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First and Second Zagreb polynomials of $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$nanotubes

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ABSTRACT

Let $G = (V,E)$ be a simple connected graph. The sets of vertices and edges of G are denoted by $V = V(G)$ and $E = E(G)$, respectively. There exist many topological indices and connectivity indices in graph theory. The First and Second Zagreb indices were first introduced by *Gutman* and *Trinajstić* in 1972. It is reported that these indices are useful in the study of anti-inflammatory activities of certain chemical instances, and in elsewhere. In this paper, we focus on the structure of "$G = VC_5C_7[p,q]$" and "$H = HC_5C_7[p,q]$" nanotubes and counting First Zagreb index $Zg_1(G) = \sum_{v\in V(G)} d_v^2$ and Second Zagreb index $Zg_2(G) = \sum_{e=uv\in E(G)} (d_u \times d_v)$ of G and H, as well as First Zagreb polynomial $Zg_1(G,x) = \sum_{e=uv\in E(G)} x^{d_u+d_v}$ and Second Zagreb polynomial $Zg_2(G,x) = \sum_{e=uv\in E(G)} x^{d_u\times d_v}$.

***Keywords*:** Nanotubes; Molecular graph; Zagreb index; Zagreb Polynomial

1. INTRODUCTION

Let G be a simple molecular graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, the distance between the vertices u and v of G is denoted by $d_G(u,v)$ (or $d(u,v)$ for short) and it is defined as the number of edges in a minimal path connecting vertices u and v [3,16,17].

In graph theory, we have many different connectivity index and topological index of arbitrary graph G. A topological index is a numeric quantity from the structural graph of a molecule which is invariant under graph automorphisms. Usage of topological indices in chemistry began in 1947 when chemist *Harold Wiener* developed the most widely known topological descriptor.

The Wiener index $W(G)$ is the oldest topological indices, (based structure descriptors) [4,10,14,15,18,19], which have very chemical applications, mathematical properties and defined as follow:

$$W(G)=\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} d(u,v)$$

An important topological index introduced more than forty years ago by *I. Gutman* and *Trinajstić* is Zagreb index $Zg_1(G)$ (or, more precisely, the First Zagreb index, because there exists also a Second Zagreb index, $Zg_2(G)$[17]). First Zagreb index $Zg_1(G)$ of the graph G is defined as the sum of the squares of the degrees of all vertices of G. They are defined as:

$$Zg_1(G) = \sum_{v\in V(G)} d_v^2 \text{ or } \sum_{e=uv\in E(G)} \left(d_u + d_v\right)$$

$$Zg_2(G) = \sum_{e=uv\in E(G)} \left(d_u \times d_v\right)$$

where d_u and d_v are the degrees of u and v, respectively.

Also, we have *First Zagreb polynomial* $Zg_1(G,x)$ and *Second Zagreb polynomial* $Zg_2(G,x)$ for two above topological indices. They are defined as [1,6-9]:

$$Zg_1(G,x) = \sum_{e=uv\in E(G)} x^{d_u+d_v}$$

$$Zg_2(G,x) = \sum_{e=uv\in E(G)} x^{d_u d_v}$$

The mathematical properties of these topological indices can be found in some recent papers [1-3,6-9,17]. In this paper, we focus on First Zagreb polynomial, Second Zagreb polynomial and their topological indices of "$G = VC_5C_7[p,q]$" and "$H = HC_5C_7[p,q]$" nanotubes.

2. RESULTS AND DISCUSSION

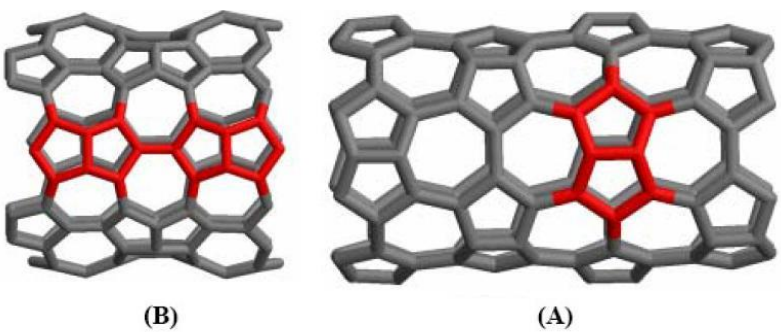

Fig. 1. The Molecular graph of VC_5C_7 (A) and HC_5C_7 (B) nanotubes.

