IJPSR (2017), Vol. 8, Issue 1 **(Research Article)**

INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES AND RESEARCH

Received on 08 July, 2016; received in revised form, 09 September, 2016; accepted, 12 October, 2016; published 01 January, 2017

FIRST AND SECOND ZAGREB INDICES AND POLYNOMIALS OF V-PHENYLENIC NANOTUBES AND NANOTORI

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Keywords:

V-Phenylenic Nanotubes and Nanotori; Molecular graph; Zagreb index; Zagreb Polynomial.

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ABSTRACT: Let *G* be a simple molecular graph with vertex and edge sets *V(G)* and *E(G)*, respectively. In 1972*, Gutman* and *Trinajstić* introduced the First and Second Zagreb topological indices of molecular graphs. These topological indices are useful in the study of anti-inflammatory activities of certain chemical instances, and in elsewhere. In this present study, compute the First Zagreb index $Zg_1(G)=\sum_{v\in V(G)} d_v^2$ and Second Zagreb index $Zg_2(G)=\sum_{e=uv\in E(G)}(d_u\times d_v)$ and the First Zagreb polynomial $Zg_1(G,x)=\sum_{e=uv\in E(G)} x^{d_u+d_v}$ and the Second Zagreb polynomial $Zg_2(G,x)=\sum_{e=uv\in E(G)} x^{d_u\times d_v}$ of *V-Phenylenic Nanotubes* and *Nanotori*.

INTRODUCTION: Let *G=(V,E)* be a simple connected graph. In chemical graphs, 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). In mathematics chemistry, there exist many topological indices and connectivity indices in graph theory. A topological index is a numeric quantity from the structural graph of a molecule which is invariant under graph automorphisms. As usual, the distance between the vertices *u* and *v* of *G* is denoted by *d(u,v)* and it is defined as the number of edges in a minimal path connecting vertices *u* and *v* [1-5].

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DOI: 10.13040/IJPSR.0975-8232.8(1).330-33

Article can be accessed online on: www.ijpsr.com

DOI link: http://dx.doi.org/10.13040/IJPSR.0975-8232.8 (1).330-33

One of the oldest graph invariants is the *Wiener index W(G)*, introduced by the chemist *Harold Wiener* [5] in 1947. It is defined as the sum of topological distances *d(u,v)* between any two atoms in the molecular graph *G*

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

An important topological index introduced more than forty years ago by *I. Gutman* and N. *Trinajstić* is the Zagreb index $Zg_1(G)$ (or, more precisely, the First Zagreb index, because there exists also a Second Zagreb index, $Zg_2(G)$ [6-8]). First Zagreb index $Zg_1(G)$ of the graph *G* is defined as the sum of the squares of the degrees of all vertices of *G*. the First and Second topological indices are defined as:

$$Zg_1(G)=\sum_{v\in V(G)} d_v^2 \text{ or } \sum_{e=uv\in E(G)}(d_u+d_v)$$

$$Zg_2(G)=\sum_{e=uv\in E(G)}(d_u\times d_v)$$

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

The First Zagreb polynomial $Zg_1(G,x)$ and the Second Zagreb polynomial $Zg_2(G,x)$ for these topological indices and are defined as:

$$Zg_1(G,x)=\sum_{e=uv\in E(G)} x^{d_u+d_v}$$

$$Zg_2(G,x)=\sum_{e=uv\in E(G)} x^{d_u d_v}$$

In Refs [6-34] these topological indices and their polynomials of some Nanotubes and Nanotorus are computed. In this paper, we focus on the First and Second Zagreb indices and their topological polynomials of *V-Phenylenic Nanotubes* and *Nanotori*.

RESULTS AND DISCUSSION: The goal of this section is computing a closed formula of the First Zagreb index $Zg_1(G)=\sum_{v\in V(G)} d_v^2$ and Second Zagreb index $Zg_2(G)=\sum_{e=uv\in E(G)} (d_u\times d_v)$ and the First Zagreb polynomial $Zg_1(G,x)=\sum_{e=uv\in E(G)} x^{d_u+d_v}$ and the Second Zagreb polynomial $Zg_2(G,x)=\sum_{e=uv\in E(G)} x^{d_u\times d_v}$ for *V-Phenylenic Nanotubes* and *Nanotori*. Following *M.V. Diudea* 35 we denote a V-Phenylenic Nanotubes and V-Phenylenic Nanotorus by $G=VPHX[m,n]$ and $H=VPHY[m,n]$, respectively (are shown in **Fig. 1** and **Fig. 2**).

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 by different compound. The novel Phenylenic and Naphthylenic lattices proposed can be constructed from a square net embedded on the toroidal surface. For a review, historical details and further bibliography see the references [36-44]. Before presenting the main results, let us introduce following definition.

