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<http://journals.up4sciences.org>Computation of the fifth Geometric-Arithmetic Index for Polycyclic Aromatic Hydrocarbons PAH_k Mehdi Alaeiyan¹, Mohammad Reza Farahani¹ [†], Muhammad Kamran Jamil².

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Abstract

Let G be a simple connected graph. The *geometric-arithmetic index* of G is defined as $GA_1(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$, where $d(u)$ represents the degree of the vertex u in the graph G . Recently, Graovac defined the fifth version of geometric-arithmetic index of a graph G as $GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_v S_u}}{S_v + S_u}$, where S_u is the sum of degrees of all neighbors of vertex u in the graph G . In this paper, we compute the fifth geometric arithmetic index of Polycyclic Aromatic Hydrocarbons (PAH_k).

Keywords: Molecular graphs, chemical structures Polycyclic Aromatic Hydrocarbon (PAH_k), enzenoid, Topological indices, fifth Geometric-Arithmetic Index.

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1 Introduction

Let $G(V, E)$ be a simple connected graph, where V and E represent the set of vertices and the set of edges, respectively. The number of elements in V and E are called the *order* and the *size* of the graph G , respectively. The *distance* between the vertices u and v is the length of the shortest path connecting them. The maximum

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distance between u and any other vertex of the graph G is called *eccentricity* of u . For a vertex $v \in V$, the number of vertices attached to v is called the degree of the vertex v . It is denoted as $d(v)$. The notation S_v is the summation of degrees of all neighbors of vertex v in G , i.e. $S_v = \sum_{uv \in E(G)} d(u)$. More details about the standard notations from the graph theory in the paper can refer to [1]–[3].

A topological index is a function (TI) from the set of finite simple graphs to the set of real numbers, with the property that $TI(G) = TI(H)$ if both the graph G and H are isomorphic. There are hundreds of topological indices being introduced. *M. Randić* [4] introduced the first degree based topological index named as *Randić index*. The Randić index of a graph G is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}.$$

A widely used connectivity topological index is *geometric-arithmetic index* (GA) introduced by Vukicevic [5] and it can be defined as

$$GA_1(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}.$$

The second member of this family of index was introduced by *Fath-Tabar* [6]

$$GA_2(G) = \sum_{uv \in E(G)} \frac{2\sqrt{n_v n_u}}{n_v + n_u},$$

where n_u is the number of vertices of graph G lying closer to the vertex u than that to the vertex v for the edge $uv \in E(G)$.

Bo-Zhou [7] proposed the *third geometric-arithmetic index* of a graph G

$$GA_3(G) = \sum_{uv \in E(G)} \frac{2\sqrt{m_v m_u}}{m_v + m_u},$$

where m_u is the number of edges of graph G lying closer to the vertex u than that to the vertex v for the edge $uv \in E(G)$.

The *fourth geometric-arithmetic index* was proposed by *Ghorbani* [8]. This index is defined as

$$GA_4(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\varepsilon_v \varepsilon_u}}{\varepsilon_v + \varepsilon_u},$$

where ε_u is the number of eccentricity of vertex u .

Recently, *Graovac* [9] defined the fifth version of geometric-arithmetic index as

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_v S_u}}{S_v + S_u}.$$

For history and further results on this family of topological indices, please refer to [10]–[16].

Chemical graph theory is the branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena. This theory has vital effect on the development of the chemical sciences.

Polycyclic Aromatic Hydrocarbons PAH_k are obtained from the burning of organic material, and naturally as a result of thermal geological reaction. For many years, they attracted much attention, because some of them are strong carcinogens. The Polycyclic Aromatic Hydrocarbons consist of several copies of benzene on circumference. The first three members of this family are shown in Figure 1. For further details, please refer to [17]–[43].

In this paper, we compute the fifth geometric-arithmetic index of Polycyclic Aromatic Hydrocarbons.

Fig. 1 The first three members of Polycyclic Aromatic Hydrocarbons family PAH_k .

2 Computation Techniques and Main Results

In this section, we computed the fifth version of Polycyclic Aromatic Hydrocarbon (PAH_k).

