4} x^{[d_T(u)+d_T(v)]^a} + \sum_{E_5} x^{[d_T(u)+d_T(v)]^a} + \sum_{E_6} x^{[d_T(u)+d_T(v)]^a} \\ &= 6x^{4^a} + (16n-4)x^{5^a} + (7n-4)x^{6^a}. \end{aligned}$$

Corollary 1.1: The first Zagreb polynomial of a linear [n]-tetracene graph T is

$$M_1(T,x) = M_1^1(T,x) = 6x^4 + (16n-4)x^5 + (7n-4)x^6.$$

Corollary 1.2: The first hyper-Zagreb polynomial of a linear [n]-tetracene graph T is

$$HM_1(T,x) = M_1^2(T,x) = 6x^{16} + (16n-4)x^{25} + (7n-4)x^{36}.$$

Theorem 2: The general second Zagreb polynomial of a linear [n]-tetracene graph T is

$$M_2^a(T,x) = 6x^{4^a} + (16n-4)x^{6^a} + (7n-4)x^{9^a}.$$

Proof: For the general second Zagreb polynomial of a linear [n]-tetracene graph T, we have

$$\begin{aligned} M_2^a(T,x) &= \sum_{uv\in E(T)} x^{[d_T(u)d_T(v)]^a} \\ &= \sum_{E_4} x^{[d_T(u)d_T(v)]^a} + \sum_{E_5} x^{[d_T(u)d_T(v)]^a} + \sum_{E_6} x^{[d_T(u)d_T(v)]^a} \\ &= 6x^{4^a} + (16n-4)x^{6^a} + (7n-4)x^{9^a}. \end{aligned}$$

Corollary 2.1: The second Zagreb polynomial of a linear [n]-tetracene graph T is

$$M_2(T,x) = M_2^1(T,x) = 6x^4 + (16n-4)x^6 + (7n-4)x^9.$$

Corollary 2.2: The first hyper-Zagreb polynomial of a linear [n]-tetracene graph T is

$$HM_2(T,x) = M_2^2(T,x) = 6x^{16} + (16n-4)x^{36} + (7n-4)x^{81}.$$

Theorem 3: The F-polynomial of a linear [n]-tetracene graph T is

$$F(T,x) = 6x^8 + (16n-4)x^{13} + (7n-4)x^{18}.$$

Proof: For the F-polynomial of a linear [n]-tetracene graph T, we have

$$F(T,x) = \sum_{uv\in E(G)} x^{d_T(u)^2 + d_T(v)^2}$$

$$= \sum_{E_4} x^{d_T(u)^2+d_T(v)^2} + \sum_{E_5} x^{d_T(u)^2+d_T(v)^2} + \sum_{E_6} x^{d_T(u)^2+d_T(v)^2}$$
$$= 6x^8 + (16n-4)x^{13} + (7n-4)x^{18}.$$

3. NANOSTRUCTURE $F = F[p, q]$

The molecular graph of a nanostructure $F = F[p, q]$ with $p = 2$ and $q = 4$ is shown in Figure 2.

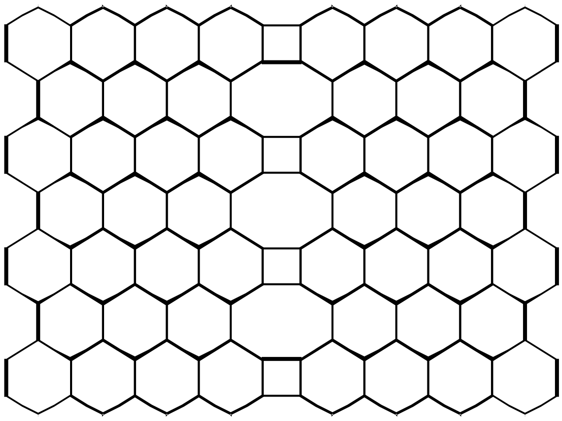

Figure-2: The graph of a nanostructure $F = F[2, 4]$

Let F be the graph of a nanostructure $F = F[p, q]$. By algebraic method, we see that F has $18p$ vertices and $27pq - 2q - 4p$ edges. We have three partitions of the edge set $E(F)$ as follows:

$E_4 = \{uv \in E(F) \,/\, d_F(u) = d_F(v) = 2\}$, $|E_4| = 2q + 4$,
$E_5 = \{uv \in E(F) \,/\, d_F(u) = 2,\ d_F(v) = 3\}$, $|E_5| = 16p + 4q - 8$.
$E_6 = \{uv \in E(F) \,/\, d_F(u) = d_F(v) = 3\}$, $|E_6| = 27pq - 20p - 8q + 4$.

