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Generalized Zagreb index of V-phenylenic nanotubes and nanotori

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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. A topological index of a graph is a number related to a graph which is invariant under graph automorphisms. In chemical graph theory, we have many invariant polynomials and topological indices for a molecular graph. In 1972, Gutman and Trinajstić introduced the First and Second Zagreb topological indices of molecular graphs. The First and Second Zagreb indices are equal to $M_1(G)=\sum_{v\in V(G)} d_v^2$ *and* $M_2(G)=\sum_{uv\in E(G)} (d_u\times d_v)$*, respectively. These topological 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 V-Phenylenic Nanotubes and Nanotori and compute the Generalized Zagreb index of these Nanostructures.*

Keywords: Topological index; Zagreb indices; Generalized Zagreb index; V-Phenylenic Nanotubes; V-Phenylenic Nanotori.

INTRODUCTION

Let $G=(V,E)$ be a simple connected graph of finite order $n=|V|=|V(G)|$ with the set of vertices and the set of edges $E=E(G)$. We denote by d_v, the degree of a vertex v of G which is defined as the number of edges incident to v. A general reference for the notation in graph theory is [1]. A molecular graph is a simple finite graph such that its vertices correspond to the atoms and the edges to the bonds. A topological index of a graph G is a number related to a graph which is invariant under graph automorphisms. In graph theory, we have many different topological indices of G [1-5].

One of the oldest graph invariants is the *Wiener index W(G)*, introduced by the chemist *Harold Wiener* [6] in 1947. It is defined as the sum of topological distances $d(u,v)$ between any two atoms in the graph G

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

The distance $d(u,v)$ between the vertices u and v of the graph G is equal to the length of (number of edges in) the shortest path that connects u and v [6-8].

An important topological index introduced more than forty years ago by *I. Gutman* and N. *Trinajstić* is the Zagreb index $M_1(G)$ (or, more precisely, the First Zagreb index, because there exists also a Second Zagreb index, $M_2(G)$ [9]). The First Zagreb index of G is defined as the sum of the squares of the degrees of all vertices of G. The first and second Zagreb indices of G are defined as follows:

$$M_1(G)=\sum_{v\in V(G)} d_v^{\,2}=\sum_{e=uv\in E(G)} (d_u+d_v)$$
$$M_2(G)=\sum_{e=uv\in E(G)} (d_u\times d_v)$$

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

The *First Zagreb polynomial* $M_1(G,x)$ and the *Second Zagreb polynomial* $M_2(G,x)$ for these topological indices and are defined as:

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

In Refs [10-27] these topological indices and their polynomials of some Nanotubes and Nanotorus are computed. Recently in 2011, A. Iranmanesh *et.al* [28] introduced the generalized Zagreb index of a connected graph G, based on degree of vertices of G. Let G be a graph with the set of vertices $V(G)$ and the set of edges $E(G)$ and r and s are two arbitrary non-negative integer, then the *Generalized Zagreb index* of G is defined as:

$$M_{\{r,s\}}(G)=\sum_{e=uv\in E(G)} (d_u^{\,r}d_v^{\,s}+d_u^{\,s}d_v^{\,r})$$

In this paper, we focus on the structure of *V-Phenylenic Nanotubes* and *Nanotori* and compute the Generalized Zagreb index of these Nanostructures.

RESULTS AND DISCUSSION

Molecular graphs V-Phenylenic Nanotubes $VPHX[m,n]$ and V-Phenylenic Nanotorus $VPHY[m,n]$ are two families of Nano-structures that their structure are consist of cycles with length four, six and eight. The novel Phenylenic and Naphthylenic lattices proposed can be constructed from a square net embedded on the toroidal surface. Geranial representations of V-Phenylenic Nanotubes $G=VPHX[m,n]$ and V-Phenylenic Nanotorus $H=VPHY[m,n]$ are shown in Figure 1 and Figure 2, respectively.

The aim of this section is to compute a closed formula of the generalized Zagreb index $M_{\{r,s\}}(G)$ of *V-Phenylenic Nanotubes* and *Nanotori.*

Some studies about Nanostructure, *Nanotubes* and *Nanotori* are presented in many papers. For a review, historical details and further bibliography please refer [29-37].

