NEW FRONT. CHEM. (**2014**)
Volume 23, Number 2, pp. 141-147
ISSN 2393-2171; ISSN-L 2393-2171

Former: Ann. West Univ. Timisoara – Series Chem.
ISSN: 1224-9513

Article

A NEW VERSION OF ZAGREB INDEX OF CIRCUMCORONENE SERIES OF BENZENOID

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ABSTRACT

Let $G=(V,E)$ be a graph, where $V(G)$ is a non-empty set of vertices and $E(G)$ is a set of edges. One of the best known and widely used is Zagreb topological index M_1 introduced in 1972 by *Gutman* and *Trinajstić*. Recently (in 2012), we know two new version of First Zagreb index as $M^*_1(G)=\sum_{uv\in E(G)} (ecc(v)+ecc(u))$, that introduced by *Ghorbani* and *Hosseinzadeh* and $ecc(u)$ is the largest distance between u and any other vertex v of G. In this paper we compute this new topological index of Circumcoronene series of benzenoid H_k.

Keywords: Cut Method, Orthogonal Cut, Zagreb Topological index, Eccentricity Connectivity index, Molecular Graph, Circumcoronene series of benzenoid.

1. INTRODUCTION

All of the graphs in this paper are simple. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds.

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [1-3]. This theory had an important effect on the development of the chemical sciences.

A topological index of a graph is a number related to a graph which is invariant under graph automorphisms and is a numeric quantity from the structural graph of a molecule.

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One of the best known and widely used is the Zagreb topological index M_1 introduced in 1972 by *I. Gutman* and *N. Trinajstić* and is defined as the sum of the squares of the degrees of all vertices of G [1,2].

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

where d_u denotes the degree (number of first neighbors) of vertex u in G. Mathematical properties of the first Zagreb index for general graphs can be found in [4-8].

Recently, *M. Ghorbani* and *M.A. Hosseinzadeh* introduced a new version of first Zagreb index in 2012 [9] as follows:

$$M^*_1(G)=\sum_{e=uv\in E(G)}(ecc(v)+ecc(u))$$

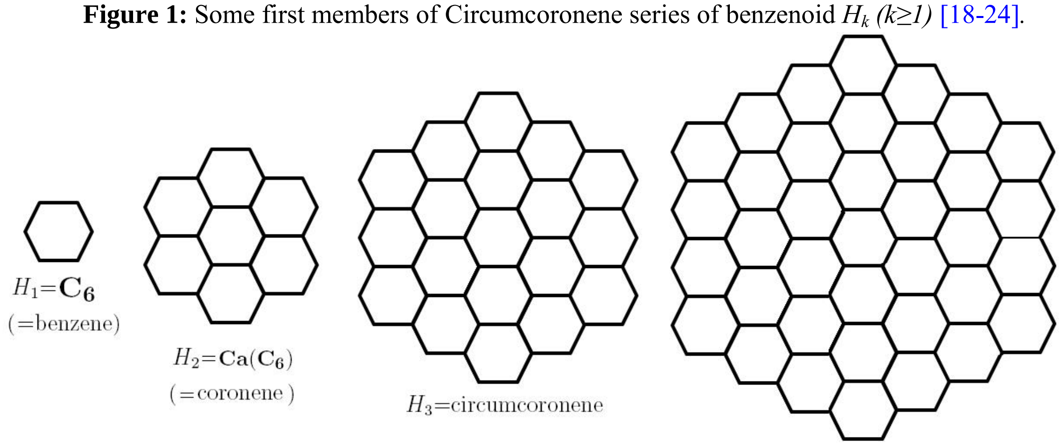
where $ecc(v)$ is eccentricity of vertex v. Let $x,y\in V(G)$ then the distance $d(x,y)$ between x and y is defined as the length of any shortest path in G connecting x and y [10-12].

In other words,

$$ecc(v)=Max\{d(u,v)|\ \forall u\in V(G)\}$$

In this paper, we call this index by *Third Zagreb index* as $M^*_1(G)=M_3(G)$ and compute this new topological index for Circumcoronene series of benzenoid H_k $(k\geq 1)$. The Circumcoronene series of benzenoid is family of molecular graph, which consist several copy of benzene C_6 on circumference. Reader can see some first members of this family in Figure 1 and its structure in general case is shown in Figure 2 (see [13-24]).

Figure 1: Some first members of Circumcoronene series of benzenoid H_k $(k\geq 1)$ [18-24].