Theorem 4: The general first Zagreb polynomial of a nanostructure graph F is
$$M_1^a(F,x) = (2q+4)x^{4^a} + (16p+4q-8)x^{5^a} + (27pq-20p-8q+4)x^{6^a}.$$

Proof: For the general first Zagreb polynomial of a nanostructure graph F, we have
$$M_1^a(F,x) = \sum_{uv\in E(F)} x^{[d_F(u)+d_F(v)]^a}$$
$$= \sum_{E_4} x^{[d_F(u)+d_F(v)]^a} + \sum_{E_5} x^{[d_F(u)+d_F(v)]^a} + \sum_{E_6} x^{[d_F(u)+d_F(v)]^a}$$
$$= (2q+4)x^{4^a} + (16p+4q-8)x^{5^a} + (27pq-20p-8q+4)x^{6^a}.$$

Corollary 4.1: The first Zagreb polynomial of a nanostructure graph F is
$$M_1(F,x) = M_1^1(F,x) = (2q+4)x^4 + (16p+4q-8)x^5 + (27pq-20p-8q+4)x^6.$$

Corollary 4.2: The first hyper-Zagreb polynomial of a nanostructure graph F is
$$HM_1(F,x) = M_1^2(F,x) = (2q+4)x^{16} + (16p+4q-8)x^{25} + (27pq-20p-8q+4)x^{36}.$$

Theorem 5: The general second Zagreb polynomial of a nanostructure graph F is
$$M_2^a(F,x) = (2q+4)x^{4^a} + (16p+4q-8)x^{6^a} + (27pq-20p-8q+4)x^{9^a}.$$

Proof: For the general second Zagreb polynomial nanostructure graph F, we have
$$M_2^a(F,x) = \sum_{uv\in E(F)} x^{[d_F(u)d_F(v)]^a}$$
$$= \sum_{E_4} x^{[d_F(u)d_F(v)]^a} + \sum_{E_5} x^{[d_F(u)d_F(v)]^a} + \sum_{E_6} x^{[d_F(u)d_F(v)]^a}$$
$$= (2q+4)x^{4^a} + (16p+4q-8)x^{6^a} + (27pq-20p-8q+4)x^{9^a}.$$

Corollary 5.1: The second Zagreb polynomial of a nanostructure graph F is

$$M_2(F,x) = M_2^1(F,x) = (2q+4)x^4 + (16p+4q-8)x^6 + (27pq-20p-8q+4)x^9.$$

Corollary 5.2: The first hyper-Zagreb polynomial of a nanostructure graph F is

$$HM_2(F,x) = M_2^2(F,x) = (2q+4)x^{16} + (16p+4q-8)x^{36} + (27pq-20p-8q+4)x^{81}.$$

Theorem 6: The F-polynomial of a nanostructure graph F is

$$F(F,x) = (2q+4)x^8 + (16p+4q-8)x^{13} + (27pq-20p-8q+4)x^{18}.$$

Proof: For the F-polynomial of a nanostructure graph F, we have

$$\begin{aligned} F(F,x) &= \sum_{uv\in E(F)} x^{d_F(u)^2+d_F(v)^2} \\ &= \sum_{E_4} x^{d_F(u)^2+d_F(v)^2} + \sum_{E_5} x^{d_F(u)^2+d_F(v)^2} + \sum_{E_6} x^{d_F(u)^2+d_F(v)^2} \\ &= (2q+4)x^8 + (16p+4q-8)x^{13} + (27pq-20p-8q+4)x^{18}. \end{aligned}$$

4. NANOSTRUCTURE $G = G[p, q]$

The molecular graph of a nanostructure $G = G[p, q]$ with $p = 2$ and $q = 4$ is shown in Figure 3.

