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The Geometric-Arithmetic Index of Benzenoid Systems and Phenylenes

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Abstract

The geometric-arithmetic index of graph G is defined as $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$, d_u (or d_v) is the degree the vertex u (or v). The GA index of benzenoid systems and phenylenes are computed, a simple relation is established between the geometric-arithmetic of a phenylene and the corresponding hexagonal squeeze in this paper.

Mathematics Subject Classification: 05C05, 05C12

Keywords: Geometric-arithmetic index; Phenylene; Hexagonal squeeze

1 Introduction

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [1-3]. This theory had an important effect on the development of the chemical sciences. Numbers reflecting certain structural features of organic molecules that are obtained from the molecular graph are usually called graph invariants or more commonly topological indices. The oldest and most thoroughly examined use of a topological index in chemistry was by Wiener [1] in the study of paraffin boiling points, and the topological index was called Wiener index.

Randić proposed a structural descriptor called the branching index [4] that later became the well-known Randić connectivity index. Motivated by the definition of Randić connectivity index based on the end-vertex degrees of edges

in a graph, Vukičević and Furtula [5] proposed a topological index named the *geometric-arithmetic index* GA. Let G be a connected graph with the vertex-set $V(G)$ and edge-set $E(G)$, respectively. $|V(G)| = n$, $|E(G)| = m$ are the number of vertices and edges. The degree of a vertex $v \in V(G)$ is the number of vertices joining to v and denoted by $deg(v)$ (or simply as d_v, $d(v)$). The *geometric-arithmetic index* of G is defined as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \tag{1}$$

For physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and acentric factor, it is noted in [5] that the predictive power of GA index is somewhat better than predictive power of the Randić connectivity index. In [6], Vukičević and Furtula gave the lower and upper bounds for the GA index, determined the trees with the minimum, the second and the third minimum, as well as the second and the third maximum GA indices.

In this report, we investigate the geometric-arithmetic index of benzenoid systems and phenylenes.

2 Preliminaries

A $i-$ vertex denotes a vertex degree i, and a $(j,k)-$edge stands for an edge connecting a $j-$vertex with a $k-$vertex, and let n_i denote the number of $i-$vertex, m_{jk} be the number of $(j,k)-$edge, respectively.

In the case of a benzenoid system S, which possesses only $(2,2)-$, $(2,3)-$, and $(3,3)-$ edges, the formula (1) reduces to

$$GA(G) = m_{22} + \frac{2\sqrt{6}}{5} m_{23} + m_{33} \tag{2}$$

For the simplicity of the expression (2), we only need calculate m_{22}, m_{23}, m_{33}. Therefore, before our main results, we introduce some notions in benzenoid systems.

As described in [7], we introduce the number of inlets, r, a novel parameter related in the manner to the structure of benzenoid systems and/or phenylenes proposed by Cyvin *et al* [8-10], and show that the geometric-arithmetic index is the function of r. Thus, B=number of simple bays, C=number of coves, F=number of fjords, f=number of fissures, L=number of lagoons. b=number of regions.

Note that Bays, coves, and fjords, fissures and lagoons are structural characteristics of the perimeter of the benzenoid systems playing some role in their theory. An illustrative example is depicted in Figure 1.

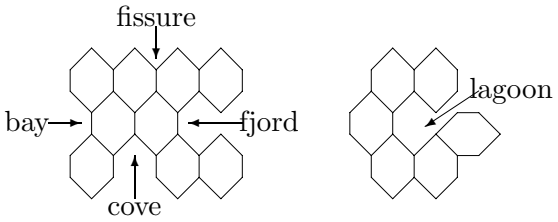


Figure 1. Types of inlets occurring on the perimeter of a benzenoid system

Let r be the total number of inlets on the perimeters of a benzenoid system described above, it is easy to see that: $b = B + 2C + 3F + 4L$, $r = B + C + F + f + L$.

