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THE SECOND ZAGREB ECCENTRICITY INDEX OF POLYCYCLIC AROMATIC HYDROCARBONS PAHK

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ABSTRACT

Let G be a molecular graph, the vertex and edge sets of which are represented by V(G) and E(G), respectively. The eccentric connectivity index is one of topological invariants that have been recently used in the quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies. The Eccentric Connectivity index ξ(G) is defined as $\xi(G)=\sum_{v\in V} d_v\times \varepsilon(v)$ *where* d_v *denotes the degree of a vertex v in G and* $\varepsilon(v)$ *is the largest distance between u and any other vertex v of G. And the Second Zagreb index is equal to* $M_2(G)=\sum_{e=uv\in E(G)}(d_v\times d_v)$*. In this paper, we compute the Second Zagreb Eccentric index* $EM_2(G)=\sum_{e=uv\in E(G)}\varepsilon(v)\times\varepsilon(u)$ *for famous molecular graph Polycyclic Aromatic Hydrocarbons* PAH_k *(* $\forall k\geq 0$*).*

Keywords: Vertex Degree; Zagreb Eccentricity Indices; Polycyclic Aromatic Hydrocarbons.
2000 Mathematics Subject Classification: 05C05, 92E10

INTRODUCTION

All graphs in this paper are finite, simple and connected. For terms and concepts that are not defined here we refer the reader to any of the standard monographs [1-4].

Let *G* be a simple and connected graph, we denote the vertex and the edge set of *G* by *V(G)* and *E(G)*, respectively. For two vertices *u* and *v* of *V(G)*, we define their *distance d(u;v)* as the length of a shortest path connecting *u* and *v* in *G*. For a given vertex *u* of *V(G)* its *eccentricity u* is the largest distance between *u* and any other vertex *v* of *G*. In other works, $\varepsilon(G)=Max_{v\in V(G)}\, d(u,v)$. The maximum eccentricity over all vertices of *G* is called the *Diameter* of *G* and is denoted by *D(G);* the minimum eccentricity among the vertices of *G* is called radius of *G* and is denoted by *R(G).* In other works,

$$D(G)=Max_{v\in V(G)}\, d(u,v)|\, \forall u\in V(G)\}$$
$$r(G)=Min_{v\in V(G)}\{\, Max\, \{d(u,v)|\, \forall u\in V(G)\}\}$$

The vertex *u* is called a central vertex if $\varepsilon(u)=r(G)$. The center of *G*, *C(G)* is defined as

$$C(G)=\{u\in V(G)|\varepsilon(u)=r(G)\}.$$

The eccentric connectivity index is one of topological invariants that have been recently used in the quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies.
The *Eccentric Connectivity index* $\zeta(G)$ of a graph G is defined as

$$\zeta(G)=\sum_{v\in V(G)} d_v\times\varepsilon(v)$$

where d_v denotes the degree of vertex v in G, i. e., the number of its neighbors in G. The eccentric connectivity index was introduced by *Sharma, Goswami* and *Madan* [6] and used in a series of papers concerned with QSAR/QSPR studies [5]The study of its mathematical properties started only recently [6-21].

The Zagreb indices have been introduced more than forty years ago in 1972 by *I. Gutman* and N. *Trinajstić* [2, 22-26]. The first and second Zagreb indices are defined as

$$M_1(G)=\sum_{e=uv\in E(G)} (d_v+d_v)$$

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

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

Recently, *M. Ghorbani* and *M.A. Hosseinzadeh* introduced new versions of Zagreb indices in 2012 [27], one of them is the Second Zagreb Eccentric index that is equal to:

$$M_2^*(G)=EM_2(G)=\sum_{e=uv\in E(G)} \varepsilon(v)\times\varepsilon(u)$$

where $\varepsilon(v)$ denotes the eccentricity of vertex $v\in V(G)$ [28-31].

The goal of this paper is computing the Second Zagreb Eccentric index $EM_2(G)$ of a famous molecular graph which named "*Polycyclic Aromatic Hydrocarbons* PAH_k" that k is positive integer number.

