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Research Article

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The Second Zagreb Eccentricity Index of Polycyclic Aromatic Hydrocarbons PAH_k

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ABSTRACT

A topological index is a real number related to a molecular graph, it does not rely on the labeling or pictorial representation of a graph. The first and second Zagreb indices are defined as $M_1(G)=\sum_{v\in V(G)} d(v)^2$ *and* $M_2(G)=\sum_{uv\in E(G)} d(u)d(v)$, *respectively. Recently, Nilanjan introduced the first and second Zagreb eccentricity indices as* $\prod E_1(G)=\prod_{v\in V(G)} \varepsilon(v)^2$ *and* $\prod E_2(G)=\prod_{uv\in E(G)} \varepsilon(u)\times\varepsilon(v)$. *In this paper, we compute the first and second Zagreb indices of Polycyclic Aromatic Hydrocarbons (PAHk).*

Keywords: Molecular graph, Topological index, Eccentric connectivity index, Zagreb eccentricity indices, Polycyclic Aromatic hydrocarbons (PAHk).

INTRODUCTION

Let *G* be a simple connected graph with vertex set *V(G)* and edge set *E(G)*. The number of elements in *V(G)* and *E(G)* is called the *order* and *size*, respectively. Let *u,v*∈ *V(G),* the *degree* of *v*, *d(v)*, is the number of vertices adjacent with *v*, and the *distance* between *u* and *v*, *d(u,v)*, is the length of the shortest path connecting them. The *eccentricity* of *v*, $\varepsilon(v)$, is the distance between *v* and a vertex farthest from *v*. The maximum and minimum eccentricities among all vertices of G are known as the *diameter* and *radius* of *G*.

Gutman et. al. introduced the *Zagreb indices* [1]. The first and second Zagreb indices are one of the oldest and widely studied topological indices. The first and second Zagreb indices are defined as $M_1(G)=\sum_{v\in V(G)} d(v)^2$ and $M_2(G)=\sum_{uv\in E(G)} d(u)d(v)$, respectively. Theses topological indices have many applications in QSAR\QSPR. Interested reader can found more history in [2-5].

Todeschini et. al. proposed the *multiplicative version of Zagreb indices* [6-9,13,14]. The first and second multiplicative Zagreb indices are defined as $\prod M_1(G)=\prod_{v\in V(G)} d(v)^2$ and $\prod M_2(G)=\prod_{uvE(G)} d(u)d(v)$, respectively.

Recently, *Nilanjan De* proposed *the multiplicative Zagreb eccentricity indices* [10] as follows:

$$\prod E_1(G)=\prod_{v\in V(G)} \varepsilon(v)^2$$
$$\prod E_2(G)=\prod_{uv\in E(G)} \varepsilon(u)\times\varepsilon(v)$$

Some recent results on these topological indices can be found in [11-12].

Polycyclic Aromatic Hydrocarbons (PAH_k) are a group of different chemicals that are formed during the incomplete burning of organic substances. Polycyclic Aromatic Hydrocarbon can be pictured as a small piece of graphene sheets with the free valances of dangling bond saturated by Hydrogen (H). Recently, some topological indices has found of Polycyclic Aromatic Hydrocarbons [15-17].

RESULTS AND DISCUSSION

In this section, we computed the second Zagreb eccentricity index of the Polycyclic Aromatic Hydrocarbons *(PAH_k)*. We used the Ring cut method [18-20] to obtain the final result. A general representation of PAH_k is shown in Figure 1.

Theorem 1: Let the graph of Polycyclic Aromatic Hydrocarbon (PAH_k), then the second Zagreb eccentricity index of PAH_k is given as

$$\prod E_2(PAH_k)=2^{18i+6k-12}(4k+1)^{6k}\prod_{i=1}^{k}\left[(2k+2i-1)^{18i}(2k+2i-2)^{12(i-1)}(k+i)^{6(i+1)}\right]$$

