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TOPOLOGICAL INDICES BASED END-VERTEX DEGREES OF EDGES ON NANOTUBES

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Abstract. In this research, we give some theoretical results, for the first, second, third and modified second Zagreb indices, Randić index, geometric-arithmetic index, atom-bond connectivity index and Zagreb polynomials of $VAC_5C_6C_7$ and $HAC_5C_6C_7$ nanotubes.

Keywords: Vertex-degree-based indices, Zagreb indices, connectivity indices, $VAC_5C_6C_7$ nanotube, $HAC_5C_6C_7$ nanotube.

AMS Subject Classification: 05C07, 13A99**.**

1. Introduction

Chemical graph theory is a branch of graph theory whose focus of interest is finding topological indices of chemical graphs (i.e. graphs that represent chemical molecules) which correlate well with chemical properties of the corresponding molecules. A molecular graph is a collection of points representing the atoms in the molecule and set of lines representing the covalent bonds. These points are named vertices and the lines are named edges in graph theory language. A topological index is a map from the set of chemical compounds represented by molecular graphs to the set of real numbers. Many topological indices are closely correlated with some physico-chemical character -istics of the underlying compounds. Carbon nanotubes are nano-objects that have raised great expectations in a number of different applications, including field emission, energy storage, molecular electronics, atomic force microscopy, and many others. In recent years, there has been considerable interest in the general problem of determining topological indices different research area [3, 11, 13, 17].

The aim of the present article is to compute the some topological indices and polynomials in a famous family of nanotubes.

2. Preliminaries

We present the basic definitions related to the topological indices chosen for the present study. All graphs considered in this study are finite, simple and connected graphs (without loops and multiple edges). For a connected graph G, $V(G)$ and $E(G)$ denote the set of vertices and edges, and $|V(G)|$ and $|E(G)|$ the numbers of vertices and edges, respectively. The degree d_u of a vertex $u \in V(G)$ is the number of vertices of G adjacent to u. In the early work of the Zagreb Mathematical Chemistry Group on the topological basis of the π-electron energy, two terms appeared in the topological formula for the total π-energy of conjugated molecules [9], which were first used as branching indices [10] and later as topological indices in QSPR and QSAR studies.

For a (molecular) graph G, the *first Zagreb index* is equal to the sum of the squares of the degrees of the vertices, and the *second Zagreb index* is equal to the sum of the products of the degrees of pairs of adjacent vertices. In fact,

$$M_1(G) = \sum_{u \in V(G)} {d_u}^2, \quad M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v).$$

Also, one can rewrite the *first Zagreb index* as:

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v).$$

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

$$M_1(G,x) = \sum_{uv \in E(G)} x^{(d_u+d_v)}, \quad M_2(G,x) = \sum_{uv \in E(G)} x^{(d_u \times d_v)},$$

where *x* is a dummy variable. For more study about polynomial in graph theory you can see [1, 2, 6, 8, 12].

A recently proposed variant of the second Zagreb index, which is defined as [14]:

$$M_2^*(G) = \sum_{uv \in E(G)} \frac{1}{d_u \times d_v},$$

is known under the name *modified second Zagreb index*.

The *third Zagreb index* were first introduced by Fath-Tabar [7]. This index is defined as follows:

$$M_3(G) = \sum_{uv \in E(G)} |d_u - d_v|.$$

Among topological indices, connectivity indices are very important and they have a prominent role in chemistry. Oldest topological connectivity index is Randić *index* of a connected graph G and introduced by M. Randić [15] (in 1975), who has shown this index to reflect molecular branching and was defined as follows:

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

The *geometric-arithmetic index* is another topological index based on degrees of vertices defined by Vukičević and Furtula [16]:

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

Estrada et al. [4, 5] introduced *atom-bond connectivity index*, which it has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows:

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

3. Main results

In this section, we calculated the first, second, third and modified second Zagreb indices, Randić index, geometric-arithmetic index and atom-bond connectivity index and Zagreb polynomials of $VAC_5C_6C_7$ and $HAC_5C_6C_7$ nano tubes. Before we proceed to our main results, we will express two remarks which will be useful later.

