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F-INDEX AND REFORMULATED ZAGREB INDEX OF CERTAIN NANOSTRUCTURES

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ABSTRACT

Chemical graph theory is a branch of graph theory whose focus of interest is to finding totological indices of chemical graphs, which correlate well with chemical properties of the chemical molecules. In this paper, we determine the F-index, reformulated first Zagrab index and general reformulated Zagreb index of linear [n]- Tetracene, V-Tetracenic nanotube, H-Tetracenic nanotube and Tetracenic nanotori.

Mathematics Subject Classification: *05C12, 05C35, 05C90.*

Key works: *molecular graph, F-index, reformulated first Zagreb index, nanostructures.*

1. INTRODUCTION

Let G be a finite, simple and connected graph with a vertex set $V(G)$ and an edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. The degree of an edge $e = uv$ in G is defined by $d_G(e) = d_G(u) + d_G(v) - 2$. We refer to [1] for undefined term and notation.

A molecular graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edges to the bonds between atoms. A topological index is a numerical parameter mathematically derived from the graph structure. These indices are useful for establishing correlation between the structure of a molecular compound and its physico-chemical properties.

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

$$M_1(G) = \sum_{v\in V(G)} d_G(v)^2,$$

$$M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v).$$

These indices were introduced by Gutman *et al*. in [2].

Another vertex degree based topological index was defined in [2], where the Zagreb indices were proposed and that was shown to influence the total π-electron energy (ε). Recently it was studied by Furtula *et al.* in [3]. They named this index as forgotten topological index or *F*-index. This index is defined as

$$F(G) = \sum_{v\in V(G)} d_G(v)^3.$$

It is easy to see that

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

Miličević *et al* [5] reformulated the first Zagreb index in terms of edge-edge instead of vertex degree:

$$EM_1(G) = \sum_{e\in E(G)} d_G(e)^2.$$

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The use of these descriptors in *QSPR* study was discussed in their paper [5]. The reformulated Zagreb indices were studied for example in [6, 7]. Many other topological indices were studied, for example, in [8, 9, 10, 11, 12, 13, 14, 15 16, 17, 18, 19, 20]

The general reformulated Zagreb index of a graph *G* is defined as

$$EM_1^a(G) = \sum_{e \in E(G)} d_G(e)^a,$$

where *a* is a real number.

In this paper, we compute the *F*-index, general reformulated Zagreb index of certain nanostructures.

2. RESULTS FOR LINEAR [*n*]-TETRACENE

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

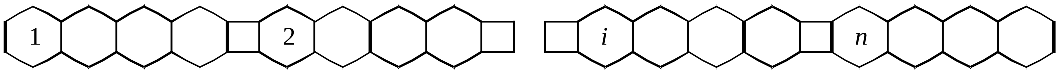

Figure-1: The molecular graph of a linear [*n*]-Tetracene

We determine the exact values of *F*-index and general reformulated first Zagreb index of a linear [*n*]- Tetracane.

Theorem 2.1: Let *T* be a linear [*n*]-Tetracene. Then

(i) $F(T) = 334\,n - 76$ (1)

(ii) $EM_1^a(T) = 6 \times 2^a + (16n-4) \times 3^a + (7n-4)\,4^a.$ (2)

Proof: Let *T* be the graph of a linear [*n*]-Tetracene. From Figure 1, one can easily check that $V(T) = 18n$ and $E(T) = 23n - 2$. In *T*, there are three types of edges based on the degree of the vertices of each edge. Further, by algebraic method, the edge degree partition of a linear [*n*]-tetracene *T* is given in Table 1.

$d_T(u), d_T(v) \setminus e = uv \in E(T)$	$E_4 = (2,2)$	$E_5 = (3,2)$	$E_6 = (3,3)$
$d_T(e)$	2	3	4
Number of edges	6	$16n - 4$	$7n - 4$

Table-1: Edge degree partition of *T*.

(i) Now to compute $F(T)$, we see that

$$F(T) = \sum_{uv \in E_4} \left(d_T(u)^2 + d_T(v)^2\right) + \sum_{uv \in E_5} \left(d_T(u)^2 + d_T(v)^2\right) + \sum_{uv \in E_6} \left(d_T(u)^2 + d_T(v)^2\right)$$

$$= (2^2+2^2)\times 6 + (3^2+2^2)(16n-4) + (3^2+3^2)(7n-4) = 334n - 76.$$

(ii) To compute $EM_1^a(T)$, we see that

$$EM_1^a(T) = \sum_{e \in E(G)} d_T(e)^a = \sum_{e \in E_4} d_T(e)^a + \sum_{e \in E_5} d_T(e)^a + \sum_{e \in E_6} d_T(e)^a$$

$$= 2^a \times 6 + 3^a(16n-4) + 4^a(7n-4).$$

An immediate corollary is the reformulated first Zagreb index of a linear [*n*]-Tetracene.

