Iranian Journal of Mathematical Chemistry, Vol. 1, No. 1, April 2010, pp. 95 – 103

IJMC

Second and Third Extremals of Catacondensed Hexagonal Systems with respect to the PI Index

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(Received, February 10, 2010)

ABSTRACT

The Padmakar-Ivan (*PI*) index is a Wiener-Szeged-like topological index which reflects certain structural features of organic molecules. The PI index of a graph G is the sum of all edges uv of G of the number of edges which are not equidistant from the vertices u and v. In this paper we obtain the second and third extremals of catacondensed hexagonal systems with respect to the PI index.

Keywords: Topological index; PI index; catacondensed hexagonal system.

1. INTRODUCTION

A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. If the vertices $u, v \in V(G)$ are connected by an edge e then we write $e=uv$. In chemical graphs, each vertex represents an atom of the molecule, and covalent bonds between atoms are represented by edge between the corresponding vertices. This shape derived from a chemical compound is often called its molecular graph. Molecular structure descriptors, frequently called *topological indices*, are used in theoretical chemistry for the design of chemical compounds with given physico-chemical properties or given pharmacologic and biological activities. Here, we consider a topological index named the Padmakar-Ivan index, see [1-6].

For an edge $e = uv$ of a graph G set

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$$G_1(e) = \{x \in V(G) | d_G(x,u) < d_G(x,v)\}$$
$$G_2(e) = \{x \in V(G) | d_G(x,v) < d_G(x,u)\},$$

It is easy to see, $G_1(e)$ is the set of vertices closer to u than to v while $G_2(e)$ consists of those vertices that are closer to v. Note that the roles of G_1(e) and $G_2(e)$ would be interchanged if the edge e would be considered as $e = vu$. Since these two sets will always be considered in pairs, this imprecision in the definition will cause no problem. Observe that if G is bipartite then for any edge e of G, G_1(e) and $G_2(e)$ form a partition of $V(G)$. If G is bipartite graph, then $m_1(e|G)$ (resp., $m_2(e|G)$) be the number of edges in the subgraph of G induced by $G_1(e)$ (resp.,$G_2(e)$). Again, the roles $m_1(e|G)$ and $m_2(|G)$ could be interchanged, but since only the sum $m_1(e|G) + m_2(e|G)$ will be considered, such a definition suffices. Now, the PI index of G is defined as

$$PI(G) = \sum_{e \in E(G)} \left[m_1(e | G) + m_2(e | G)\right].$$

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 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.

Lemma 1 (See [7]). For any hexagonal system with n vertices, m edges and h hexagons and n_i internal vertices,

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

It is easy to see that all catacondensed hexagonal systems with h hexagons have $4h+1$ vertices and $5h+1$ edges. In a series of papers [8-14], Khadikar and his co-authors defined and then computed the PI index of some chemical graphs. In this paper we use the method that is established by Klavžar to obtain the second and third extremals of catacondensed hexagonal systems with respect to PI index [15]. Our notation is standard and mainly taken from [16, 17].

2. MAIN RESULT AND DISCUSSION

In what follows a method given by Klavžar is described. Using this method, it is possible to obtain extremals of catacondensed hexagonal systems with respect to the PI index. Let G be a graph, then we say that a partition $E_1,\ldots, E_k$ of $E(G)$ is a *PI*-partition of G if for any i, $1 \le i \le k$, and for any $e, f \in E_i$, we have $G_1(e) = G_1(f)$ and $G_2(e) = G_2(f)$.

Lemma 2 (See [17]). Let $E_1,\ldots, E_k$ be a *PI*-partition of a bipartite graph G. Then

$$PI(G) = |E(G)|^2 - \sum_{i=1}^{k} |E_i|^2 .$$

Since hexagonal systems are bipartite, then by Lemmas 1 and 2, we can see that if X is a catacondensed hexagonal system with h hexagons, $PI(X) = (5h+1)^2 - \sum_{i=1}^{k} |E_i|^2$, where $E_1,\ldots, E_k$ is a PI-partition of X. One can see that in a hexagonal system with h hexagons and *PI*-partition $E_1, \ldots, E_k$ for each i, $1 \le i \le k$, $2 \le |E_i| \le h+1$.

