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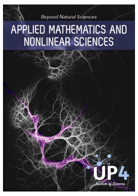

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Computing Eccentric Version of Second Zagreb Index of Polycyclic Aromatic Hydrocarbons (PAHk)

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Abstract

ARecently, Ghorbani et. al. introduced the eccentric versions of first and second Zagreb indices called third and fourth Zagreb indices defined as$M_3(G) = \sum_{uv\in E(G)} (\varepsilon(u)+\varepsilon(v))$ $and\, M_4(G) = \sum_{v\in V(G)} \varepsilon(v)^2$, respectively, where $\varepsilon(v)$is the eccentricity of the vertex v. In this paper, we compute the closed formula for third Zagreb index of Polycyclic Aromatic Hydrocarbons (PAH$_k$).

Keywords: Molecular graph, Eccentricity, Zagreb Indices, Polycyclic Aromatic Hydrocarbons (PAHk)
AMS 2010 codes: 05C05; 92E10.

1 Introduction

Let G be simple connected *graph* with vertex set *V(G)* and edge set *E(G).* The number of elements in the set *V(G)* and *E(G)* are called the *order* and *size* of the graph G, respectively. In a graph G, the *distance* between two vertices is the shortest length path connecting them. For a vertex $v\in V(G)$, the *eccentricity* of v is the maximum

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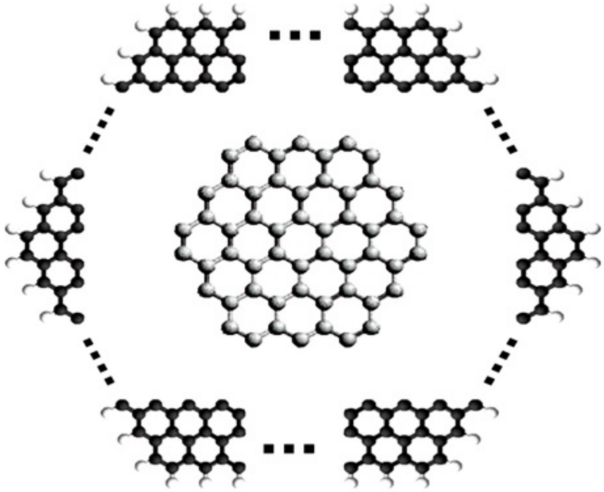

Fig. 1 A general representation of Polycyclic Aromatic Hydrocarbons PAH_k.

distance between v and any other vertex of G denoted as $\varepsilon(v)$. The maximum eccentricity is called the diameter and the minimum eccentricity is called the radius of the graph G. In a graph G the *degree* of a vertex v is the number of its first neighbors, $d(v)$.

Topological index is a numerical descriptor of the molecular structure derived from the corresponding molecular graph. Many topological indices are widely used for quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies.

Gutman et.al. [1] proposed vertex degree based topological indices of a graph, named as first Zagreb index $M_1(G)$ and second Zagreb index $M_2(G)$. These are defined as:

$$M_1(G) = \sum_{v\in V(G)} d(v)^2$$
$$M_2(G) = \sum_{uv\in V(G)} d(u)\cdot d(v)$$

In 2010, *Todeschini* et. al. [2] and [3] introduced the multiplicative versions of the above Zagreb indices named as multiplicative Zagreb indices, which are defined as follows:

$$\prod_1(G) = \prod_{v\in V(G)} d(v)^2$$
$$\prod_2(G) = \prod_{uv\in E(G)} d(u)\cdot d(v)$$

More history and results on Zagreb and multiplicative Zagreb indices can be found in [4]– [10].

Recently, Ghorbani and Hosseinzadeh [11] defined the eccentric versions of Zagreb indices. These are named as third and fourth Zagreb indices and defined as follows:

$$M_3(G) = \sum_{uv\in E(G)} (\varepsilon(u) + \varepsilon(v))$$
$$M_4(G) = \sum_{v\in V(G)} \varepsilon(v)^2$$

The Polycyclic Aromatic hydrocarbons PAH_k for all positive integer number k is ubiquitous combustion products. They have been implicated as carcinogens and play a role in graphitization of organic materials. A general representation of Polycyclic Aromatic Hydrocarbons is shown in Figure 1. For more details see [12]– [16].

In this paper, we compute the third Zagreb index of Polycyclic Aromatic Hydrocarbons PAH_k.

2 Computation Techniques and Main Results

In this section, we discussed the techniques to find the eccentricity of vertices of the Polycyclic Aromatic Hydrocarbons PAH_k and gave the closed formula of third Zagreb index of PAH_k. We use the ring cut method [17,18]

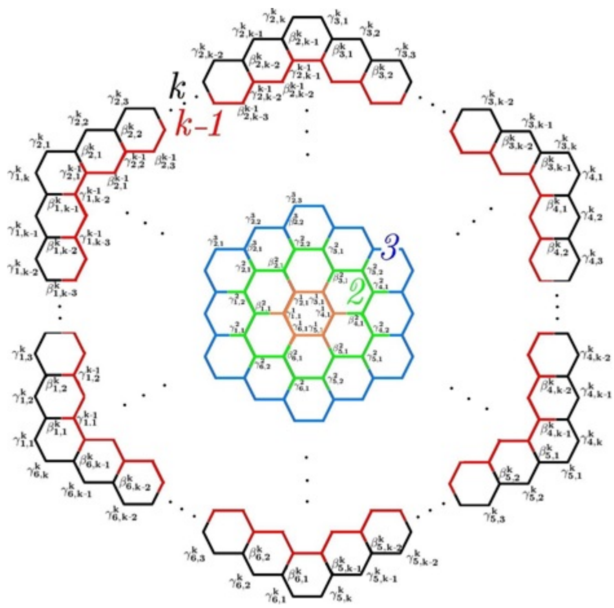

Fig. 2 Another representation of Polycyclic Aromatic Hydrocarbons (PAHk).

