Molecular graphs with extremal first geometric-arithmetic index

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Abstract. Let $MG(i,n)$ be a connected molecular graph without multiple edges on n vertices whose the minimum degree of vertices is i, where $1 \leq i \leq 4$. One of the newest topological indices is the first Geometric-Arithmetic index. In this paper we determine the graph with the minimum and the maximum value of first Geometric-Arithmetic index in the family of graphs $MG(i,n)$, $1 \leq i \leq 3$.
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1. Introduction

All graphs G considered in this paper are undirected and finite on n vertex, loops and multiple edges do not occur. The number of vertices of G is denoted by n. Two vertices are adjacent iff they are connected by an edge; two edges are adjacent iff they have an end vertex in common.

For given graph G, it is called a molecular graph if the maximum degree of every vertex reaches to four. Molecular graphs are significantly important in showing the mathematical applications in chemistry. Molecules properties description is of a great value in the science of chemistry and pharmacology. A topological index is a numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. In an exact phrase, if Λ denotes the class of all finite graphs then a topological index is a function Top from Λ into real numbers with this property that Top(G) = Top(H), if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological index. The *Wiener index* [1] is the first reported distance based topological index defined as half sum of the distances between all the pairs of vertices in a molecular graph [2]. *Topological indices* are abundantly being used in the *QSPR* and *QSAR* researches. So far, many various types of topological indices have been described. One of the newest and the most efficient indices of this type is the first *Geometric-Arithmetic index* defined as follows:

$$GA_1(G) = \sum_{uv \in E(G)} 2\sqrt{d_u d_v}/(d_u + d_v),$$

where, d_u is the vertex degree of u for an edge uv. In [3] by studding the 18 octane isomers it has been indicated that the first Geometric-Arithmetic index is an efficient

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tools in the description of molecules physic-chemical characteristics. For more studies the reader is referred to the papers presented by [4, 5].

Vukicević and Furtula have obtained the lower and upper boundaries for GA_1 index in [3]. Yuan and Colleagues determined those molecular graphs possessing the minimum and maximum value of the GA_1 [4]. They also determined the molecular trees having the lowest, second lowest and third lowest value of GA_1 and highest, second highest and third highest value of GA_1 as well. From among other researches on the first Geometric - Arithmetic index, the description of the first general Geometric - Arithmetic by Elyasi and Iranmanesh can be pointed out. They obtained higher and lower boundaries for general GA_1index. For more information and new researches on the first geometric-arithmetic index, refer to [9-14].

In the current study we consider the molecular graphs with the lowest degrees of 1, 2, and 3. In the second section of the article, we present the preliminary concepts and definitions which will be used in the following sections and subsections. In the third section, we determine those molecular graphs having the lowest value of GA_1 index and the highest value of GA_1 among all of the molecular graphs with the lowest degree equal to 1. In the fourth section, those graphs having the lowest and the highest first Geometric - Arithmetic index are determined among all of the molecular graphs with the lowest degree of 2. And, finally in the fifth section extremal graphs are determined for molecular graphs with the lowest degree of 3.

2. Results and Discussions

Let $G(m)$ be a connected molecular graph on n vertices and m edges, where $V=\{v_1,v_2,\ldots,v_n\}$. Clearly, $n - 1\leq m \leq 2n$. Suppose also, n_i is the number of vertices of degree i, $i = 1, 2, 3, 4$ and x_{ij} is the number of edges connecting a vertex of degree i to a vertex of degree j. So, the first Geometric - Arithmetic index of a given molecular graph can be reformulated as follows:

$$GA_1(G)=\sum_{1\leq i\leq j\leq 4}\frac{2\sqrt{ij}}{i+j}x_{ij} \tag{1}$$

Denoted by $MG(i,n)$ means the set of all connected molecular graphs G, having n vertices with the lowest degree i, $i = 1,2,3$.

