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Research Article

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Computation on the fourth Zagreb index of Polycyclic Aromatic Hydrocarbons (PAHk)

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ABSTRACT

The first and second Zagreb indices is defined as $\sum_{v\in V(G)} d(v)^2$ *and* $\sum_{uv\in E(G)} d(u)d(v)$*, respectively, where d(v) is the degree of the vertex v. Recently, Ghorbani et. al. proposed the eccentric version of Zagreb index called fourth Zagreb index as* $\sum_{v\in V(G)} \varepsilon(v)^2$ *, where* $\varepsilon(v)$ *is the eccentricity of the vertex v. In this paper, we compute the exact formulae for the Polycyclic aromatic hydrocarbon (*PAH_k*).*

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

INTRODUCTION

Mathematical chemistry is the area of research busy in novel application of mathematics to chemistry. It concern with the mathematical modeling of chemical phenomena [1]. Mathematical chemistry has also sometimes been called computer chemistry. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [2]. The pioneers of the chemical graph theory are *A. Balaban*, *A. Graovac*, *I. Gutman*, *H. Hosoya*, *M. Ranić* and *N. Rrinajstić* [3].

Polycyclic aromatic hydrocarbons (PAHk) are a group of more than 100 different chemicals that are released from burning oil, trash, gasoline, wood or other organic substance such as charcoal broiled meat. They are also called polynuclear aromatics hydrocarbons. They can occur naturally when they are released from forest fires and volcanoes and can be manufactured.

Let G be a simple connected graph with set of vertices $V(G)$ and set of edges $E(G)$. The number of vertices adjacent to a vertex v is called its degree, denoted as $d(v)$. The *distance* between two vertices is the length of shortest path connecting them. For a vertex $v\in V$, the maximum distance between v and any other vertex of G is called *eccentricity* of *v*, denoted as, $\varepsilon(G)$. *Diameter* and *radius* is the maximum and minimum, respectively, eccentricity of a graph *G*.

In 1971, *Gutman* and co-authors defined the *first* and *second Zagreb indices* for a graph *G* as [4]:

$$M_1(G)=\sum_{v\in V(G)} d(v)^2 \quad \textit{and} \quad M_2(G)=\sum_{uv\in E(G)} d(u)d(v)$$

More about their applications and properties see [5-9,16].

Sharma and co-authors introduced the *eccentric connectivity index* of a graph *G* as [10]:

$$\zeta^c(G)=\sum_{v\in V(G)} d(v).\varepsilon(v)$$

Gupta and co-authors proposed the *connective eccentric index* of *G* as [11,12]:

$$C^{\zeta}(G)=\sum_{v\in V(G)} \frac{d(v)}{\varepsilon(v)}$$

For physico-chemical properties and mathematical properties of these indices can be found in [13-15].

By seeing the great application of Zagreb indices and eccentricity indices *Ghorbani* and *Hosseinzadeh* introduces the *fourth version of Zagreb indices* defined as [17]:

$$M_4(G)=\sum_{v\in V(G)} \varepsilon(v)^2$$

RESULTS AND DISCUSSION

In this section, we compute the fourth Zagreb index of Polycyclic aromatic hydrocarbons *(PAHk)*. *PAHk* contains carbon (degree 3) and hydrogen (degree 1) atoms, a general representation are shown in Figure 1 [18-31]. The *ring cut method* partition the set of vertices. We use the ring cut method to obtain the required result [32, 33].

Theorem 1: Consider the graph of polycyclic aromatic hydrocarbons. Then the fourth Zagreb index of polycyclic aromatic hydrocarbons is equal to

$$M_4(PAH_k)=96k^3+72k^2+54k+24+\sum_{i=2}^{k} 6i\left(8k^2+8i^2+8ki-4i-4k+1\right)$$

Proof: To obtain the result we will use the ring cut method on the structure on Circumcoronene homologous series of Benzenoid as shown in Figure 2. From Figure it is clear that we have only two types of vertices, vertex with degree 3 and vertex with degree 1. We named these vertices as α for vertices of degree 1 and β and γ for vertices of degree 3. So we have,

$$V(PAH_k)=\{\alpha_{z,l}\ ,\ \beta^i_{z,l}\ ,\ \gamma^i_{z,j}\ :l=1,...,k,\ j\in Z_i\ ,\ l\in Z_{i-1}\ \&\ z\in Z_6\}$$

where Z_i={1,2,…,i}.

