STUDIA UBB CHEMIA, LVI, 3, 2011 (p. 59 - 70)

GENERALIZED ZAGREB INDEX OF GRAPHS

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ABSTRACT. In this paper, we introduce the generalized Zagreb index of a connected graph and express some of the properties of this index. Then we find the generalized Zagreb index of some nanotubes and nanotori.

Keywords: *The first and second Zagreb indices, Generalized Zagreb index, Nanotubes, Nanotori.*

INTRODUCTION

Throughout this paper, we consider only simple, undirected, connected and finite graphs. A simple graph is a graph without any loops or multiple edges. Let G be a graph with the set of vertices $V(G)$ and the set of edges $E(G)$. We denote by $\deg_G(u)$, the degree of a vertex u of G which is defined as the number of edges incident to u.

A topological index of G is a real number related to G and it is invariant under all graph isomorphism. In Chemistry, graph invariants are known as topological indices.

Wiener index, introduced by Harold Wiener in 1947, is the first topological index in Chemistry [1-2]. Wiener index of G is defined as the sum of distances between all pairs of vertices of G.

Zagreb indices were defined about forty years ago by Gutman and Trinajestic [3]. The first and second Zagreb indices of G are denoted by $M_1(G)$ and $M_2(G)$, respectively and defined as follows:

$$M_1(G) = \sum_{u \in V(G)} \deg_G(u)^2 \text{ and } M_2(G) = \sum_{uv \in E(G)} \deg_G(u)\deg_G(v).$$

We refer the reader to [4-9], for more information about these indices.

In this paper, we introduce the generalized Zagreb index of a connected graph and express some of the properties of this index. Then we find the generalized Zagreb index of some nano-structures.

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DEFINITIONS AND PRELIMINARIES

Let G be a graph with the set of vertices $V(G)$ and the set of edges $E(G)$.

Definition 2.1 Generalized Zagreb index of G is defined as follows: If r and s are arbitrary nonnegative integers, then

$M_{\{r,s\}}(G) = \sum_{uv \in E(G)} (\deg_G(u)^r \deg_G(v)^s + \deg_G(u)^s \deg_G(v)^r)$ and

$M_{\{0,-1\}}(G) = |V(G)|$.

In the next Theorem, we express some of the properties of this index. Its proof follows immediately from the definition, so is omitted.

Theorem 2.2 The generalized Zagreb index of a graph G satisfies the following conditions.

(i) $M_{\{r,s\}}(G) = M_{\{s,r\}}(G)$;

(ii) $M_{\{0,0\}}(G) = 2|E(G)|$;

(iii) $M_{\{1,0\}}(G) = M_1(G)$;

(iv) $M_{\{1,1\}}(G) = 2M_2(G)$;

(v) $M_{\{r-1,0\}}(G) = \sum_{u \in V(G)} \deg_G(u)^r$;

(vi) $M_{\{r,r\}}(G) = 2 \sum_{uv \in E(G)} (\deg_G(u) \deg_G(v))^r$.

Let P_n, C_n, S_n, K_n and W_n denote the n-vertex path, cycle, star, complete graph and wheel respectively. Let $K_{a,b}$ be complete bipartite graph on $a+b$ vertices. Determining the generalized Zagreb index of these graphs is a matter of simple counting, so the proof of the next Theorem is also omitted.

Theorem 2.3

(i) $M_{\{r,s\}}(P_n) = 2^{r+1} + 2^{s+1} + (n-3)2^{r+s+1}$;

(ii) $M_{\{r,s\}}(C_n) = n2^{r+s+1}$;

(iii) $M_{\{r,s\}}(S_n) = (n-1)^{r+1} + (n-1)^{s+1}$;

(iv) $M_{\{r,s\}}(K_n) = n(n-1)^{r+s+1}$;

(v) $M_{\{r,s\}}(W_n) = (n-1)[2\times 3^{r+s} + 3^r(n-1)^s + 3^s(n-1)^r]$;

(vi) $M_{\{r,s\}}(K_{a,b}) = a^{r+1}b^{s+1} + a^{s+1}b^{r+1}$.