Definition 1: [20, 21] Let $G=(V;E)$ be a simple connected graph and d_v is degree of vertex $v\in V(G)$ (Obviously $1\le \delta \le d_v \le \Delta \le n-1$, such that $\delta=Min\{d_v|v\in V(G)\}$ and $\Delta=Max\{d_v|v\in V(G)\}$). We divide the edge set $E(G)$ and the vertex set $V(G)$ of graph G to several partitions, as follow:

$$\forall k: \delta\le k\le\Delta,\ V_k=\{v\in V(G)|\ d_v=k\}$$
$$\forall i: 2\delta\le i\le 2\Delta,\ E_i=\{e=uv\in E(G)|d_u+d_v=i\}$$
$$\forall j: \delta^2\le j\le\Delta^2,\ E_j^*=\{uv\in E(G)|d_u\times d_v=j\}.$$

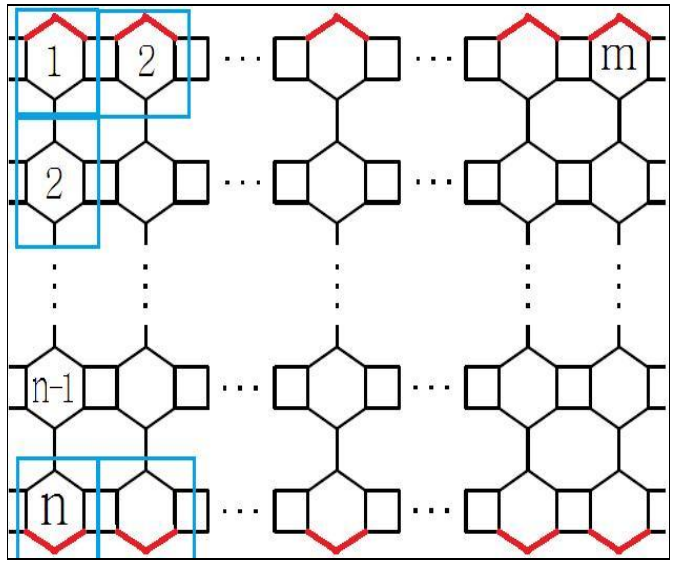

FIG. 1: 2-DIMENSIONAL LATTICE OF THE V-PHENYLENIC NANOTUBES VPHX [m,n].

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

The First Zagreb polynomial of G is equal to

$Zg_1(VPHX[m,n], x)=(9mn-5m)x^6+(4m)x^5$

So the First Zagreb index of G is $Zg_1(VPHX[m,n])=54mn-10m$

The Second Zagreb polynomial of G is equal to

$Zg_2(VPHX[m,n], x)=(9mn-5m)x^9+(4m)x^6$

So the Second Zagreb index of G is $Zg_2(VPHX[m,n])=81mn+3m$

Proof: $\forall m,n\in\mathbb{N}$, consider Nanotubes $G=VPHX[m,n]$, where m and n be the number of hexagon in the first row and column in this Nanotubes. Thus the number of vertices in this Nanotubes is equal to $|V(VPHX[m,n])|=6mn$ ($\forall m,n\in\mathbb{N}$) Since $|V_2|=m+m$ and $|V_3|=6mn-2m$ and the number of edges of $G=VPHX[m,n]$ is equal to

$$|E(VPHX[m,n])|=\frac{2(2m)+3(6mn-2m)}{2}=9mn-m.$$

Now by using the structure of V-Phenylenic Nanotubes *VPHX[m,n]* in **Fig. 1**, we mark the edges of E_5, E_6^* by red color and the edges of E_6, E_9^* by black color.

Therefore, we have the number of $2m+2m$ edges in the edge partition E_5 (or E_6*) and $9mn-5m$ members in the edge partition E_6 (or E_9*) of $G=VPHX[m,n]$, respectively.

Thus, by according to Definition 1 and using the definitions of Zagreb polynomials, one can see that

$$Zg_1(G,x)=\sum_{e\in E(G)} x^{d_u+d_v}=\sum_{e\in E_6} x^6+\sum_{e\in E_5} x^5$$

$$Zg_2(G,x)=\sum_{e\in E(G)} x^{d_u\times d_v}=\sum_{e\in E_6} x^9+\sum_{e\in E_5} x^6$$

Finally, the First Zagreb polynomial of $G=VPHX[m,n]$ is equal to

$$Zg_1(VPHX[m,n], x)=(9mn-5m)x^6+(4m)x^5$$

and the Second Zagreb polynomial of $G=VPHX[m,n]$ is equal to

$$Zg_2(VPHX[m,n], x)=(9mn-5m)x^9+(4m)x^6$$

Now, it is easy to see that

$$Zg_1(VPHX[m,n])=\left.\frac{\partial Zg_1(VPHX[m,n],x)}{\partial x}\right|_{x=1}=(9mn-5m)\times 6+(4m)\times 5=54mn-10m$$

And

$$Zg_2(VPHX[m,n])=\left.\frac{\partial Zg_2(VPHX[m,n],x)}{\partial x}\right|_{x=1}=(9mn-5m)\times 9+(4m)\times 6=81mn+3m$$

Here, we complete the proof of Theorem 1.