2. 1. Extremal graphs in $MG(i,n)$

In the current subsection, we construct the extremal graphs in class of $MG(1,n)$. According to Eq. (1) and by substituting terms $a_{ij}=2\sqrt{ij}/(i+j)$ in GA_1 index we have:

$$GA_1(G)=a_{12}x_{12}+a_{13}x_{13}+a_{14}x_{14}+x_{22}+a_{23}x_{23}+a_{24}x_{24}+x_{33}+a_{34}x_{34}+x_{44} \tag{2}$$

Also, the following relations hold for every graph G with the lowest degree 1,

$$
\begin{aligned}
&2x_{11}+x_{12}+x_{13}+x_{14}=n_1\\
&x_{12}+2x_{22}+x_{23}+x_{24}=2n_2\\
&x_{13}+x_{23}+x_{33}+x_{34}=2n_3\\
&x_{14}+x_{24}+x_{34}+2x_{44}=4n_4\\
&n_1+n_2+n_3+n_4=n
\end{aligned}
\tag{3}
$$

Yuan and Colleagues determined the upper and the lower bounds for the molecular graphs [4, Theorem 4] and they determined the molecular trees possessing the lowest value of GA_1 index. Therefore, according to the Yuan and Colleagues' results one can deduce that the molecular graphs with the lowest value of GA_1 index in MG(1,n) are the same as those molecular trees with the lowest value of GA_1 index. For finding the graph with the highest GA_1 index, according to [3, Theorem 1], $n_1 = n_3 = 1$ and clearly, $x_{33} = 0$. So in this case by applying Eq.(3) we have:

$$
\begin{aligned}
&x_{13}=1-x_{12}-x_{14},\\
&x_{34}=2+x_{12}+x_{14}-x_{23},\\
&x_{44}=2n-5-\frac{3}{2}x_{12}-x_{14}-2x_{22}-\frac{1}{2}x_{23}-\frac{3}{2}x_{24}.
\end{aligned}
$$

By replacing the above equations in (2), we have

$$
\begin{aligned}
GA_1(G)=&\,2n-5+\frac{8\sqrt{3}}{7}+\frac{\sqrt{3}}{2}+\left(a_{12}-a_{13}+a_{34}-\frac{3}{2}\right)x_{12}+\left(-a_{13}+a_{14}+a_{34}-1\right)x_{14}-x_{22}\\
&+\left(a_{23}-a_{34}-\frac{1}{2}\right)x_{23}+\left(a_{24}-\frac{3}{2}\right)x_{24}.
\end{aligned}
$$

By a simple calculation, we can see all of the coefficients $x_{12}, x_{14}, x_{22}, x_{23}, x_{24}$ are negative. So, for every $n \geq 7$, graph G with $n_1 = n_3 = 1, n_4 = n-2, n_2 = 0, x_{13} = 1, x_{34} = 2, x_{44} = 2n-5$ and $x_{11} = x_{12} = x_{14} = x_{22} = x_{23} = x_{24} = x_{33} = 0$ is a graph which owns the highest value of GA_1 index. Immediately, we can conclude the following theorem:

Theorem 1. Among all of the molecular graphs with n vertices having minimum degree 1 we have:

I. If $n \equiv 2 \pmod 3$, then for $n \geq 5$, the molecular tree with only degrees 1 and 4 is a molecular tree with the minimum value of GA_1 index. In this case $x_{14} = \frac{2}{3}(n+1)$ and $x_{44} = \frac{1}{3}(n-5)$ then the value of GA_1 is equal to $13n/15 - 17/15$. Note that the molecular tree is not unique.

II. If $n \equiv 1 \pmod 3$, then for $n \geq 13$, the molecular tree with a single vertex of degree three adjacent to three vertices of degree four, and without vertices of degree two is a molecular tree with the minimum value of GA_1 index. In this case $x_{14} = \frac{1}{3}(2n+1)$, $x_{34} = 3$ and $x_{44} = \frac{1}{3}(n-13)$ then the value of GA_1 is equal to $\frac{13}{15}n + \frac{12\sqrt{3}}{7} - \frac{61}{15}$. Note that the molecular tree is not unique.

III. If $n \equiv 0 \pmod 3$, then for $n \geq 9$, the graph with a single vertex of degree two adjacent to two vertices of degree four, and without vertices of degree three is a molecular tree with the minimum value of GA_1 index. In this case $x_{14} = 2n/3$, $x_{24} = 2$ and $x_{44} = (n-9)/3$ then the value of GA_1 is equal to $13n/15 + 4\sqrt{2}/3 - 3$. Note that the molecular tree is not unique.