3 The geometric-arithmetic index of benzenoid systems

Theorem 3.1 *Let S be a benzenoid system with n vertices, h hexagons and r inlets. Then*

$$GA(S) = n + h + \frac{4\sqrt{6} - 10}{5}r - 1$$

Proof. By the definition of an inlet, an inlet corresponds to a sequence of vertices on the perimeter, of which the first and the last are 2-vertices and all other 3-vertices, thus, we have $m_{23} = 2r$. The number of 3-vertices in a benzenoid system S is $n_3 = 2(h - 1)$ and it follows that $m_{23} + m_{33} = 3n_3 = 6h - 6$. By combing above results, we have $m_{33} = 3h - r - 3$.

In benzenoid systems, $m_{22} + m_{23} + m_{33} = m$ is the total number of edges, and $m = n + h - 1$. Therefore, we arrive at $m_{22} = n - 2h - r + 2$.

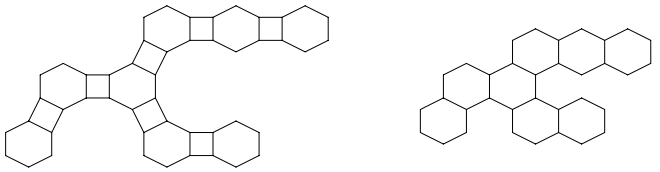
Finally, we obtain the desired result.

This completes the proof.

4 The geometric-arithmetic index of phenylenes

Phenylenes are a class of chemical compounds in which the carbon atoms form 6- and 4-membered cycles. Each 4-membered cycle(=square) is adjacent to two disjoint 6-membered cycles(=hexagons), and no two hexagons are adjacent[11]. By eliminating, "squeezing out", the squares from a phenylene, a catacondensed hexagonal system (which may be jammed) is obtained, called the hexagonal squeeze of the respective phenylene ([12]). Clearly, there is a one-to-one correspondence between a phenylene (PH) and its hexagonal squeeze (HS). Both possess the same number (h) of hexagons. In addition, a phenylene with h hexagons possesses h-1 squares. The number of vertices of PH and HS are 6h and 4h+2, respectively; The number of edges of PH and HS are 8h-2

and 5h+1, respectively. An example of phenylene and its hexagonal squeeze is shown in Figure 2.



PH HS

Figure 2. A phenylene (PH) and its hexagonal squeeze (HS).

For phenylenes and their hexagonal squeezes, some results related to the mathematical properties of Wiener index, Randić index, the second order Randić index, PI index have been reported in the literatures([13-15]).

In the case of phenylenes, a fissure, bay, cove, fjord, and lagoon are defined in full analogy to the benzenoid systems: A fissure (*resp.* a bay, cove, fjord, or lagoon) corresponds to a sequence of four (*resp*, six, eight, ten, and twelve) consecutive vertices on the perimeter, of which the first and the last are 2-vertices and the rest are 3-vertices.

Similar to the discussion of Theorem 1, we have

Theorem 4.1 *Let PH be a phenylene with h hexagons and r inlets. Then*

$$GA(PH) = 8h + \frac{4\sqrt{6} - 10}{5}r - 2.$$

Proof. The proof is analogous to the proof of Theorem 1. This time the number of 3-vertices is $n_3 = 4(h-1)$, whereas the number of edges is $m = n + (2h-1) - 1 = 8h - 2$. Thus,

$$m_{22} = 2h - r + 4 \tag{3}$$

$$m_{23} = 2r \tag{4}$$

$$m_{33} = 6h - r - 6 \tag{5}$$

Substituting relations (3)-(5) into the equation (2), we arrive at the result.

5 A relation between the geometric-arithmetic index between PH and HS

In the following, we establish a relation between the geometric-arithmetic index of a phenylene and the corresponding hexagonal squeeze.

For the hexagonal squeeze HS of a phenylene, HS may be jammed (which possesses lagoons). Since a phenylene with n vertices has $\frac{n}{6}$ hexagons, its hexagonal squeeze has $4 \cdot \frac{n}{6} + 2$ vertices.

Comparing Theorem 3.1 with Theorem 4.1, we have

Theorem 5.1 *Let PH be a phenylene with h hexagons and HS its hexagonal squeeze. Then*

$$GA(PH) = GA(HS) + 3(h-1).$$

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