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

The First Zagreb polynomial and its index of H are equal to

$$Zg_1(VPHY[m,n], x)=(9mn)x^6$$
$$Zg_1(VPHY[m,n])=54mn$$

The Second Zagreb polynomial and its index of H are equal to

$$Zg_2(VPHY[m,n], x)=(9mn)x^9$$
$$Zg_2(VPHY[m,n])=81mn$$

Proof: Consider V-Phenylenic Nanotori $H=VPHY[m,n]$ ($\forall m,n\in\mathbb{N}$), 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 **Fig. 2**, one can see that this Nanotorus is a member of *Cubic* graph families and all vertices have degree three. Therefore, $H=VPHY[m,n]$ has $6mn$ vertices with degree three and alternatively number of edge in H is $|E(VPHY[m,n])|=9mn$.

Now, by according to definitions of Zagreb polynomials, we will have:

The First and Second Zagreb polynomials of V-Phenylenic Nanotori $H=VPHY[m,n]$ are equal to

$$Zg_1(VPHY[m,n], x)=(9mn)x^6$$
$$Zg_2(VPHY[m,n], x)=(9mn)x^9$$

And obviously, the First and Second Zagreb indices of $VPHY[m,n]$ are equal to

$$Zg_1(VPHY[m,n])=(9mn)\times 6=54mn$$

And

$$Zg_2(VPHY[m,n])=(9mn)\times 9=81mn.$$

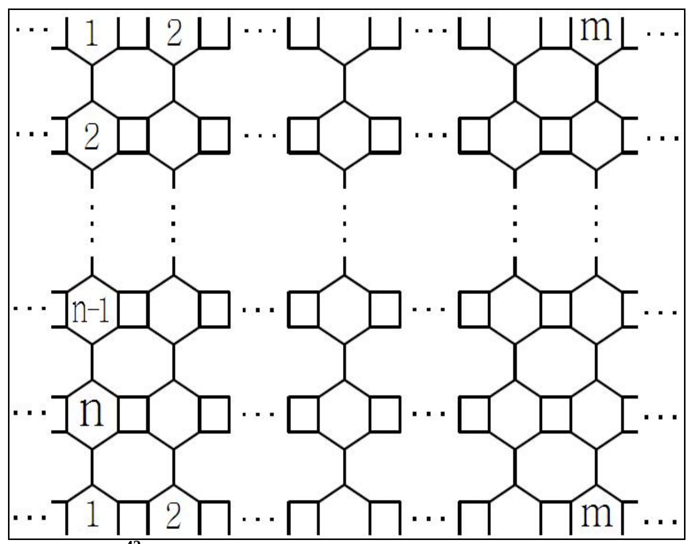

FIG. 2: [42] 2-DIMENSIONAL LATTICE OF THE V-PHENYLENIC NANOTORI *H=VPHY [m,n]*.

CONCLUSIONS: In this report, we study some properties of some of oldest topological indices and polynomials of (molecular) graphs that called the First and Second Zagreb topological indices, First and Second Zagreb polynomials. In continue, closed analytical formulas for First and Second Zagreb topological indices of a physico chemical structure of Phenylenic Nanotubes and Nanotorus are given. These nano structures are V-Phenylenic Nanotube *VPHX[m,n]* and V-Phenylenic Nanotorus *VPHY[m,n]*.

The structures of V-Phenylenic Nanotube and V-Phenylenic Nanotorus consist of several $C_4C_6C_8$ net. A $C_4C_6C_8$ net is a trivalent decoration made by alternating C_4, C_6 and C_8. Phenylenes are polycyclic conjugated molecules, composed of four-and six-membered rings such that every four membered ring (= square) is adjacent to two six-membered rings (= hexagons). In other words, a composition of four-, six-and eight-membered rings in the structures of *VPHX[m,n]* and *VPHY[m,n]* is a $C_4C_6C_8$ net.

ACKNOWLEDGMENTS*:* The authors are thankful to Prof. Mircea V. Diudea from Faculty of Chemistry and Chemical Engineering Babes-Bolyai University (Romania) for their helpful comments and suggestions.

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How to cite this article:
Farahani MR, Kumar RP and Kanna MRR: First and second zagreb indices and polynomials of V-phenylenic nanotubes and nanotori. Int J Pharm Sci Res 2017; 8(1): 330-33.doi: 10.13040/IJPSR.0975-8232.8(1).330-33.