Received: 13 June 2021 | Revised: 10 August 2021 | Accepted: 14 August 2021
DOI: 10.22034/ecc.2021.295046.1204

Eurasian Chemical Communications
SAMI

FULL PAPER

The geometric arithmetic (GA) index of certain trees and bicyclic graphs

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The geometric arithmetic (GA) index is one of the recently most investigated degree-based molecular structure descriptors that have applications in chemistry. For a graph G, the (GA) index is defined as $GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_u d_v}}{d_u+d_v}$, where d_u denotes the degree of a vertex u in G. In this paper, we obtain the general formulas of geometric arithmetic GA index for two types of trees graphs. Also, we provide the general formulas to the bicyclic graphs after attaching branches of B_i for all vertices. Finally, we computed the geometric arithmetic GA index to the molecular graph representing the molecular structure of the bicyclic chemical graphs.

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KEYWORDS

The geometric arithmetic (GA) index; bicyclic graphs; bicyclic chemical graph; molecular graph; tree.

Introduction

Molecular descriptors have found a wide application in quantitative structure-activity relationship analysis (QSAR) and quantitative structure-property relationship (QSPR) targets the estimation of specific characteristics based on the structures of the compounds under study [1]. Among them, topological indices have a prominent place. One of the best known and widely used is the connectivity χ index, introduced in 1975 by Milan Randić [2,3], who has shown this index to reflect molecular branching. The introduction of graph theoretic concepts in chemistry is well known, and the reader is referred to the following references for definitions and notations [4,5]. The first geometric–arithmetic index GA was proposed by Vukičević and Futuna [6]. This index is defined as $GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_u d_v}}{d_u+d_v}$. It was demonstrated [6], on the example of octane isomers, that the GA index is well correlated with a variety of physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation and acentric factor. Moreover, the quality of these correlations was found to be better than for other often employed molecular descriptors [1]. The mathematical properties of the GA and other indices were reported [7–16]. Das and Trinajstić [10] compared the ABC index and the GA indices for molecular graphs and general graphs. The (chemical) trees, unicyclic, bicyclic graph(s) with maximal ABC index were determined [3,17-22, 29-40]. Recently, In 2016 Mohanad et al. studied the general formula for ABC index of some special trees graphs, also in the same paper provided a general formula of ABC index of bicyclic graphs [22]. In this paper we have three sections, the first one, we present the general formula of geometric arithmetic GA index of some special trees. In the second section, we provided a general formula of geometric arithmetic GA index of bicyclic graphs. Finally, we computed the geometric arithmetic GA index of molecular graph associated with molecular structure of the bicyclic chemical graphs.

Preliminaries

A vertex of a graph is said to be a pendant if its neighbourhood contains exactly one vertex. An edge of a graph is said to be a pendant if one of its vertices is a pendant vertex.

Let G be a graph and $u, v \in V(G)$. A $(u,v)-walk$ is a finite sequence of vertices $a_\circ, a_1, a_2, \dots, a_k$, with $k \geq 0, u = a_\circ$ and $v = a_k$, such that $a_{i-1}a_i \in E(G)$ for each $i = 1,2,3,\dots,k$. The length of the walk is k that is the number of edges in it. A $(u,v)-walk$ is called a path if no vertices are repeated.

Let B_i be a branch of a tree T formed by attaching i pendant path of length 2 to the vertex v such that the degree of v in T is $i+1$ (see Figure 1. for an illustration), the minimal-ABC trees were fully characterized by Hosseini, Ahmadi and Gutman [23].

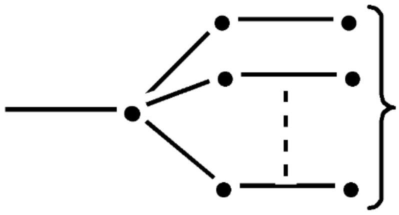

FIGURE 1 The branche B_i

The Curtain graph [22] is a tree graph obtained by attaching m branches of B_k to each vertex of path P_n, we denote such graph by $T(n, B_k^m)$ (Figure 2).

