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A Note on the First Geometric–Arithmetic Index of Hexagonal Systems and Phenylenes

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ABSTRACT

The first geometric-arithmetic index was introduced in the chemical theory as the summation of $2\sqrt{d_u d_v}/(d_u + d_v)$ overall edges of the graph, where d_u stand for the degree of the vertex *u*. In this paper we give the expressions for computing the first geometric-arithmetic index of hexagonal systems and phenylenes and present new method for describing hexagonal system by corresponding a simple graph to each hexagonal system.

Keywords: Geometric-arithmetic index, hexagonal system, phenylenes.

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1. INTRODUCTION

Throughout this paper *G* is a simple connected graph with vertex and edge sets *V*(*G*) and *E*(*G*), respectively. A topological index is a numeric quantity from the structural graph of a molecule. The concept of the first geometric-arithmetic index was introduced in the chemical graph theory. This index is defined as

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

where *uv* is an edge of the molecular graph *G* and d_u stand for the degree of the vertex *u*, see [1].

A hexagonal 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. This figure divides the plane into one infinite external region and a number of finite internal all internal region must be regular hexagons. Hexagonal systems are considerable importance in theoretical chemistry because they are the natural graph

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representation of benzenoid hydrocarbon. A vertex of a hexagonal system belongs to at most three hexagons. A vertex shared by three hexagons is called an internal vertex; the number of internal vertices of a hexagonal system is denoted by n_i. A hexagonal system is called catacondensed if $n_i=0$, otherwise ($n_i>0$), it is called precondensed, For more details and new results about hexagonal systems, see [2−9].

Lemma 1.1. (See [4]). For any hexagonal system with *n* vertices, *m* edges and *h* hexagons and n_i internal vertices,

$$n=4h+2-n_i \text{ and } m=5h+1-n_i.$$

Phenylenes are a class of chemical compounds in which the carbon atoms form squares and hexagons. Each square is adjacent to two disjoint hexagons, and no two hexagons are adjacent. Their respective molecular graphs are also referred to as phenylenes. By eliminating, squeezing out, the squares from a phenylene, a catacondensed benzenoid system (which may be jammed) is obtained, called the hexagonal squeeze of the respective phenylene. 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 such a PH and its HS are 6h and 4h + 2, respectively. We recall some concept about hexagonal systems that will be used in the paper. A hexagon *H* of a catacondensed hexagonal system has either one, two or three neighboring hexagons. If *H* has one neighboring hexagon, it is called terminal, and if it has three neighboring hexagons it is called branched. A hexagon *H* adjacent to exactly two other hexagons posses two vertices of degree 2. If these two vertices are adjacent, *H* is angularly connected. Each branched and angularly connected hexagons in a catacondensed hexagonal system is said to be kink, in Figure 1(a) the kinks are marked by K. The linear chain L_h with h hexagons is the catacondensed system without kinks, see Figure 1(b). Our notation is standard and mainly taken from [10, 11].

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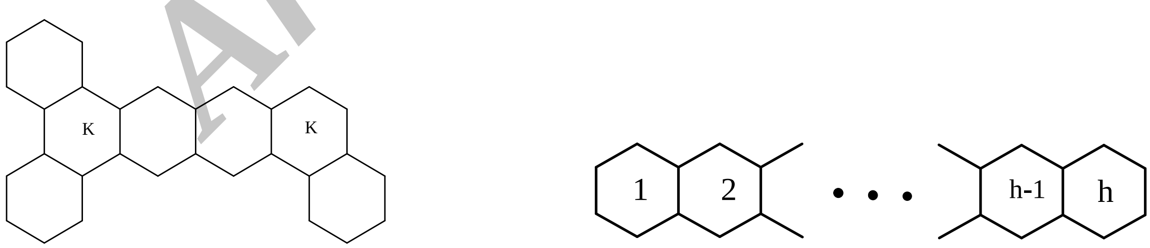

(a) (b)

Figure 1. (a) The Kinks, (b) A Linear Chain L_h.

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2. MAIN RESULT AND DISCUSSION

At first we define a concept related to a hexagonal system and use it to obtain the GA index of a hexagonal system.