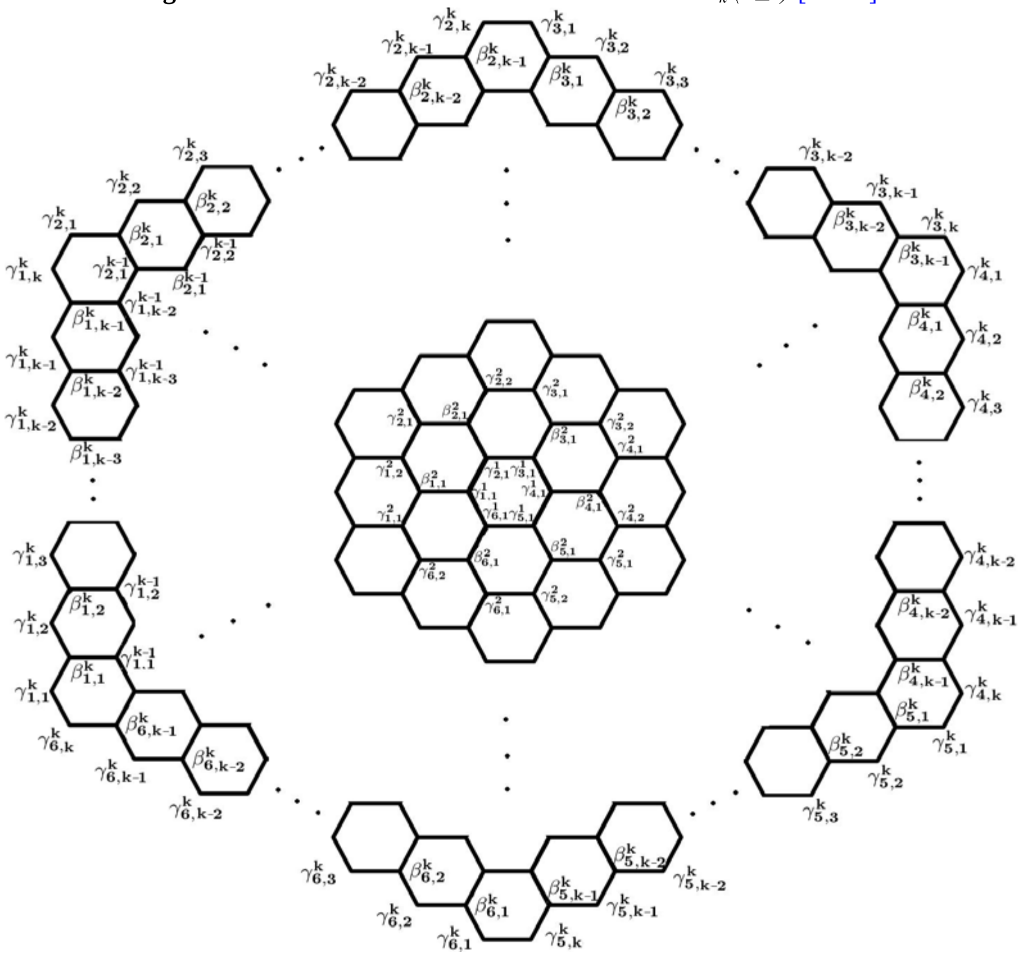


2. Results and Discussion

In this sections, we compute the third Zagreb index $M_3(G)$ for Circumcoronene series of benzenoid H_k $\forall k\geq 1$. For achieve to our aims, we use of Ring-cut Method. Definition of the Cut Method and some its properties are presented in [17].

We encourage readers that lock at to Figure 3 and see ring-cuts of Circumcoronene series of benzenoid, for example.

Figure 2: The Circumcoronene Series of benzenoid H_k $(k\geq 1)$ [18-24].



Now, we can exhibit the closed formula of third Zagreb index $M_3(H_k)$ in following theorem.

Theorem 1. The First Zagreb index of Circumcoronene series of benzenoid H_k $(k\geq 1)$ is equal to [24]

$$M_1(H_k)=54k^2-30k$$

Theorem 2. Let G be the Circumcoronene series of benzenoid H_k $(k\geq 1)$. Then the third Zagreb index of H_k is equal to

$$M_3(H_k)=60k^3-33k^2+9k$$

Proof of Theorem 2. Consider circumcoronene series of benzenoid G=Hk (k≥1), as shown in Figure 2. Here, we denote its vertices by following notations (At first, suppose $\mathbb{Z}6$ is the cycle finite group of order 6 and I coming from $\mathbb{Z}_k$):

1) Consider Benzene C6 (or sub-graph H_1 of H_k) and call vertices by $\gamma^{1}_{z,1}$ for every all z∈ $\mathbb{Z}_6$, respectively.

