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Geometric arithmetic index of Alkanes and Unicyclic chemical graphs

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Abstract

The geometric arithmetic GA index is one of the most investigated degree based molecular structure descriptors that have applications in chemistry. For a graph G, the geometric arithmetic GA index is defined as $GA(G) = \sum\limits_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$, where d_u denotes the degree of a vertex u in G. In this paper, we obtain the general formula for the geometric arithmetic GA index for certain trees and unicyclic graphs with application such as Alkanes, Isomerism of Alkanes and more classes of Cycloalkanes.

Keywords: Degree of vertex, Graph, Geometric arithmetic index.

1. Introduction

Description of the structure or shape of molecules is very helpful in predicting activity and properties of molecules in complex experiments. For that purpose, the molecular descriptors [1] as mathematical quantities are particularly useful. Among the molecular descriptors, the so-called topological indices [2] play a significant role. The topological indices can be classified by the structural properties of graphs used for their calculation. The Randić connectivity index [3] depend on the degrees of vertices, while the Hosoya index [4] is calculated by the counting of non-incident edges in a graph. On the other hand, there is a group of so-called information indices that are based on information functional [5]. Let $G = (V, E)$ be a simple graph of order n. The first geometric-arithmetic index GA was proposed in [6].

This index is defined as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

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It was demonstrated [6], on the example of octane isomers, that 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 [7]. Bhanumathi *et al.,* investigated the Geometric-arithmetic GA index of some graphs and an infinite class of Nanostar dendrimers [8]. Rodrigueza and Sigarreta obtained new inequalities involving GA index and characterize graphs extremal with respect to them [9]. Sigarreta obtained new inequalities involving the geometric-arithmetic index and other well known topological indices such as relate the geometric-arithmetic index of a graph G with its first Zagreb index, its second Zagreb index, its modified Zagreb index and its Randić index [10]. Alaeiyan *et al.,* computed the fifth geometric arithmetic index of Polycyclic Aromatic Hydrocarbons [11]. Abdelgader *et al.,* computed the geometric arithmetic and atom bond connectivity indices of special graphs such as Cayley tree, Square lattice and Complete bipartite [12]. Sardar *et al.,* computed the geometric arithmetic of the line graphs of graphs such as Banana tree and Firecracker graph [13]. Farahani and Rajesh Kanna computed the geometric-arithmetic and anther index to $V-$phenylenic Nanotubes and Nanotori [14]. The mathematical properties of the geometric arithmeticGA and other indices were reported in [15, 16, 17, 18].

The (chemical) trees, unicycle, graph(s) with ABC index were determined in [19]. Recently, In 2016 Mohanad *et al.,* studied the general formula for ABC index of some special trees graphs and provided a general formula of ABC index of unicyclic graphs [18].

In this paper we have two sections. In the first section, we present the general formula of the geometric arithmetic GA index of certain tree graphs and their representing in Chemistry such as Alkane and Isomerism of Alkanes. The second section provides the general formula of GA index of special Unicyclic graphs with application in Unicycle chemical graphs such as cycloalkanes and more types of it.

The special graphs considered here are obtained from the path and the cycle by adding a certain tree to each vertex in a uniform way.

2. Preliminaries

A connected graph with maximum vertex degree of at most 4 is said to be a 'molecular graph'. Its graphical representation may resemble a structural formula of some (usually organic) molecule. That was a primary reason for employing graph theory in Chemistry. Nowadays this area of Mathematical Chemistry is called chemical graph theory.

A tree in which the maximum vertex degree does not exceed 4 is said to be a 'chemical tree'. A vertex of a graph is said to be pendant if its neighborhood contains exactly one vertex. An edge of a graph is said to be pendant if one of its vertices is a pendant vertex to be pendant if one of its vertices is a pendant vertex. Let G be a graph and $v \in V(G)$. A $(u,v)-walk$ is a finite sequence of vertices $v_1, v_2, \ldots, v_k$, with $k \geq 1$, $u = v_1$ and $v = v_k$, such that $v_{i-1}v_i \in E(G)$ for each $i = 1, 2, \ldots, k$. The length of the walk is $k-1$, that is the number of edges in it. A $(u,v)-walk$ is called a path if no vertices are repeated.

