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On Multiplicative and Redefined Version of Zagreb Indices of V-Phenylenic Nanotubes and Nanotorus

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Authors' contributions

This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.

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Abstract

Let G be an arbitrary simple and 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 similarly, 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 $M_2(G)$ and define them as $PM_1(G)=\prod_{e=uv\in E(G)}(d_v+d_v)$ and

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$PM_2(G) = \prod_{e=uv\in E(G)} (d_v \times d_v)$, respectively. And then we compute these Multiple Zagreb indices of V-Phenylenic Nanotubes *VPHX[p,q]* and V-Phenylenic Nanotorus *VPHY[p,q]* ($\forall p,q\in \mathbb{N}-\{1\}$). Furthermore, we present the redefined 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 graph without loops, multiple, or directed edges. In chemical graphs, a molecular graph is a simple graph such that the vertices of the graph can 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 *respectively*). 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 researches 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 which was defined in 1972 by Gutman and 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 the degree of vertices of G) has been introduced recently by Gutman [6], Ghorbani and his co-authors [7] as follows:

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

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

We encourage the readers to refer to [1,5-26] for historical backgrounds, computational techniques, and mathematical properties of these topological Zagreb indices.

The following definitions on redefined Zagreb indices are borrowed from [27]:

- The first redefined Zagreb index of a graph G is defined by

$$\mathrm{Re}\,ZG_1(G)=\sum_{uv\in E(G)}\frac{d_u+d_v}{d_u\times d_v}.$$

- The second redefined Zagreb index of a graph G is defined by

$$\mathrm{Re}\,ZG_2(G)=\sum_{uv\in E(G)}\frac{d_u\times d_v}{d_u+d_v}.$$

- The third redefined Zagreb index of a graph G is defined by

$$\mathrm{Re}\,ZG_3(G)=\sum_{uv\in E(G)}(d_u\times d_v)(d_u+d_v).$$

Although there have been several advances in Zagreb index of molecular graphs, the study of multiplicative Zagreb indices and redefined Zagreb indices of special chemical structures have been largely limited. In addition, as widespread and critical chemical structures, V-Phenylenic Nanotubes, and V-Phenylenic Nanotorus are widely used in medical science and pharmaceutical field. For these reasons, we have attracted tremendous academic and industrial interests to research the multiplicative Zagreb indices and redefined Zagreb indices of these molecular structures from a mathematical point of view.

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. As a supplement, three classes of redefined Zagreb indices of V-Phenylenic Nanotubes *VPHX[p,q]* and V-Phenylenic Nanotorus *VPHY[p,q]* ($\forall p,q\in\mathbb{N}-\{1\}$) are determined.

2 Main Results and Proofs

The novel Phenylenic and Naphthylenic lattices proposed can be constructed from a square net embedded on the toroidal surface. Following Diudea [28], we denote V-Phenylenic Nanotubes and V-Phenylenic Nanotorus as *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] belong to* two different families of Nano-structures whose structures are made up of cycles with length four, six and eight. These molecular graphs have been presented in many papers which can be referred to the paper series [17,29-39]. A general representation of V-Phenylenic Nanotubes *VPHX[p,q]* and V-Phenylenic Nanotorus *VPHY[p,q]* are shown in Figs. 1 and 2, respectively.

In this section, we focus on the structures of molecular graph "*V-Phenylenic Nanotubes* and *Nanotori*" and count 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* are the number of hexagon in the first row and column in this Nanotubes. In general case of this Nanotubes, there are *6pq* vertices/atoms and *9pq-p* edges/bonds, see Fig. 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 follows:

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

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

On the other hand, from the structure of *G=VPHX[p,q]*, *w*e have two partitions of the edge set of Nanotubes *G* (E_5 and E_6) as follows:

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

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

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

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

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

$$PM_2(VPHX[p,q])=\prod_{uv\in E(G)}\left(d_v\times d_v\right)=\prod_{uv\in E_6^*}\left(d_v\times d_v\right)\times\prod_{uv\in E_9^*}\left(d_v\times d_v\right)$$

$$=\left(6\right)^{4p}\times\left(9\right)^{(9q-5)p}=\left(2\right)^{4p}\times\left(3\right)^{(18q-6)p}.$$

