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Geometric Arithmetic Index of Alkanes and Unicyclic chemical graphs

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Abstract

The Geometric–Arithmetic (GA) index has emerged as one of the most actively studied degree-based molecular structure descriptors due to its significant relevance in chemical graph theory. For a graph Γ, the GA index is given by $GA(\Gamma) = \sum_{\mu\nu \in E(\Gamma)} \frac{2\sqrt{\lambda_\mu \lambda_\nu}}{\lambda_\mu + \lambda_\nu}$. Here, λ_μ denotes the degree of the vertex μ in the graph Γ.

In this research, we develop general expressions for the Geometric–Arithmetic index for various families of trees and uni–cyclic graphs, with illustrative applications to chemical structures such as alkanes, their isomers, and broader classes of cycloalkanes.

Keywords: Geometric–Arithmetic GA Index, Unicyclic Graph, Isomerism of Alkanes.

1. Introduction

In chemical graph theory, a molecular structure can be represented by a simple graph that the vertices correspond to atoms and the edges represent the chemical bonds between them [1]. This approach makes it possible to study chemical compounds by means of algebraic and combinatorial techniques instead of direct laboratory methods. Numerical quantities obtained from such graphs are known as topological indices, and they have an important role in the expansion of QSARs/QSPRs, where mathematical invariants are used to predict physical and chemical behavior [2].

Among the many families of topological indices, those that belonged on the degrees of the vertices are of particular interest because of their ease of computation and their strong discriminating ability between different molecular structures [3]. The Geometric-Arithmetic GA index is one such degree based index. It is calculated by using the degrees of the two vertices that are connected by each edge of the graph. The GA has been shown to correlate well with several physical and thermodynamic characteristics of organic

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compounds [4]. Alkanes provide a fundamental example in this context. The molecular graphs of alkanes are represented by chemical trees in which each vertex has degree at most four. Structural variations among alkanes, particularly branching, influence the value of the GA index, making it useful for distinguishing between different isomers that share the same molecular formula [5].

Let Γ be a simple graph with vertex set V and edge set E, such that $|V(\Gamma)| = n$ and $|E(\Gamma)| = m$. The first Geometric–Arithmetic GA_1 index was introduced by Vukićević and Furtula [6] and formula as:

$$GA_1(\Gamma) = \sum_{\mu\nu \in E(\Gamma)} \frac{2\sqrt{\lambda_\mu \lambda_\nu}}{\lambda_\mu + \lambda_\nu}.$$

Rodrigueza and Sigarreta established new bounds for the GA index and identified the extremal graphs attaining these inequalities [7]–[9].

Sigarreta subsequently derived further inequalities involving the GA index together with several classical topological indices, establishing connections between $GA(\Gamma)$ and indices such as a group of degree based topological indices [10]. Prof. Alaeiyan et al. presented the fifth GA index for Polycyclic aromatic hydrocarbon (PAH) [11]. Prof. Abdelgader et al. evaluated both the GA index and the ABC index for specific classes of graphs [12]. Sardar et al. investigated the GA index of line graphs associated with structures such as the banana tree and the firecracker graph [13]. Farahani determined the GA index and several related indices for V-phenylenic Nanotubes and nanotorii [14]. Additional mathematical developments linking the GA index with other topological indices can be found in [15]–[19]. Further studies of chemical graph structures such as trees, unicyclic graphs, and families examined via the atom–bond connectivity index appear in [20]–[23].

In this research, we obtain expressions of the GA index for several classes of tree and unicyclic graphs that correspond to alkanes, isomeric forms of alkanes, cycloalkanes, and cycloalkanes with alkyl substitutions. These results contribute to the theoretical framework of chemical graph theory and provide useful formulas for the characterization of molecular structure.

2. Preliminaries

A graph can be used to represent the structural framework of a molecule by assigning a vertex to each atom and an edge to each bond connecting two atoms. When the maximum degree of every vertex in the graph does not exceed four, the graph is regarded as a molecular graph because it reflects the bonding limitations of carbon based compounds. This representation allows the structural properties of chemical compounds to be studied through graph theoretic methods. A tree satisfying the same degree restriction is called a chemical tree. For two vertices μ and ν in a graph Γ, a walk from μ to ν is a finite sequence of vertices in which consecutive vertices are adjacent. If no vertex appears more than once in this sequence, the walk is called a path. These basic concepts will be used throughout the following sections [24].