Molecular graphs ”$VC_5C_7[p,q]$” and ”$HC_5C_7[p,q]$” are tow family of nanotubes, such that their structure are consist of cycles with length five and seven by different compound. In other words, a C_5C_7 net is a trivalent decoration made by alternating C_5 and C_7. It can cover either a cylinder or a torus. For a review, historical details and further bibliography see the 3-dimensional lattice of ”$VC_5C_7[p,q]$” and ”$HC_5C_7[p,q]$” nanotubes in Figure 1 and their 2-dimensional lattice in Figure 2 and Figure 3, respectively and references [6,11-13].

On the other hands, to achieve our aims and counting our favorites indices of ”$VC_5C_7[p,q]$” and ”$HC_5C_7[p,q]$” nanotubes, we need to the following definition.

Definition 1.

[5,6] Let $G = (V;E)$ be a simple connected graph and d_v is degree of vertex $v\in V(G)$ (Obviously $1\leq \delta \leq d_v \leq \Delta \leq n-1$, such that $\delta = Min\{ d_v|v\in V(G)\}$ and $\Delta = Max\{d_v|v\in V(G)\}$). We divide the edge set $E(G)$ and the vertex set $V(G)$ of graph G to several partitions, as follow:

$$\forall k: \delta\leq k\leq \Delta,\ V_k = \{v\in V(G)|\ d_v = k\}$$
$$\forall i: 2\delta\leq i\leq 2\Delta,\ E_i = \{e = uv\in E(G)|d_u + d_v = i\}$$
$$\forall j: \delta^2\leq j\leq \Delta^2,\ E_j{}^* = \{uv\in E(G)|d_u\times d_v = j\}.$$

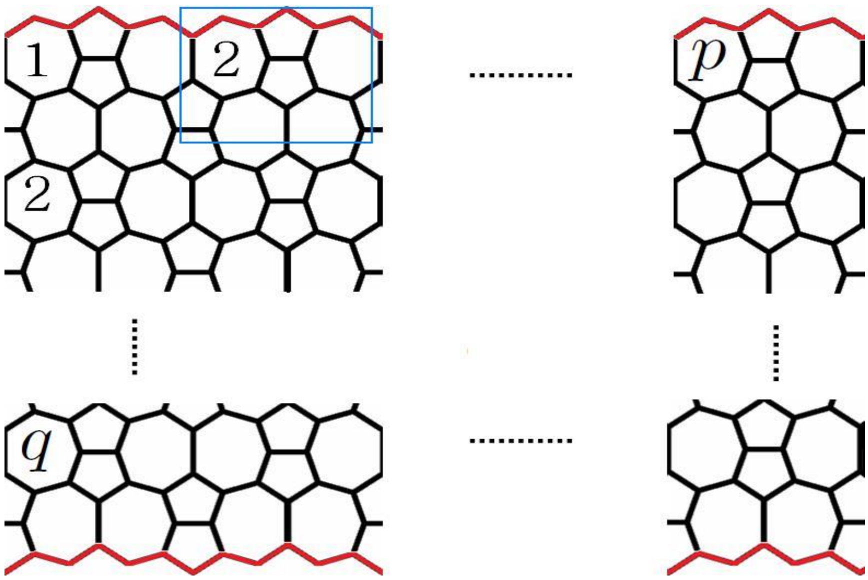

Fig. 2. 2-Dimensional Lattice of G = $VC_5C_7[p,q]$.

Now, by these terminologies, we have following theorems.