3. GA index of certain trees with application to alkanes and isomerism of alkanes

In this section, we provide the general formula for geometric arithmetic GA index of some trees graphs.

Let T_n^m be a tree graph obtained by attaching m vertices to each vertex of path P_n as shown Figure 1.

Theorem 3.1. *Let n and m be a positive integers such that $n \geq 3, m \geq 1$. The geometric arithmetic GA index of the graph $G = T_n^m$ is:*

$$GA(T_n^M) = \frac{4m\sqrt{m+1}}{m+2} + \frac{2m(n-2)\sqrt{m+2}}{m+3} + \frac{4\sqrt{(m+1)(m+2)}}{2m+3} + n - 3.$$

Proof. We have two types of edges: In the first type, we have mn edges, $2m$ edges of them are incident on two vertices of degree 1 and degree $(m+1)$. The remaining $m(n-2)$ edges are incident on two vertices of degrees 1 and degree $(m+2)$.

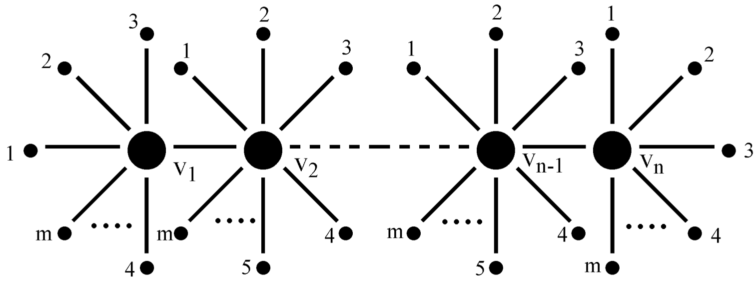

Figure 1: The tree graph T_n^m

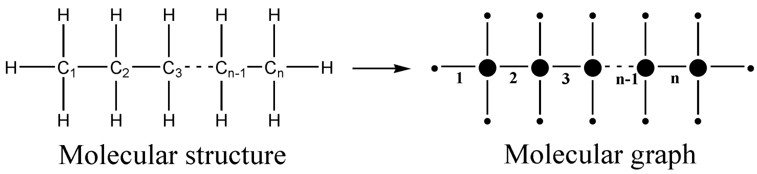

Figure 2: Molecular structure of AlkanesC_nH_{2n+2} and Molecular graph representing the chemical compound of Alkanes

In the second type, we have $(n-1)$ edges of path P_n, 2 edges of them contain two vertices, the first one degree $(m+1)$ and the second of degree $(m+2)$. The remaining $(n-3)$ edges are incident on two vertices of the same degrees $(m+2)$.

Now, we have,

$E_1 = uv \in E(G)|d_u = 1d_v = m+1 = 2m.$

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

$E_3 = uv \in E(G)|d_u = m+1d_v = m+2 = 2.$

$E_4 = uv \in E(G)|d_u = d_v = m+2 = n-3.$

By using the definition of geometric arithmetic (GA) index of G, we have following computation for the geometric-arithmetic GA index of T_n^m as follow:

$$\begin{aligned}
GA(T_n^M) &= \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \\
&= \sum_{e=uv\in E_1} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \sum_{e=uv\in E_2} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \sum_{e=uv\in E_3} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \sum_{e=uv\in E_4} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \\
&= E_1\frac{2\sqrt{1\times(m+1)}}{1+m+1} + E_2\frac{2\sqrt{1\times(m+2)}}{1+m+2} + E_3\frac{2\sqrt{(m+1)(m+2)}}{m+1+m+2} + E_4\frac{2\sqrt{(m+2)\times(m+2)}}{m+2+m+2} \\
&= \frac{4m\sqrt{m+1}}{m+2} + \frac{2m(n-2)\sqrt{m+2}}{m+3} + \frac{4\sqrt{(m+1)(m+2)}}{2m+3} + n-3.
\end{aligned}$$

□

Many applications of trees are found in Chemistry. Some of them are applied to the class of alkanes. We will establish the geometric arithmetic GA index for it. Alkanes are hydrocarbons with only a single bond between the atoms and it has a general formula C_nH_{2n+2}, where the numbers of covalent bonds are four for Carbon and one for Hydrogen as shown in Figure 2.