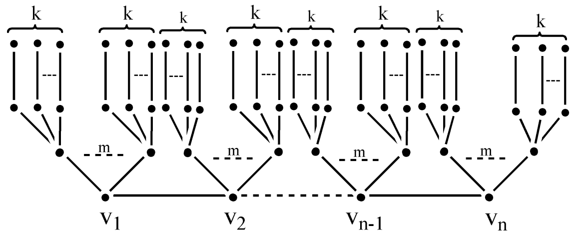

FIGURE 2 The Curtain graph $T(\text{n}, B_k^m)$

Geometric Arithmetic (GA) index of two types of trees

In this section, we provide the general formula for geometric arithmetic (GA) index of two types of trees graphs, and the first one is associated with the Curtain tree $T(n, B_k^m)$ as follows.

Before proving the main results in all Theorem in this paper, let us introduce the following definition.

Definition 3.1. [24-28] For a connected graph $G = (V(G), E(G))$ with the minimum and maximum of degrees $\delta = Min\{d_v | v \in V(G)\}$ and $\Delta = Max\{d_v | v \in V(G)\}$, respectively, there exist vertex/atom and edge/bond partitions as follows:

$$\forall k: \delta \leq k \leq \Delta, Vk = \{v \in V(G) | \, d_v = k\}$$

$$\forall i: 2\delta \leq i \leq 2\Delta, E_i = \{e = uv \in E(G) | d_u + d_v = i\}$$

$$\forall j: \delta^2 \leq j \leq \Delta^2, E_j^* = \{uv \in E(G) | d_u \times d_v = j\}.$$

Theorem 3.1. Let n, k, m be positive integers such that $n \geq 3, k \geq 2$ and $m \geq 1$, the geometric arithmetic (GA) index of the Curtain graph $G = T(n, B_k^m)$ is

$$GA(G) = 2\sqrt{2}mnk\left(\frac{(k+3)+3\sqrt{k+1}}{3(k+3)}\right) + \frac{4m\sqrt{(m+1)(k+1)}}{m+k+2} + 2m(n-2)\frac{\sqrt{(m+2)(k+1)}}{m+k+3} + \frac{4\sqrt{(m+1)(m+2)}}{2m+3} + n - 3$$

Proof: Relying on the structure of Curtain graph $T(n, B_k^m)$ in Figure 2, we have mn of branches B_k. Firstly, we will mark all edges in those branches as follows:

The branch of B_k contains $2k$ edges, with k of them containing two vertices, the first one of degree one and the second of degree two. Other k edges also contain two vertices, the first of degree two and the second of degree $k+1$. Also, we have mn edges linking branches of B_k with vertices of the path with $2m$ of them containing two vertices; the first is degree $m+1$ and the second of degree $k+1$. The remaining $(n-2)m$ edges also contain two vertices: The first degree $k+1$, and the second degree $m+2$.

Now, it remains only the edges of the path. This path contains $n-1$ edges. Two of them contain two vertices, the first of degree $m+1$ and the second of degree $m+2$. The remaining $n-3$ edges also contain two vertices that have the same degree $m+2$. Now, we have,

$$E_1 = \{uv \in E(G) | d_u = 1 \,\&\, d_v = 2\} = kmn.$$

$$E_2 = \{uv \in E(G) | d_u = k+1 \,\&\, d_v = 2\} = kmn.$$

$$E_3 = \{uv \in E(G) | d_u = m+1 \,\&\, d_v = k+1\} = 2m.$$

$$E_4 = \{uv \in E(G) | d_u = k+1 \,\&\, d_v = m+2\} = m(n-2).$$

$$E_5 = \{uv \in E(G) | d_u = m+1 \,\&\, d_v = m+2\} = 2.$$

$$E_6 = \{uv \in E(G) | d_u = d_v = m+2\} = n-3.$$

By using the definition of geometric arithmetic (GA) index of G, we have the following computation for the geometric-arithmetic GA index of $T(n, B_k^m)$ as follows:

$$GA(T(n, B_k^m)) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

$$= \sum_{e=uv \in E_1} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{e=uv \in E_2} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{e=uv \in E_3} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

$$+ \sum_{e=uv \in E_4} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{e=uv \in E_5} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{e=uv \in E_6} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