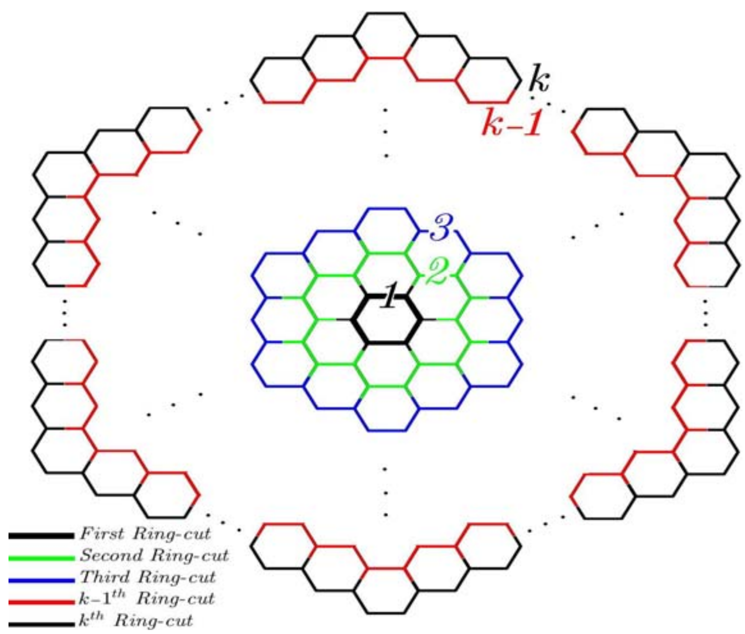
2) Name all $\gamma^{1}_{z,j}$'s adjacent vertices (without name) by $\beta^{2}_{z,j}$, such that j is constant (=1) and z∈$\mathbb{Z}_6$.

3) Name two remaining $\beta^{2}_{z,j}$'s adjacent vertices by $\gamma^{2}_{z,j}, \gamma^{2}_{z,j+1}$ (j=1, z∈ $\mathbb{Z}$6) such that edges $\beta^{2}_{z,j}\gamma^{2}_{z,j}, \beta^{2}_{z,j}\gamma^{2}_{z,j+1}$ be the in E(Hk); see Figure 3.

4) Name all $\gamma^{i}_{z,j}$'s adjacent vertices (without name) by $\beta^{i}_{z,j}$, such that j=1,…,I and j∈$\mathbb{Z}$i & z∈$\mathbb{Z}$6.

5) Name two remaining $\beta^{i}_{z,j}$'s adjacent vertices by $\gamma^{i}_{z,j}, \gamma^{i}_{z,j+1}$ such that j∈$\mathbb{Z}$i-1 & z∈$\mathbb{Z}$6 and insert two edges $\beta^{i}_{z,j}\gamma^{i}_{z,j}$, $\beta^{i}_{z,j}\gamma^{i}_{z,j+1}$ into E(Hk); see Figure 3.

Figure 3. The Ring-cuts of Circumcoronene series of benzenoid. [18-24].



Thus, by above notations, the sets of vertices and edges of Circumcoronene series of benzenoid $G=H_k$ $(k\geq 1)$ are equal to:

$$V(H_k)=\{V(H_k)=\{\gamma^i_{z,j},\beta^i_{z,l}\ |i\in\mathbb{Z}_k\ \&\ j\in\mathbb{Z}_i\ \&\ z\in\mathbb{Z}_6\},$$

$$E(H_k)=\{\beta^i_{z,j}\gamma^i_{z,j},\beta^i_{z,j}\gamma^i_{z,j+1},\beta^i_{z,j}\gamma^{i-1}_{z,j}\ and\ \gamma^i_{z,i}\gamma^i_{z+1,1}|i\in\mathbb{Z}_k\ \&\ j\in\mathbb{Z}_i\ \&\ z\in\mathbb{Z}_6\}.$$

Also, by attention to ring cuts of H_k in Figure 3 and using above notations, it had understood that all vertices where named in step I^{th} , conditions 4) and 5) above, are in I^{th} ring cut R_i of H_k. Thus, we using of results from [17] and conclude some properties as follow:

(I) $\forall i=1,\dots,k;\ j\in\mathbb{Z}_{i-1}\ \&\ z\in\mathbb{Z}_6$: $ecc(\beta^i_{z,j})=\underbrace{\mathbf{d}(\beta^{\mathbf{i}}_{\mathbf{z},\mathbf{j}},\beta^{\mathbf{i}}_{\mathbf{z+3},\mathbf{j}})}_{4i-3}+\underbrace{\mathbf{d}(\beta^{\mathbf{i}}_{\mathbf{z+3},\mathbf{j}},\gamma^{\mathbf{k}}_{\mathbf{z+3},\mathbf{j}})}_{2(k-i)+1}=2(k+i+1)$

(II) $\forall i=1,\dots,k;\ j\in\mathbb{Z}_i\ \&\ z\in\mathbb{Z}_6$: $ecc(\gamma^i_{z,j})=\underbrace{\mathbf{d}(\gamma^{\mathbf{i}}_{\mathbf{z},\mathbf{j}},\gamma^{\mathbf{i}}_{\mathbf{z+3},\mathbf{j}})}_{4i-1}+\underbrace{\mathbf{d}(\gamma^{\mathbf{i}}_{\mathbf{z+3},\mathbf{j}},\gamma^{\mathbf{k}}_{\mathbf{z+3},\mathbf{j}})}_{2(k-i)}=2(k+i)-1$