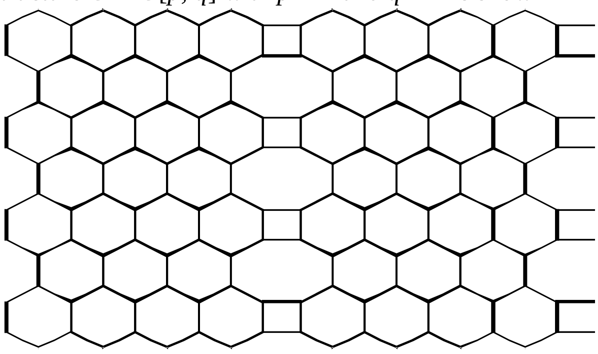

Figure-3: The graph of a nanostructure $G = G[2, 4]$

Let G be the graph of a nanostructure $G = G[p, q]$. By algebraic method, we see that G has $18pq$ vertices and $27pq - 4q$ edges. We have two partitions of the edge set $E(G)$ as follows:

$E_5 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_5| = 16p$,

$E_6 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_6| = 27pq - 20p$.

Theorem 7: The general first Zagreb polynomial of a nanostructure graph G is

$$M_1^a(G,x) = 16x^{5^a} + (27pq-20p)x^{6^a}.$$

Proof: For the general first Zagreb polynomial nanostructure graph G, we have

$$\begin{aligned} M_1^a(G,x) &= \sum_{uv\in E(G)} x^{[d_G(u)+d_G(v)]^a} \\ &= \sum_{E_5} x^{[d_G(u)+d_G(v)]^a} + \sum_{E_6} x^{[d_G(u)+d_G(v)]^a} \\ &= 16px^{5^a} + (27pq-20p)x^{6^a}. \end{aligned}$$

Corollary 7.1: The first Zagreb polynomial of a nanostructure graph G is

$$M_1(G,x) = M_1^1(G,x) = 16px^5 + (27pq-20p)x^6.$$

Corollary 7.2: The first hyper-Zagreb polynomial of a nanostructure graph G is

$$HM_1(G,x) = M_1^2(G,x) = 16px^{25} + (27pq-20p)x^{36}.$$

Theorem 8: The general second Zagreb polynomial of a nanostructure graph G is

$$M_2^a(G,x) = 16px^{6^a} + (27pq-20p)x^{9^a}.$$

Proof: For the general second Zagreb polynomial of a nanostructure graph G, we have

$$M_2^a(G,x) = \sum_{uv\in E(G)} x^{[d_G(u)d_G(v)]^a}$$
$$= \sum_{E_5} x^{[d_G(u)d_G(v)]^a} + \sum_{E_6} x^{[d_G(u)d_G(v)]^a}$$
$$= 16px^{6^a} + (27pq-20p)x^{9^a}.$$

Corollary 8.1: The second Zagreb polynomial of a nanostructure graph G is

$$M_2(G,x) = M_2^1(G,x) = 16px^6 + (27pq-20p)x^9.$$

Corollary 8.2: The second hyper-Zagreb polynomial of a nanostructure graph G is

$$HM_2(G,x) = M_2^2(G,x) = 16px^{36} + (27pq-20p)x^{81}.$$

Theorem 9: The F-polynomial of a nanostructure graph G is

$$F(G,x) = 16px^{13} + (27pq-20p)x^{18}.$$

Proof: For the F-polynomial of a nanostructure graph G, we have

$$F(G,x) = \sum_{uv\in E(G)} x^{d_G(u)^2+d_G(v)^2}$$
$$= \sum_{E_5} x^{d_G(u)^2+d_G(v)^2} + \sum_{E_6} x^{d_G(u)^2+d_G(v)^2}$$
$$= 16px^{13} + (27pq-20p)x^{18}.$$

5. NANOSTRUCTURE *K = K*[*p, q*]

The molecular graph of a nanostructure $K = K[p, q]$ with $p = 2$ and $q = 3$ is shown in Figure 4.