Lemma 2.4 If H is a subgraph of G, then $M_{\{r,s\}}(H) \leq M_{\{r,s\}}(G)$.

Proof. The proof is obvious.⌈

Theorem 2.5 If T is a tree with exactly n vertices, then $M_{\{r,s\}}(P_n) \le M_{\{r,s\}}(T) \le M_{\{r,s\}}(S_n)$.

Proof. The proof is straightforward.

Theorem 2.6 If G is a graph with n vertices, then $M_{\{r,s\}}(P_n) \le M_{\{r,s\}}(G) \le M_{\{r,s\}}(K_n)$.

Proof. Since G is simple, then $|V(G)| = n$. So for every $u \in V(G)$, $\deg_G(u) \le n-1$. Consequently,

$|E(G)| = \frac{1}{2}\sum_{u\in V(G)} \deg_G(u) \le \frac{1}{2}\sum_{u\in V(G)}(n-1) = \frac{n(n-1)}{2}$. Therefore

$$M_{\{r,s\}}(G) = \sum_{[u,v]\in E(G)} (\deg_G(u)^r \deg_G(v)^s + \deg_G(u)^s \deg_G(v)^r) \le 2\sum_{[u,v]\in E(G)} (n-1)^{r+s} =$$

$$2(n-1)^{r+s}|E(G)| \le 2(n-1)^{r+s}\frac{n(n-1)}{2} = n(n-1)^{r+s+1} = M_{\{r,s\}}(K_n).$$

It is a well-known fact that G has a subgraph T with n vertices, which is also a tree. Combining the previous Theorem and Lemma 2.4, we can obtain the desired results.

RESULTS AND DISCUSSION

Carbon nanotubes (CNTs) are allotropes of carbon with molecular structure and tubular shape, having diameters of the order of a few nanometers and lengths up to several millimeters. Nanotubes are categorized as single-walled (SWNTs) and multi-walled (MWNTs) nanotubes. In 1991, Iijima discovered carbon nanotubes as multi-walled structures [10]. When a nanotube is bent so that its ends meet a nanotorus is produced. In this section, we calculate the generalized Zagreb index of some nanotubes and their related nanotori.

3.1 Generalized Zagreb index in nanotubes and nanotori

A polyhex net is a trivalent covering made entirely by hexagons C_6. It can cover either a cylinder or a torus. Next, the polyhex covering can be modified, e.g., by the Stone-Wales isomerization [11], as shown by Diudea [12-15]. In the following, the generalized Zagreb index will be calculated in a series of nanotubes and their corresponding nanotori.

3.1.1. Polyhex nanotubes and nanotori

Let $G = TUZC_6(p,q)$ be an arbitrary zigzag polyhex nanotube, where p is the number of horizontal hexagons in each row and q is the number of zigzag lines in the molecular graph of G (see Figure 1). Then

$\left|V(G)\right| = 2pq$, $\left|E(G)\right| = 3pq - p$ and we have:

$M_{\{r,s\}}(G) = 4p(2^r 3^s + 2^s 3^r) + (3pq - 5p)(3^r 3^s + 3^s 3^r) =$

$p(2^{r+2} 3^s + 2^{s+2} 3^r + 2(3q-5)3^{r+s})$.

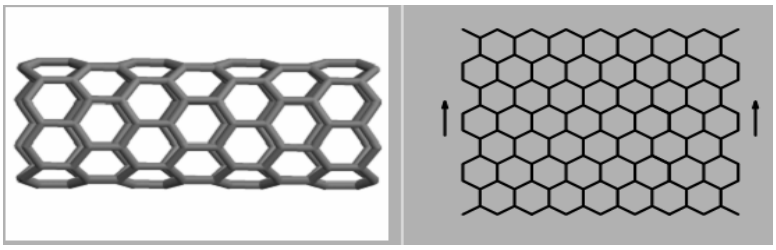

Figure 1. $TUZC_6(8,8)$

Let $T = TZC_6(p,q)$ be the nanotorus related to the nanotube TZC6(p,q). Then, $\left|V(T)\right| = 2pq$, $\left|E(T)\right| = 3pq$ and

$M_{\{r,s\}}(T) = 3pq(3^r 3^s + 3^s 3^r) = 2pq 3^{r+s+1}$.