2. Main Results

In this section, we compute a new version of two topological Second Zagreb and Eccentric indices, which called the Second Zagreb Eccentric index $EM_2(G)=\sum_{e=uv\in E(G)} \varepsilon(v)\times\varepsilon(u)$ of famous Hydrocarbon molecular graph "*Polycyclic Aromatic Hydrocarbons* PAH_k ($\forall k\geq 0$)".

Polycyclic Aromatic Hydrocarbons PAH_k is a family of hydrocarbon molecules, such that its structure is consisting of *Benzene* C_6 on circumference and is ubiquitous combustion products, which some its first members are PAH_1=*benzene* (C_6), PAH_2=*Coronene* and PAH_3=*Circumcoronene* (reader can see Figure 1).

In Refs [32-46] some properties and more historical details of this family of hydrocarbon molecules are studied. Also polycyclic aromatic hydrocarbons *PAHn* family is very similar properties to one of famous family of *Benzenoid* system "*Circumcoronene Homologous Series of Benzenoid* H_k". The properties and applications of Benzenoid system are presented in many papers; reader can see references [20, 26, 47].

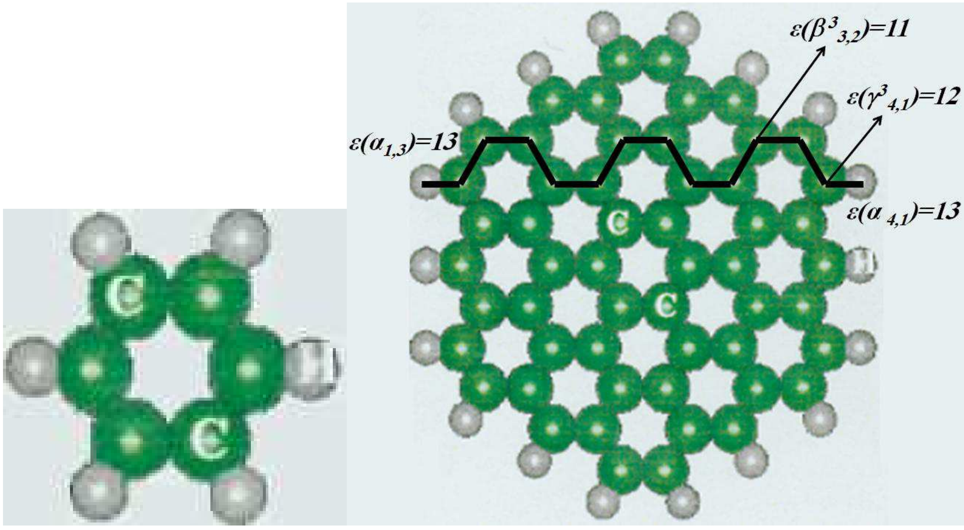

Figure 1. Two examples of first members of *Polycyclic Aromatic Hydrocarbons PAH$_k$*.

Theorem 1. Let G be the *Polycyclic Aromatic Hydrocarbons PAH$_k$*, $\forall k\geq 0$. The Second Eccentricity Zagreb index of *PAHn* is equal to

$$EM_2(PAH_k)=126k^4+108k^3-40k^2-2k.$$

Proof of Theorem 1. $\forall k\geq 0$, Consider the *Polycyclic Aromatic Hydrocarbons PAH$_k$*, as shown in Figure 1. At first, we using Notation 1 and name all vertices of PAH_k as follow, such that its vertex set and edge set will be

$$V(PAH_k)=\{\alpha_{z,j},\gamma^i_{z,j},\beta^i_{z,j}\ |i=1,\ldots,k.\ j\in\mathbb{Z}_i,\ l\in\mathbb{Z}_{i-1},\ z\in\mathbb{Z}_6\}=A_k\cup B_k\cup\Gamma_k$$