$$= E_1 \frac{2\sqrt{1 \times 2}}{1+2} + E_2 \frac{2\sqrt{2(k+1)}}{2+k+1} + E_3 \frac{2\sqrt{(m+1)(k+1)}}{m+1+k+1} + E_4 \frac{2\sqrt{(m+2)(k+1)}}{m+2+k+1}$$

$$+ E_5 \frac{2\sqrt{(m+1)(m+2)}}{m+1+m+2} + E_6 \frac{2\sqrt{(m+2)(m+2)}}{m+2+m+2}$$

$$= 2mnk \frac{\sqrt{2}}{3} + 2mnk \frac{\sqrt{2(k+1)}}{k+3} + \frac{4m\sqrt{(m+1)(k+1)}}{m+k+2}$$

$$+ 2m(n-2) \frac{\sqrt{(m+2)(k+1)}}{m+k+3} + \frac{4\sqrt{(m+1)(m+2)}}{2m+3} + (n-3)$$

$$= 2\sqrt{2}mnk \left(\frac{(k+3)+3\sqrt{k+1}}{3(k+3)} \right) + \frac{4m\sqrt{(m+1)(k+1)}}{m+k+2}$$

$$+ 2m(n-2) \frac{\sqrt{(m+2)(k+1)}}{m+k+3} + \frac{4\sqrt{(m+1)(m+2)}}{2m+3} + n - 3 \ \blacksquare$$

Geometric arithmetic GA index of two types of bicyclic graphs

In this section, we provide the general formula for geometric arithmetic (GA) index of some bicyclic graphs; first, we have the following assertion associated with the Jellyfish graph $B^{B_k}(n, r, m)$ as follows.

A bicyclic graph is a connected graph in which the number of its edges is one more than the number of its vertices. The Jellyfish graph [20] is obtained by joining a cycle of length n with another cycle of length m by a path of length r followed by putting branches of B_k at each vertex in two cycles and path except the terminal vertices in the path where we put one of B_k, we denote such graph by $B^{B_k}(n, r, m)$ as shown in Figure 3.

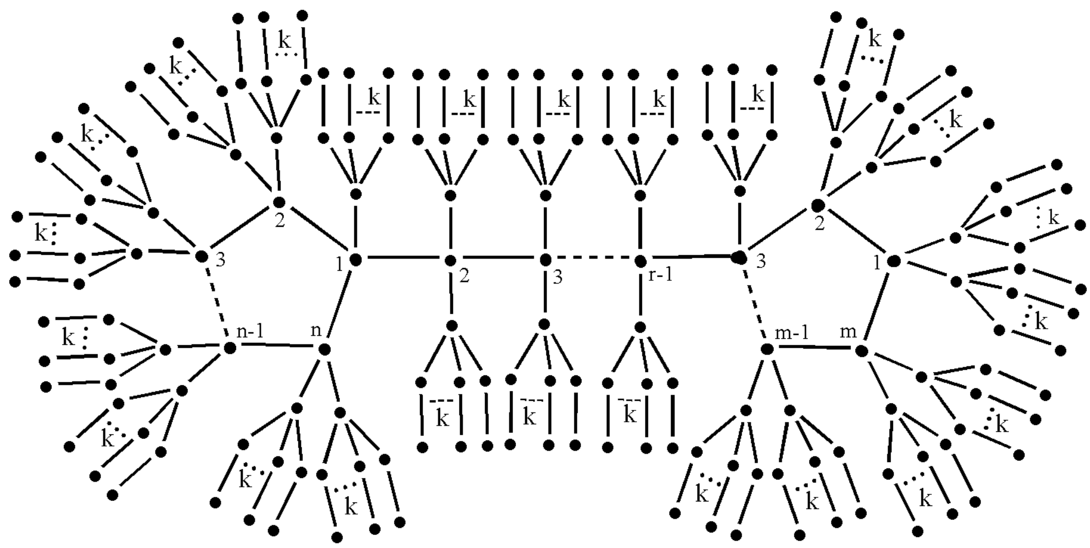

FIGURE 3 The Jellyfish graph $B^{B_k}(n,r,m)$

Theorem 4.1. Let n,m,k,r be a positive integer such that $n,m \geq 3, k,r \geq 2$, the geometric arithmetic (GA) index of a graph $G = B^{B_k}(n,r,m)$ is

$$GA(G) = 2(n+m+r-3)\left[\frac{2k\sqrt{2}}{3} + \frac{2k\sqrt{2(k+1)}}{k+3} + \frac{4\sqrt{k+1}}{k+5}\right] + n+m+r-1.$$