Theorem 1. Let G and H be the V-Phenylenic Nanotubes $VPHX[m,n]$ and V-Phenylenic Nanotorus $VPHY[m,n]$ $(\forall m,n\in\mathbb{N}-\{1\})$, respectively. Then:

The Generalized Zagreb index of G is equal to

$$M_{\{r,s\}}(VPHX[m,n])=(3^r2^{s+2}+3^s2^{r+2})m+2(3^{r+s})(9n-5)m$$

The Generalized Zagreb index of H is equal to

$$M_{\{r,s\}}(VPHY[m,n])=2mn(3^{r+s+2})$$

Before prove Theorem 1, let us introduce some definitions.

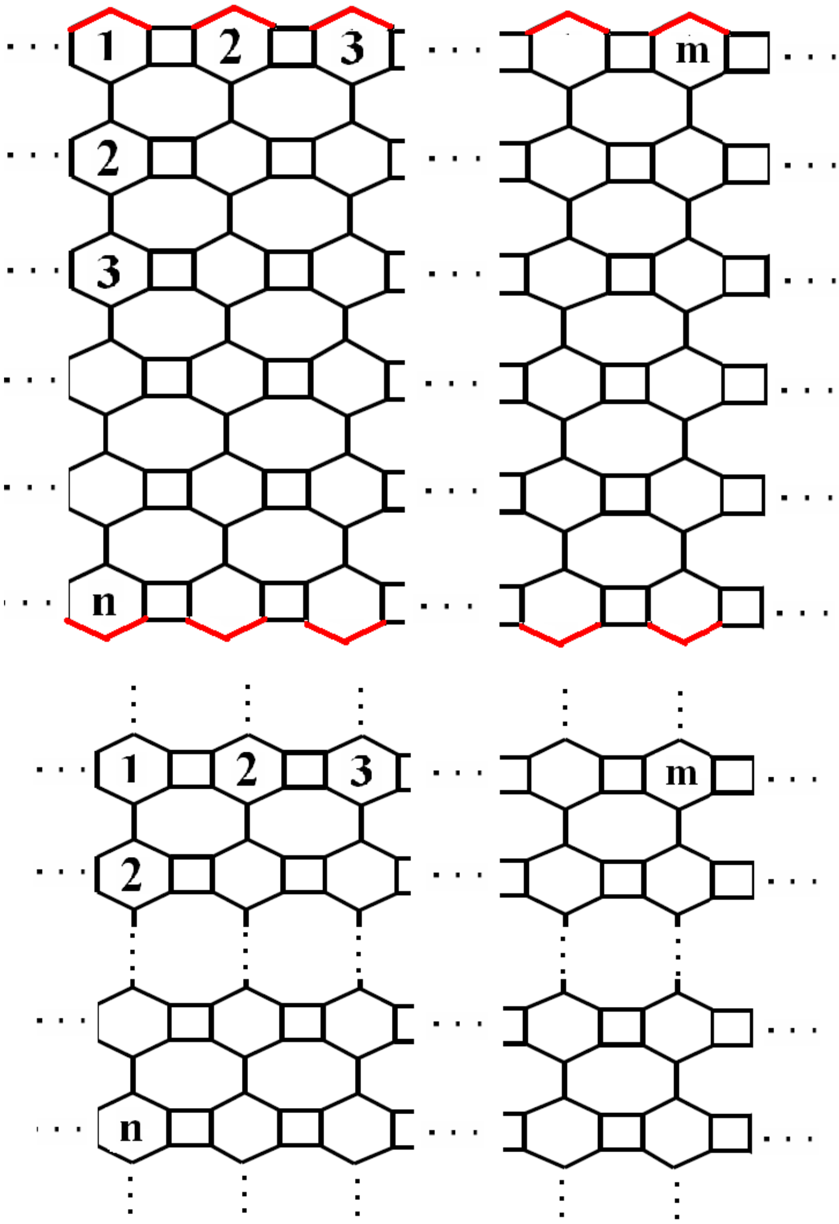

Figure 1. Geranial representations of V-Phenylenic Nanotubes *G=VPHX[m,n]* and V-Phenylenic Nanotorus *H=VPHY[m,n]* $\forall m,n\in\mathbb{N}-\{1\}$

Definition 1. Let G and d_v $(1\leq d_v\leq n-1)$ be a simple connected molecular graph and the degrees of vertices/atom v in G. We divide the vertex set $V(G)$ and edge set $E(G)$ of G into several partitions as follows

$$\forall\ i,j \text{ and } k:\ \delta\leq i,j,k\leq\Delta:$$
$$V_{\{k\}}=\{v\in V(G)|\ d_v=k\}$$
$$E_{\{i,j\}}=\{e=uv\in E(G)|d_u=j\ \&\ d_v=i\}$$

where δ and Δ are the minimum and maximum of d_v for all $v\in V(G)$, respectively.