Theorem 3.2. *Let n be a positive integer such that $n \geq 1$. Then the geometric arithmeticGA index of a graph $G = C_nH_{2n+2}$ is:*

$$GA(C_nH_{2n+2}) = \frac{13n}{5} + \frac{3}{5}.$$

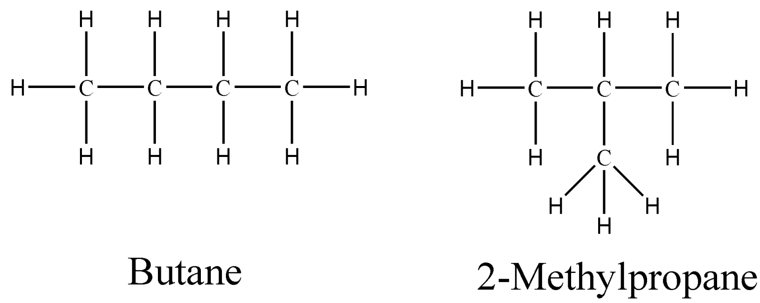

Figure 3: Structural formula C_4H_{10} having the same molecular formula

Proof. We have two types of edges: In the first type, we have $E_1 = (2n+2)$ edges are incident on two vertices of degree 1 and degree 4.

In the second type, we have $E_2 = (n-1)$ edges between the vertices of carbon, the edges contain two vertices of the same degree four.

Now, we have,

$E_1 = \{uv \in E(G) \in d_u = 1d_v = 4\} = 2n+2.$

$E_2 = \{uv \in E(G) \in d_u = d_v = 4\} = n-1.$

By using the definition of geometric arithmetic (GA) index of G, we have following computation for the geometric-arithmetic GA index of C_nH_{2n+2} as follow:

$$\begin{aligned} GA(C_nH_{2n+2}) &= \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \\ &= \sum_{e=uv\in E_1} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \sum_{e=uv\in E_2} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \\ &= E_1\frac{2\sqrt{1\times 4}}{1+4} + E_2\frac{2\sqrt{4\times 4}}{4+4} \\ &= \frac{8}{5}(n+1) + n - 1 \\ &= \frac{13n}{5} + \frac{3}{5}. \end{aligned}$$

□

In$n-$alkanes, no carbon is bonded to more than two other carbons, giving rise to a linear chain. When a carbon is bonded to more than two other carbons, a branch is formed. The smallest branched alkane isisobutane.Notice that isobutane has the same molecular formula C_4H_{10}, as n-butane but has a different structural formula. Two different molecules which have the same molecular formula are isomers as shown in Figure 3.

Remark 3.3. Let G be Isomerism of alkanes. The general formula of geometric arithmetic GA index of G is the same as the general formula of alkanes above. That is $GA(C_nH_{2n+2}) = \frac{13n}{5} + \frac{3}{5}$.

Proof. Computing GA index for G will depend on the number of edges and the degree of vertices in the structural formula associated with G. Since isomerism of alkanes have the same numbers of Carbon and Hydrogen atoms, it follows that they have the same numbers of edges and the degree of vertices so the general formula (C_nH_{2n+2}) of alkanes.

The proof of this remark then follows the same method as in the proof of Theorem 3.2. □

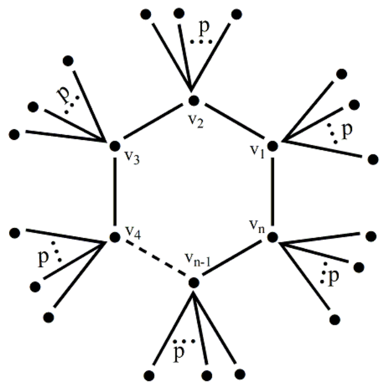

Figure 4: A unicyclic graph U_n^p

4. GA index of certain unicyclic graphs and their representing in chemistry

In this section, we provide the general formula for geometric arithmetic index of certain Unicyclic graphs and Unicyclic chemical graphs.

A unicyclic graph U is any connected graph where the number of vertices n equals the number of edges of$U$. The length of the cycle in U equals the girth of U.

Let $U_n^pU_n^p$ be a unicyclic graph, which is obtained from a cycle of length n by attaching p pendant vertices to each vertex of the cycle as shown in Figure 4.