Proof: Relying on the structure of the Jellyfish graph $B^{B_k}(n,r,m)$ in Figure 3, we have $2(n+m+r-3)$ of branches B_k. Firstly, we will mark all edges in those branches as follows:
The branch of B_k contains $2k$ edges, with k of them containing two vertices, the first one of degree one and the second of degree two. Another k edge of them also contains two vertices, the first of degree two and the second of degree $k+1$.

Also, we have $2(n+m+r-3)$ edges linking branches of B_k with vertices of two cycles and path, each contains two vertices, the first one of degree four and the second of degree $k+1$.

Likewise, we have $n+m+r-1$ of edges that contain vertices it degree four.
Now, we have,

$$E_1 = \{uv \in E(G) | d_u = 1 \,\&\, d_v = 2\} = 2k(n+m+r-3).$$

$$E_2 = \{uv \in E(G) | d_u = k+1 \,\&\, d_v = 2\} = 2k(n+m+r-3).$$

$$E_3 = \{uv \in E(G) | d_u = 4 \,\&\, d_v = k+1\} = 2(n+m+r-3).$$

$$E_4 = \{uv \in E(G) | d_u = d_v = 4\} = n+m+r-1.$$

By using the definition of geometric arithmetic (GA) index of G. We have the following computation for this index GA of $B^{B_k}(n,r,m)$ as follows:

$$GA(B^{B_k}(n,r,m)) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$$

$$= \sum_{e=uv\in E_1} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \sum_{e=uv\in E_2} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \sum_{e=uv\in E_3} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$$

$$+ \sum_{e=uv\in E_4} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$$

$$= E_1 \frac{2\sqrt{1\times 2}}{1+2} + E_2 \frac{2\sqrt{2(k+1)}}{2+k+1} + E_3 \frac{2\sqrt{4(k+1)}}{4+k+1} + E_4 \frac{2\sqrt{4\times 4}}{4+4}$$

$$= \frac{4k\sqrt{2}}{3}(n+m+r-3) + 4k(n+m+r-3)\frac{\sqrt{2(k+1)}}{k+3}$$

$$+ (m+n+r-3)\frac{8\sqrt{(k+1)}}{k+5} + n+m+r-1$$

$$= 2(n+m+r-3)\left[\frac{2k\sqrt{2}}{3} + \frac{2k\sqrt{2(k+1)}}{k+3} + \frac{4\sqrt{k+1}}{k+5}\right] + n+m+r-1 \blacksquare$$

Geometric arithmetic *GA* index of bicyclic chemical graph

In section three, we computed geometric arithmetic index for sure of bicyclic graphs. Here we introduce the application to the bicyclic graph in Chemistry, such as polycyclic alkanes, as shown in Figure 4, to find a general formula to geometric arithmetic for it.

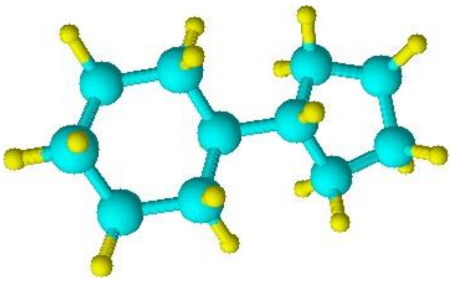

FIGURE 4 Some types of polycyclic alkanes

Polycyclic alkanes, which are molecules contain two or more cycloalkanes that are joined, forming multiple rings. The cycloalkanes are cyclic hydrocarbons, meaning that the carbons of the molecule are arranged in the form of a ring. Cycloalkanes are also saturated, meaning that all of the carbons atoms that make up the ring are single bonded to other atoms (no double or triple bonds).