Definition 2. 1. A hexagon in a hexagonal system is called cubic hexagon if the degree of all vertices are equal to 3.

Throughout this paper, we suppose that *HS* is a hexagonal system with *n* vertices, *m* edges, *h* hexagons, h_i cubic hexagons and n_i internal vertices. If we partition the edge set of *HS* into three subsets E_1, E_2 and E_3, as follows:

$$E_1 = \{e = uv \mid d_u + d_v = 4\},$$
$$E_2 = \{e = uv \mid d_u + d_v = 5\},$$
$$E_3 = \{e = uv \mid d_u + d_v = 6\}.$$

Therefore,

$$GA_1(HS) = m + (\frac{2\sqrt{6}}{5} - 1)|E_2|. \qquad (1)$$

Theorem 2. 2. Let *HS* be a hexagonal system, then the first geometric-arithmetic index is computed as follows:

$$GA_1(HS) = (3 + \frac{4\sqrt{6}}{5})h + (2 - \frac{4\sqrt{6}}{5})h_i + (\frac{4\sqrt{6}}{5} - 2)k_i - n_i + 1,$$

where k_i is the number of hexagons with exactly two parallel edges in E_3.

Proof. Let *H* be a hexagon in a hexagonal system such that it has at least one vertex of degree 2. There are six cases, see Figure 2(a)-(f). In cases (a)-(e), there are two edges in E_2 and in case (f), there are four edges in E_2. In case (f) a hexagon with two vertices of degree 2, has just two edges in E_3 such that these edges are parallel. Suppose k_i is the number of these hexagons (the hexagon with exactly two parallel edges in E_3). Then,

$|E_2| = 2(h - h_i) + 2k_i = 2(h - h_i + k_i)$. By Eq(1) we have:

$$GA_1(HS) = m + (\frac{2\sqrt{6}}{5} - 1) \times 2(h - h_i + k_i)$$
$$= 5h - n_i + 1 + 2(\frac{2\sqrt{6}}{5} - 1)(h - h_i + k_i)$$
$$= (3 + \frac{4\sqrt{6}}{5})h + (2 - \frac{4\sqrt{6}}{5})h_i + (\frac{4\sqrt{6}}{5} - 2)k_i - n_i + 1.$$

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Set $\alpha = 3 + \frac{4\sqrt{6}}{5}$ and $\beta = 2 - \frac{4\sqrt{6}}{5}$, therefore $GA_1(HS) = \alpha h + \beta h_i - \beta k_i - n_i + 1$. □