Theorem 1. Consider the graph of Polycyclic Aromatic Hydrocarbons (PAH_k), then the fifth geometric-arithmetic index of Polycyclic Aromatic Hydrocarbon is equal to

$$GA_5(PAH_k) = 9k^2 + k \left(6\frac{\sqrt{21}}{5} + \frac{9\sqrt{7}}{2} - 15 \right) + \left(12 - \frac{9\sqrt{7}}{2} \right).$$

Proof. A graphical representation of Polycyclic Aromatic Hydrocarbons is shown in Figure 2. It contains $6k^2 + 6k$ vertices and $9k^2 + 3k$ edges. In this structure, there are two types of vertices, vertices with degree 1 and degree 3. We denote the sets of vertices with degree 1 as $V_1 = \{v \in V(G) | d_v = 1\}$ and degree 3 as $V_3 = \{v \in V(G) | d_v = 3\}$. On the basis of degrees of the vertices we divide the edge set into a partition $E_4 = \{uv \in E(PAH_k) | d_u + d_v = 4\}$, $E_6 = \{uv \in E(PAH_k) | d_u + d_v = 6\}$ and $|E_4| = 6k$, $|E_6| = 9k^2 - 3k$.

The sum of degrees of vertices for each edge of PAH_k is represented as follows:

1. There are k edges $e = uv$ for which, $S_u = 3, S_v = 7$ when $u \in V_1, v \in V_3$ and $uv \in E_4$.
2. There are 6 edges $e = uv$ for which, $S_u = S_v = 7$ when $u, v \in V_6$ and $uv \in E_6$.
3. There are $9k^2 - 15k + 6$ edges $e = uv$ for which, $S_u = S_v = 9$ when $u, v \in V_3$ and $uv \in E_6$.

Now, we apply these calculations to the definition of the fifth geometric-arithmetic index which can be demonstrated as follows,

$$\begin{aligned} GA_5(PAH_k) &= \sum_{e=uv \in E(H_k)} \frac{2\sqrt{S(v)S(u)}}{S(v)+S(u)} \\ &= 6k \frac{2\sqrt{3 \times 7}}{3+7} + 6 \frac{2\sqrt{7 \times 7}}{7+7} + 12(k-1) \frac{2\sqrt{7 \times 9}}{7+9} + (9k^2 - 15k + 6) \frac{2\sqrt{9 \times 9}}{9+9} \\ &= 6k \frac{\sqrt{21}}{5} + 6 + (k-1) \frac{9\sqrt{7}}{2} + (9k^2 - 15k + 6) \\ &= 9k^2 + k \left(6\frac{\sqrt{21}}{5} + \frac{9\sqrt{7}}{2} - 15 \right) + \left(12 - \frac{9\sqrt{7}}{2} \right) \end{aligned}$$

which is the required result.

Example 2. The reader can find some values of the fifth geometric-arithmetic index of Polycyclic Aromatic Hydrocarbons (PAH_k) for integer $k=1, 2, 3, \dots, 10^{12}$ in following table.

Fig. 2 General representation of Polycyclic Aromatic Hydrocarbons (PAH_k).

Table 1. Computing GA_5 index for Polycyclic Aromatic Hydrocarbons PAH_k ($\forall k = 1, 2, 3, \dots, 10^{12}$):