IV. For $n \geq 7$, the graph with a single vertex of degree three adjacent to one vertex of degree one and two vertex of degree four, and without vertices of degree two is a molecular graph with the maximum value of GA_1 index. In this case $x_{13} = 1$, $x_{34} = 2$ and $x_{44} = 2n-4$ then the value of GA_1 is equal to $2n - 5 + 23\sqrt{3}/14$. Note that the molecular tree is not unique.

2. 2. Extremal graphs in MG(2,n)

Here, we determine those graphs having the lowest and the highest value of GA_1 in class of MG(2,n) graphs. If m be the number of the edges of an arbitrary molecular graph with the lowest vertex degree of 2, then it is obvious that $n \leq m \leq 2n$. For every $G \in MG(2,n)$ the following relations are true:

$$
\begin{aligned}
2x_{22} + x_{23} + x_{24} &= 2n_2 \\
x_{23} + 2x_{33} + x_{34} &= 3n_3 \\
x_{24} + x_{34} + x_{44} &= 4n_4 \\
n_2 + n_3 + n_4 &= n
\end{aligned} \tag{4}
$$

Regarding the $a_{ij} = \frac{2\sqrt{ij}}{i+j}$, the value of GA_1 index can be calculated as follows:

$$GA_1(G) = x_{22} + a_{23}x_{23} + a_{24}x_{24} + x_{33} + a_{34}x_{34} + x_{44} \tag{5}$$

For finding a graph with the lowest value of GA_1 in MG(2,n), based on the equations in (4) we have:

$$x_{22} = n - \frac{5}{6}x_{23} - \frac{3}{4}x_{24} - \frac{2}{3}x_{33} - \frac{7}{12}x_{34} - \frac{1}{2}x_{44}.$$

Now, by replacing x_{22} in (5) we obtain:

$$GA_1(G) = n + \left(a_{14} - \frac{5}{6}\right)x_{23} + \left(a_{24} - \frac{3}{4}\right)x_{24} + \left(1 - \frac{2}{3}\right)x_{33} + \left(a_{34} - \frac{7}{12}\right)x_{34} + \left(1 - \frac{1}{2}\right)x_{44}.$$

By a simple calculation, we can see all of terms $x_{23}, x_{24}, x_{33}, x_{34}, x_{44}$ are positive, so for every $n \geq 3$, graph G with $n_2 = n$ and $x_{22} = n$, is a graph that owns the lowest value of the GA_1 index.

According to [3, Theorem 1] we can consider that $n_2 = 1$, and obviously $x_{22} = 0$. For finding a graph which possesses the highest value of GA_1 index in MG(2,n) and according to the equations in (4) as well we have:

$$x_{24} = 2 - x_{23},$$
$$x_{44} = 2n - 3 - \frac{1}{6}x_{23} - \frac{4}{3}x_{33} - \frac{7}{6}x_{34}.$$

Now, by replacing x_{24} and x_{44} in (5) we have

$$GA_1(G) = 2n - 3 + \frac{4\sqrt{2}}{3} + \left(a_{14} - a_{24} - \frac{1}{6}\right)x_{23} + \left(-\frac{1}{3}\right)x_{33} + \left(a_{34} - \frac{7}{6}\right)x_{34}.$$

By a simple calculation, we can see all of the coefficients x_{23}, x_{33} and x_{34} in the above equation are negative; therefore the highest value of GA_1 is obtained. Hence, for every $n \geq 6$, a graph with $n_2 = 1$, $n_4 = n - 1$, $x_{24} = 2$, $x_{44} = 2n - 3$ and the other $x_{ij} = 0$, is a graph with the highest value of GA_1. In other words, we proved the following theorem:

Theorem 2 Among the molecular graphs having n number of vertices considering two as the minimum degree for every vertex:
(I) For $n \geq 3$, the graph with only degrees two and without vertices of degree three and four is a unique molecular graph with the minimum GA_1 index, which is equal to n. In this case $G \cong C_n$.