Corollary 2.2: Let T be a linear [*n*]-Tetracene. Then

$$EM_1(T) = 256n - 76.$$

Proof: Put $a = 2$ in equation (2), we get the desired result.

3. RESULTS FOR NANOSTRUCTURE *F = F[p, q]*

The molecular graph of 2-*D* lattice with of $F = F[p, q]$ with $p = 2$ and $q = 4$ is shown in Figure 2.

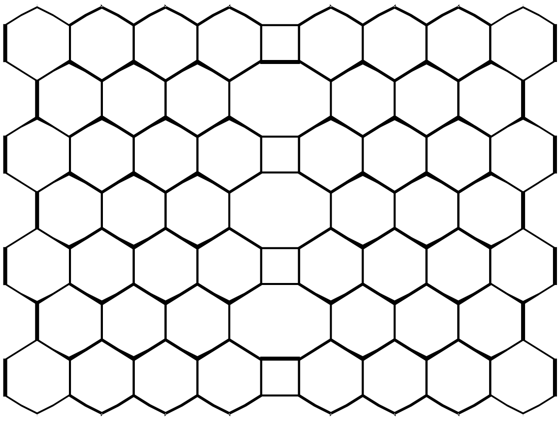

Figure-2: The graph of 2-D lattice of $F = F[p, q]$ with $p = 2$ and $q = 4$

We compute the F-index and general reformulated first Zagreb index of a nanostructure $F = F[p, q]$.

Theorem 3.1: Let $F = F[p, q]$ be a nanostructure. Then

(i) $F(F[p, q]) = 486\,pq - 152p - 76q.$ (3)

(ii) $EM_1^a\left(F\left[p,q\right]\right) = 27\times 4^a\,pq + \left(16\times 3^a - 20\times 4^a\right)p + \left(2\times 2^a + 4\times 3^a - 8\times 4^a\right)q + 4\times 2^a - 8\times 3^a + 4\times 4^a$ (4)

Proof: Let $F = F\,[p, q]$ be a nanostructure as shown in Figure 2. By algebraic method, we have $|V(F)| = 18p$ and $|E(F)| = 27pq - 2q - 4p$. Further, the edge degree partition of a nanostructure F is given in Table 2.

$d_F(u), d_F(v) \setminus e = uv \in E(F)$	$E_4 = (2,2)$	$E_5 = (3,2)$	$E_6 = (3,3)$
$d_F(e)$	2	3	4
Number of edges	$2q + 4$	$16p+4q - 8$	$27pq - 20p - 8q + 4$

Table-2: Edge degree partition of $F = F(p, q)$

(i) Now to determine $F(F)$, we see that

$$F(F) = \sum_{uv\in E(F)} \left(d_F(u)^2 + d_F(v)^2\right)$$

$$= \sum_{uv\in E_4} \left(d_F(u)^2 + d_F(v)^2\right) + \sum_{uv\in E_5} \left(d_F(u)^2 + d_F(v)^2\right) + \sum_{uv\in E_6} \left(d_F(u)^2 + d_F(v)^2\right)$$

$$= \left(2^2 + 2^2\right)\left(2q+4\right) + \left(3^2 + 2^2\right)\left(16p + 4q - 8\right) + \left(3^2 + 3^2\right)\left(27pq - 20p - 8q + 4\right)$$

$$= 486pq - 152p - 76q.$$

(ii) To determine $EM_1^a(F)$, we see that

$$EM_1^a(F) = \sum_{e\in E(F)} d_F(e)^2 = \sum_{e\in E_4} d_F(e)^2 + \sum_{e\in E_5} d_F(e)^2 + \sum_{e\in E_6} d_F(e)^2$$

$$= 2^a\left(2q+4\right) + 3^a\left(16p + 2q - 8\right) + 4^a\left(27pq - 20p - 8q + 4\right)$$

$$= 27\times 4^a\,pq + \left(16\times 3^a - 20\times 4^a\right)p + \left(2\times 2^a + 4\times 3^a - 8\times 4^a\right)q + 4\times 2^a - 8\times 2^a + 4\times 4^a.$$

An immediate corollary is the reformulated first Zagreb index of a nanostructure F.

Corollary 3.2: Let $F = F[p, q]$ be a nanostructure. Then

$$EM_1(F[p,q]) = 432pq - 176p - 84q + 8.$$

Proof: Put $a = 2$ in equation (4), we get the desired result.

4. RESULTS FOR NANOSTRUCTURE $G = G\,[p, q]$.

The modular graph of 2-D lattice of $G=G[p, q]$ with $p = 2$ and $q = 4$ is shown in Figure 3.