Theorem 4.1. *Let n, p be positive integers such that $n \geq 3, p \geq 1$. Then the geometric arithmetic GA index of a graph $G = U_n^p$ is:*

$$GA(U_n^p) = \frac{n(p + 2p\sqrt{p+2} + 3)}{p+3}.$$

Proof. We have two types of edges: In the first type, we have np pendant edges are incident on two vertices of degree 1 and degree $p + 2$.

In the second type, we have n edges between the vertices of cycle, the edges contain two vertices of the same degree $p + 2$.

Now, we have,

$E_1 = \{uv \in E(G) \in d_u = 1 d_v = p + 2\} = np.$

$E_2 = \{uv \in E(G) \in d_u = d_v = p + 2\} = n.$

By using the definition of geometric arithmetic (GA) index of G, we have following computation for the geometric-arithmetic GA index of U_n^p as follow:

$$\begin{aligned}
GA(U_n^p) &= \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\
&= \sum_{e=uv \in E_1} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{e=uv \in E_2} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\
&= E_1 \frac{2\sqrt{1 \times (p+2)}}{1 + p + 2} + E_2 \frac{2\sqrt{(p+2) \times (p+2)}}{p + 2 + p + 2} \\
&= \frac{2np\sqrt{p+2}}{p+3} + \frac{2n(p+2)}{2(p+2)} \\
&= \frac{n(p + 2p\sqrt{p+2} + 3)}{p+3}.
\end{aligned}$$

□

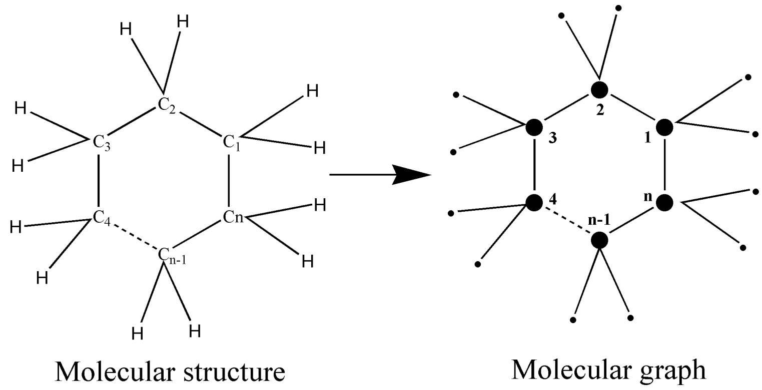

Figure 5: Molecular structure of Cycloalkanes (C_nH_{2n}) and Molecular graph representing the chemical compound of Cycloalkanes

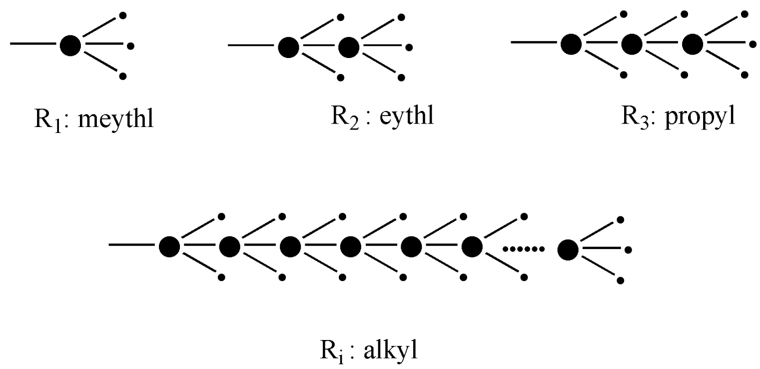

Figure 6: Some types of branches of Alkyl

A Unicyclic chemical graph UU is the Unicyclic graph that has no vertex with degree greater than 4.

In Theorem 4.1 if p equals two we get the chemical compounds that is cycloalkanes, which we denote by $U_n^2U_n^2$ where Cycloalkanes (C_nH_{2n}) as shown in Figure 5.

The next corollary corresponds to the case $p = 2$ of Theorem 4.1. We give an alternative proof after stating the theorem.

Corollary 4.2. *Let U_n^2 be classes of cycloalkane. Then the geometric arithmetic GA index of U_n^2 is*

$$GA(U_n^2) = \frac{13}{5}n.$$

Proof. The proof clearly follows from the above Theorem 4.1 by letting $p = 2$. □

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 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 6.