Proof of Theorem 1. $\forall m,n\in\mathbb{N}-\{1\}$, consider Nanotubes $G=VPHX[m,n]$, where m and n be the number of hexagon in the first row and column in this Nanotubes. From the structure of the V-Phenylenic Nanotubes $VPHX[m,n]$, one can see that the number of vertices in $VPHX[m,n]$ is equal to $6mn$ $(=|V(VPHX[m,n])|)$.

Because

$$|V_{\{2\}}|=|\{v\in V(VPHX[m,n])|\ d_v=2\}|=m+m$$
$$|V_{\{3\}}|=|\{v\in V(VPHX[m,n])|\ d_v=3\}|=6mn-2m$$

and these imply that the number of edges of G $(|E(VPHX[m,n])|)$ is equal to

$$\frac{2(2m)+3(6mn-2m)}{2}=9mn-m.$$

From the structure of the V-Phenylenic Nanotubes $VPHX[m,n]$, it is easy to see that the edge set of graph G can be dividing to two partitions $E_{\{2,3\}}$ and $E_{\{3,3\}}$. In Figure 1, we mark all members of edge partition $E_{\{2,3\}}$ by red color and all members of edge partition $E_{\{3,3\}}$ by black color. Thus, there exist $2m+2m$ edges in $E_{\{2,3\}}$ and $9mn-5m$ members in $E_{\{3,3\}}$ of $G=VPHX[m,n]$. In other words,

$$E_{\{2,3\}}=\{e=uv\in E(G)|\ d_u=3\ \&d_v=2\} \rightarrow |E_{\{2,3\}}|=4m$$
$$E_{\{3,3\}}=\{e=uv\in E(G)|\ d_u=d_v=3\} \rightarrow |E_{\{3,3\}}|=9mn-5m$$

Therefore, by according to the definition of the generalized Zagreb index of graph, we can compute this index for the V-Phenylenic Nanotubes $VPHX[m,n]$ as follows:

$$M_{\{r,s\}}(VPHX[m,n])=\sum_{uv\in E(VPHX[m,n])}(d_u^r d_v^s+d_u^s d_v^r)$$
$$=\sum_{uv\in E_{\{2,3\}}}(3^r2^s+3^s2^r)+\sum_{uv\in E_{\{3,3\}}}(3^r3^s+3^s3^r)$$
$$=\sum_{uv\in E_{\{2,3\}}}(3^r2^s+3^s2^r)+\sum_{uv\in E_{\{3,3\}}}2(3^{r+s})$$
$$=4m\times(3^r2^s+3^s2^r)+(9mn-5m)\times 2(3^{r+s})$$

Now, consider V-Phenylenic Nanotori $H=VPHY[m,n]$ with $6mn$ vertices/atoms and $9mn$ edges/bonds $(\forall m,n\in\mathbb{N}-\{1\})$, where m and n be the number of hexagon in the first row and column in H. From the structure of this V-Phenylenic Nanotori in Figure1, we can see that Nanotorus $VPHY[m,n]$ is a member of *Cubic* graph families and all vertices have degree three. In other words,

$$|V_{\{3\}}|=|\{v\in V(VPHY[m,n])|d_v=3\}|$$
$$=6mn=|V(VPHY[m,n])|$$

$$E_{\{3,3\}}|=|\{e=uv\in E(VPHY[m,n])|\ d_u=d_v=3\}|$$
$$=9mn=|E(VPHY[m,n])|$$

Thus, the generalized Zagreb index of V-Phenylenic Nanotori $VPHY[m,n]$ is equal to

$$M_{\{r,s\}}(VPHY[m,n])=\sum_{uv\in E(VPHY[m,n])}(d_u^r d_v^s+d_u^s d_v^r)$$
$$=\sum_{uv\in E_{\{3,3\}}}(3^r3^s+3^s3^r)$$
$$=(9mn)\times 2(3^{r+s})$$
$$=2mn(3^{r+s+2})$$

Here, we complete the proof of the Theorem 1.■

CONCLUSION

In this present study, we compute the Generalized Zagreb index $M_{\{r,s\}}(G)=\sum_{e=uv\in E(G)}(d_u^r d_v^s+d_u^s d_v^r)$ for two families of Nanostructures namely "*V-Phenylenic Nanotubes* and *Nanotori*" and defined as.

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