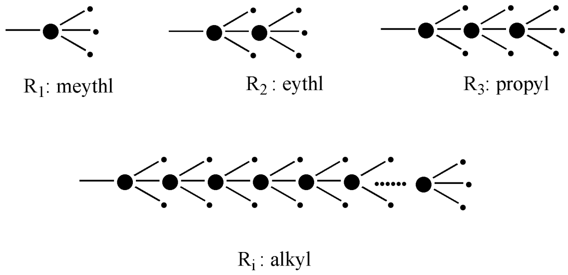

FIGURE 5 Some types of branches of Alkyl.

The group of Alkyl or branches of Alkyl are classes of alkanes with one hydrogen atom removed. It has the general formula C_nH_{2n+1}. If n is greater than or equal to 1, it will contain the branches of Alkyl. For example:

Methyl (CH_3), ethyl (C_2H_5) and propyl (C_3H_7) contain two branches and butyl (C_4H_9) as shown in Figure 5.

When we join two different Chemical compounds as cycloalkanes by a branch of Alkyl, we will get a new type of bicyclic chemical graph.

The molecular graph representing the molecular structure of the bicyclic chemical graphs is denoted by $C_{n,m}^{R_i}$, where n, m, r is the number of carbon atoms, as shown in Figure 6.

The following Theorem gives the geometric arithmetic GA index associated with bicyclic chemical graphs $C_{n,m}^{R_i}$.

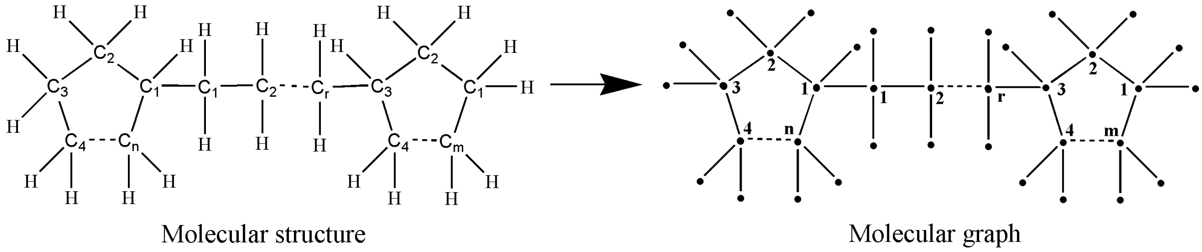

FIGURE 6 Molecular structure and molecular graph representing the bicyclic chemical graphs $C_{n,m}^{R_i}$.

Theorem 4.3. Let n, m, r be a positive integer such that $n, m \geq 3, r \geq 1$, the geometric arithmetic GA index of a graph $G = C_{n,m}^{R_i}$ is $GA(C_{n,m}^{R_i}) == \frac{13}{5}(n + m + r - 1)$

Proof: According to the structure of the bicyclic chemical graphs $C_{n,m}^{R_i}$ in Figure 6, we have two types of edges. Firstly, we will mark all edges in this graph as follows:

In the first type, we have $n + m + r - 1$ edges containing two vertices that have the same degree four.

In the second type, we have $2(n + m + r - 1)$ edges that are incident on two vertices of degree one and degree four.

Now, we have,

$$E_1 = \{uv \in E(G) | d_u = d_v = 4\}$$
$$= n + m + r - 1.$$

$E_2 = \{uv \in E(G) | d_u = 1 \; \& \; d_v = 4\}$
$= 2(n + m + r - 1).$

By using the definition of geometric arithmetic (GA) index of G. We have the following computation for this index GA of $C_{n,m}^{R_i}$ as follows:

$GA(\, C_{n,m}^{R_i}) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$

$= \sum_{e=uv \in E_1} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{e=uv \in E_2} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$

$= E_1 \frac{2\sqrt{4\times4}}{4+4} + E_2 \frac{2\sqrt{1\times4}}{1+4}$

$= n + m + r - 1 + \frac{8}{5}(n + m + r - 1)$

$= \frac{13}{5}(n + m + r - 1)$ ■

Let $C_{n,r,m}^{R_s}$ be a bicyclic graph associated with molecular graph to some classes of chemical compound. The molecular structure of this class is obtained by joining two different cycloalkanes of length n and m by a branch of Alkyl of length r. When attaching branches of Alkyl R_s to each hydrogen atom, we get a new class of bicyclic chemical graphs, as shown in Figure 7, and the molecular graph representing the bicyclic chemical graphs $C_{n,r,m}^{R_s}$, as shown in Figure 8.