Remark 1. We denote the 2-dimensional lattice of $VAC_5C_6C_7[4p, 2q]$ by G (Figure 1). Now we consider the molecular graph G. It is easy to see that $|V(G)| = 16pq$ and $|E(G)| = \frac{49pq-7p}{2} - q + 1$. We partition the edges of G into three subsets $E_1(G), E_2(G)$ and $E_3(G)$. The following table gives the three types and gives the number of edges in each type.

Table 1. Computing the Number of edges for molecular graph G.

(d_u, d_v) **where** $uv \in E(G)$	**Total Number of Edges**
$E_1 = [2,2]$	$2p$
$E_2 = [2,3]$	$8p$
$E_3 = [3,3]$	$\frac{49pq-27p}{2} - q + 1$

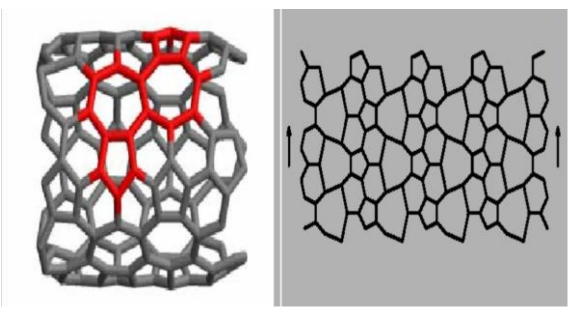

Figure 1. 3D and 2D lattice of $VAC_5C_6C_7[16,8]$ nanotube.

Remark 2. We denote the 2-dimensional lattice of $HAC_5C_6C_7[4p,2q]$ by K (Figure 2). Now we consider the molecular graph K. It is easy to see that $|V(K)| = 16pq$ and $|E(K)| = 24pq - 2p$. We partition the edges of K into two subsets $E_1(K)$ and $E_2(K)$. The following table gives the two types and gives the number of edges in each type.

Table 2. Computing the Number of edges for molecular graph K.

(d_u, d_v) **where** $uv \in E(K)$	**Total Number of Edges**
$E_1 = [2,3]$	$8p$
$E_2 = [3,3]$	$24pq - 10p$

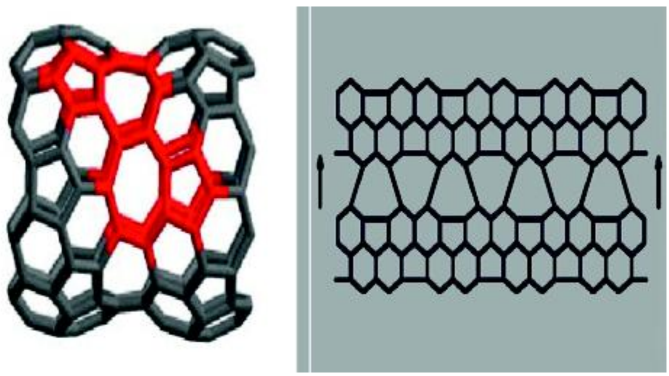

Figure 2. 3D and 2D lattice of $HAC_5C_6C_7[16,8]$ nanotube.

From these tables, we give an explicit computing formula for some topological indices of nanotubes, as shown in Figures 1 and 2. By using the before calculations, we have following theorems. These theorems are main result in this paper.

Theorem 1. *Let G be* $VAC_5C_6C_7[4p,2q]$ *nanotube, we have*

i. $M_1(G,x) = \left(\frac{49pq-27p}{2} - q + 1\right)x^6 + 8px^5 + 2px^4.$

ii. $M_2(G,x) = \left(\frac{49pq-27p}{2} - q + 1\right)x^9 + 8px^6 + 2px^4.$

Proof. By definitions of first and second Zagreb polynomials and partition of edges described in the Table 1 of Remark 1, we can see that:

i. $$M_1(G,x) = \sum_{uv\in E(G)} x^{(d_u+d_v)} = \sum_{uv\in E_1(G)} x^4 + \sum_{uv\in E_2(G)} x^5 + \sum_{uv\in E_3(G)} x^6$$
$$= \left(\frac{49pq-27p}{2} - q + 1\right)x^6 + 8px^5 + 2px^4.$$

ii. $M_2(G,x) = \sum_{uv\in E(G)} x^{(d_u\times d_v)} = \sum_{uv\in E_1(G)} x^4 + \sum_{uv\in E_2(G)} x^6 + \sum_{uv\in E_3(G)} x^9$
$= \left(\frac{49pq-27p}{2} - q + 1\right)x^9 + 8px^6 + 2px^4.$

Next we calculate the first and second Zagreb indices for $VAC_5C_6C_7[4p,2q]$ nanotube.