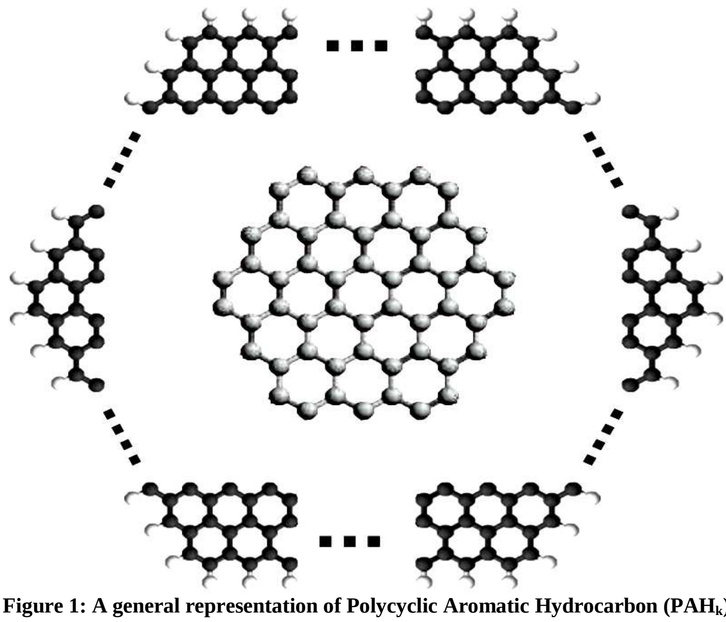

Figure 1: A general representation of Polycyclic Aromatic Hydrocarbon (PAH_k)

Proof: From Figure 1 it is clear that the structure of PAH_k has $6n^2$ vertices\atoms of degree 3 and 6n vertices\atoms of degree 1 and $9k^2$-3k edges. The vertices of degree 1 are denoted by α and the vertices of degree 3 are denoted by β and γ, as shown in Figure 2. Clearly, the vertex set is $V(PAH_k)=\{\alpha_{z,l}\ ,\ \beta^i_{z,l}\ ,\ \gamma^j_{z,j}\ :l=1,...,k,\ j\in Z_i\ ,\ l\in Z_{i-1}\ \&\ z\in Z_6\}$, where $Z_i=\{1,2,\ldots,i\}$. Also, the edge set is $E(H_k)=\{\gamma^i_{z,j}\beta^i_{z,j}, \gamma^i_{z,j+1}\beta^i_{z,j}, \gamma^{i-1}_{z,j}\beta^i_{z,j}$ and $\gamma^i_{z,j}\gamma^i_{z,j+1} | i\in\mathbb{Z}_k\ \&\ j\in\mathbb{Z}_i\ \&\ z\in\mathbb{Z}_6\}$.

To obtain the final result we partitions the vertex set and edge set the help of ring cut for illustration see Figure 2 and [20]. We have

- For all vertices $\alpha_{z,j}$ of PAH_k $\left(j\in Z_k, z\in Z_6\right)$

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

- For all vertices $\beta^i_{z,j}$ of PAH_k ($\forall i=1,..,k;\ z\in\mathbb{Z}_6,\ j\in\mathbb{Z}_{i-1}$)

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

- For all vertices $\gamma^j_{z,j}$ of PAH_n ($\forall i=1,..,k;\ z\in\mathbb{Z}_6,\ j\in\mathbb{Z}_i$)

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

We now apply the above calculation on the definition of second Zagreb eccentricity index to obtain the final result as:

$$\prod E_2(PAH_k)=\prod_{uv\in E(G)}\varepsilon(u)\times\varepsilon(v)$$

$$=\left(\prod_{\beta^i_{z,j}\gamma^i_{z,j}\in E(H_k)}\varepsilon(\beta^i_{z,j})\varepsilon(\gamma^i_{z,j})\right)\times\left(\prod_{\beta^i_{z,j}\gamma^i_{z,j+1}\in E(H_k)}\varepsilon(\beta^i_{z,j})\varepsilon(\gamma^i_{z,j+1})\right)$$

$$\times\left(\prod_{\beta^i_{z,j}\gamma^{i-1}_{z,j}\in E(H_k)}\varepsilon(\beta^{i+1}_{z,j})\varepsilon(\gamma^{i-1}_{z,j})\right)\times\left(\prod_{\gamma^i_{z,i}\gamma^i_{z+1,1}\in E(H_k)}\varepsilon(\gamma^i_{z,i})\varepsilon(\gamma^i_{z+1,1})\right)\times\left(\prod_{\alpha_{z,j}\gamma^k_{z,j}}\varepsilon(\alpha_{z,j})\varepsilon(\gamma^k_{z,j})\right)$$