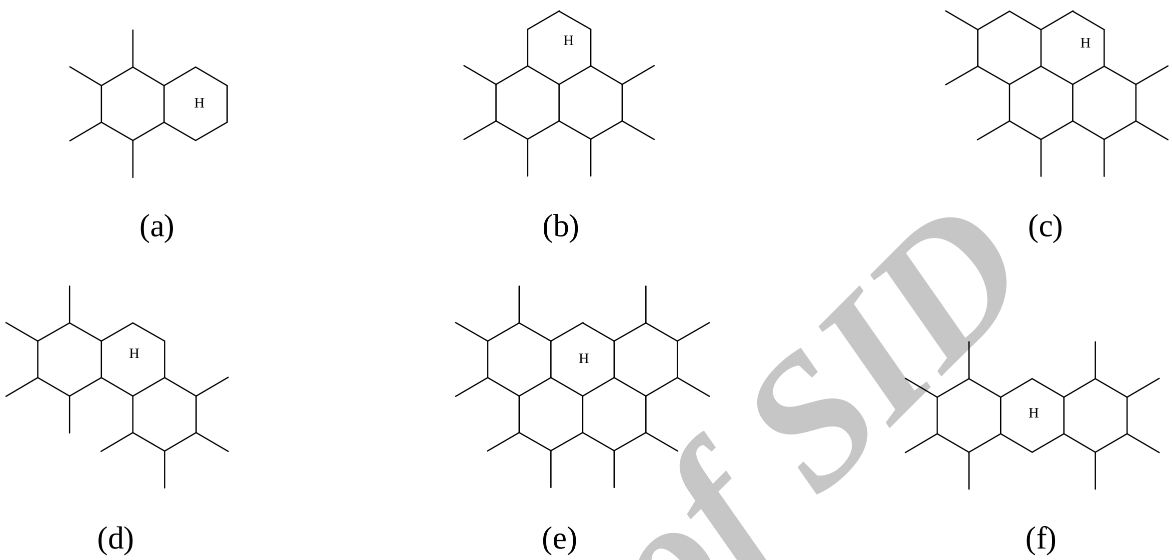

Figure 2. Six Different Cases for a Hexagon in HS with at Least One Vertex of Degree 2.

Corollary 2. 3. Let *CHS* be a catacondensed hexagonal system with *h* hexagons. Then

$$GA_1(CHS) = \alpha h + \beta h_i - \beta k_i + 1.$$

Definition 2. 4. For each *HS* the related graph G_{HS} is defined as follows:

$$V(G_{HS}) = \{H \mid H \text{ be a hexagon in hexagonal system}\},$$
$$E(G_{HS}) = \{H_1H_2 \mid \exists e \in E(X),\ H_1 \cap H_2 = \{e\}\}.$$

Example 2. 5. In Figure 3 the hexagonal systems L_5, *HS*, X_{10} and E_{12} with their related graphs are shown.

It is easy to see that for each hexagonal system *HS*, G_{HS} is simple planner graph and $\Delta(G_{HS}) \leq 6$.

Lemma 2. 6. (i) The hexagonal system *HS* is catacondensed if and only if G_{HS} is a tree, such that $\Delta(G_{HS}) \leq 3$.

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(ii) A hexagon H, in a catacondensed system is a cubic hexagon if and only if $\deg_{G_{HS}} H = 3$.

Proof. By definition of catacondensed hexagonal system and related graph, the proof is straightforward. □