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

Also, we divide the vertex set of the *Polycyclic Aromatic Hydrocarbons PAH$_k$* in following partitions as:

$$A_k=\{\alpha_{z,j}\ |j=1,\ldots,k,\ z\in\mathbb{Z}_6\}$$
$$\Gamma_k=\{\gamma^i_{z,j}\ |i=1,\ldots,k.\ j\in\mathbb{Z}_i, z\in\mathbb{Z}_6\}$$
$$B_k=\{\beta^i_{z,j}\ |i=2,\ldots,k,\ j\in\mathbb{Z}_{i-1},\ z\in\mathbb{Z}_6\}$$

From Figure 1, it is easy to see that the degree of vertices of Γ_k and B_k is three (set of carbon (C) atoms) and the degree of vertices of A_k is one (set of hydrogen (H) atoms). Also the size of vertex partitions Γ_k, B_k and A_k are equal to $3k(k+1)$, $3k(k-1)$ and $6k$, respectively.

Obviously, the number of vertices of PAH_k is equal to

$$|V(PAH_k)|=\sum\Gamma_k+\sum B_k+\sum A_k=6k^2+6k$$

On the other hands, the number of edges of PAH_k is equal to

$$|E(PAH_k)|=½[3\sum\Gamma_k+3\sum B_k+1\sum A_k]=½[3(6k^2)+6k]=9k^2+3k.$$

Now, by using of results from [20, 46, 47], we attend to properties of Ring-cut method and mixed with above notation of the *Polycyclic Aromatic Hydrocarbons PAH$_k$*, we can calculate the following results $\varepsilon(v)$ for all $v\in V(PAH_k)$.

$\forall i=2,\ldots,k;\ j\in\mathbb{Z}_{i-1}\ \&\ z\in\mathbb{Z}_6$:

$$\varepsilon(\beta^{i}_{z,j})=\underbrace{d(\beta^{i}_{z,j},\beta^{i}_{z+3,j})}_{4i-3}+\underbrace{d(\beta^{i}_{z+3,j},\gamma^{k}_{z+3,j})}_{2(k-i)+1}+\underbrace{d(\gamma^{k}_{z+3,j},\alpha_{z+3,j})}_{1}=2k+2i-1$$

$\forall i=1,\dots,k;\ j\in\mathbb{Z}_i\ \&\ z\in\mathbb{Z}_6$:

$$\varepsilon(\gamma^{j}_{z,j})=\underbrace{d(\gamma^{i}_{z,j},\gamma^{i}_{z+3,j})}_{4i-1}+\underbrace{d(\gamma^{i}_{z+3,j},\gamma^{k}_{z+3,j})}_{2(k-i)}+\underbrace{d(\gamma^{k}_{z+3,j},\alpha_{z+3,j})}_{1}=2(k+i)$$

$\forall j=1,\dots,k\ \&\ z\in\mathbb{Z}_6$:

$$\varepsilon(\alpha_{z,j})=d(\alpha_{z,j},\gamma^{k}_{z,j})+d(\gamma^{k}_{z,j},\gamma^{k}_{z',j'})+d(\gamma^{k}_{z',j'},\alpha_{z',j'})=4k+1.$$

Now, from Figure 1 and by refer [46], the Second Eccentricity Zagreb index of Polycyclic Aromatic Hydrocarbons $EM_2(PAH_k)$ $(k\geq 0)$ is equal to

$$EM_2(PAH_k)=\sum_{uv\in E(PAH_k)}\varepsilon(v)\times\varepsilon(u)$$

$$=\sum_{\beta^{i}_{z,j}\gamma^{j}_{z,j}\in E(PAH_k)}\varepsilon(\beta^{i}_{z,j})\times\varepsilon(\gamma^{j}_{z,j})+\sum_{\beta^{i}_{z,j}\gamma^{j}_{z,j+1}\in E(PAH_k)}\varepsilon(\beta^{i}_{z,j})\times\varepsilon(\gamma^{j}_{z,j+1})+\sum_{\beta^{i}_{z,j}\gamma^{j-1}_{z,j}\in E(PAH_k)}\varepsilon(\beta^{i}_{z,j})\times\varepsilon(\gamma^{j-1}_{z,j})$$