Theorem 2. *Let* G *be* $VAC_5C_6C_7[4p,2q]$ *nanotube, we have*

i. $M_1(G) = 147pq - 33p - 6q + 6.$

ii. $M_2(G) = 220.5pq - 65.5p - 9q + 9.$

Proof. We know the first and second Zagreb indices will be the first derivative of $M_1(G,x)$ and $M_2(G,x)$ evaluated at $x=1$, respectively. Thus,

i. $M_1(G) = \frac{\partial M_1(G,x)}{\partial x}|_{x=1} = \left(\frac{49pq-27p}{2} - q + 1\right)\times 6 + (8p\times 5) + (2p\times 4)$
$= 147pq - 33p - 6q + 6.$

ii. $M_2(G) = \frac{\partial M_2(G,x)}{\partial x}|_{x=1} = \left(\frac{49pq-27p}{2} - q + 1\right)\times 9 + (8p\times 6) + (2p\times 4)$
$= 220.5pq - 65.5p - 9q + 9.$

However, the definitions of the first and second Zagreb indices can be obtained from the above formulas.

Theorem 3. The first and second Zagreb indices of $\mathrm{HAC_5C_6C_7[4p,2q]}$ nanotube is computed as*:*

$M_1(K,x) = (24pq - 10p)x^6 + 8px^5$ $M_1{}'(K,1) = 144pq - 20p$
$M_2(K,x) = (24pq - 10p)x^9 + 8px^6$ $M_2{}'(K,1) = 216pq - 42p$

Proof. It is proved by the similar method in the proof of Theorem 1 and Theorem 3.

Theorem 4. The modified second and third Zagreb indices of $\mathrm{VAC_5C_6C_7[4p,2q]}$ and $\mathrm{HAC_5C_6C_7[4p,2q]}$ nano tubes are computed as:

Zagreb indices	$\boldsymbol{VAC_5C_6C_7[4p,2q]}$	$\boldsymbol{HAC_5C_6C_7[4p,2q]}$
M_2^*	$\frac{49}{18}pq + \frac{1}{3}p - \frac{1}{9}q + \frac{1}{9}$	$\frac{8}{3}pq + \frac{2}{9}p$
M_3	$8p$	$8p$

Proof. The formulas follow immediately from apply the precedent definitions, Remark 1 and Remark 2.

Finally, we calculate the Randić index, geometric-arithmetic index and atom-bond connectivity index of $VAC_5C_6C_7[4p,2q]$ and $HAC_5C_6C_7[4p,2q]$ by use an algebraic method.

Theorem 5. The connectivity indices of $\mathrm{VAC_5C_6C_7[4p,2q]}$ and $\mathrm{HAC_5C_6C_7[4p,2q]}$ nanotubes are computed as:

Connectivity indices	$\boldsymbol{VAC_5C_6C_7[4p,2q]}$	$\boldsymbol{HAC_5C_6C_7[4p,2q]}$
χ	$\frac{49}{6}pq+\left(\frac{8\sqrt{6}-21}{6}\right)p-\frac{1}{3}q+\frac{1}{3}$	$8pq+\left(\frac{4\sqrt{6}-10}{3}\right)p$
GA	$24.5pq+\left(\frac{32\sqrt{6}-115}{10}\right)p-q+1$	$24pq+(\frac{16\sqrt{6}}{5}-10)p$
ABC	$\frac{49}{3}pq+(5\sqrt{2}-9)p-\frac{2}{3}q+\frac{2}{3}$	$16pq+(4\sqrt{2}-\frac{20}{3})p$

Proof. By direct calculation.

