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

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ABSTRACT. The geometric-arithmetic index is a 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 denotes the degree of vertex 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: benzenoid graph, geometric-arithmetic index, GA_5 index.

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

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$e = uv$ 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 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, i.e., the number of its neighbors in 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,

$$GA_4(G) = \sum_{uv\in E(G)} \frac{2\sqrt{\varepsilon_u\,\varepsilon_v}}{\varepsilon_u + \varepsilon_v} \text{ and } GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{\delta_u\,\delta_v}}{\delta_u + \delta_v}.$$

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 graph 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 compute them for some benzenoid graphs.

2. MAIN RESULTS

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

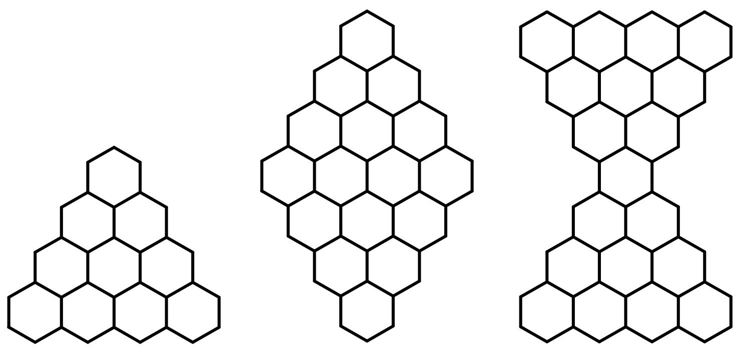

Figure 1: The benzenoid graphs T_4, R_4 and X_4 from left to right.

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

Theorem 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 in 5 subsets. All of m_{22} edges have a vertex u with $\delta(u)=5$ and a vertex v with $\delta(v)=6$ I .n 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. *For 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 theorem 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 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 1.

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

n	$GA(T_n)$	$GA(R_n)$	$GA(X_n)$
2	14.879	18.838	25.838
3	26.758	37.677	49.596
4	41.636	62.515	79.354
5	59.515	93.354	115.11
6	80.394	130.19	156.87
7	104.27	173.03	204.63

n	$GA_5(T_n)$	$GA_5(R_n)$	$GA_5(X_n)$
2	14.856	18.832	61.792
3	26.814	37.776	103.71
4	41.774	62.721	151.63
5	59.731	93.667	205.54
6	80.691	130.61	265.46
7	331.38	173.56	331.38

Table I.

Corollary 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 5. Let G_n be one of the benzenoid graphs T_n, R_n *or* X_n, we have:

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

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