When we attach alkyl or branches of alkyl in place of all hydrogen atoms or some of them in Cycloalkanes we will get a new class of Unicyclic chemical graphs, denoted by U_n^{alkyl} where n is the number of Carbon atoms as in Figure 7.

The following theorem gives the geometric arithmetic GA index associated with unicyclic chemical graph U_n^{alkyl}.

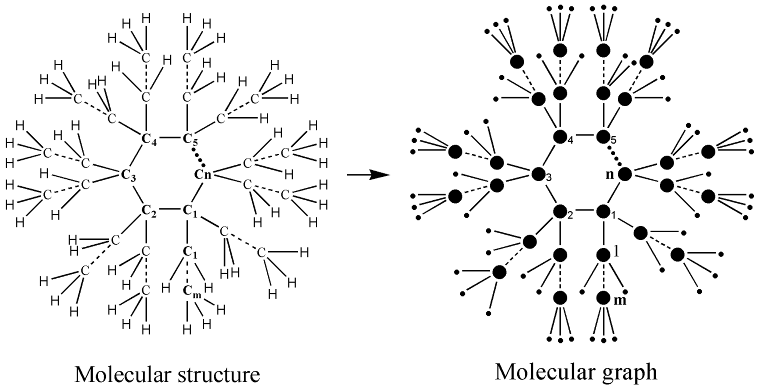

Figure 7: Molecular structure of U_n^{alkyl} and molecular graph representing the chemical compound of U_n^{alkyl}

Theorem 4.3. *Let n be a positive integer such that $n \geq 4$. Then the geometric arithmetic GA index of a graph $G = U_n^{alkyl}$ is*

$$GA(U_n^{alkyl}) = \frac{13n(2m+1)}{5}.$$

Proof. We have two types of edges: In the first type, we have $2n$ of brenches of alkyl, each of them contain $E_1 = 2m+1$ pendant edges are incident on two vertices of degree 1 and degree 4. Also, it has $E_2 = m-1$ edges are incident on two vertices of the same degrees 4.

In the second type, we have $E_3 = 3n$ edges, $2n$ edges of them linking the branches of alkyl with the vertices of cycle and the remaining n edges of the cycle. All of them are incident on two vertices of the same degrees four.

Now, we have,

$E_1 = \{uv \in E(G) \in d_u = 1 d_v = 4\} = 2n(2m+1)$.

$E_2 = \{uv \in E(G) \in d_u = d_v = 4\} = 2n(m-1) + 3n$.

$E_3 = uv \in E(G) | d_u = d_v = 4 = 3n$.

By using the definition of geometric arithmetic (GA) index of G, we have following computation for the geometric-arithmetic GA index of U_n^{alkyl} as follow:

$$\begin{aligned}
GA(U_n^{alkyl}) &= \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\
&= \sum_{e=uv \in E_1} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{e=uv \in E_2} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\
&= E_1 \frac{2\sqrt{1 \times 4}}{1+4} + E_2 \frac{2\sqrt{4 \times 4}}{4+4} \\
&= \frac{8n}{5}(2m+1) + 2n(m-1) + 3n \\
&= \frac{16nm}{5} + \frac{8n}{5} + 2nm + n \\
&= \frac{26nm}{5} + \frac{13n}{5} \\
&= \frac{13n(2m+1)}{5}.
\end{aligned}$$

□

5. Conclusion

Description of the structure or shape of molecules is very helpful in predicting activity and properties of molecules in complex experiments. For that purpose, the molecular descriptors as mathematical quantities are particularly useful. Among the molecular descriptors, the so-called topological indices play a significant role. In this paper we tackled the problem to find general formula for the geometric arithmetic GA index for certain trees and their representing as classes of chemical tree. Also, we provide the general formula for geometric arithmetic index of certain Unicyclic graphs associated with Unicyclic chemical graph as cycloalkanes. after that we attach alkyl or branches of alkyl in place of all hydrogen atoms or some of them in Cycloalkanes to find a new general formula for it. Such results can be of great impact as there is a strong need to understand the mathematical structure to get this formula there has been nearly no related work conducted in this area. More generally speaking, this could serve as a characterization of chemical graph structures according to a notion of on chemical graph theory.

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