Let $G = TUAC_6(p,q)$ be an arbitrary armchair polyhex nanotube, where p is the number of horizontal hexagons in one row and q is the number of rows in the molecular graph of G (see Figure 2). Then $\left|V(G)\right| = 2pq$, $\left|E(G)\right| = 3pq - 2p$ and we have:

$M_{\{r,s\}}(G) = 4p(2^r 3^s + 2^s 3^r) + 2p(2^r 2^s + 2^s 2^r) + (3pq - 8p)(3^r 3^s + 3^s 3^r) =$

$p(2^{r+2} 3^s + 2^{s+2} 3^r + 2^{r+s+2} + 2(3q-8)3^{r+s})$.

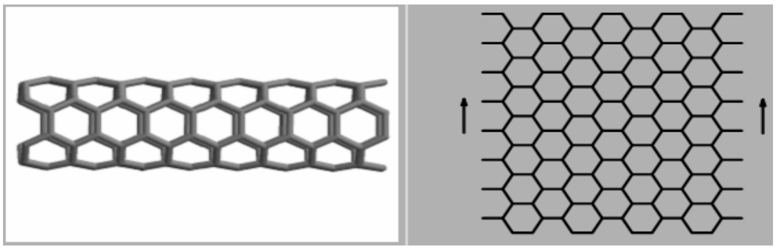

Figure 2. $TUAC_6(4,16)$

Let $T = TAC_6(p,q)$ be the nanotorus related to G. Then $\left|V(T)\right| = 2pq$, $\left|E(T)\right| = 3pq$ and $M_{\{r,s\}}(T) = 3pq(3^r 3^s + 3^s 3^r) = 2pq 3^{r+s+1}$.

3.1.2 $C_4C_8(p,q)$ nanotubes and nanotori

A C_4C_8 net is a trivalent decoration made by alternating C_4 and C_8. It can cover either a cylinder or a torus.

Let $G = TURC_4C_8(p,q)$ (R means rhomb, see Figure 3). We denote the number of rhombs in each row by p and the number of rhombs in each column by q. Then $|V(G)| = 4pq$, $|E(G)| = p(6q-1)$ and we have:

$$M_{\{r,s\}}(G) = 4p(2^r3^s + 2^s3^r) + (6pq - 5p)(3^r3^s + 3^s3^r) =$$
$$p(2^{r+2}3^s + 2^{s+2}3^r + 2(6q-5)3^{r+s}).$$

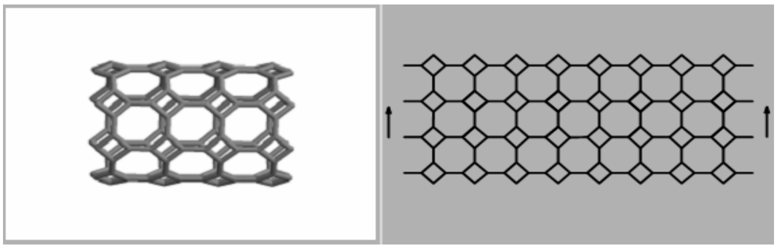

Figure 3. $TURC_4C_8(8,4)$

Now, let $T = TRC_4C_8(p,q)$ be the nanotorus related to G. Then $|V(T)| = 4pq$, $|E(T)| = 6pq$ and $M_{\{r,s\}}(T) = 6pq(3^r3^s + 3^s3^r) = 4pq3^{r+s+1}$.

Let $G = TUSC_4C_8(p,q)$ (S means square, see Fgure 4). We denote the number of squares in one row by p and the number of rows by q ($q \geq 2$). Then $|V(G)| = 4pq$, $|E(G)| = p(6q-2)$ and we have:

$$M_{\{r,s\}}(G) = 4p(2^r3^s + 2^s3^r + 2^{r+s} + (3q-4)3^{r+s}).$$

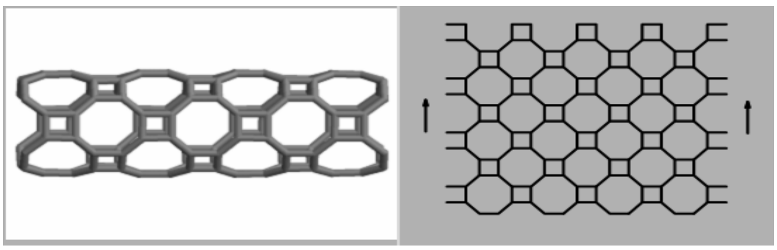

Figure 4. $TUSC_4C_8(4,8)$

Now, let $T = TSC_4C_8(p,q)$ be the nanotorus related to G. Then $\left|V(T)\right| = 4pq$, $\left|E(T)\right| = 6pq$ and $M_{\{r,s\}}(T) = 6pq(3^r3^s + 3^s3^r) = 4pq3^{r+s+1}$.

3.1.3 $C_5C_7(p,q)$ nanotubes and nanotori

A C_5C_7 net is a trivalent covering made by alternating C_5 and C_7. It can cover either a cylinder or a torus.

Let $G = TUHC_5C_7(2p,q)$ (see Figure 5), where 2p is the number of pentagons in each row. In this nanotube, the four first rows of vertices and edges are repeated, alternatively. We denote the number of this repetition by q. In each period of this nanotube, there are 16p vertices and we have q periods. So $\left|V(G)\right| = 16pq$. Also, the number of edges in each period is equal to 24p except from the last period which has 22p edges. So $\left|E(G)\right| = 24pq - 2p$ and we have:

$$M_{\{r,s\}}(G) = 8p(2^r3^s + 2^s3^r) + (24pq - 10p)(3^r3^s + 3^s3^r) =$$
$$4p(2^{r+1}3^s + 2^{s+1}3^r + 3^r + 3^s + (12q-5)3^{r+s}).$$

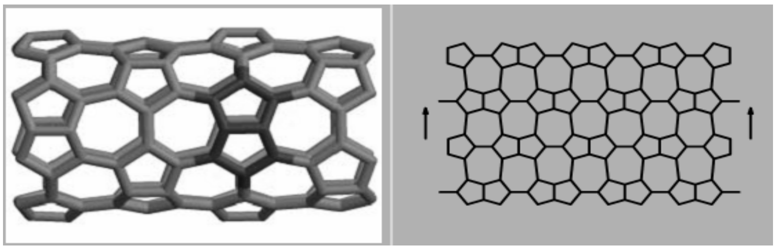

Figure 5. $TUHC_5C_7(8,2)$

Let $T = THC_5C_7(2p,q)$ be the nanotorus related to G. Then $\left|V(T)\right| = 16pq$, $\left|E(T)\right| = 24pq$ and $M_{\{r,s\}}(T) = 24pq(3^r3^s + 3^s3^r) = 16pq3^{r+s+1}$.

Let $G = TUVC_5C_7(2p,q)$ (see Figure 6), where 2p is the number of heptagons in each row. In this nanotube, the four first rows of vertices and edges are repeated, alternatively. We denote the number of this repetition by q. In each period of this nanotube, there are 16p vertices and we have q periods. So $\left|V(G)\right| = 16pq$. Also, the number of edges in each period is equal to 24p expect from the last period which has 21p edges. So

$\left|E(G)\right| = 24p(q-1)+21p = 24pq-3p$ and we have:

$M_{\{r,s\}}(G) = 10p(2^r3^s + 2^s3^r) + p(2^r2^s + 2^s2^r) + (24pq-14p)(3^r3^s + 3^s3^r) =$
$2p(5(2^r3^s + 2^s3^r) + 2^{r+s} + 2(12q-7)3^{r+s})$.

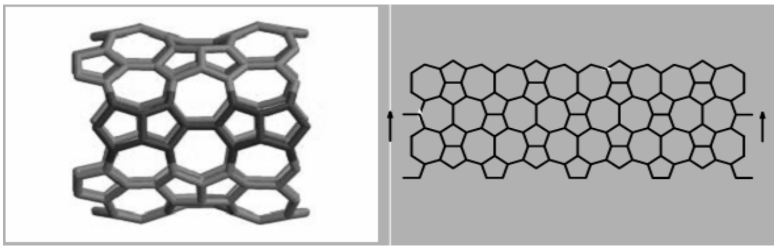

Figure 6. $TUVC_5C_7(8,2)$

Let $T = TVC_5C_7(2p,q)$ be the nanotorus related to G. Then $\left|V(T)\right| = 16pq$, $\left|E(T)\right| = 24pq$ and $M_{\{r,s\}}(T) = 24pq(3^r3^s + 3^s3^r) = 16pq3^{r+s+1}$.