$$=\prod_{z=1}^{6}\left(\prod_{i=2}^{k}\prod_{j=1}^{i}\varepsilon(\beta^i_{z,j})\varepsilon(\gamma^i_{z,j})\right)\times\prod_{z=1}^{6}\left(\prod_{i=2}^{k}\prod_{j=1}^{i}\varepsilon(\beta^i_{z,j})\varepsilon(\gamma^i_{z,j+1})\right)$$

$$\times\prod_{z=1}^{6}\left(\prod_{i=1}^{k-1}\prod_{j=1}^{i}\varepsilon(\beta^{i+1}_{z,j})\varepsilon(\gamma^{i-1}_{z,j})\right)\times\prod_{z=1}^{6}\left(\prod_{i=2}^{k}\varepsilon(\gamma^i_{z,i})\varepsilon(\gamma^i_{z+1,1})\right)$$

$$\times\prod_{z=1}^{6}\prod_{i=1}^{k}\left(\varepsilon(\alpha_{z,i})\varepsilon(\gamma^k_{z,i})\right)$$

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

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

$$\times\prod_{i=1}^{k}\left[(4k+1)(2k+2i)\right]^{6}$$

$$=\prod_{i=1}^{k}\left[(2k+2i-1)(2k+2i-2)\right]^{12(i-1)}\times\prod_{i=1}^{k}\left[2(2k+2i-1)(k+i)\right]^{6i}\times\prod_{i=1}^{k}\left[(2k+2i-1)\right]^{12}$$

$$\times\prod_{i=1}^{k}\left[(4k+1)(2k+2i)\right]^{6}$$

$$=2^{12i-12+6i+6k}(4k+1)^{6k}\prod_{i=1}^{k}\left[(2k+2i-1)^{12i-12+6i+12}(2k+2i-2)^{12(i-1)}(k+i)^{6i+6}\right]$$

$$=2^{18i+6k-12}(4k+1)^{6k}\prod_{i=1}^{k}\left[(2k+2i-1)^{18i}(2k+2i-2)^{12(i-1)}(k+i)^{6(i+1)}\right]$$

Hence, the proof is complete.■

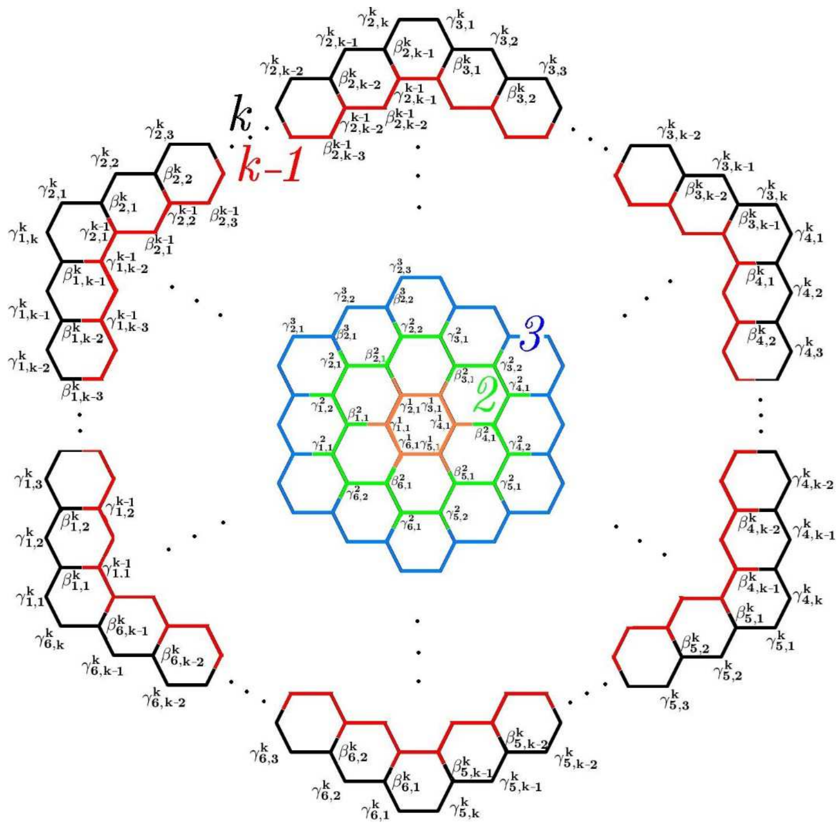

Figure 2: A general vertices representation of Polycyclic Aromatic Hydrocarbons *(PAHk)*

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