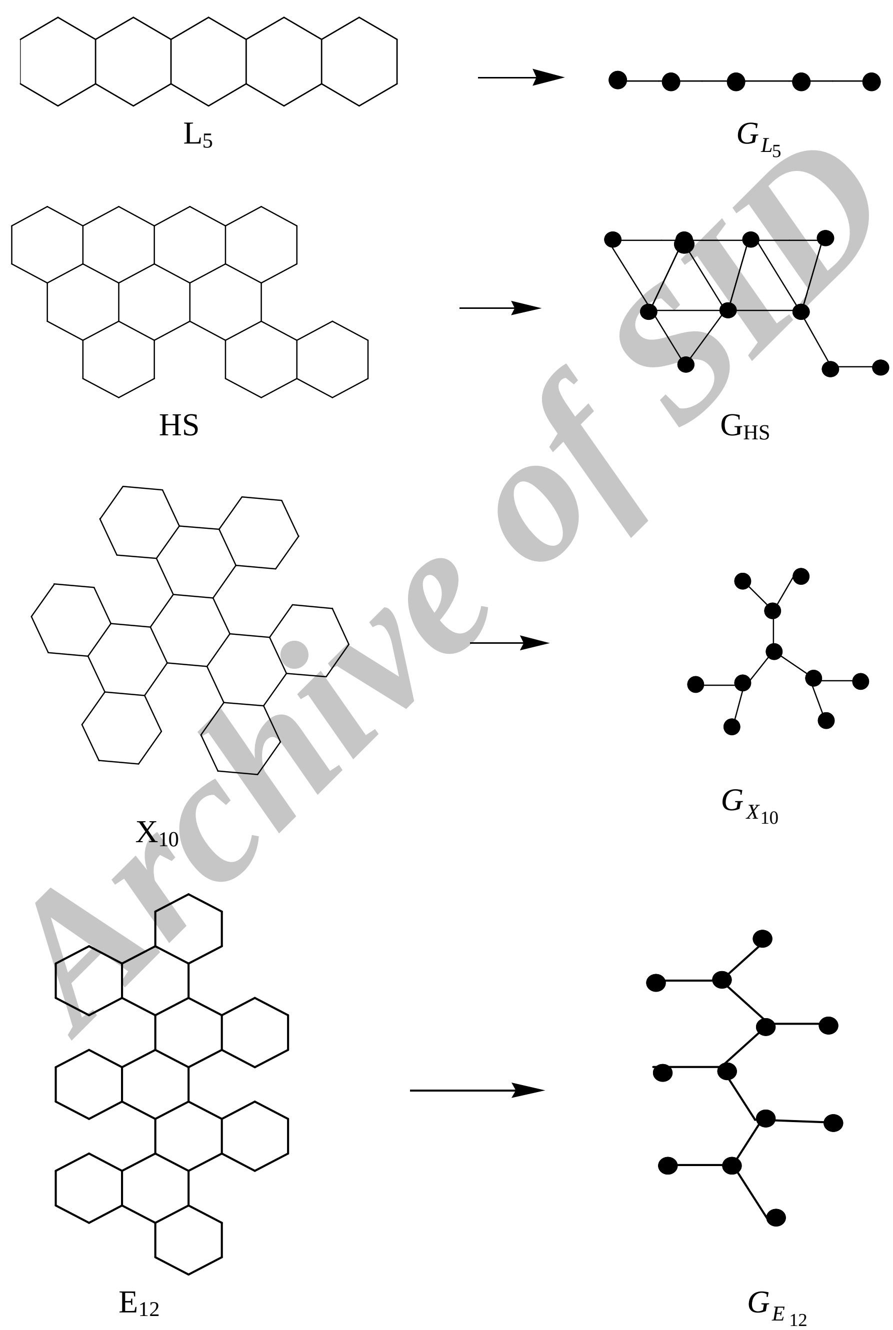

Figure 3. Hexagonal Systems with Related Graphs.

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Theorem 2. 7. Let *CHS* be a catacondensed hexagonal system with h hexagons, then $GA_1(L_h) \le GA_1(CHS) \le GA_1(X_h)$.

Proof. By Corollary 2.3 and since $\beta > 0$, then minimum value of GA_1 for catacondensed hexagonal systems with *h* hexagons, is happened for a catacondensed hexagonal system, such that $h_i=0$ and k_i has maximum value. In a linear chain with *h* hexagons, it is easy to see that $h_i=0$ and $k_i=h-2$ there is no hexagonal system such that $k_i=h$ *or* $h-1$, for $h \ge 3$ then $GA_1(L_h) \le GA_1(CHS)$. Also the maximum value of GA_1 for catacondensed hexagonal systems with *h* hexagons, is happened for a catacondensed hexagonal system, such that h_i has maximum value and $k_i=0$. A catacondensed hexagonal system X_h has the maximum value of h_i if and only if the tree G_{X_h} has maximum number of vertices of degree 3. By Lemma 2.6, for a catacondensed hexagonal system *X*, $\Delta_{G_X} \le 3$. The maximum number of vertices of degree 3 in G_X is equal to $[(h-2)/2]$, in fact $h_i = [(h-2)/2]$ for h=1 it is trivial that $h_i=0$ and for $h \ge 2$ by induction on *h*, see Figures 4 (a)-(d). Therefore, $GA_1(CHS) \le GA_1(X_h)$ and this completes the proof. □

Theorem 2. 8. Let *PH* be a Phenylenes with h hexagons, then the geometric-arithmetic index is computed as follows:

$$GA_1(PH) = (6+\frac{4\sqrt{6}}{5})h + (2-\frac{4\sqrt{6}}{5})h_i + (\frac{4\sqrt{6}}{5}-2)k_i - 2,$$

where k_i is the number of hexagons with exactly two parallel edges in E_3.