Let $G = TUSC_5C_7(p,q)$ (S means spiral, see Figure 7). We denote the number of pentagones in the first row by p. In this nanotube, the two first rows of vertices and edges are repeated, alternatively. We denote the number of this repetition by q. In each period of this nanotube, there are 8p vertices except from the last period which has 6p vertices. Hence $\left|V(G)\right| = 8p(q-1)+6p = 8pq-2p$. Also, the number of edges in each period is equal to 12p except from the last period which has 7p edges. So $\left|E(G)\right| = 12p(q-1)+7p = 12pq-5p$ and we have:

$M_{\{r,s\}}(G) = 6p(2^r3^s + 2^s3^r) + p(2^r2^s + 2^s2^r) + (12pq-12p)(3^r3^s + 3^s3^r) =$
$p(2^{r+1}3^{s+1} + 2^{s+1}3^{r+1} + 2^{r+s+1} + 8(q-1)3^{r+s+1})$.

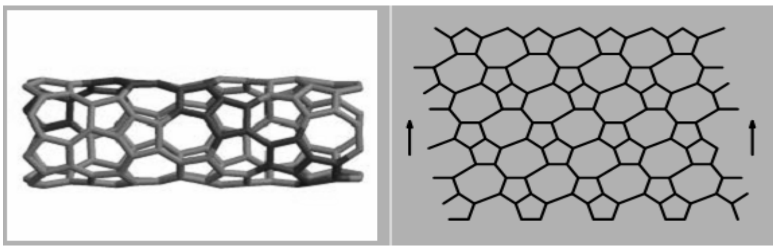

Figure 7. $TUSC_5C_7(4,4)$

Let $T = TSC_5C_7(p,q)$ be the nanotorus related to G. Then $|V(T)| = 8pq$, $|E(T)| = 12pq$ and $M_{\{r,s\}}(T) = 12pq(3^r3^s + 3^s3^r) = 8pq3^{r+s+1}$.

3.1.4. $XAC_5C_7(p,q)$ nanotubes and nanotori

Let $G = TUHAC_5C_7(p,q)$ (see Figure 8). We denote the number of heptagons in the first row by p. In this nanotube, the three first rows of vertices and edges are repeated, alternatively. The number of this repetition is denoted by q. In each period of this nanotube, there are 8p vertices and we have q periods. Hence $|V(G)| = 8pq$. Also, the number of edges in each period is equal to 12p except from the last period which has 11p edges. So $|E(G)| = 12p(q-1) + 11p = 12pq - p$ and we have:

$$M_{\{r,s\}}(G) = 4p(2^r3^s + 2^s3^r) + (12pq - 5p)(3^r3^s + 3^s3^r) =$$
$$2p(2^{r+1}3^s + 2^{s+1}3^r + (12q-5)3^{r+s}).$$

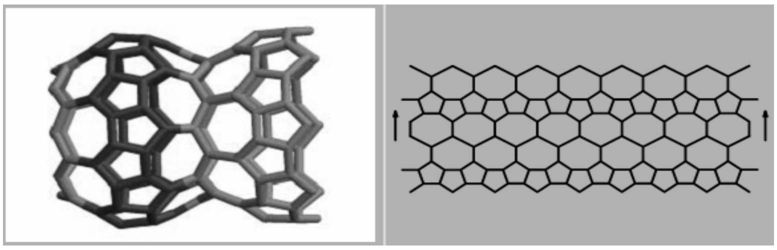

Figure 8. $TUHAC_5C_7(8,2)$

Let $T = THAC_5C_7(p,q)$ be the nanotorus related to G. Then $|V(T)| = 8pq$, $|E(T)| = 12pq$ and $M_{\{r,s\}}(T) = 12pq(3^r3^s + 3^s3^r) = 8pq3^{r+s+1}$.

