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Research Paper

Computing Two Types of Geometric-Arithmetic Indices of Some Benzenoid Graphs

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Abstract. The well-known geometric-arithmetic index is a famous topological index was defined as $GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u\,d_v}}{d_u+d_v}$, where $d_u = deg(u)$ in G. By replacing $\delta_u = \sum_{v\sim u} d_v$ instead of d_u in $GA(G)$, we have a new version of this index that defined as $GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{\delta_u\,\delta_v}}{\delta_u+\delta_v}$. In this paper, we present exact formulas of these indices for some benzenoid graphs.

Keywords: Connected graph, benzenoid graph, geometric-arithmetic index, GA_5 index
Mathematics Subject Classification (2010): Primary 05C90; Secondary 92E10.

1 Introduction

Let G be a simple connected graph. A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. In chemical graph theory, the vertices and edges of a graph also correspond to the atoms and bonds of the molecular graph, respectively. If e is an edge/bond of G, connecting the vertices/atoms $u$and v, then we write $e = uv$ say " u and v are adjacent". Chemical graph theory is an important branch of graph theory and Mathematical chemistry, which applies graph theory to mathematical modeling of chemical phenomena [7, 9, 10, 12]. A chemical topological index is a numeric quantity from the structural graph of a molecule and is invariant on the automorphism of the graph. The concept of geometric-arithmetic

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indices was introduced in the chemical graph theory. These indices generally are defined as:

$$GA_{general}(G) = \sum_{uv \in E(G)} \frac{2\sqrt{Q_u\, Q_v}}{Q_u + Q_v},$$

where Q_u is some quantity that in a unique manner can be associated with the vertex u of graph G. The first member of this class was considered by Vukičević and Furtula [11], by setting Q_u to be d_u, we have:

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

in which d_u denotes the degree of vertex u in G, namely, the number of its neighbors G.

The second member of this class was considered by Fath-Tabar *et al.* [2], by setting Q_u to be the number n_u of vertices of G lying closer to the vertex u than to the vertex v for the edge uv of the graph G,

$$GA_2(G) = \sum_{uv \in E(G)} \frac{2\sqrt{n_u\, n_v}}{n_u + n_v}.$$

The third member of this class was considered by Bo Zhou et al. [14], by setting Q_u to be the number m_u of edges of G lying closer to the vertex u than to the vertex v for the edge uv of the graph G,

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

The fourth and fifth members of this class was considered by Ghorbani et al. [3,4], by setting Q_u to be ε_u, the eccentricity of vertex u (the largest distance between u and any other vertex of graphs) and δ_u, the summation of degree of neighbors of vertex u, $GA_4(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\varepsilon_u\, \varepsilon_v}}{\varepsilon_u + \varepsilon_v}$ and $GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\delta_u\, \delta_v}}{\delta_u + \delta_v}$.

For a comprehensive survey of the mathematical properties and chemical properties of these indices see papers series and books [1, 5, 6, 8, 13].

A benzenoid system is a connected geometric figure obtained by arranging congruent regular hexagons in a plane, so that two hexagons are either disjoint or have a common edge. Benzenoid graphs are simple, plane, and bipartite. The vertices lying on the border of the unbounded face of a benzenoid graphs are called external and other vertices, if present, are called internal. In this paper, we focus on the first and fifth geometric-arithmetic indices are computed them for some benzenoid graphs.

2 Results

In this section, we compute first and fifth geometric-arithmetic indices for some benzenoid graphs as shown in Figure 1.

The first class of benzenoid graphs we consider is triangular benzenoids such as shown in Figure 1. We denote this graph by T_n in which n is the number of hexagons in the base

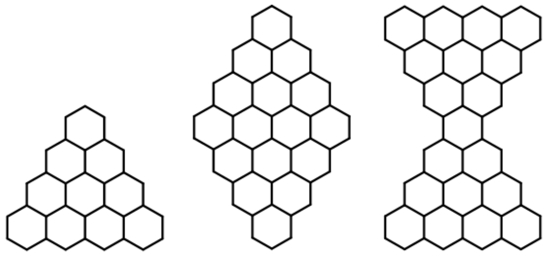

Figure 1. The benzenoid graphs T_4, R_4 and X_4 from left to right.

of graph. Obviously, the total number of hexagons in T_n is $\frac{n(n+1)}{2}$. Also T_n, has $|V(T_n)| = n^2 + 4n + 1$ vertices and $|E(T_n)| = \frac{3}{2}n(n+3)$ edges.