Chemical trees are trees that have no vertex with degree greater than 4. A *pendant* vertex is adjacent to exactly one other vertex, and its edge is termed *pendant*.

Let $\nu \in V(\Gamma)$ of a graph Γ. A (μ, ν)-walk is a finite sequence of vertices

$$\nu_1, \nu_2, \ldots, \nu_k, \qquad k \geq 1,$$

such that $\mu = \nu_1$, $\nu = \nu_k$, and $\nu_{i-1}\nu_i \in E(\Gamma)$ for every $i = 2, \ldots, k$. The length of this walk is $k - 1$, corresponding to the number of edges it traverses. A (μ, ν)-walk is called a *path* if all the vertices in the sequence are distinct.

3. GA index of certain Alkanes graphs and their chemical properties

In this section, we derive the general expression for the GA index of certain classes of tree graphs.

Let T_n^m (or equivalently $T_n^{B_k}$) denote the tree obtained by attaching m pendant vertices to each vertex of the path P_n, as illustrated in Figure 1.

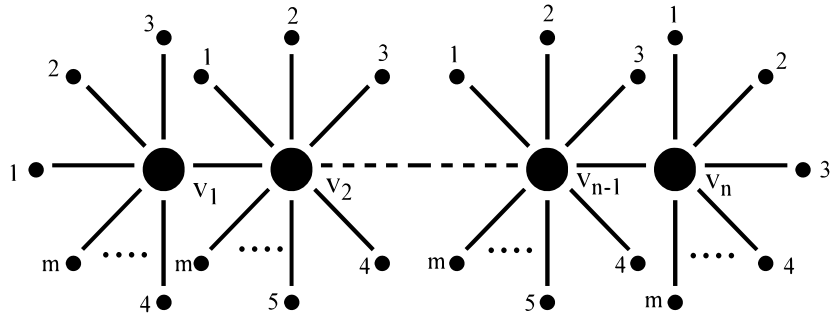

Figure 1: The tree graph T_n^m

Theorem 3.1. *Consider two integers $n \geq 3$ and $\tau \geq 1$. For the graph $\Gamma = T_n^\tau$, the Geometric-Arithmetic index is given by $GA\,(T_n^\tau) = \frac{4\tau\sqrt{\tau+1}}{\tau+2} + \frac{2\tau(n-2)\sqrt{\tau+2}}{\tau+3} + \frac{4\sqrt{(\tau+1)(\tau+2)}}{2\tau+3} + n - 3$.*

Proof. The edges of the graph can be classified into two types. In the first type, there are mn edges in total. Among these, 2τ edges join a vertex of degree 1 to a vertex of degree $(\tau + 1)$, while the remaining $\tau(n - 2)$ edges connect a vertex of degree 1 to a vertex of degree $(\tau + 2)$.

In the second category, which corresponds to the $(n - 1)$ edges of the path P_n, two of these edges have endpoints of degrees $(\tau+1)$ and $(\tau+2)$, respectively. The remaining $(n-3)$ edges each connect two vertices whose degrees are both equal to $(\tau + 2)$. Thus

$$\begin{aligned}
|E_1 =&\{\mu\nu \in E(\Gamma)|\lambda_\mu = 1\&\lambda_\nu = \tau + 1\}| = 2\tau.\\
|E_2 =&\{\mu\nu \in E(\Gamma)|\lambda_\mu = 1\&\lambda_\nu = \tau + 2\}| = \tau(n - 2).\\
|E_3 =&\{\mu\nu \in E(\Gamma)|\lambda_\mu = \tau + 1\&\lambda_\nu = \tau + 2\}| = 2.\\
|E_4 =&\{\mu\nu \in E(\Gamma)|\lambda_\mu = \lambda_\nu = \tau + 2\}| = n - 3.
\end{aligned}$$