$GA_5(PAH_1)$	11.4991	$GA_5(PAH_{10})$	924.1441
$GA_5(PAH_2)$	40.9041	$GA_5(PAH_{20})$	3648.1941
$GA_5(PAH_3)$	88.3091	$GA_5(PAH_{30})$	8172.2441
$GA_5(PAH_4)$	153.7141	$GA_5(PAH_{40})$	14496.2941
$GA_5(PAH_5)$	237.1191	$GA_5(PAH_{50})$	22620.3441
$GA_5(PAH_6)$	338.5241	$GA_5(PAH_{60})$	32544.3941
$GA_5(PAH_7)$	457.9291	$GA_5(PAH_{70})$	44268.4441
$GA_5(PAH_8)$	595.3341	$GA_5(PAH_{80})$	57792.4941
$GA_5(PAH_9)$	750.7391	$GA_5(PAH_{90})$	73116.5441
$GA_5(PAH_{100})$	90240.5941	$GA_5(PAH_{1000})$	9002405.0941
$GA_5(PAH_{200})$	360481.0941	$GA_5(PAH_{2000})$	36004810.0941
$GA_5(PAH_{300})$	810721.5941	$GA_5(PAH_{3000})$	81007215.0941
$GA_5(PAH_{400})$	1440962.0941	$GA_5(PAH_{4000})$	144009620.0941
$GA_5(PAH_{500})$	2251202.5941	$GA_5(PAH_{5000})$	225012025.0941
$GA_5(PAH_{600})$	3241443.0941	$GA_5(PAH_{6000})$	324014430.0941
$GA_5(PAH_{700})$	4411683.5941	$GA_5(PAH_{7000})$	441016835.0941
$GA_5(PAH_{800})$	5761924.0941	$GA_5(PAH_{8000})$	576019240.0941
$GA_5(PAH_{900})$	7292164.5941	$GA_5(PAH_{9000})$	729021645.0941

$GA_5(PAH_{10000})$	900024050.0941
$GA_5(PAH_{20000})$	3600048100.0941
$GA_5(PAH_{30000})$	8100072150.0941
$GA_5(PAH_{40000})$	14400096200.0941
$GA_5(PAH_{50000})$	22500120250.0941
$GA_5(PAH_{60000})$	32400144300.0941
$GA_5(PAH_{70000})$	44100168350.0941
$GA_5(PAH_{80000})$	57600192400.0941
$GA_5(PAH_{90000})$	72900216450.0941
$GA_5(PAH_{100000})$	90000240500.0941
$GA_5(PAH_{200000})$	360000481000.094
$GA_5(PAH_{300000})$	810000721500.094
$GA_5(PAH_{400000})$	1440000962000.09
$GA_5(PAH_{500000})$	2250001202500.09
$GA_5(PAH_{600000})$	3240001443000.09
$GA_5(PAH_{700000})$	4410001683500.09
$GA_5(PAH_{800000})$	5760001924000.09
$GA_5(PAH_{900000})$	7290002164500.09
$GA_5(PAH_{1000000})$	9000002405000.09
$GA_5(PAH_{2000000})$	36000004810000.1
$GA_5(PAH_{3000000})$	81000007215000.1
$GA_5(PAH_{4000000})$	144000009620000
$GA_5(PAH_{5000000})$	225000012025000
$GA_5(PAH_{6000000})$	324000014430000
$GA_5(PAH_{7000000})$	441000016835000
$GA_5(PAH_{8000000})$	576000019240000
$GA_5(PAH_{9000000})$	729000021645000
$GA_5(PAH_{10000000})$	900000024050000
$GA_5(PAH_{20000000})$	$3.6000000481 \times 10^{15}$
$GA_5(PAH_{30000000})$	$8.10000007215 \times 10^{15}$
$GA_5(PAH_{40000000})$	$1.44000000962 \times 10^{16}$
$GA_5(PAH_{50000000})$	$2.250000012025 \times 10^{16}$
$GA_5(PAH_{60000000})$	$3.24000001443 \times 10^{16}$
$GA_5(PAH_{70000000})$	$4.410000016835 \times 10^{16}$
$GA_5(PAH_{80000000})$	$5.76000001924 \times 10^{16}$
$GA_5(PAH_{90000000})$	$7.290000021645 \times 10^{16}$
$GA_5(PAH_{100000000})$	$9.00000002405 \times 10^{16}$
$GA_5(PAH_{200000000})$	$3.60000000481 \times 10^{17}$
$GA_5(PAH_{300000000})$	$8.100000007215 \times 10^{17}$
$GA_5(PAH_{400000000})$	$1.440000000962 \times 10^{18}$
$GA_5(PAH_{500000000})$	$2.2500000012025 \times 10^{18}$
$GA_5(PAH_{600000000})$	$3.240000001443 \times 10^{18}$
$GA_5(PAH_{700000000})$	$4.4100000016835 \times 10^{18}$
$GA_5(PAH_{800000000})$	$5.760000001924 \times 10^{18}$
$GA_5(PAH_{900000000})$	$7.2900000021645 \times 10^{18}$