$$+\sum_{\gamma^{j}_{z,i}\gamma^{j}_{z+1,1}\in E(PAH_k)}\varepsilon(\gamma^{j}_{z,i})\times\varepsilon(\gamma^{j}_{z+1,1})+\sum_{\alpha_{z,j}\gamma^{k}_{z,j}\in E(PAH_k)}\varepsilon(\gamma^{k}_{z,j})\times\varepsilon(\alpha_{z,j})$$

$$=\underbrace{\sum_{i=2}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}\varepsilon(\beta^{i}_{z,j})\times\varepsilon(\gamma^{j}_{z,j})+\sum_{i=2}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}\varepsilon(\beta^{i}_{z,j})\times\varepsilon(\gamma^{j}_{z,j+1})}+\underbrace{\sum_{i=2}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}\varepsilon(\beta^{i}_{z,j})\times\varepsilon(\gamma^{j-1}_{z,j})}$$

$$+\underbrace{\sum_{z=1}^{6}\sum_{i=1}^{k}\varepsilon(\gamma^{j}_{z,i})\varepsilon(\gamma^{j}_{z+1,1})}+\underbrace{\sum_{z=1}^{6}\sum_{j=1}^{k}\varepsilon(\gamma^{k}_{z,j})\varepsilon(\alpha_{z,j})}$$

$$=2\times[6\sum_{i=2}^{k}(i-1)(2k+2i-2)(2k+2i-1)]+6\sum_{i=2}^{k}(i-1)(2k+2i-2)(2k+2(i-1)-1)$$

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

$$=6\sum_{i=1}^{k}2(i-1)(4k^2+4i^2+8ki-6k-6i+2)+6\sum_{i=1}^{k}(i-1)(4k^2+4i^2+8ki-10k-10i+6)$$

$$+6\sum_{i=1}^{k}(4k^2+4i^2+8ki-4k-4i+1)+24k^2(4k+1)$$

$$=24k^2(4k+1)+6\sum_{i=1}^{k}[8k^2i+8i^3+16ki^2-12ki-12i^2+4i-4k^2-4i^2-8ki+4k+4i-1]$$

$$+[4k^2i+4i^3+8ki^2-10ki-10i^2+6i-4k^2-4i^2-8ki+10k+10i-6]+[4k^2+4i^2+8ki-4k-4i+1]$$

$$=24k^2(4k+1)+6\sum_{i=1}^{k}[(12)i^3+(16k-12-4+8k-10-4+4)i^2$$

$$+(8k^2-12k+4-8k+4+4k^2-10k+6-8k+10+8k-4)i+(-4k^2+4k-1-4k+10k^2-6+4k^2-4k+1)]$$

$$=24k^2(4k+1)+6\sum_{i=1}^{k}[12i^3+(24k-26)i^2+(12k^2-30k+20)i+(10k^2-4k-6)]$$

$$=6[12\left(\frac{k^4}{4}+\frac{k^3}{2}+\frac{k^2}{4}\right)+(24k-26)\left(\frac{k^3}{2}+\frac{k^2}{3}+\frac{k}{6}\right)+(12k^2-30k+20)\left(\frac{k^2}{2}+\frac{k}{2}\right)$$

$$+(10k^2-4k-6)(k)+(16k^3+4k^2)]$$

$$=6[(3k^4+6k^3+3k^2)+(12k^4+8k^3+4k^2-13k^3-\frac{26}{3}k^2-\frac{13}{3}k)$$

$$+(6k^4+6k^3-15k^3-15k^{2+}10k^2+10k)+(10k^3-4k^2-6k)+(16k^3+4k^2)]$$

$$=6(21k^4+18k^3-{}^{20}\!/_{3}k^2-{}^{1}\!/_{3}k)$$

Here, we complete the proof of Theorem 1. □

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