Theorem 1. Let G be $VC_5C_7[p,q]$ nanotubes. Then:

- First Zagreb polynomial of G is equal to

$$Zg_1\ (VC_5C_7[p,q],x) = (24pq - 6p)x^{\,6} + (12p)x^{\,5}.$$

So First Zagreb index of G is $Zg_1(VC_5C_7[p,q])$ = 144pq + 24p.

- Second Zagreb polynomial of G is equal to

$$Zg_2(VC_5C_7[p,q],x) = (24pq - 6p)x^{9} + (12p)x^{6}$$

So Second Zagreb index of G is $Zg_2(VC_5C_7[p,q]) = 216pq + 18p$.

Proof.

Consider nanotubes $G = VC_5C_7[p,q]$, wedenote the number of pentagons in the first row by p, in this nanotubes the four first rows of vertices and edges are repeated alternatively, we denote the number of this repetition by q. Hence the number of vertices in this nanotubes is equal to $(\forall p,q \in N)\ n = |V(VC_5C_7[p,q])| = 16pq + 6p$. Since $|V_2| = 3p + 3p$ and $|V_3| = 16pq$, thus $e = |E(VC_5C_7[p,q])| = \frac{1}{2}(2(6p) + 3(16pq)) = 24pq + 6p$.

So, we mark the edges of $E5$, E_6* by red color and the edges of $E6$, E_9* by black color, in Figure 2. Thus, we have the number of $6p+6p$ and $24pq-6p$ members edges of edge set E_5 (or E_6*) and E_6 (or E_9*) of $G=VC_5C_7[p,q]$, respectively. Now, by according to Definition 1;

$$Zg_1(G,x) = \sum_{e \in E(G)} x^{d_u + d_v} = \sum_{e \in E_6} x^6 + \sum_{e \in E_5} x^5.$$

So, First Zagreb polynomial of $VC_5C_7[p,q]$ is

$$Zg_1(VC_5C_7[p,q], x) = (24pq - 6p)x^{6} + (12p)x^{5}$$

and Second Zagreb polynomial of $VC_5C_7[p,q]$ is equal to

$$Zg_2(VC_5C_7[p,q], x) = (24pq - 6p)x^{9} + (12p)x^{6}$$

By according to the definition of First Zagreb index and Second Zagreb index, we have following equations:

$$Zg_1(VC_5C_7[p,q]) = \sum_{v \in V(G)} d_v^2 = 6p \times (2^2) + 16pq \times (3^2) = 144pq + 24p.$$

and

$$Zg_2(VC_5C_7[p,q]) = \frac{\partial Zg_2(G,x)}{\partial x}\Big|_{x=1} = (24pq - 6p) \times 9\} + 12p \times 6\} = 216pq + 18p$$

Here, we complete the proof of Theorem 1.

Theorem 2.

Let H be"$HC_5C_7[p,q]$"nanotubes. Then:

- First Zagreb polynomial of H is equal to

$$Zg_1(HC_5C_7[p,q], x) = (12pq - 4p)x^6 + (8p)x^5 + (p)x^4.$$

So First Zagreb index of H is $Zg_1(HC_5C_7[p,q]) = 72pq + 20p$

- Second Zagreb polynomial of H is equal to

$$Zg_2(HC_5C_7[p,q], x) = (12pq - 4p)x^9 + (8p)x^6 + (p)x^4.$$

So Second Zagreb index of H is $Zg_2(HC_5C_7[p,q]) = 108pq + 16p$.