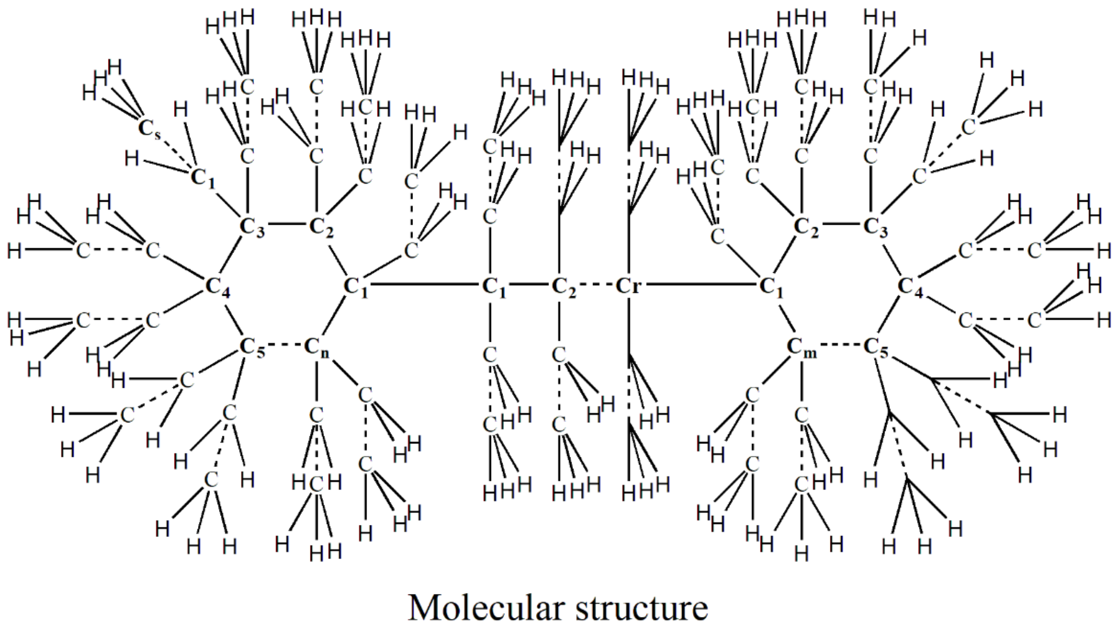

FIGURE 7 Molecular structure of bicyclic chemical graphs $C_{n,r,m}^{R_s}$

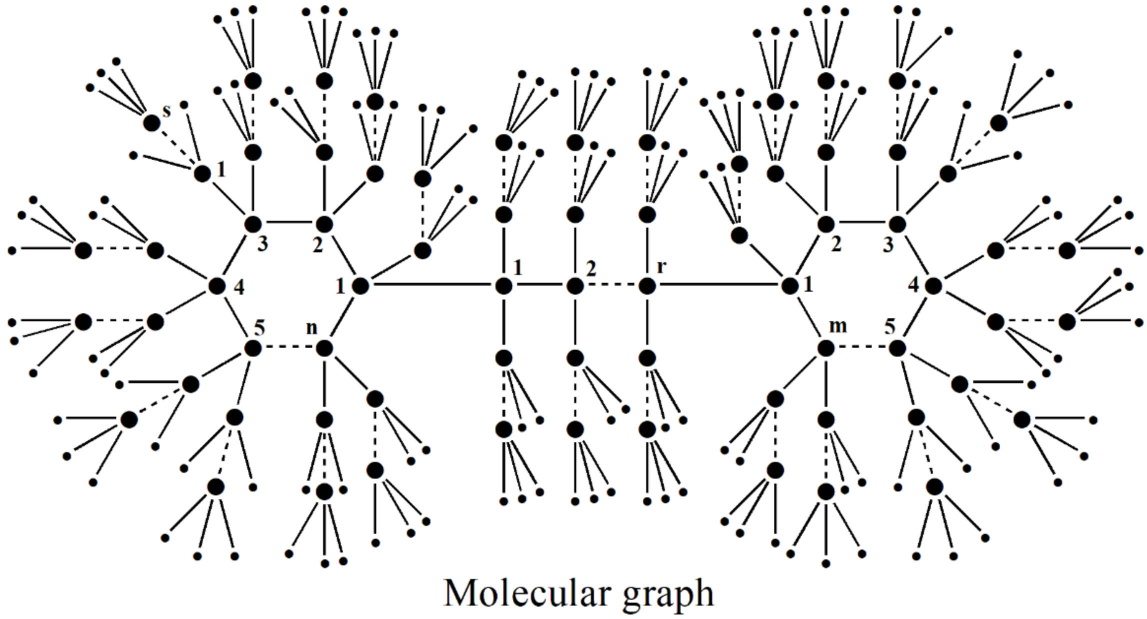

FIGURE 8 Molecular graph representing the bicyclic chemical graphs $C_{n,r,m}^{R_s}$

Theorem 4.3. Let n, m, r, s be a positive integer such that $n, m \geq 3$; $r, s \geq 1$, the geometric arithmetic GA index of a graph $G = C_{n,r,m}^{R_s}$ is $GA(C_{n,r,m}^{R_s}) = \frac{13}{5}(2s+1)(n+m+r) - \frac{26}{5}s - \frac{13}{5}$

Proof: Considering the structure of the bicyclic graph $G = C_{n,r,m}^{R_s}$ in Figure 8, we have $2(n+m+r-1)$ branches R_s. Firstly, we will mark all edges in these branches as follows:

The branch of R_s contains $3s$ edges, with $2s+1$ of them containing two vertices, the first one of degree 1 and the second vertex of degree 4. The remaining $s-1$ edges also contain two vertices that have the same degree 4.

Also, we have $2(n+m+r-1)$ edges linking branches of R_s with vertices of two cycles and a joining path, each containing two vertices of the same degree 4.

Likewise, we have $n+m+r+1$ of edges which made two cycles and the joining path for it—all edges in this case contain two vertices of the same degree 4.

Now, we have,

$$E_1 = \{uv \in E(G) | d_u = 1 \; \& \; d_v = 4\} = (4s+2)(n+m+r-1).$$

$$E_2 = \{uv \in E(G) | d_u = d_v = 4\} = (2s+1)(n+m+r) - 2s + 1.$$

By using the definition of geometric arithmetic (GA) index of G., we have the following computation for this index GA of $B^{B_k}(n, r, m)$, as follows:

$$GA(B^{B_k}(n, r, m)) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

$$= \sum_{e=uv \in E_1} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{e=uv \in E_2} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

$$= E_1 \frac{2\sqrt{1 \times 4}}{1+4} + E_2 \frac{2\sqrt{4 \times 4}}{4+4}$$

$$= \frac{4}{5}(4s+2)(n+m+r-1) + (2s+1)(n+m+r) - 2s + 1$$

$$= \frac{13}{5}(2s+1)(n+m+r) - \frac{26}{5}s - \frac{13}{5} \blacksquare$$

Conclusion

In conclusion, this study reveals three findings: First, we established the general formulas of geometric arithmetic (GA) index for two types of trees graphs. Second, we provided the general formulas to the bicyclic graphs after attaching branches of B_i. For all vertices. Finally, we showed that the bi-cyclic graph $C_{n,m}^{R_i}$, $C_{n,r,m}^{R_s}$ is associated with some bicyclic chemical graphs to find a general formula to geometric arithmetic.

Acknowledgments

The authors extend their real appreciation to the reviewers for their insightful comments and technical suggestions to enhance quality of the article.

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How to cite this article: Mohanad Ali Mohammed, Hasan H. Mushatet. The geometric arithmetic (GA) index of certain trees and bicyclic graphs. *Eurasian Chemical Communications*, 2021, 3(9), 635-643. **Link:** http://www.echemcom.com/article_135211.html