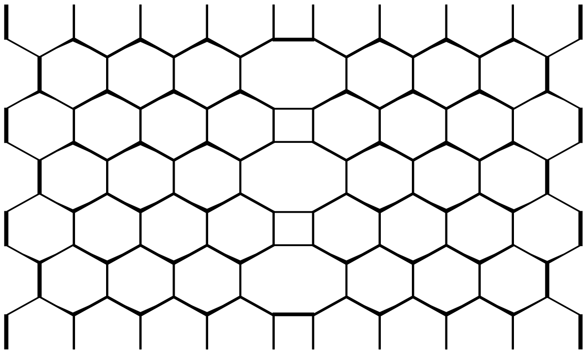

Figure-4: The graph of a nanostructure $K = K[2, 3]$

Let K be the graph of a nanostructure $K = K[p, q]$. By algebraic method, we see that K has $18pq$ vertices and $27pq - 2q$ edges. We have three partitions of the edge set $E(K)$ as follows:

$E_4 = \{uv . E(K) / d_K(u) = d_K(v) = 2\}$, $|E_4| = 2q$.
$E_5 = \{uv . E(K) / d_K(u) = 2, d_K(v) = 3\}$, $|E_5| = 4q$.
$E_6 = \{uv . E(K) / d_K(u) = d_K(v) = 3\}$, $|E_6| = 27pq - 8q$.

Theorem 10: The general first Zagreb polynomial of a nanostructure graph K is

$$M_1^a(K,x) = 2qx^{4^a} + 4qx^{5^a} + (27pq-8q)x^{6^a}.$$

Proof: For the general first Zagreb polynomial of a nanostructure graph K, we have

$$M_1^a(K,x) = \sum_{uv\in E(K)} x^{[d_K(u)+d_K(v)]^a}$$
$$= \sum_{E_4} x^{[d_K(u)+d_K(v)]^a} + \sum_{E_5} x^{[d_K(u)+d_K(v)]^a} + \sum_{E_6} x^{[d_K(u)+d_K(v)]^a}$$
$$= 2qx^{4^a} + 4qx^{5^a} + (27pq-8q)x^{6^a}.$$

Corollary 10.1: The first Zagreb polynomial of a nanostructure graph *K* is

$$M_1(K,x) = M_1^1(K,x) = 2qx^4 + 4qx^5 + (27pq - 8q)x^6.$$

Corollary 10.2: The first hyper-Zagreb polynomial of a nanostructure graph *K* is

$$HM_1(K,x) = M_1^2(K,x) = 2qx^{16} + 4qx^{25} + (27pq - 8q)x^{36}.$$

Theorem 11: The general second Zagreb polynomial of a nanostructure graph *K* is

$$M_2^a(K,x) = 2qx^{4^a} + 4qx^{6^a} + (27pq - 8q)x^{9^a}.$$

Proof: For the general second Zagreb polynomial of a nanostructure graph *K*, we have

$$M_2^a(K,x) = \sum_{uv\in E(K)} x^{[d_K(u)d_K(v)]^a}$$
$$= \sum_{E_4} x^{[d_K(u)d_K(v)]^a} + \sum_{E_5} x^{[d_K(u)d_K(v)]^a} + \sum_{E_6} x^{[d_K(u)d_K(v)]^a}$$
$$= 2qx^{4^a} + 4qx^{6^a} + (27pq - 8q)x^{9^a}.$$

Corollary 11.1: The second Zagreb polynomial of a nanostructure graph *K* is

$$M_2(K,x) = M_2^1(K,x) = 2qx^4 + 4qx^6 + (27pq - 8q)x^9.$$

Corollary 11.2: The first hyper-Zagreb polynomial of a nanostructure graph *K* is

$$HM_2(K,x) = M_2^2(K,x) = 2qx^{4^a} + 4qx^{6^a} + (27pq - 8q)x^{9^a}.$$

Theorem 12: The *F*-polynomial of a nanostructure graph *K* is

$$F(K,x) = 2qx^8 + 4qx^{13} + (27pq - 8q)x^{18}.$$

Proof: For the *F*- polynomial of a nanostructure graph *K*, we have

$$F(K,x) = \sum_{uv\in E(K)} x^{d_K(u)^2 + d_K(v)^2}$$
$$= \sum_{E_4} x^{d_K(u)^2 + d_K(v)^2} + \sum_{E_5} x^{d_K(u)^2 + d_K(v)^2} + \sum_{E_6} x^{d_K(u)^2 + d_K(v)^2}$$
$$= 2qx^8 + 2qx^{13} + (27pq - 8q)x^{18}.$$