For $n \geq 6$, the graph with a single vertex of degree two adjacent to one vertex of degree four, and without vertices of degree three is a molecular graph with the maximum value of GA_1 index. In this case $x_{24} = 2$ and $x_{44} = 2n-3$ then the value of GA_1 is equal to $2n-3+\frac{4\sqrt{2}}{3}$. Note that the molecular tree is not unique.

2. 3 Extremal graphs in MG(3,n)

In the present section, we determine those molecular graphs having the lowest and the highest value of GA_1 index with the lowest degree 3. For every molecular in MG(3,n) the following relations hold:

$$\begin{aligned} 2x_{33}+x_{34} &= 3n_3 \\ x_{34}+x_{44} &= 4n_4 \\ n_3+n_4 &= n \end{aligned} \tag{6}$$

The value of GA_1 index for every arbitrary molecular graph in MG(3,n) can be calculated as follows:

$$GA_1(G)=x_{33}+\frac{4\sqrt{3}}{7}x_{34}+x_{44} \tag{7}$$

For finding the graph with the lowest GA_1 index in MG(3,n) we consider the two cases:

Case 1 Suppose that $n_4 = 1$. In this case $n_3 = n-1$ and it is apparent that n should be an odd number. It is clear that x_{44}=0, so according to (6) we have:

$$x_{34}=4,\ x_{33}=\frac{3(n-1)}{2}-2.$$

Therefore, in this case if n be an odd number, then the graphs $x_{34} = 4$, $x_{33} = \frac{3(n-1)}{2}-2$ and $x_{44} = 0$ have the lowest value of GA_1 index.

Case 2. Suppose that $n_4 = 2$. In this case $n_3 = n-2$ and it is clear that n should be an even number. In this case according to (6) we have:

$$x_{34}=8-2x_{44},\ x_{33}=\frac{3(n-1)}{2}-4+x_{44}.$$

Now, by replacing the above Eq. in (7), we have:

$$GA_1(G)=\frac{3}{2}n-7+\frac{32\sqrt{3}}{7}+2(1-a_{34})x_{44}.$$

By a simple calculation, we can see that the coefficient X_{44}, in the above equation is positive. So, in this case for every $n \geq 8$, the graphs with $x_{34} = 8$, $x_{33} = \frac{3}{2}n - 7$ and $x_{44} = 0$ are those having the lowest value of GA_1.

For finding the graph with the highest value of GA_1 index in MG(3,n), according to [3, Theorem 1], we should consider the graph having the highest number of edges as possible. So we assume that $n_3 = 2$, therefore in this case the two graphs can be considered as follows:

G_1: $x_{33} = 0$, $x_{34} = 6$, $x_{44} = 2n - 7$.

and

G_2: $x_{33} = 1$, $x_{34} = 4$, $x_{44} = 2n - 6$.

Now, by comparing GA_1 index, for these one can see that G_2 has the maximum GA_1 index in MG(3,n).

Theorem 3 Among all of the molecular n vertex graphs and with the minimum vertex degree of 3:
(I) If $n \equiv 1$ (mod 2), then for every $n \geq 5$, the graph with a single vertex of degree four adjacent to four vertices of degree three and other edges connecting the vertex of degree three to the vertex of the degree three, is a molecular graph that has the minimum values of GA_1 index, which is equal to $\frac{3(n-1)}{2} - 2 + \frac{16\sqrt{3}}{7}$. Note that the molecular tree is not unique.

(II) If $n \equiv 0$ (mod 2), then for every $n \geq 8$, the graph with two vertices of degree four, each adjacent to four vertices of degree three, and other edges connect a vertex of degree three to the vertex of degree three, is a molecular graph that possesses the minimum values of GA_1 index and this value is equal to $\frac{3}{2}n - 7 + \frac{32\sqrt{3}}{7}$. Note that the molecular tree is not unique.

(III) For $n \geq 6$, the graph with a single vertex of degree three adjacent to one vertex of degree three, two vertices of degree three, each adjacent to two vertices of degree four, and other edges connect a vertex of degree four to the vertex of degree four, is a molecular graph that possesses the maximum values of GA_1 index and this value is equal to $2n - 5 + \frac{16\sqrt{3}}{7}$. Note that the molecular tree is not unique.

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