Let $G = TUVAC_5C_7(p,q)$ (see Figure 9). In this nanotube, the three first columns of vertices and edges are repeated, alternatively. We denote the number of this repetition by q and the number of vertical lines in the first column of each period by p. In each period, there are 8p vertices and 12p-3 edges. So $|V(G)| = 8pq$ and $|E(G)| = (12p-3)q$ and we have:

$$M_{\{r,s\}}(G) = 8q(2^r3^s + 2^s3^r) + 2q(2^r2^s + 2^s2^r) + (12p-13)q(3^r3^s + 3^s3^r) =$$
$$2q(2^{r+2}3^s + 2^{s+2}3^r + 2^{r+s+1} + (12p-13)3^{r+s}).$$

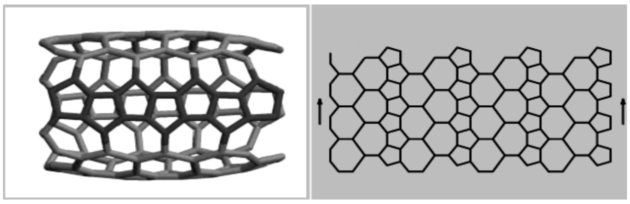

Figure 9. $TUVAC_5C_7(4,4)$

Now, let $T = TVAC_5C_7(p,q)$ be the nanotorus related to G. Then $|V(T)| = 8pq$, $|E(T)| = 12pq$ and $M_{\{r,s\}}(T) = 12pq(3^r3^s + 3^s3^r) = 8pq3^{r+s+1}$.

3.1.5 $C_5C_6C_7(p,q)$ nanotubes and nanotori

A $C_5C_6C_7$ net is a trivalent decoration made by alternating C_5, C_6 and C_7. It can cover either a cylinder or a torus.

Let $G = TUHAC_5C_6C_7(p,q)$ (see Figure 10). We denote the number of pentagons in the first row by p. In this nanotube, the three first rows of vertices and edges are repeated, alternatively. We denote the number of this repetition by q. In each period of this nanotube, there are 16p vertices and we have q periods. So $|V(G)| = 16pq$. Also, the number of edges in each period is equal to 24p expect from the last period which has 22p edges. So $|E(G)| = 24p(q-1) + 22p = 24pq - 2p$ and we have:

$$M_{\{r,s\}}(G) = 8p(2^r3^s + 2^s3^r) + (24pq - 10p)(3^r3^s + 3^s3^r) =$$
$$4p(2^{r+1}3^s + 2^{s+1}3^r + (12q-5)3^{r+s}).$$

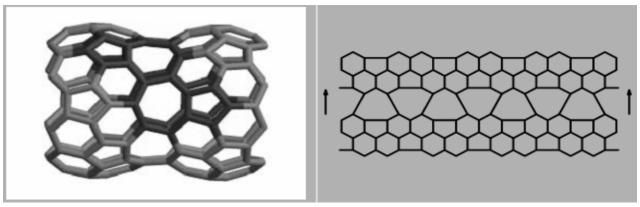

Figure 10. $HAC_5C_6C_7(4,2)$

Now, let $T = THAC_5C_6C_7(p,q)$ be the nanotorus related to G. Then $|V(T)| = 16pq$, $|E(T)| = 24pq$ and

$$M_{\{r,s\}}(T) = 24pq(3^r3^s + 3^s3^r) = 16pq3^{r+s+1}.$$

Let $G = TUVAC_5C_6C_7(p,q)$ (see Figure 11). In this nanotube, the three first columns of vertices and edges are repeated, alternatively. We denote the number of this repetition by q and the number of pentagons in each period by p. In each period of this nanotube, there are 16p vertices and 24(p-1)+21 edges and we have q periods. So $|V(G)| = 16pq$ and $|E(G)| = 24pq - 3q$ and we have:

$M_{\{r,s\}}(G) = 8q(2^r3^s + 2^s3^r) + 2q(2^r2^s + 2^s2^r) + (24pq - 14q)(3^r3^s + 3^s3^r) =$
$2q(2^{r+1}3^s + 2^{s+1}3^r + 2^{r+s+1} + (24p-13)3^{r+s})$.