Therefore, we have following computations for third Zagreb index $M_3(H_k)$ as:

$$M^*_1(H_k)=\sum_{e=uv\in E(H_k)}(ecc(v)+ecc(u))\Rightarrow$$

$$\begin{aligned}M_3(H_k)=&\sum_{\beta^i_{z,j}\gamma^i_{z,j}\in E(H_k)}[\mathrm{ecc}(\beta^i_{z,j})+\mathrm{ecc}(\gamma^i_{z,j})]+\sum_{\beta^i_{z,j}\gamma^i_{z,j+1}\in E(H_k)}[\mathrm{ecc}(\beta^i_{z,j})+\mathrm{ecc}(\gamma^i_{z,j+1})]\\&+\sum_{\beta^i_{z,j}\gamma^{i-1}_{z,j}\in E(H_k)}[\mathrm{ecc}(\beta^i_{z,j})+\mathrm{ecc}(\gamma^{i-1}_{z,j})]+\sum_{\gamma^i_{z,i}\gamma^i_{z+1,1}\in E(H_k)}[\mathrm{ecc}(\gamma^i_{z,i})+\mathrm{ecc}(\gamma^i_{z+1,1})]\\&=\sum_{i=2}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}[\mathrm{ecc}(\beta^i_{z,j})+\mathrm{ecc}(\gamma^i_{z,j})]+\sum_{i=2}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}[\mathrm{ecc}(\beta^i_{z,j})+\mathrm{ecc}(\gamma^i_{z,j+1})]\\&+\sum_{i=1}^{k-1}\sum_{j=1}^{i}\sum_{z=1}^{6}[\mathrm{ecc}(\beta^{i+1}_{z,j})+\mathrm{ecc}(\gamma^i_{z,j})]+\sum_{i=1}^{k}\sum_{z=1}^{6}[\mathrm{ecc}(\gamma^i_{z,i})+\mathrm{ecc}(\gamma^i_{z+1,1})]\end{aligned}$$

Now, using properties (I) and (II) above, where $ecc(\beta^i_{z,j})=2k+2i-2$ and $ecc(\gamma^i_{z,j})=2k+2i-2$, respectively. Obviously $\sum_{z=1}^{6}1=6$.

$$M_3(H_k)=2\left(\sum_{i=2}^{k}6(i-1)[2k+2i-1+2k+2i-2]\right)+\sum_{i=1}^{k-1}6i[2k+2i-1+2k+2(i+1)-2]+\sum_{i=1}^{k}6(4k+4i-2)$$

$$=2\left(\sum_{i=1}^{k-1}6i(4k+4i+1)\right)+\sum_{i=1}^{k-1}6i(4k+4i-1)+\sum_{i=1}^{k}(24k+24i-12)$$

$$=\ldots$$

$$=\sum_{i=1}^{k-1}72i^2+\sum_{i=1}^{k-1}(72k+30)i+\sum_{i=1}^{k-1}(24k-12)+48k-12$$

$$=72\left(\frac{k(k-1)(2k-1)}{6}\right)+(72k+30)\left(\frac{k(k-1)}{2}\right)+(k-1)(24k-12)+48k-12$$

$$=(24k^3-36k^2+12k)+(36k^3-21k^2-15k)+(24k^2-36k+12)+48k-12.$$

Finally, $\forall k\in\mathbb{Z}$ the third Zagreb index is equal to

$$M_3(H_k)=60k^3-33k^2+9k. \blacksquare$$

4. CONCLUSION(S)

In Theoretical Chemistry, the topological indices and molecular structure descriptors are used for modeling physical-chemical, toxicological, biological and other properties of chemical compounds and nano structure analyzing.

In this paper, we were counting one of new molecular structure descriptors of Circumcoronene series of Benzenoid. The First eccentricity Zagreb index (third Zagreb index) $M^*_1(G)= M_3(G)=\sum_{uv\in E(G)}(ecc(v)+ecc(u))$ was introduced by *Ghorbani* and *Hosseinzadeh* in 2012. This new topological index is useful to surveying the structure of molecular graphs.

ACKNOWLEDGMENTS

The author is thankful to Professor Dr. *Mehdi Alaeiyan* from Department of Mathematics, Iran University of Science and Technology (IUST), and Professor Dr. *Mircea V. Diudea* from the Faculty of Chemistry and Chemical Engineering of Babes-Bolyai University (Romania) and *Dr. Miranda Petronella Vlad* from the Dimitrie Cantemir University, Bucharest, Faculty of Economic Sciences (Romania) for their precious support and suggestions

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