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**Research Article**

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# Fourth Geometric Arithmetic Index of Polycyclic Aromatic Hydrocarbons ($PAH_k$)

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**Abstract** The *geometric-arithmetic* index of a graph *G* is defined as $GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$. Recently, *Ghorbani* et. al. introduced the eccentric version of the geometric-arithmetic index as $GA_4(G)=\sum_{uv\in E(G)}\frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}$, where $\varepsilon(u)$ is the *eccentricity* of the vertex *u*. In this paper, we compute the *fourth geometric-version* of *Polycyclic aromatic hydrocarbons ($PAH_k$).*

**Keywords** Geometric-arithmetic, Topological indices, Zagreb indices, Polycyclic Aromatic Hydrocarbons

**Introduction**

Let *G(V,E)* be a graph, where *V* and *E* represent the *vertex set* and *edge set*, respectively. The *degree* of a vertex *v* in a graph *G* is the number of vertices adjacent with *v* and denoted as *d(v).* The *maximum degree* in a graph *G* is denoted as $\Delta(G)$ and the *minimum degree* as $\delta(G)$. A vertex with degree 1 is called a *pendent vertex*. The *distance* between *u* and *v* in a graph *G* is the length of the shortest path between them denoted as *d(u,v)* and the *eccentricity* of a vertex *v* is the largest distance between *v* and any other vertex *u* of *G* i.e. $\varepsilon(v)=Max\{d(v,u)\,|\,\forall u\in V(G)\}$. Among the eccentricity over all vertices of *G* the minimum and maximum are called the *radius* and *diameter* of *G*.

*Topological indices* are the numerical value associated with chemical constitution professes for correlation of chemical structure with various physical properties, chemical and biological activity. The topological index of a molecule is a non-empirical numerical quantity that quantifies the structure and the branching pattern of molecule. There are hundreds of degree based and distance based topological indices have been introduced up to now.

The *Zagreb indices* have been introduced more than thirty years ago by *Gutman* and *Trinajstić* [1]. They are defined as:

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

The *geometric-arithmetic* index of a graph *G*, *GA(G)*, proposed by *Vukivević* and *Furtula* [2] as:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$$

In 2010, *M. Ghorbani* and *A. Khaki* [3] defined the eccentric version of geometric-arithmetic index named as *geometric-arithmetic eccentricity* index and defined as

$$GA_4(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}$$

For history and more results about the geometric-arithmetic indices reader may see [4-10].

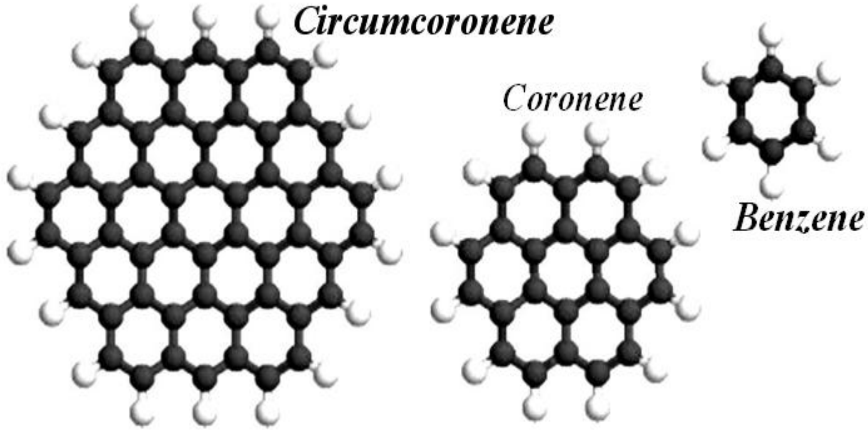


*Figure 1: First few members of Polycyclic aromatic hydrocarbons (PAHk).*

*Polycyclic Aromatic Hydrocarbons ($PAH_k$)* discussed here is a family of hydrocarbon molecules, which consists of several copies of benzene on circumference and is ubiquitous combustion products. They are of interest as molecular analogues of graphite as candidates for interstellar species and as building blocks of functional materials for device applications. This can be thought as small pieces of graphene sheets with the free valences of the dangling bonds saturated by Hydrogen. Figure 1 shows first few members of this family and Figure 2 is its general representation. Further information can be found in [11-16].