$GA_5(PAH_{10000000000})$	$9.000000002405 \times 10^{18}$
$GA_5(PAH_{20000000000})$	$3.600000000481 \times 10^{19}$
$GA_5(PAH_{30000000000})$	$8.1000000007215 \times 10^{19}$
$GA_5(PAH_{40000000000})$	$1.4400000000962 \times 10^{20}$
$GA_5(PAH_{50000000000})$	$2.25000000012025 \times 10^{20}$
$GA_5(PAH_{60000000000})$	$3.2400000001443 \times 10^{20}$
$GA_5(PAH_{70000000000})$	$4.41000000016835 \times 10^{20}$
$GA_5(PAH_{80000000000})$	$5.7600000001924 \times 10^{20}$
$GA_5(PAH_{90000000000})$	$7.29000000021645 \times 10^{20}$
$GA_5(PAH_{100000000000})$	$9.0000000002405 \times 10^{20}$
$GA_5(PAH_{200000000000})$	$3.6000000000481 \times 10^{21}$
$GA_5(PAH_{300000000000})$	$8.10000000007215 \times 10^{21}$
$GA_5(PAH_{400000000000})$	$1.44000000000962 \times 10^{22}$
$GA_5(PAH_{500000000000})$	$2.25000000001202 \times 10^{22}$
$GA_5(PAH_{600000000000})$	$3.24000000001443 \times 10^{22}$
$GA_5(PAH_{700000000000})$	$4.41000000001683 \times 10^{22}$
$GA_5(PAH_{800000000000})$	$5.76000000001924 \times 10^{22}$
$GA_5(PAH_{900000000000})$	$7.29000000002165 \times 10^{22}$
$GA_5(PAH_{1000000000000})$	$9.00000000002405 \times 10^{22}$
$GA_5(PAH_{2000000000000})$	$3.60000000000481 \times 10^{23}$
$GA_5(PAH_{3000000000000})$	$8.10000000000721 \times 10^{23}$
$GA_5(PAH_{4000000000000})$	$1.44000000000096 \times 10^{24}$
$GA_5(PAH_{5000000000000})$	$2.25000000000012 \times 10^{24}$
$GA_5(PAH_{6000000000000})$	$3.240000000000144 \times 10^{24}$
$GA_5(PAH_{7000000000000})$	$4.410000000000168 \times 10^{24}$
$GA_5(PAH_{8000000000000})$	$5.760000000000192 \times 10^{24}$
$GA_5(PAH_{9000000000000})$	$7.290000000000217 \times 10^{24}$
$GA_5(PAH_{10000000000000})$	$9.00000000000024 \times 10^{24}$
$GA_5(PAH_{20000000000000})$	$3.600000000000048 \times 10^{25}$
$GA_5(PAH_{30000000000000})$	$8.100000000000072 \times 10^{25}$
$GA_5(PAH_{40000000000000})$	$1.440000000000001 \times 10^{26}$
$GA_5(PAH_{50000000000000})$	$2.2500000000000012 \times 10^{26}$
$GA_5(PAH_{60000000000000})$	$3.2400000000000014 \times 10^{26}$
$GA_5(PAH_{70000000000000})$	$4.4100000000000017 \times 10^{26}$
$GA_5(PAH_{80000000000000})$	$5.7600000000000019 \times 10^{26}$
$GA_5(PAH_{90000000000000})$	$7.2900000000000022 \times 10^{26}$
$GA_5(PAH_{100000000000000})$	$9.0000000000000024 \times 10^{26}$

Corollary 3. Consider the molecular graph Polycyclic Aromatic Hydrocarbons (PAH_k) shown in Figure 1, thus Theorem 1 and Table 1 imply that for enough large integer number k , the approach fifth geometric-arithmetic index of PAH_k is equal to

$$GA_5(\widehat{PAH_k}) = 9k^2.$$

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