Using the definition of (GA) index for a graph Γ, we obtain the following computation for the graph T_n^τ:

$$\begin{aligned}
GA(T_n^\tau) =& \sum_{\mu\nu\in E(\Gamma)} \frac{2\sqrt{\lambda_\mu\lambda_\nu}}{\lambda_\mu + \lambda_\nu}\\
=& \sum_{e=\mu\nu\in E_1} \frac{2\sqrt{\lambda_\mu\lambda_\nu}}{\lambda_\mu + \lambda_\nu} + \sum_{e=\mu\nu\in E_2} \frac{2\sqrt{\lambda_\mu\lambda_\nu}}{\lambda_\mu + \lambda_\nu} + \sum_{e=\mu\nu\in E_3} \frac{2\sqrt{\lambda_\mu\lambda_\nu}}{\lambda_\mu + \lambda_\nu} + \sum_{e=\mu\nu\in E_4} \frac{2\sqrt{\lambda_\mu\lambda_\nu}}{\lambda_\mu + \lambda_\nu}\\
=& E_1\frac{2\sqrt{1\times(\tau+1)}}{1+\tau+1} + E_2\frac{2\sqrt{1\times(\tau+2)}}{1+\tau+2} + E_3\frac{2\sqrt{(\tau+1)(\tau+2)}}{\tau+1+\tau+2} + E_4\frac{2\sqrt{(\tau+2)\times(\tau+2)}}{\tau+2+\tau+2}\\
=& \frac{4\tau\sqrt{\tau+1}}{\tau+2} + \frac{2\tau(n-2)\sqrt{\tau+2}}{\tau+3} + \frac{4\sqrt{(\tau+1)(\tau+2)}}{2\tau+3} + n - 3.
\end{aligned}$$

Alkanes are hydrocarbons in which every carbon atom forms four covalent bonds, whereas each hydrogen atom forms a single covalent bond. Their general molecular formula is given by C_nH_{2n+2}, as depicted in Figure 2 [22].

□

Theorem 3.2. *For a integer $n \geq 1$, and the Geometric-Arithmetic index of $\Gamma = C_nH_{2n+2}$ is $GA(C_nH_{2n+2}) = \frac{13n}{5} + \frac{3}{5}$.*

Proof. Two distinct categories of edges arise within this structure.

The first category consists of $|E_1| = 2n + 2$ edges, each connecting two vertices of degrees 1 and 4.

The second category comprises $|E_2| = n - 1$ edges, each joining two carbon vertices, both of which have degree 4. Thus

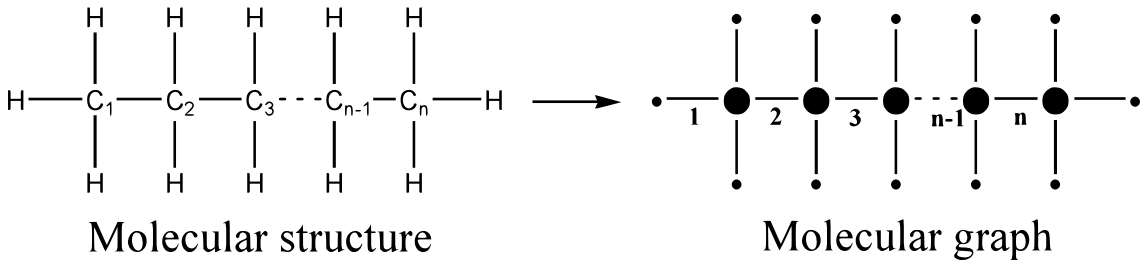

Figure 2: Molecular structure of Alkanes C_nH_{2n+2}

$$|E_1 = \{\mu\nu \in E(\Gamma) \in \lambda_\mu = 1 \& \lambda_\nu = 4\}| = 2n + 2.$$
$$|E_2 = \{\mu\nu \in E(\Gamma)\lambda_\mu = \lambda_\nu = 4\}| = n - 1.$$

Using the definition of GA index of $\Gamma = C_nH_{2n+2}$, we will have:

$$GA(C_nH_{2n+2}) = \sum_{\mu\nu \in E(\Gamma)} \frac{2\sqrt{\lambda_\mu \lambda_\nu}}{\lambda_\mu + \lambda_\nu} = \sum_{e=\mu\nu \in E_1} \frac{2\sqrt{\lambda_\mu \lambda_\nu}}{\lambda_\mu + \lambda_\nu} + \sum_{e=\mu\nu \in E_2} \frac{2\sqrt{\lambda_\mu \lambda_\nu}}{\lambda_\mu + \lambda_\nu}$$
$$= E_1 \frac{2\sqrt{1 \times 4}}{1+4} + E_2 \frac{2\sqrt{4 \times 4}}{4+4} = \frac{8}{5}(n+1) + n - 1 = \frac{13n}{5} + \frac{3}{5}.$$

□

Isomerism of alkanes: In η-alkanes, each carbon atom is bonded to at most two other carbon atoms, forming a linear chain structure. The simplest branched alkane is isobutane, which shares the molecular formula C_4H_{10} with η-butane but differs in its structural arrangement, as illustrated in Figure 3 [22].