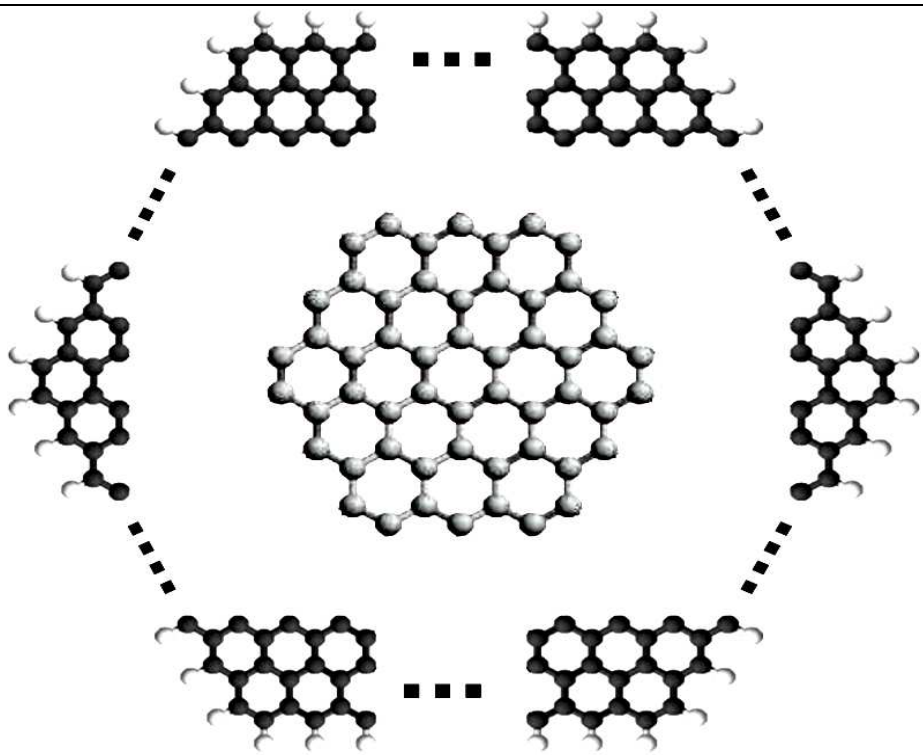

Figure 1: A general representation of polycyclic aromatic hydrocarbon (PAH_k)

With the help of ring cut method we divide the vertices, and i^{th} ring cut has $6i+6(i-1)$ vertices of type $\beta^i_{z,j}\ \gamma^i_{z,j}\ \ (\forall i=1,...,k; z\in Z_6\ ,\ j\in Z_i)$. Form Figure 2 it is clear that $d(\gamma^i_{z,j},\ \gamma^k_{z,j})=d(\beta^i_{z,j},\beta^k_{z,j})=2(k-i).$ Also, we found that

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

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

Now we apply the above calculation on fourth Zagreb index to obtain the result

$$M_4(G)=\sum_{v\in V(G)}\varepsilon(v)^2$$

$$=\sum_{\alpha_{z,j}\in V(PAH_k)}\varepsilon^2(\alpha_{z,j})+\sum_{\beta^i_{z,j}\in V(PAH_k)}\varepsilon^2(\beta^i_{z,j})+\sum_{\gamma^i_{z,j}\in V(PAH_k)}\varepsilon^2(\gamma^i_{z,j})$$

$$=\sum_{z=1}^{6}\sum_{j=1}^{k}\varepsilon^2(\alpha_{z,j})+\sum_{i=2}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}\varepsilon^2(\beta^i_{z,j})+\sum_{i=1}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}\varepsilon^2(\gamma^i_{z,j})$$

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

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

$$=96k^3+72k^2+54k+24+\sum_{i=2}^{k}6i\left(8k^2+8i^2+8ki-4i-4k+1\right)$$

This is the desired result.■

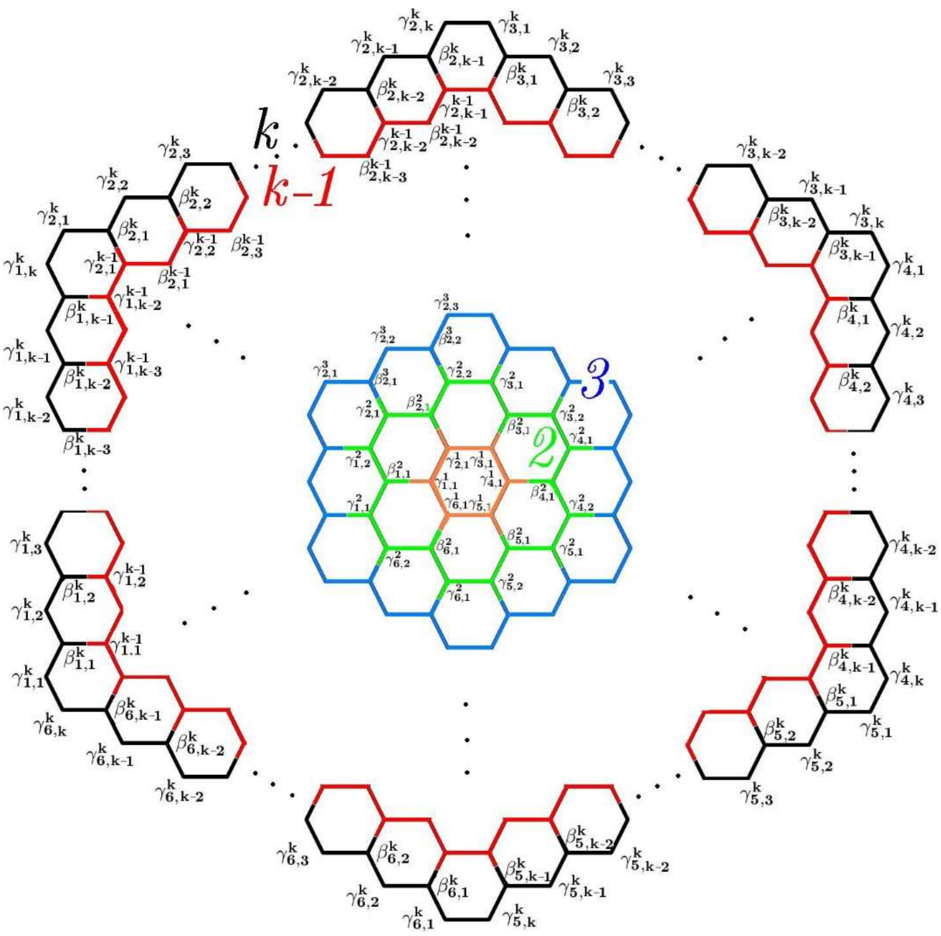

Figure 2: Vertex wise general representation of PAH_k structure

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