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A Note on General Third Geometric-arithmetic Index of Special Chemical Molecular Structures

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Abstract: In theoretical chemistry, the geometric-arithmetic indices were introduced to measure the stability of alkanes and the strain energy of cycloalkanes. In this note, we report the general third geometric-arithmetic index of unilateral polyomino chain and unilateral hexagonal chain. Also, the third geometric-arithmetic index of these chemical structures are presented.
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1 Introduction

One of the most important applications of chemical graph theory is to measure chemical, physical and pharmaceutical properties of molecules called alkanes. Several indices relied on the graphical structure of the alkanes are defined and employed to model both the melting point and boiling point of the molecules. Molecular graph is a topological representation of a molecule such that each vertex represents an atom of molecule, and covalent bounds between atoms are represented by edges between the corresponding vertices.

Specifically, topological index can be regarded as a score function $f : G \to \mathbf{R}^+$ with this property that $f(G_1) = f(G_2)$ if two molecular graphs G_1 and G_2 are isomorphic. There are several vertex distance-based and degree-based indices which are introduced to analyze the chemical properties of molecule graph. For instance, Wiener index, PI index, Szeged index, atom-bond connectivity index and geometric-arithmetic index. Several papers contributed

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to determine the indices of special molecular graphs (see [1]–[9]).

All (molecular) graphs considered in this paper are finite, loopless, and without multiple edges. Let G be a (molecular) graph with vertex set $V(G)$ and edge set $E(G)$. All graph notations and terminologies used but undefined in this paper can be found in [10].

By considering the degrees of vertices in G, Vukicevic and Furtula[11] developed the geometric-arithmetic index, shortly GA index, which is defined by

$$GA(G) = \sum_{e=uv} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)},$$

where $d(u)$ denotes the degree of vertex $u \in V(G)$.

Yuan *et al.*[12] obtained the lower and upper bounds for GA index of molecular graphs in terms of the numbers of vertices and edges. They also determined the n-vertex molecular trees with the minimum, the second and the third minimum, as well as the second and the third maximum GA indices. Das *et al.*[13] obtained the lower and upper bounds on GA indices and characterize molecular graphs for which these bounds are best possible. Moreover, they discussed the effect on GA index of inserting an edge into a molecular graph. Madanshekaf and Moradi[14] calculated the geometric-arithmetic index of two infinite classes of dendrimers.

Fath-Tabar *et al.*[15] defined a new version of the geometric-arithmetic index, i.e., the second geometric-arithmetic index:

$$GA_2(G) = \sum_{e=uv} \frac{2\sqrt{n(u)n(v)}}{n(u)+n(v)},$$

where $n(u)$ is the number of vertices closer to vertex u than vertex v and $n(v)$ defines similarly. In [16], the maximum and the minimum second geometric-arithmetic index of the star-like tree are learned in view of an increasing or decreasing transformation of the second geometric arithmetic index of trees. Furthermore, they determine the corresponding extremal trees.

Let $e = uv$ be an edge of the molecular graph G. The number of edges of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $m_u(e)$. Analogously, $m_v(e)$ is the number of edges of G whose distance to the vertex v is smaller than the distance to the vertex u. Zhou *et al.*[17] proposed a third class of geometric-arithmetic index:

$$GA_3(G) = \sum_{e=uv} \frac{2\sqrt{m_u(e)m_v(e)}}{m_u(e)+m_v(e)}.$$

For more chemical engineering applications, the extension version of geometric-arithmetic indices are given by researches. Eliasi and Iranmanesh[18] defined the ordinary geometric-arithmetic index (or, general geometric-arithmetic index) as follows:

$$OGA_\gamma(G) = \sum_{e=uv} \left[\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}\right]^\gamma,$$

where γ is a real number. For a real number γ, the general second geometric-arithmetic