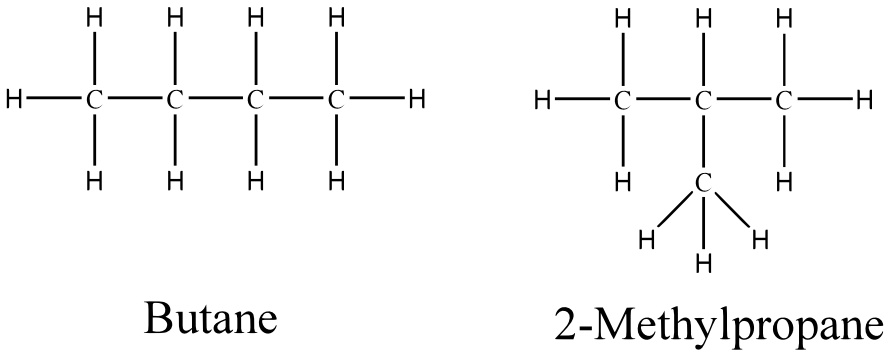

Figure 3. The difference between structural and molecular formulas of C_4H_{10} Structural formula C_4H_{10} having the same molecular formula.

Remark 3.3. The Geometric-Arithmetic index of Isomerism of alkanes is equal to $GA(C_\eta H_{2\eta+2}) = \frac{13\eta}{5} + \frac{3}{5}$.

Proof. Two types of edges can be identified in this structure.

The first type consists of $|E_1| = 2\eta + 2$ edges, each linking two vertices of degree 1 and 4.

The second type consists of $|E_2| = \eta - 1$ edges, where each edge connects two carbon vertices, both having degree 4. □

4. *GA* index of certain Uni–cyclic graphs and their chemical properties

In this section, we study a family of unicyclic chemical graphs and derive a general expression for their Geometric-Arithmetic index. Such graphs play an important role in chemical graph theory, as many

molecular structures can be represented within this class, particularly those whose properties depend on vertex degrees.

Let $\Gamma = U_n^p$ be a connected uni-cyclic graph such that the number of vertices and edges are equals, i.e., $|V(\Gamma)| = |E(\Gamma)|$ and constructed from a cycle of length n by adding p pendant vertices to each vertex of the cycle, as illustrated in Figure 4.

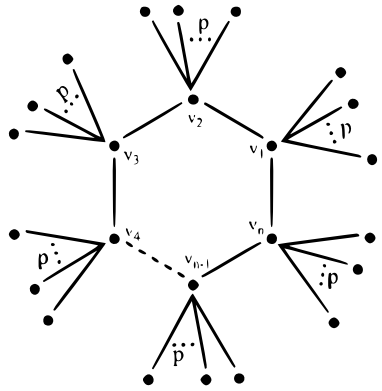

Figure 3: A unicyclic graph U_n^p

Theorem 4.1. *Consider two integers $n \geq 3$ and $p \geq 1$. For the graph $\Gamma = U_n^p$, the GA index is given by* $GA(U_n^p) = \frac{n\left(p+2p\sqrt{p+2}+3\right)}{p+3}$.

Proof. The edges of the graph can be categorized into two types.

In the first type, there are np pendant edges, that joining two vertices of degree 1 and $p+2$.

