

On Multiplicative Version of Zagreb indices of V-Phenylenic Nanotubes and Nanotorus

ABSTRACT

Let G is an arbitrary simple, connected, graph, with the vertex set $V(G)$ and edge set $E(G)$. The first Zagreb index of a graph G is defined as $M_1(G) = \sum_{v \in V(G)} d_v^2$, where d_u and d_v are the degrees of u and v , respectively. An alternative expression for $M_1(G)$ is $\sum_{e=uv \in E(G)} (d_u + d_v)$. And also the Second Zagreb index $M_2(G) = \sum_{e=uv \in E(G)} (d_u \times d_v)$. In this paper, we consider a multiplicative version of $M_1(G)$ and $M_2(G)$ defined as $PM_1(G) = \prod_{e=uv \in E(G)} (d_u + d_v)$ and $PM_2(G) = \prod_{e=uv \in E(G)} (d_u \times d_v)$, respectively. And computed these Multiple Zagreb indices of V-Phenylenic Nanotubes $VPHX[p, q]$ and V-Phenylenic Nanotorus $VPHY[p, q]$ ($\forall p, q \in \mathbb{N} - \{1\}$).

Keywords: Topological index; Zagreb index; Multiple Zagreb indices; V-Phenylenic Nanotubes; V-Phenylenic Nanotorus.

1. INTRODUCTION

Let $G=(V, E)$ be a finite graphs without loops, multiple, or directed edges. In chemical graphs, a molecular graph is a simple graph such that the vertices of the graph correspond to the atoms of molecules while the edges represent chemical bonds ($V(G)$ and $E(G)$ are the vertex and edge set of G). For a vertex $v \in V(G)$, the degree d_v is the number of vertices of G adjacent to v . A general reference for the notation in graph theory is [1-4].

In theoretical Chemistry, molecular structure descriptors, the topological indices are used for modeling physico-chemical, toxicologic, biological and other properties of chemical compounds. Many of the topological indices of current interest in mathematical chemistry are defined in terms of vertex degrees of the molecular graph.

The first Zagreb index of a graph G is among the oldest graph invariant and defined in 1972 by *I. Gutman* and *N. Trinajstić* [5] as

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

where d_u and d_v are the degrees of u and v , respectively. An alternative expression for $M_1(G)$ is $\sum_{e=uv \in E(G)} (d_u + d_v)$. Also the Second Zagreb index

$$M_2(G) = \sum_{e=uv \in E(G)} (d_u \times d_v)$$

The multiplicative version of these Zagreb indices of a graph G (based on degree of vertices of G) introduced recently by *I. Gutman* [6] and *M. Ghorbani* and his co-authors [7] as:

$$PM_1(G) = \prod_{e=uv \in E(G)} (d_u + d_v)$$

$$PM_2(G) = \prod_{e=uv \in E(G)} (d_u \times d_v)$$

We encourage the reader to consult [6-28] for historical background, computational techniques, and mathematical properties of these topological Zagreb indices. In this paper, we focus on the structure of V-Phenylenic Nanotubes $VPHX[p,q]$ and V-Phenylenic Nanotorus $VPHY[p,q]$ ($\forall p,q \in \mathbb{N}-\{1\}$) and compute their Multiplicative Zagreb indices.

3. RESULTS AND DISCUSSION

The novel phenylenic and naphthylenic lattices proposed can be constructed from a square net embedded on the toroidal surface. Following *M.V. Diudea* [29] we denote a V-Phenylenic nanotube and V-Phenylenic nanotorus by $G=VPHX[p,q]$ and $H=VPHY[p,q]$, respectively. Molecular graphs V-Phenylenic Nanotubes $VPHX[p,q]$ and V-Phenylenic Nanotorus $VPHY[p,q]$ are two families of Nano-structures that their structure are consist of cycles with length four, six and eight. These molecular graphs are presented in many papers; see the paper series [30-38]. A general representation of V-Phenylenic Nanotubes $VPHX[p,q]$ and V-Phenylenic Nanotorus $VPHY[p,q]$ are shown in Figures 1 and 2, respectively. In this section, we focus on the structures of molecular graph "V-phenylenic Nanotubes and Nanotori" and counting their First Multiple Zagreb and Second Multiple Zagreb indices.

Theorem 1. Let G be V-Phenylenic Nanotubes $VPHX[p,q]$ ($\forall p,q \in \mathbb{N}-\{1\}$). Then:

The First Multiple Zagreb index of G is equal to

$$PM_1(VPHX[p,q]) = (5)^{4p} \times (6)^{(9q-5)p}$$

The Second Multiple Zagreb index of G is equal to

$$PM_2(VPHX[p,q]) = (2)^{4p} \times (3)^{(18q-6)p}$$

Proof. Let G be V-Phenylenic Nanotubes $VPHX[p,q]$, where p and q be the number of hexagon in the first row and colupq in this Nanotubes. In general case of this Nanotubes, there are $6pq$ ($|V(VPHX[p,q])|$) vertices/atoms and $9pq-p$ ($|E(VPHX[p,q])|$) edges/bonds, see Figure 1.