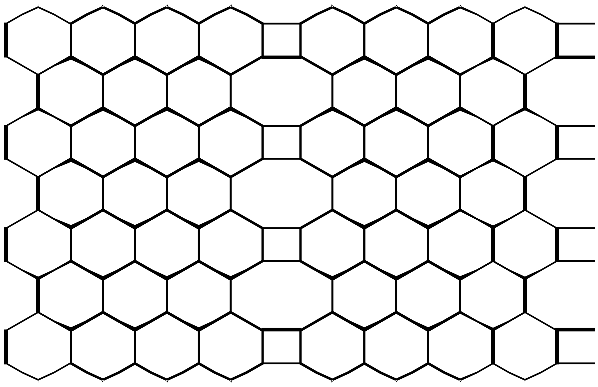

Figure-3: The graph of 2-*D* lattice of $G = G\,[p, q]$ with $p = 2$ and $q = 4$

We determine the *F*-index and general reformulated first Zagreb index of a nonstructure $G = G[p, q]$.

Theorem 4.1: Let $G = G\,[p, q]$ be a nanostructure. Then

(i) $F(G) = 486pq - 152p.$ (5)

(ii) $EM_1^{a}(G) = 27 \times 4^a pq + (16 \times 3^a - 20 \times 4^a)p.$ (6)

Proof: Let $G = G[p, q]$ be a nanostructure as shown in Figure 3. By Algebraic method, we have $|V(G)| = 18pq$ and $E(G) = 27pq - 4q$. In G, there are two types of edges based on the degree of the vertices of each edge. Further, by algebraic method, the edge degree partition of a nanostructure G is given in Table 3.

$d_G(u), d_G(v) \backslash e = uv \in E(G)$	$E_5 = (3, 2)$	$E_6 = (3, 3)$
$d_G(e)$	3	4
Number of edges	$16p$	$27pq - 20p$

Table-3: Edge degree partition of G

(i) Now to compute $F(G)$,we see that

$$F(G) = \sum_{uv \in E(G)} \left(d_G(u)^2 + d_G(v)^2\right) = \sum_{uv \in E_5} \left(d_G(u)^2 + d_G(v)^2\right) + \sum_{uv \in E_6} \left(d_G(u)^2 + d_G(v)^2\right)$$

$$= (3^2+2^2)16p + (3^2 + 3^2)(27pq - 20p) = 486pq - 152p.$$

(ii) To compute $EM_1^{a}(G)$, we see that

$$EM_1^a(G) = \sum_{e \in E(G)} d_G(e)^a = \sum_{e \in E_5} d_G(e)^a + \sum_{e \in E_6} d_G(e)^a$$

$$= 3^a \times 16p + 4^a \times (27pq - 20p) = 27 \times 4^a pq + (16 \times 3^a - 20 \times 4^a)\, p.$$

An immediate corollary is the reformulated first Zagreb index of a nanostructure G.

Corollary 4.2: Let $G = G[p, q]$ be a nanostructure. Then

$$EM_1(G) = 432\,pq - 176\,p$$

Proof: Put $a = 2$ in equation (6), we get the desired result.

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

The molecular graph of 2-*D* lattice of $K = K\,[p, q]$ with $p = 2$ and $q = 3$ is shown in Figure 4.

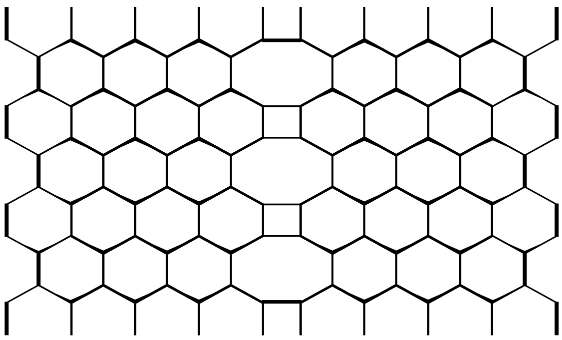

Figure 4: The graph of 2-D lattice of $K = K[p, q]$ with $p = 2$ and $q = 3$

In the following theorem, we compute the F-index and general reformulated first Zagreb index of a nanostructure $K = K[p, q]$.

Theorem 5.1: Let $K = K[p, q]$ be a nanostructure. Then

(i) $F(K[p, q]) = 486pq - 76q$. (7)

(ii) $EM_1^a (K[p, q]) = 27 \times 4^a (pq) + (2 \times 2^a + 4 \times 3^a - 8 \times 4^a)q$. (8)

Proof: Let $K = K[p, q]$ be a nanostructure as shown in Figure 4. By algebraic method, we have $|V(K)| = 18pq$ and $|E(K)| = 27pq - 2q$. In K, there are three types of edges based on the degree of the vertices of each edge. Further, by algebraic method, the edge degree partition of a nanostructure K is given in Table 4.