Theorem 2.1. *For graph T_n we have*

$$GA(T_n) = \frac{3}{2}n(n-1) + 6 + \frac{12\sqrt{6}}{5}(n-1),$$

$$GA_5(T_n) = \frac{3}{2}n(n-3) + 3 + \sqrt{35} + \frac{8\sqrt{5}}{3} + \frac{12\sqrt{42}}{13}(n-2) + \frac{9\sqrt{7}}{8}(n-1).$$

Proof. Let m_{ij} is an edge that connects a vertex of degree i to a vertex of degree j. So in graph T_n for external vertices we have $|m_{22}| = 6$, $|m_{23}| = 6(n-1)$ and for internal vertices that all of them are from degree 3, $|m_{33}| = \frac{3}{2}n(n-1)$, then we have

$$GA(T_n) = \frac{3}{2}n(n-1) + 6 + \frac{12\sqrt{6}}{5}(n-1).$$

For compute $GA_5(T_n)$, we partition the edges of graph into five subsets. All of m_{22}edges have a vertex u with $\delta(u) = 5$ and a vertex v with $\delta(v) = 6$. In m_{23} edges, we consider two cases: one set is contain edges with $\delta(u) = 5$and $\delta(v) = 7$, that these edges have a common vertex with a m_{22}. So the number of these edges are equal to 6. Other edges with two external vertices have $\delta(u) = 6$ and $\delta(v) = 7$, that the number of these edges are equal to $6(n-2)$. Edges with an external vertex and an internal vertex are equal to $3(n-1)$and have $\delta(u) = 7$and $\delta(v) = 9$. Finally the number of edges with two internal vertices are $\frac{3}{2}n(n-3) + 3$ and $\delta(u) = \delta(v) = 9$. Then we have

$$GA_5(T_n) = \frac{3}{2}n(n-3) + 3 + \sqrt{35} + \frac{8\sqrt{5}}{3} + \frac{12\sqrt{42}}{13}(n-2) + \frac{9\sqrt{7}}{8}(n-1)$$

which completes the proof. □

A benzenoid rhombus R_n is obtained from two copies of a triangular benzenoid T_n by identifying hexagons in one of their base rows that is shown in Figure 1. Consequently, $|V(R_n)| = 2n(n+2)$ and $|E(R_n)| = 3n^2 + 4n - 1$.

Theorem 2.2. *or graph R_n we have*

$$GA(R_n) = 3n^2 - 4n + 7 + \frac{16\sqrt{6}}{5}(n-1),$$

$$GA_5(R_n) = 3n^2 - 8n + 7 + \frac{8\sqrt{20}}{9} + \frac{4\sqrt{35}}{3} + \frac{16\sqrt{42}}{13}(n-2) + \frac{\sqrt{63}}{2}(n-1).$$

Proof. The proof is similar to that of Theorem 2.1. □

Third benzenoid graph that we consider is benzenoid hourglass. A benzenoid hourglass X_n is obtained from two copies of T_n by overlapping their extremal hexagons in the way shown in Figure 1. The number of vertices and edges of X_n is given by $|V(X_n)| = 2(n^2 + 4n - 2)$ and $|E(X_n)| = 3n^2 + 9n - 4$.

Theorem 2.3. *For graph X_n we have*

$$GA(X_n) = 3n^2 - 3n + 12 + \frac{8\sqrt{6}}{5}(3n-4),$$

$$GA_5(X_n) = 3n^2 + 9n + 10 + \frac{16\sqrt{20}}{9} + \frac{16\sqrt{35}}{12} + \frac{24\sqrt{42}}{13}(n-2) + \frac{12\sqrt{63}}{16}(n-1).$$

Proof. The proof is similar to Theorem 2.1. □

Corollary 2.4. *For benzenoid graphs in Figure 1 we have the following statements*

$$GA(R_n) - GA(T_n) \approx 1.5n^2 - 0.5404n - 0.9596,$$

$$GA(X_n) - GA(T_n) \approx 1.5n^2 + 4.3788n - 3.798,$$

$$GA(X_n) - GA(R_n) \approx 4.9192n - 2.8384,$$

$$GA(X_n) - 2GA(T_n) \approx -3.9192,$$

$$GA_5(T_n) - GA(T_n) \approx 0.0801n - 0.1834,$$

$$GA_5(R_n) - GA(R_n) \approx 0.1074n - 0.2193,$$

$$GA_5(X_n) - GA(X_n) \approx 18.160n - 0.366.$$

Corollary 2.5. *Let G_n be one of the benzenoid graphs T_n,R_n or X_n, we have*

$$\lim_{n\to\infty} \frac{GA(G_n)}{GA(G_{n-1})} = 1.$$

In Table 1, we compute $GA(G)$ and $GA_5(G)$ for three graphs in Figure 1, $(2 \le n \le 7)$.

Table 1.

n	$GA(T_n)$	$GA(R_n)$	$GA(X_n)$	$GA_5(T_n)$	$GA_5R_n)$	$GA_5(X_n)$
2	14.879	18.838	25.838	14.856	18.832	61.792
3	26.758	37.677	49.596	26.814	37.776	103.71
4	41.636	62.515	79.354	41.774	62.721	151.63
5	59.515	93.354	115.11	59.731	93.667	205.54
6	80.394	130.19	156.87	80.691	130.61	265.46
7	104.27	173.03	204.63	331.38	173.56	331.38

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