From the structure of V-Phenylenic Nanotubes $VPHX[p,q]$, it is easy to see that there are $p+p$ vertices of G with degree 2 and alternatively $6pq-2p$ vertices of G with degree three. In other words, we have two partitions of the vertex set $V(VPHX[p,q])$ as follow:

$$V_2 = \{v \in V(VPHX[p,q]) \mid d_v = 2\} \rightarrow |V_2| = 2p$$

$$V_3 = \{v \in V(VPHX[p,q]) \mid d_v = 3\} \rightarrow |V_3| = 2p(3q-1)$$

On the other hands, from the structure of $G=VPHX[p,q]$, we have two partitions of the edge set of Nanotubes G (E_5 and E_6) as follow:

$$E_5 = E_6 = \{e = uv \in E(VPHX[p,q]) \mid d_u = 3 \text{ \& } d_v = 2\} \rightarrow |E_5| = |E_6| = 2p+2p$$

$$E_6 = E_9 = \{e = uv \in E(VPHX[p,q]) \mid d_u = d_v = 3\} \rightarrow |E_6| = |E_9| = 9pq-5p$$

Therefore, the first Multiple Zagreb index of V-Phenylenic Nanotubes $G=VPHX[p,q]$ is equal to

$$PM_1(VPHX[p,q]) = \prod_{uv \in E(G)} (d_v + d_v) = \prod_{uv \in E_5} (d_v + d_v) \times \prod_{uv \in E_6} (d_v + d_v) = (5)^{4p} \times (6)^{(9q-5)p}$$

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85 And the second Multiple Zagreb index of V-Phenylenic Nanotubes $G=VPHX[p,q]$ is equal to

$$PM_2(VPHX[p,q]) = \prod_{uv \in E(G)} (d_v \times d_v) = \prod_{uv \in E_5^*} (d_v \times d_v) \times \prod_{uv \in E_6^*} (d_v \times d_v) = (6)^{4p} \times (9)^{(9q-5)p} \\ = (2)^{4p} \times (3)^{(18q-6)p}$$

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89 And these completed the proof of Theorem 1. ■

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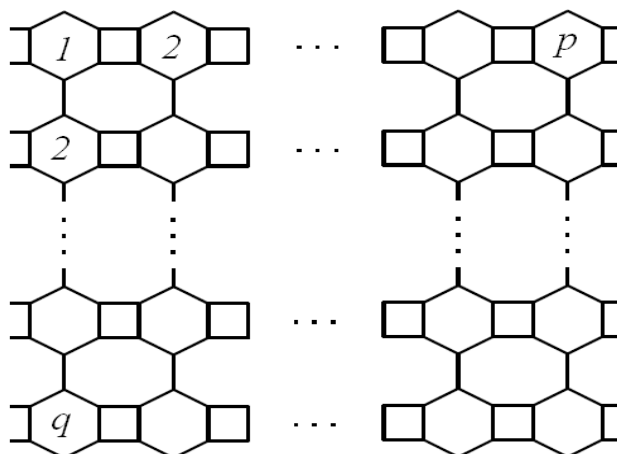


Figure 1. A general case of V-Phenylenic Nanotubes $G=VPHX[p,q]$, $\forall p,q \in \mathbb{N}-\{1\}$.

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95 **Lemma 1.** Let H be V-Phenylenic Nanotorus $VPHY[p,q]$ ($\forall p,q \in \mathbb{N}-\{1\}$). Then:

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97 The First Multiple Zagreb index of G is equal to

$$PM_1(VPHY[p,q]) = 6^{9pq}$$

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100 The Second Multiple Zagreb index of G is equal to

$$PM_2(VPHY[p,q]) = 3^{18pq}$$

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103 *Proof.* Consider Nanotorus $H=VPHY[p,q]$, where p and q be the number of hexagon in the

104 first row and colupq in this Nanotorus.

105 Now by using the structure of $VPHX[p,q]$ in Figure 2, one can see that the number of vertices

106 and edges in this Nanotorus is equal to $|V(VPHX[p,q])|=6pq$ and $|E(VPHX[p,q])|=9pq$,

107 respectively ($\forall p,q \in \mathbb{N}-\{1\}$). Since in $H=VPHY[p,q]$, $|V_2|=0$ and $|V_3|=6pq$.

108 Thus, the first and second Multiple Zagreb indices of V-Phenylenic Nanotorus $H=VPHY[p,q]$

109 is equal to

$$PM_1(VPHY[p,q]) = \prod_{uv \in E(H)} (d_v + d_v) = \prod_{uv \in E_6} (d_v + d_v) = 6^{9pq}$$

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112 And

$$PM_2(VPHY[p,q]) = \prod_{uv \in E(H)} (d_v \times d_v) = \prod_{uv \in E_6^*} (d_v \times d_v) = 3^{18pq}$$

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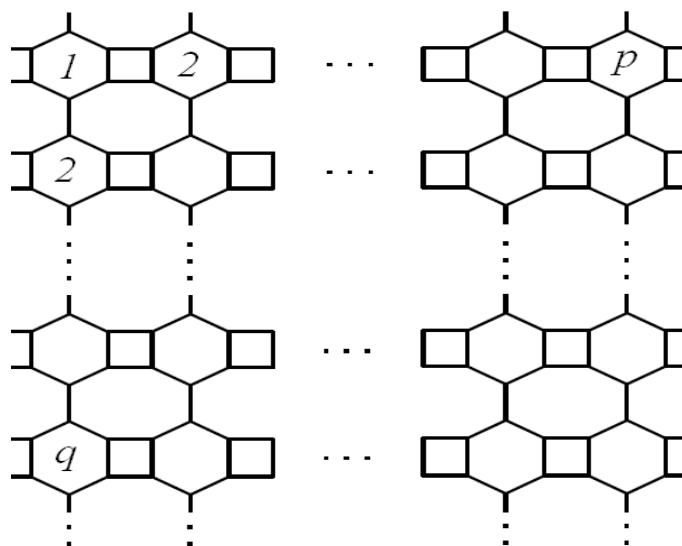


Figure 2. A general case of V-Phenylenic Nanotorus $H=VPHY[p,q]$, $\forall p,q \in \mathbb{N}-\{1\}$.

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