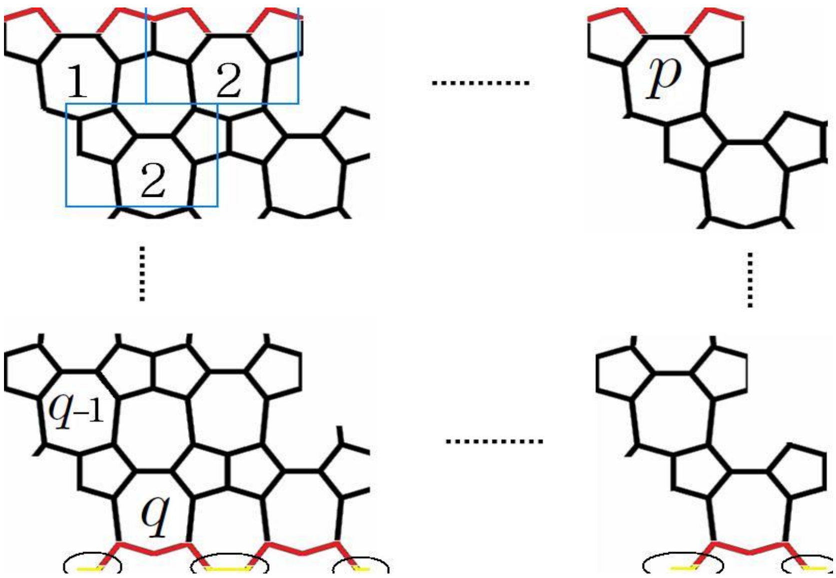

Fig. 3. 2-Dimensional Lattice of H = $HC_5C_7[p,q]$.

Proof.

Consider nanotubes $H = HC_5C_7[p,q]$. This nanotubes consists of heptagon and pentagon nets. We denote the number of heptagons in the first row by p. In this nanotubes the four first rows of vertices and edges are repeated alternatively, we denote the number of this repetition by q. Hence the number of vertices in this nanotubes is equal to $n = |V(HC_5C_7[p,q])| = 8pq + 5p$, then $(\forall p,q \in N)$ $e = |E(HC_5C_7[p,q])| = 12pq + 5p$. Because $|V_2| = 2p + 3p$ and $|V_3| = 8pq$, thus $e = \frac{1}{2}(2(5p) + 3(8pq))$.

So, we mark the members of E_4, E_4* by yellow color, the members of E_5, E_6* by red color and the members of E_6, E_9* by black color, in Figure 3. On the other hand, there are the number of p, $4p + 4p$ and $12pq - 4p$ members edges of edge set E_4 (or E_4*), E_5 (or E_6*) and E_6 (or E_9*), respectively.

Thus, we have following computations for Zagreb polynomials of $HC_5C_7[p,q]$:

$$Zg_1(H,x) = \sum_{e\in E(H)} x^{d_u+d_v} = \sum_{e\in E_6} x^6 + \sum_{e\in E_5} x^5 + \sum_{e\in E_4} x^4$$

and

$$Zg_2(H,x) = \sum_{e \in E(H)} x^{d_u + d_v} = \sum_{e \in E_9^*} x^9 + \sum_{e \in E_6^*} x^5 + \sum_{e \in E_4^*} x^4.$$

So, First Zagreb polynomial and Second Zagreb polynomial of $H=HC_5C_7[p,q]$ are equal to

$$Zg_1(H,x) = (12pq - 4p)x^6 + (8p)x^5 + (p)x^4$$

and
$$Zg_2(H,x) = (12pq - 4p)x^9 + (8p)x^6 + (p)x^4,$$

respectively. Also, we have following equations for First Zagreb index and Second Zagreb index

$$Zg_1(HC_5C_7[p,q]) = \frac{\partial Zg_1(G,x)}{\partial x}|_{x=1} = 6\times(12pq - 4p) + 5\times 8p + 4\times p = 72pq + 20p.$$

and

$$Zg_2(HC_5C_7[p,q]) = 9\times(12pq - 4p) + 6\times 8p + 4\times p = 108pq + 16p.$$

3. CONCLUSION

In this paper, we compute two important topological polynomials and their indices called ”Zagreb” of Two families of nanotubes "$VC_5C_7[p,q]$" and "$HC_5C_7[p,q]$". These topological polynomials and their indices are useful for surveying structure of nanotubes, that have relation with degrees of their vertices and communications their edges.

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