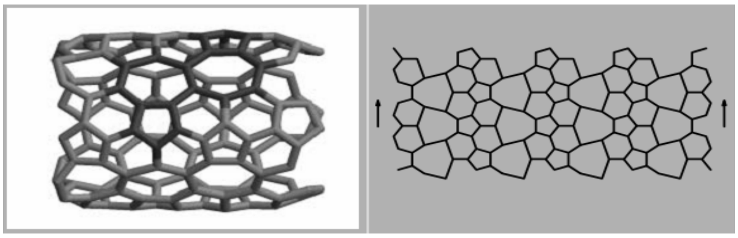

Figure 11. $VAC_5C_6C_7(2,4)$

Let $T = TVAC_5C_6C_7(p,q)$ be the nanotorus related to G. Then $|V(T)| = 16pq$, $|E(T)| = 24pq$ and

$M_{\{r,s\}}(T) = 24pq(3^r3^s + 3^s3^r) = 16pq3^{r+s+1}$.

The coverings and notations for nanotubes and nanotori are taken from Diudea's papers [11-14].

3. 2. CLASSICAL ZAGREB INDICES IN NANOTUBES AND NANOTORI

In this section, as the results of the previous section and Theorem 2.2, we derived the first and second Zagreb indices of the above-mentioned nanotubes and nanotori. They are been listed in the following tables.

Table 1. First and second Zagreb indices of some nanotubes

Nanotube G	$M_1(G) = M_{\{1,0\}}(G)$	$M_2(G) = \frac{1}{2}M_{\{1,1\}}(G)$
$TUZC_6(p,q)$	2p(9q-5)	3p(9q-7)
$TUAC_6(p,q)$	2p(9q-10)	p(27q-40)
$TURC_4C_8(p,q)$	2p(18q-5)	3p(18q-7)

$Nanotube \quad G$	$M_1(G) = \quad M_{\{1,0\}}(G)$	$M_2(G) = \frac{1}{2} M_{\{1,1\}}(G)$
$TUSC_4C_8(p,q)$	4p(9q-5)	2p(27q-20)
$TUHC_5C_7(2p,q)$	4p(36q-1)	6p(36q-5)
$TUVC_5C_7(2p,q)$	6p(24q-5)	2p(108q-31)
$TUSC_5C_7(p,q)$	2p(36q-19)	4p(27q-17)
$TUHAC_5C_7(p,q)$	2p(36q-5)	3p(36q-7)
$TUVAC_5C_7(p,q)$	6q(12p-5)	q(108p-61)
$TUHAC_5C_6C_7(p,q)$	4p(36q-5)	6p(36q-7)
$TUVAC_5C_6C_7(p,q)$	2q(72p-25)	q(216p-85)

Table 2. First and second Zagreb indices of some nanotori

$Nanotorus \quad T$	$M_1(T) = \quad M_{\{1,0\}}(G)$	$M_2(T) = \frac{1}{2} M_{\{1,1\}}(G)$
$TZC_6(p,q)$	$18pq$	$27pq$
$TAC_6(p,q)$		
$TRC_4C_8(p,q)$	$36pq$	$54pq$
$TSC_4C_8(p,q)$		
$THC_5C_7(2p,q)$	$144pq$	$216pq$
$TVC_5C_7(2p,q)$		
$TSC_5C_7(p,q)$	$72pq$	$108pq$
$THAC_5C_7(p,q)$		
$TVAC_5C_7(p,q)$		
$THAC_5C_6C_7(p,q)$	$144pq$	$216pq$
$TVAC_5C_6C_7(p,q)$		

CONCLUSIONS

The generalized Zagreb index was defined and next formulas for calculating this new topological index in some nanotubes and nanotori were derived. The classical Zagreb indices formulas for the considered nanotubes and nanotori were tabulated.

ACKNOWLEDGEMENT.

This research is partially supported by Iran National Science Foundation (INSF), (Grant No. 87040351). Authors are thankful to Professor Mircea V. Diudea, Faculty of Chemistry and Chemical Engineering, “Babes-Bolyai” University, Cluj, Romania for valuable assistance.

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