4. Examples

In this section, we give some examples in the following tables. In fact, we obtain topological indices of nanostructures by replacing different number of p and q.

Table 3. Some values of the topological indices of $VAC_5C_6C_7$.

$\boldsymbol{p}$	$\boldsymbol{q}$	$\boldsymbol{M_1}$	$\boldsymbol{M_2}$	$\boldsymbol{M_2^*}$	$\boldsymbol{\chi}$	$\boldsymbol{GA}$	$\boldsymbol{ABC}$
2	2	516	742	11.4444	31.8653	89.6767	60.8088
2	3	804	1174	16.7778	47.8653	137.6767	92.8088
2	4	1092	1606	22.1111	63.8653	185.6767	124.8088
3	2	777	1117.5	17.2222	47.9646	135.0151	91.5465
3	3	1212	1770	25.2778	72.1313	207.5151	139.8799
3	4	1647	2422.5	33.3333	96.2980	280.0151	188.2132
4	2	1038	1493	23	64.0639	180.3535	122.2843
4	3	1620	2366	33.7778	96.3973	277.3535	186.9509
4	4	2202	3239	44.5556	128.7306	374.3535	251.6176

Table 4. Some values of the topological indices of $HAC_5C_6C_7$.

$\boldsymbol{p}$	$\boldsymbol{q}$	$\boldsymbol{M_1}$	$\boldsymbol{M_2}$	$\boldsymbol{M_2^*}$	$\boldsymbol{\chi}$	$\boldsymbol{GA}$	$\boldsymbol{ABC}$
2	2	*536*	*780*	*11.1111*	*31.8653*	*91.6767*	*61.9804*

2	3	*824*	*1212*	*16.4444*	*47.8653*	*139.6767*	*93.9804*
2	4	*1112*	*1644*	*21.7778*	*63.8653*	*187.6767*	*125.9804*
3	2	*804*	*1170*	*16.6667*	*47.7980*	*137.5151*	*92.9706*
3	3	*1236*	*1818*	*24.6667*	*71.7980*	*209.5151*	*140.9706*
3	4	*1668*	*2466*	*32.6667*	*95.7980*	*281.5151*	*188.9706*
4	2	*1072*	*1560*	*22.2222*	*63.7306*	*183.3535*	*123.9608*
4	3	*1648*	*2424*	*32.8889*	*95.7306*	*279.3535*	*187.9608*
4	4	*2224*	*3288*	*43.5556*	*127.7306*	*375.3535*	*251.9608*

5. Conclusion

Among topological descriptors, topological indices are very important and they have a prominent role in chemistry. In the past years, nanostructures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications. We have mentioned here some theoretical results about the Zagreb and conectivity indices of the tubes $VAC_5C_6C_7$ and $HAC_5C_6C_7$. We have finished our work by giving some examples of graphs with of various dimensions.

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Nanoboruların kənarlarında təpələrin dərəcələri əsasında topoloji indekslər

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XÜLASƏ

Bu işdə biz birinci, ikinci, üçüncü və modifikasiya olunmuş ikinci Zagreb indeksi, Randic indeksi, həndəsi-ədədi indeks, atomların əlaqəliliyi indeksi, $VAC_5C_6C_7$ -dən olan Zaqreb çoxhədliləri və $HAC_5C_6C_7$ nonoboruları üçün bəzi nəzəri tədqiqatları verilir.

Açar sözlər: Verteks dərəcələri indeksi, Zaqreb indeksi, qoşulma indeksi, $HAC_5C_6C_7$ nanoboruları, $HAC_5C_6C_7$ nanoboruları.

Топологические индексы основанные на степеней конечных вершин краев нанотрубок

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РЕЗЮМЕ

В этом исследовании, мы приведем некоторые теоретические результаты для первый, второй, третий и модифицированного второго Загреб индекса, Randic индекса, геометрическо-арифметического индекса, индекса связности атомов и многочлены Загреба из $VAC_5C_6C_7$ и нанотрубок $HAC_5C_6C_7$.

Ключевые слова: индексы Vertex порядка, Загреб индексы, индексы подключения, нанотрубки $HAC_5C_6C_7$, нанотрубки $HAC_5C_6C_7$.