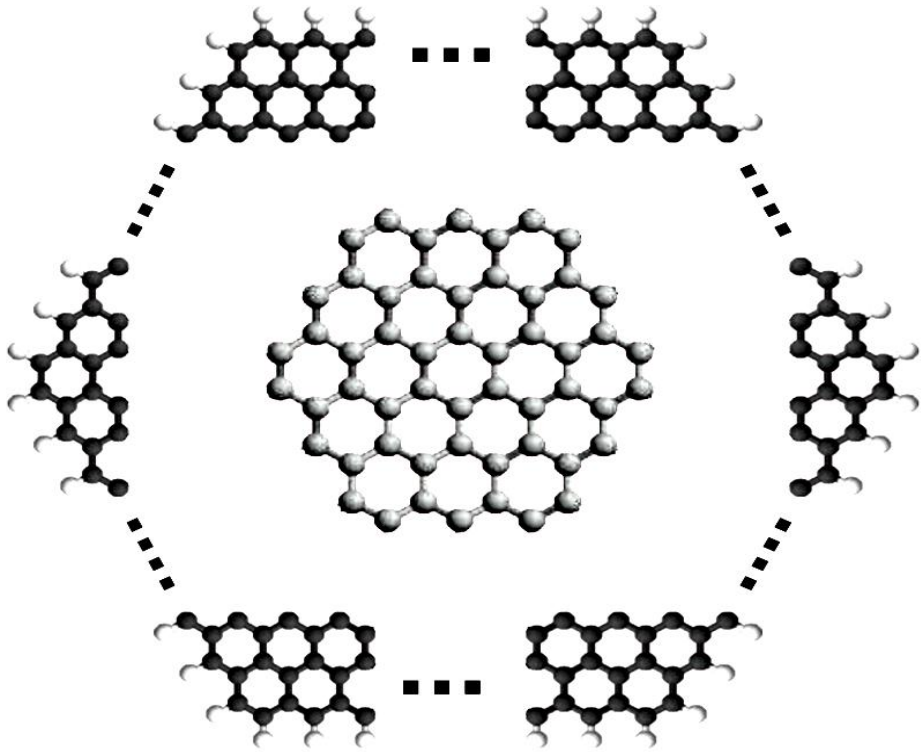

*Figure 2: The general representation of Polycyclic aromatic hydrocarbons (PAHk).*

**Results**

In this section, we computed the fourth version of geometric-arithmetic index of Polycyclic aromatic hydrocarbons *($PAH_k$)*. We used the ring cut method to divide the vertices of this structure. In ring cut method, all vertices of *G* are partitioned and we insert some vertices of *G* in a common ring-cut, such that these vertices have similar mathematical properties [17,18].

**Theorem 1:** Let the Polycyclic aromatic hydrocarbon ($PAH_k$), then the fourth geometric-arithmetic index of $PAH_k$ is given as

$$GA_4\left(PAH_k\right)=12\sum_{i=1}^{k}\left[\frac{2\left(i-1\right)\sqrt{\left(2k+2i-1\right)\left(2k+2i-2\right)}}{4k+4i-3}+\frac{i\sqrt{\left(2k+2i-1\right)\left(2k+2i\right)}}{4k+4i-1}+\frac{\sqrt{\left(4k+1\right)\left(2k+2i\right)}}{6k+2i+1}\right]$$

**Proof:** We denote the pendent vertices by $\alpha$ and the vertices of degree three by $\beta$ and $\gamma$. So the vertex set is $V(PAH_n)=\{\alpha_{z,l},\beta^{i}_{z,l},\gamma^{i}_{z,j} \mid I=1,...,k,\quad j\in\mathbb{Z}_i \quad \& \quad l\in\mathbb{Z}_{i-1} \quad \& \quad z\in\mathbb{Z}_6\}$ and $E(PAH_n)=\{\alpha_{z,j}\gamma^{k}_{z,j},\beta^{i}_{z,j}\gamma^{i}_{z,j},\beta^{i}_{z,j}\gamma^{i}_{z,j+1},\beta^{i}_{z,j}\gamma^{i-1}_{z,j}\ \&\ \gamma^{i}_{z,i}\gamma^{i}_{z+1,1} \mid i\in\mathbb{Z}_k\ \&\ j\in\mathbb{Z}_i\ \&\ z\in\mathbb{Z}_6\}$(Figure 3) , where $\mathbb{Z}_i=\{1,2,...,i\}$ is the cycle finite group of order *i*. We split the vertices in some ring cut partitions, such that i$^{th}$ ring cut contain 6i+6(i-1). All vertices of same ring cut have same eccentricity and $d(\gamma^{i}_{z,j},\gamma^{k}_{z,j})=d(\beta^{i}_{z,l},\beta^{k}_{z,l})=2(k-i)$. From the references [19-22] and Figure 3 we have the following information:

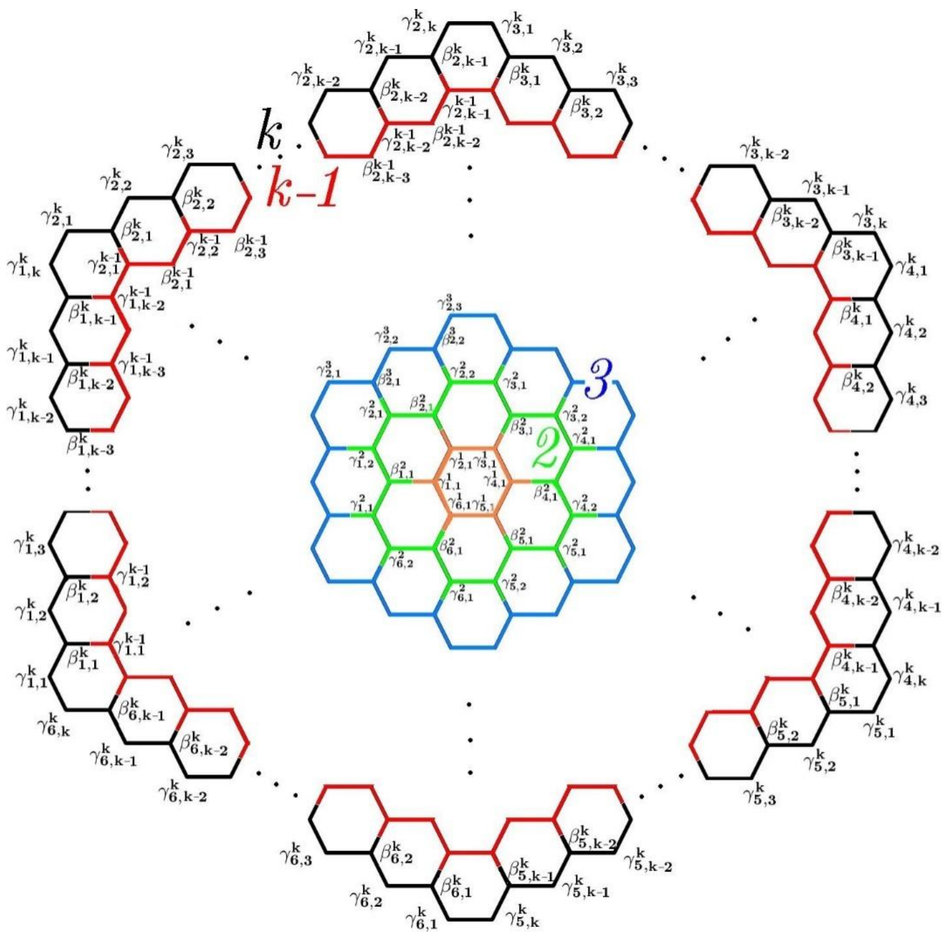


*Figure 3: A vertex wise representation of polycyclic aromatic hydrocarbons $PAH_k$.*

I. For all vertices $\alpha_{z,j}$ (hydrogen (H) atoms) of $PAH_n$ *(□j=1,..,k; z=1,..,6)*

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

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

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

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

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

To obtain the final result, we apply this information on the definition of fourth geometric-arithmetic index

$$GA_4(PAH_k) = \sum_{uv\in E(G)} \frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}$$

$$= \left(\sum_{\beta^i_{z,j}\gamma^i_{z,j}\in E(PAH_k)} \frac{2\sqrt{\varepsilon(\beta^i_{z,j})\varepsilon(\gamma^i_{z,j})}}{\varepsilon(\beta^i_{z,j})+\varepsilon(\gamma^i_{z,j})}\right) + \left(\sum_{\beta^i_{z,j}\gamma^i_{z,j+1}\in E(PAH_k)} \frac{2\sqrt{\varepsilon(\beta^i_{z,j})\varepsilon(\gamma^i_{z,j+1})}}{\varepsilon(\beta^i_{z,j})+\varepsilon(\gamma^i_{z,j+1})}\right) +$$

$$+ \left(\sum_{\beta^i_{z,j}\gamma^{i-1}_{z,j}\in E(PAH_k)} \frac{2\sqrt{\varepsilon(\beta^{i+1}_{z,j})\varepsilon(\gamma^{i-1}_{z,j})}}{\varepsilon(\beta^{i+1}_{z,j})+\varepsilon(\gamma^{i-1}_{z,j})}\right) + \left(\sum_{\gamma^i_{z,i}\gamma^i_{z+1,1}\in E(PAH_k)} \frac{2\sqrt{\varepsilon(\gamma^i_{z,i})\varepsilon(\gamma^i_{z+1,1})}}{\varepsilon(\gamma^i_{z,i})+\varepsilon(\gamma^i_{z+1,1})}\right) +$$

$$+ \left(\sum_{\alpha_{z,j}\gamma^k_{z,j}\in E(G)} \frac{2\sqrt{\varepsilon(\alpha_{z,j})\varepsilon(\gamma^k_{z,j})}}{\varepsilon(\alpha_{z,j})+\varepsilon(\gamma^k_{z,j})}\right)$$

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

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

$$+ \sum_{z=1}^{6}\left(\sum_{i=1}^{k} \frac{2\sqrt{\varepsilon(\alpha_{z,j})\varepsilon(\gamma^k_{z,j})}}{\varepsilon(\alpha_{z,j})+\varepsilon(\gamma^k_{z,j})}\right)$$

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

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

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

$$=\sum_{i=2}^{k}24(i-1)\left[\frac{\sqrt{(2k+2i-1)(2k+2i-2)}}{4k+4i-3}\right]++\sum_{i=1}^{k}12i\left[\frac{\sqrt{(2k+2i-1)(2k+2i)}}{4k+4i-1}\right]+$$

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

$$=12\sum_{i=1}^{k}\left[\frac{2(i-1)\sqrt{(2k+2i-1)(2k+2i-2)}}{4k+4i-3}+\frac{i\sqrt{(2k+2i-1)(2k+2i)}}{4k+4i-1}+\frac{\sqrt{(4k+1)(2k+2i)}}{6k+2i+1}\right]+6k$$

So, the proof is complete.■

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