$d_K(u), d_K(v) \setminus e = uv \in E(K)$	$E_4 = (2,2)$	$E_5 = (3,2)$	$E_6 = (3,3)$
$d_K(e)$	2	3	4
Number of edges	$2q$	$4q$	$27pq - 8q$

Table-4: Edge degree partition of K.

(i) Now to compute $F(K)$, we see that

$$F(K) = \sum_{uv \in E(K)} \left(d_K(u)^2 + d_K(v)^2\right)$$

$$= \sum_{uv \in E_4} \left(d_K(u)^2 + d_K(v)^2\right) + \sum_{uv \in E_5} \left(d_K(u)^2 + d_K(v)^2\right) + \sum_{uv \in E_6} \left(d_K(u)^2 + d_K(v)^2\right)$$

$$= \left(2^2 + 2^2\right)2q + \left(3^2 + 2^2\right)4q + \left(3^2 + 3^2\right)\left(27pq - 8q\right) = 486pq - 76q.$$

(ii) To compute $EM_1^a [K]$, we see that

$$EM_1^a(K) = \sum_{e \in E(K)} d_K(e)^a = \sum_{e \in E_4} d_K(e)^a + \sum_{e \in E_5} d_K(e)^a + \sum_{e \in E_6} d_K(e)^a$$

$$= 2^a \times 2q + 3^a \times 4q + 4^a \times \left(27pq - 8q\right) = 27 \times 4^a\, pq + \left(2 \times 2^a + 4 \times 3^a - 8 \times 4^a\right)q\,.$$

An immediate corollary in the reformulated first Zagreb index of a nanostructure K.

Corollary 5.2: Let $K = K[p, q]$ be a nanostructure. Then

$EM_1(K) = 432\, pq - 84\, q.$

Proof: Put $a = 2$ in equation (8), we get the desired result.

6. RESULTS FOR NANOSTRUCTURE $L = L\,[p, q]$

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

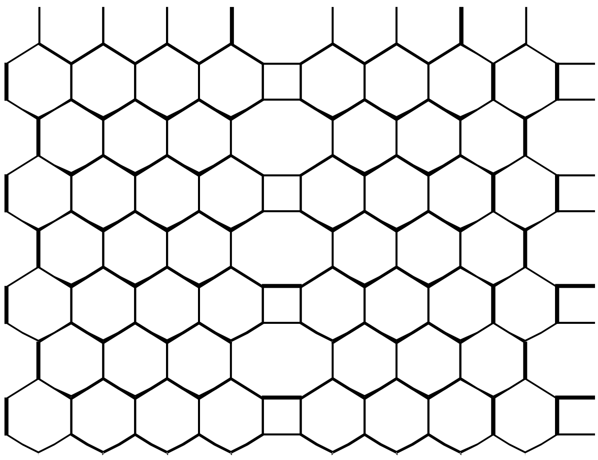

Figure-5: The graph of 2-D lattice of $L = L[p, q]$ with $p = 2$ and $q = 4$.

In the following theorem, we compute the F-index and general reformulated first Zagreb index of a nanostructure $L = L[p, q]$.

Theorem 6: Let $L = [p, q]$ be a nanostructure. Then

(i) $F(L[p, q]) = 486pq$. (9)

(ii) $EM_1^a(L[p, q]) = 4^a \times 27pq$. (10)

Proof: Let $L = L[p, q]$ be a nanostructure as shown in Figure 5. By algebraic method, we have $|V(L)| = 18pq$ and $|E(L)| = 27pq$. Further the edge degree partition of the nanostructure $L = L[p, q]$ is given in Table 5.

$d_L(u), d_L(v) \setminus e = uv \in E(L)$	$E_6 = (3,3)$
$d_L(e)$	4
Number of edges	$27pq$

Table-5: Edge partition of L.

(i) Now to compute $F(L)$, we see that

$$F(L) = \sum_{uv \in E_6} \left(d_L(u)^2 + d_L(v)^2\right) = \left(3^2 + 3^2\right) 27pq = 486pq$$

(ii) To compute $EM_1^a(L)$, we see that

$$EM_1^a(L) = \sum_{uv \in E_6} d_L(e)^a = 4^a \times 27pq.$$

An immediate corollary is the reformulated first Zagrab index of a nanostructure L.

Corollary 6.2: Let $L=L[p, q]$ be a nanostructure Then $EM_1(L) = 432pq$.

Proof: Put $a = 2$ in equation (10), we get the desired result.

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