Proof. By Eq(1) and $|E(PH)| = m = 8h-2$

$$\begin{aligned} GA_1(PH) &= m + (\frac{2\sqrt{6}}{5}-1)\times 2(h-h_i+k_i) \\ &= 8h-2+(\frac{2\sqrt{6}}{5}-1)\times 2(h-h_i+k_i) \\ &= (6+\frac{4\sqrt{6}}{5})h + (2-\frac{4\sqrt{6}}{5})h_i + (\frac{4\sqrt{6}}{5}-2)k_i - 2. \end{aligned}$$

Set $\alpha = 3+\frac{4\sqrt{6}}{5}$ *and* $\beta = 2-\frac{4\sqrt{6}}{5}$, thus $GA_1(PH) = (\alpha+3)h + \beta h_i - \beta k_i - 2.$ □

Theorem 2. 10. Let *PH* be a Phenylenes with *h* hexagons and *HS* its hexagonal squeeze. Then the geometric-arithmetic of *PH* and *HS* are related as:

$$GA_1(PH) - GA_1(HS) = 3(h-1).$$

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Proof. It easy to see that *HS* is a catacondensed hexagonal system. Then by Corollary 2.3 and Theorem 2.8,

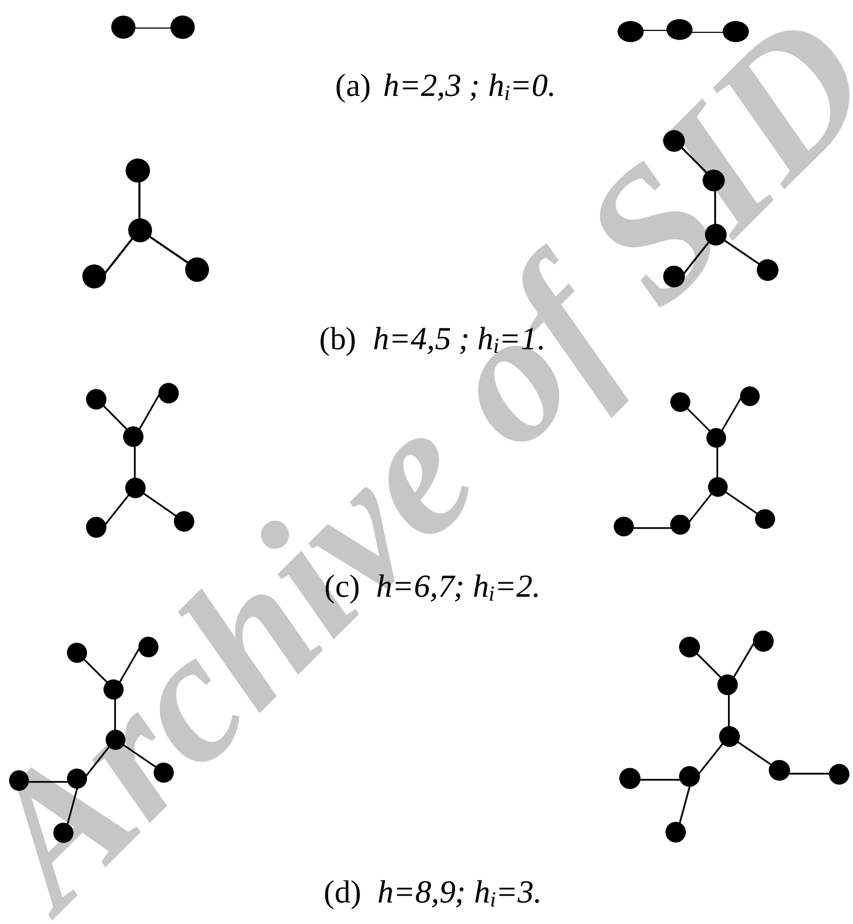
$$GA_1(HS) = \alpha\, h + \beta\, h_i - \beta\, k_i + 1$$

$$GA_1(PH) = (\alpha + 3)\, h + \beta\, h_i - \beta\, k_i - 2$$

Then we conclude that:

$$GA_1(PH) - GA_1(HS) = 3(h-1).$$

□



(a) h=2,3 ; h_i=0.

(b) h=4,5 ; h_i=1.

(c) h=6,7; h_i=2.

(d) h=8,9; h_i=3.

Figure 4. Graphs for Hexagonal Systems with h Hexagons, Maximum Value of h_i and $k_i = 0$.

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