to divide the vertices in partition sets. From Figure 2 we have the vertex set as $V(PAH_k) = \{\alpha_{z,l}\ ,\ \beta^i_{z,l}\ ,\ \gamma^i_{z,j}\ :\ l = 1,...,k,\ j \in Z_i\ ,\ l \in Z_{i-1}\ \& z \in Z_6\}$, where α, β and γ represents the vertices with degree 1, 3 and 3, respectively, and $Z_i = \{1, 2, \ldots, i\}$.

Theorem 1. *Let G be the Polycyclic aromatic hydrocarbons PAH_k. Then the third Zagreb index of PAH_k is equal to*

$$M_3(PAH_k) = 6\sum_{i=1}^{k}(12i(i+k) + 2k - 9i + 5).$$

Proof. To obtain the final result we used the ring cut method. The i-th ring cut contains $6(2i-1)$ vertices also $d(\beta^i_{z,l}, \beta^k_{z,l}) = d(\gamma^i_{z,j}, \gamma^k_{z,j}) = 2(k-i)$. So, we have

1. For all vertices $\alpha_{z,j}$ of PAH_k $(j \in Z_k, z \in Z_6)$

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

1. For all vertices $\beta^i_{z,j}$of PAH_k *(*$\forall i = 1, \cdots, k; z \in Z_6, j \in Z_{i-1}$*)*

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

1. For all vertices $\gamma^i_{z,j}$ of PAH_n *(*$\forall i = 1, \cdots, k; z \in Z_6, j \in Z_i$*.*

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

Now we apply these results on the definition of third Zagreb index to obtain the required result.

$$
\begin{aligned}
M_3(PAH_k) &= \sum_{uv\in E(G)} (\varepsilon(u)+\varepsilon(v)) \\
&= \left(\sum_{\beta^i_{z,j}\gamma^i_{z,j}\in \mathrm{E}(H_k)} (\varepsilon(\beta^i_{z,j})+\varepsilon(\gamma^i_{z,j})) \right) + \left(\sum_{\beta^i_{z,j}\gamma^i_{z,j+1}\in \mathrm{E}(H_k)} (\varepsilon(\beta^i_{z,j})+\varepsilon(\gamma^i_{z,j+1})) \right) \\
&+ \left(\sum_{\beta^i_{z,j}\gamma^{i-1}_{z,j}\in \mathrm{E}(H_k)} \left(\varepsilon\left(\beta^{i+1}_{z,j}\right)+\varepsilon\left(\gamma^{i-1}_{z,j}\right)\right) \right) + \left(\sum_{\gamma^i_{z,i}\gamma^i_{z+1,1}\in \mathrm{E}(H_k)} (\varepsilon(\gamma^i_{z,i})+\varepsilon(\gamma^i_{z+1,1})) \right) \\
&+ \left(\sum_{\alpha_{z,j}\gamma^k_{z,j}} \left(\varepsilon(\alpha_{z,j})+\varepsilon\left(\gamma^k_{z,j}\right)\right) \right) \\
&= \sum_{z=1}^{6} \left(\sum_{i=2}^{k}\sum_{j=1}^{i} (\varepsilon(\beta^i_{z,j})+\varepsilon(\gamma^i_{z,j})) \right) + \sum_{z=1}^{6} \left(\sum_{i=2}^{k}\sum_{j=1}^{i} (\varepsilon(\beta^i_{z,j})+\varepsilon(\gamma^i_{z,j+1})) \right) \\
&+ \sum_{z=1}^{6} \left(\sum_{i=2}^{k}\sum_{j=1}^{i} \left(\varepsilon\left(\beta^{i+1}_{z,j}\right)+\varepsilon\left(\gamma^{i-1}_{z,j}\right)\right) \right) + \sum_{z=1}^{6} \left(\sum_{i=2}^{k} (\varepsilon(\gamma^i_{z,i})+\varepsilon(\gamma^i_{z+1,1})) \right) \\
&+ \sum_{z=1}^{6} \left(\sum_{i=1}^{k} \left(\varepsilon(\alpha_{z,j})+\varepsilon\left(\gamma^k_{z,j}\right)\right) \right) \\
&= \sum_{i=2}^{k} 6(i-1)\left[(2k+2i-1)+(2k+2i-2)\right] + \sum_{i=2}^{k} 6(i-1)\left[(2k+2i-1)+(2k+2i-2)\right] \\
&+ \sum_{i=1}^{k} 6i\left[(2k+2i-1)+(2k+2i)\right] + \sum_{i=1}^{k} 6\left[2(2k+2i-1)\right] \\
&+ \sum_{i=1}^{k} 6\left[(4k+1)+(2k+2i)\right] \\
&= \sum_{i=1}^{k} (12(i-1)(4k+4i-3)) + \sum_{i=1}^{k} 6i(4k+4i-1) + \sum_{i=1}^{k} 12(2k+2i-1) \\
&+ \sum_{i=1}^{k} 6(6k+2i+1) \\
&= 6\sum_{i=1}^{k} (12i(i+k)+2k-9i+5)
\end{aligned}
$$

which ends the proof.

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