6. NANOSTRUCTURE *L* = *L*[*p*, *q*]

The molecular graph of a nanostructure $L = L[p, q]$ with $p = 2$ and $q = 4$ is shown in Figure 5.

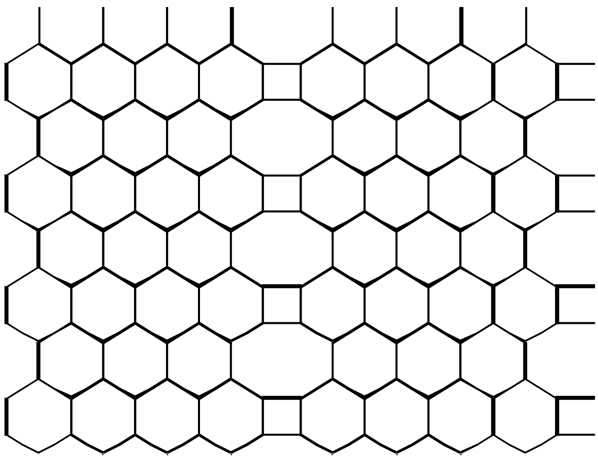

Figure-5: The graph of a nanostructure $L = L[2, 4]$

Let *L* be the graph of a nanostructure $L = L[p, q]$. By algebraic method, we see that *L* has $18pq$ vertices and $27pq$ edges. We have only one partition of the edge set $E(L)$ as follows:

$E_6 = \{uv \in E(L) \,/\, d_L(u) = d_L(v) = 3\}$, $|E_6| = 27pq$.

Theorem 13: The general first Zagreb polynomial of a nanostructure graph *L*, we have

$$M_1^a\left(L,x\right)=27\,pqx^{6^a}.$$

Proof: For the general first Zagreb polynomial of a nanostructure graph *L*, we have

$$M_1^a\left(L,x\right)=\sum_{uv\in E(L)} x^{\left[d_L(u)+d_L(v)\right]^a}=27\,pqx^{6^a}.$$

Corollary 13.1: The first Zagreb polynomial of a nanostructure graph *L* is

$$M_1\left(L,x\right)=M_1^1\left(L,x\right)=27\,pqx^{6}.$$

Corollary 13.2: The first hyper-Zagreb polynomial of a nanostructure graph *L* is

$$HM_1\left(L,x\right)=M_1^2\left(L,x\right)=27\,pqx^{36}.$$

Theorem 14: The general second Zagreb polynomial of a nanostructure graph *L*, is

$$M_2^a\left(L,x\right)=27\,pqx^{9^a}.$$

Proof: For the general second Zagreb polynomial of a nanostructure graph *L*, we have

$$M_2^a\left(L,x\right)=\sum_{uv\in E(L)} x^{\left[d_L(u)d_L(v)\right]^a}=27\,pqx^{9^a}.$$

Corollary 14.1: The second Zagreb polynomial of a nanostructure graph *L* is

$$M_2\left(L,x\right)=M_2^1\left(L,x\right)=27\,pqx^{9}.$$

Corollary 14.2: The second hyper-Zagreb polynomial of a nanostructure graph *L* is

$$HM_2\left(L,x\right)=M_2^2\left(L,x\right)=27\,pqx^{81}.$$

Theorem 15: The *F*-polynomial of a nanostructure graph *L* is

$$F\left(L,x\right)=27\,pqx^{18}.$$

Proof: For the *F*-polynomial of a nanostructure graph *L*, we have

$$F\left(L,x\right)=\sum_{uv\in E(L)} x^{d_L(u)^2+d_L(v)^2}=27\,pqx^{18}.$$

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