And these completed the proof of Theorem 1. ■

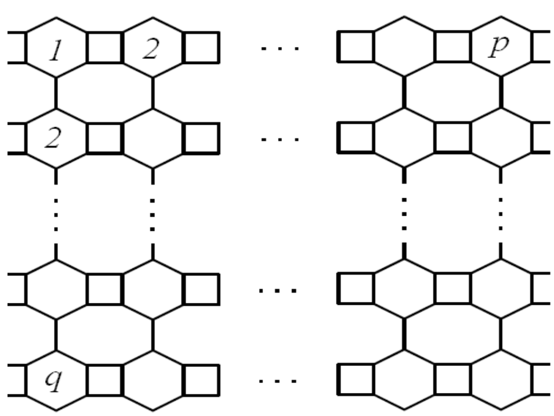

Fig. 1. A general case of V-Phenylenic Nanotubes *G=VPHX[p,q], ∀p,q∈N-{1}*

Theorem 2. Let *H* be V-Phenylenic Nanotorus *VPHY[p,q]* ($\forall p,q\in \mathbb{N}-\{1\}$). Then:

The First Multiple Zagreb index of *G* is equal to

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

The Second Multiple Zagreb index of *G* is equal to

$$PM_1(VPHY[p,q])= 3^{18pq}.$$

Proof. Consider Nanotorus *H=VPHY[p,q]*, where *p* and *q* are the number of hexagon in the first row and column in this Nanotorus.

Now by using the structure of *VPHY[p,q]* in Fig. 2, we can see that the number of vertices and edges in this Nanotorus is equal to $|V(VPHX[p,q])|=6pq$ and $|V(VPHX[p,q])|=9pq$, respectively ($\forall p,q\in \mathbb{N}-\{1\}$). Since in $H=VPHY[p,q]$, $|V_2|=0$ and $|V_3|=6pq$.

Thus, the first and second Multiple Zagreb indices of V-Phenylenic Nanotorus *H=VPHY[p,q]* is equal to

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

and

$$PM_2(VPHY[p,q])=\prod_{uv\in E(H)}\left(d_v\times d_v\right)=\prod_{uv\in E_9^*}\left(d_v\times d_v\right)=3^{18pq}.$$

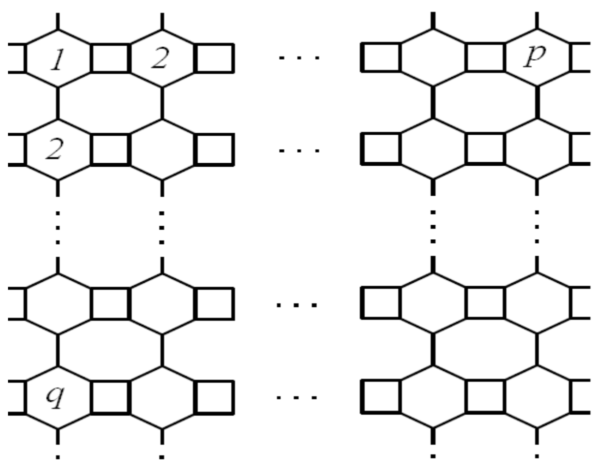

Fig. 2. A general case of V-Phenylenic Nanotorus *H=VPHY[p,q]* ($\forall p,q\in \mathbb{N}-\{1\}$)

3 Additional Findings

In this section, as a supplement conclusion, we state the first, second and third redefined Zagreb indices of V-Phenylenic Nanotubes *VPHX[p,q]* and V-Phenylenic Nanotorus *VPHY[p,q]* ($p,q\in \mathbb{N}-\{1\}$). The techniques to prove Theorem 3 and Theorem 4 are similar to what we stated in Theorem 1 and Theorem 2. Hence, we skip the detail proofs here.

Theorem 3. Let G be V-Phenylenic Nanotubes $VPHX[p,q]$ **(** $\forall p,q\in\mathbb{N}-\{1\}$**)**. Then:

$$ReZG_1(VPHX[p,q])=6pq,$$

$$ReZG_2(VPHX[p,q])=\frac{27pq}{2}-\frac{27p}{10},$$

$$ReZG_3(VPHX[p,q])=486pq-150p.$$

Theorem 4. Let H be V-Phenylenic Nanotorus $VPHY[p,q]$ ($\forall p,q\in\mathbb{N}-\{1\}$). Then:

$$ReZG_1(VPHY[p,q])=6pq,$$

$$ReZG_2(VPHY[p,q])=\frac{27}{2}pq,$$

$$ReZG_3(VPHY[p,q])=486pq.$$

4 Conclusion

The multiplicative Zagreb indices and redefined Zagreb indices that relied on the graphical structure of the alkanes are defined and employed to model both the melting point and boiling point of the molecules. In this report, we mainly obtained the multiplicative Zagreb indices of V-Phenylenic Nanotubes $VPHX[p,q]$ and V-Phenylenic Nanotorus $VPHY[p,q]$ ($\forall p,q\in\mathbb{N}-\{1\}$). And then, the redefined Zagreb indices of these structures are also considered. The promising prospects of the application for the chemical and pharmacy engineering will be illustrated in the theoretical conclusion that is obtained in this paper.

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Competing Interests

Authors have declared that no competing interests exist.

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