In the second type, there are n edges forming the cycle, with both endpoints of each edge having degree $p+2$. Thus

$$|E_1 = \{\mu\nu \in E(\Gamma)\lambda_\mu = 1 \& \lambda_\nu = p+2\}| = np.$$
$$|E_2 = \{\mu\nu \in E(\Gamma)\lambda_\mu = \lambda_\nu = p+2\}| = n.$$

Using the GA index for a graph Γ, we obtain the following computation for U_n^p:

$$\begin{aligned} GA(U_n^p) &= \sum_{\mu\nu\in E(\Gamma)} \frac{2\sqrt{\lambda_\mu\lambda_\nu}}{\lambda_\mu+\lambda_\nu} = \sum_{e=\mu\nu\in E_1} \frac{2\sqrt{\lambda_\mu\lambda_\nu}}{\lambda_\mu+\lambda_\nu} + \sum_{e=\mu\nu\in E_2} \frac{2\sqrt{\lambda_\mu\lambda_\nu}}{\lambda_\mu+\lambda_\nu} \\ &= E_1\frac{2\sqrt{1\times(p+2)}}{1+p+2} + E_2\frac{2\sqrt{(p+2)\times(p+2)}}{p+2+p+2} = \frac{2np\sqrt{p+2}}{p+3} + \frac{2n(p+2)}{2(p+2)} = \frac{n(p+2p\sqrt{p+2}+3)}{p+3}. \end{aligned}$$

□

The Theorem 4.2 provides the interpretation for the GA index that corresponding to the unicyclic chemical graph U_n^{alkyl}. In aunicyclic chemical graph U_n^{alkyl} every vertex has degree at most 4.

Theorem 4.2. *Consider two integers $n, p \geq 4$, the GA index of a graph $\Gamma = U_n^{alkyl}$ is equal to:*

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

Proof. The edges of the graph can be classified into two types.

In the first type, there are $2n$ alkyl branches. Each branch contains $|E_1| = 2p+1$ pendant edges connecting two vertices of degrees 1&4, and $|E_2| = p-1$ edges connecting two vertices of degree 4.

In the second type, there are $|E_3| = 3n$ edges associated with the cycle: $2n$ edges connect the alkyl branches to the vertices of the cycle, while the remaining n edges form the cycle itself. All these edges link vertices of degree 4. Thus

$$\begin{aligned}
|E_1 =&\{\mu\nu \in E(\Gamma)\lambda_\mu = 1\&\lambda_\nu = 4\}| = 2n(2p+1).\\
|E_2 =&\{\mu\nu \in E(\Gamma)\lambda_\mu = \lambda_\nu = 4\}| = 2n(p-1) + 3n.\\
|E_3 =&\{\mu\nu \in E(\Gamma)|\lambda_\mu = \lambda_\nu = 4\}| = 3n.
\end{aligned}$$

Using the definition of GA index for a graph Γ, we obtain the following computation for U_n^{alkyl}:

$$\begin{aligned}
GA(U_n^{alkyl}) =& \sum_{\mu\nu\in E(\Gamma)} \frac{2\sqrt{\lambda_\mu\lambda_\nu}}{\lambda_\mu+\lambda_\nu} = \sum_{e=\mu\nu\in E_1} \frac{2\sqrt{\lambda_\mu\lambda_\nu}}{\lambda_\mu+\lambda_\nu} + \sum_{e=\mu\nu\in E_2} \frac{2\sqrt{\lambda_\mu\lambda_\nu}}{\lambda_\mu+\lambda_\nu}\\
=&|E_1|\frac{2\sqrt{1\times 4}}{1+4} + |E_2|\frac{2\sqrt{4\times 4}}{4+4} + |E_3| = \frac{8n}{5}(2p+1) + 2n(p-1) + 3n\\
=&\frac{16np}{5} + \frac{8n}{5} + 2np + n = \frac{26np}{5} + \frac{13n}{5} = \frac{13n(2p+1)}{5}.
\end{aligned}$$

□

5. Conclusion

In this research, we developed general formulas for the GA index for various families of trees and their corresponding chemical tree representations. In addition, we obtained general expressions for the GA index of selected unicyclic graphs, particularly those arising from unicyclic chemical structures such as cycloalkanes. These results were further extended by incorporating alkyl groups or branches of alkyl groups in place of some or all hydrogen atoms in cycloalkanes, leading to new general formulas for the resulting modified structures.

The significance of these findings lies in the fact that the mathematical framework supporting such formulas plays a central role in chemical graph theory, yet the existing literature contains only limited results of this type.

More broadly, these developments may be viewed as contributing to the characterization of chemical graph structures within the context of chemical graph theory.

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