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 the kinks are marked by K.

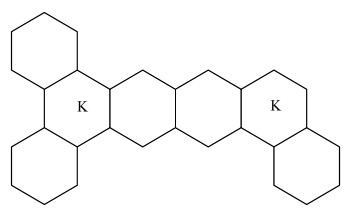

Figure 1. The kinks.

The linear chain L_h with h hexagons is the catacondensed system without kinks, see Figure 2. A segment is maximal linear chain in catacondensed system. The length of a segment is the number of its hexagons.

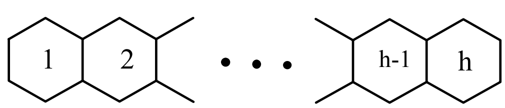

Figure 2. A Linear Chain L_h.

A zig-zag chain Z_h with h hexagons is the catacondensed hexagonal system with h-2 kinks in another word the length of its segments is equal to 1 or 2, see Figure 3.

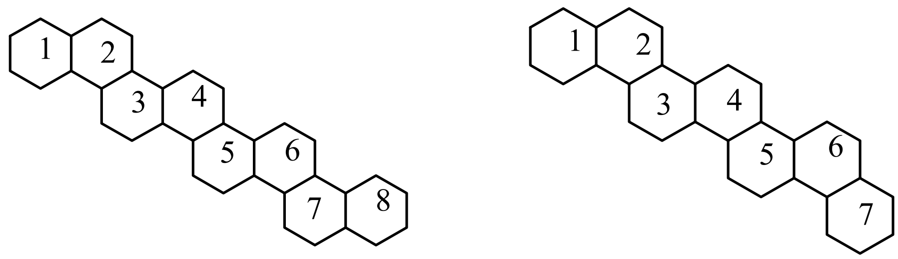

Figure 3. The Zig-Zag chains Z_8 and Z_7.

Let E_1, …, E_k be a *PI*-partition of a catacondensed hexagonal system X. Then one can see that for each $E_i, 1 \le i \le k$, there is $e_i \in E(X)$ such that $E_i = \{e \in E(X) \mid \ e \parallel e_i\}$. In Figure 4, *PI*-partition of linear chain and zig-zag chain are marked by dashed lines.

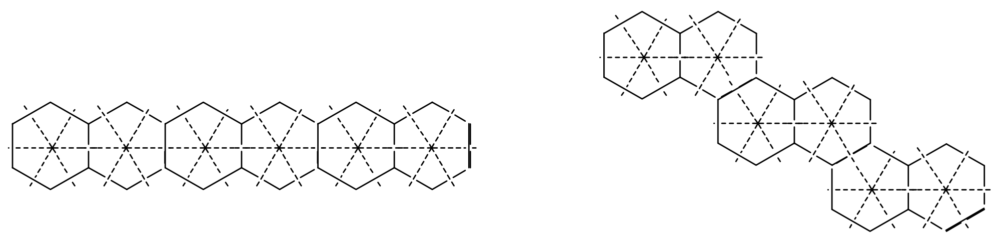

Figure 4. PI-Partitions of L_6 and Z_6.

Let E_1, … , E_k be a *PI*-partition of catacondensed hexagonal system X, with h hexagons, it is easy to see that $k = 2h + 1$ and $\sum_{i=1}^{k} |E_i| = 5h+1$. We can say that X is a linear chain L_h if there exists $1 \le i' \le k$ $|E_{i'}| = h+1$ and for $1 \le i \le k$, $i \ne i'$, $|E_i| = 2$. Also X is a zigzag chain if $|E_i| = 1 \ or \ 2$ for $1 \le i \le k$.

A transformation of type 1 for a cotacondensed hexagonal system is defined as follows: Let X be a cotacondensed hexagonal system with h hexagons. We choose a segment with maximum length containing at least one terminal hexagon. Suppose that the length of this segment is t, denoted by L_t. Remove a terminal hexagon of X (which is not in L_t) and add it to L_t, for obtaining L_{t+1}. This new hexagonal system is denoted by X_1. In Figure 5, this process is applied on X (four times) to obtain X_2, X_3 and X_4. Clearly, if X is a linear chain then X_1 is equal to X.

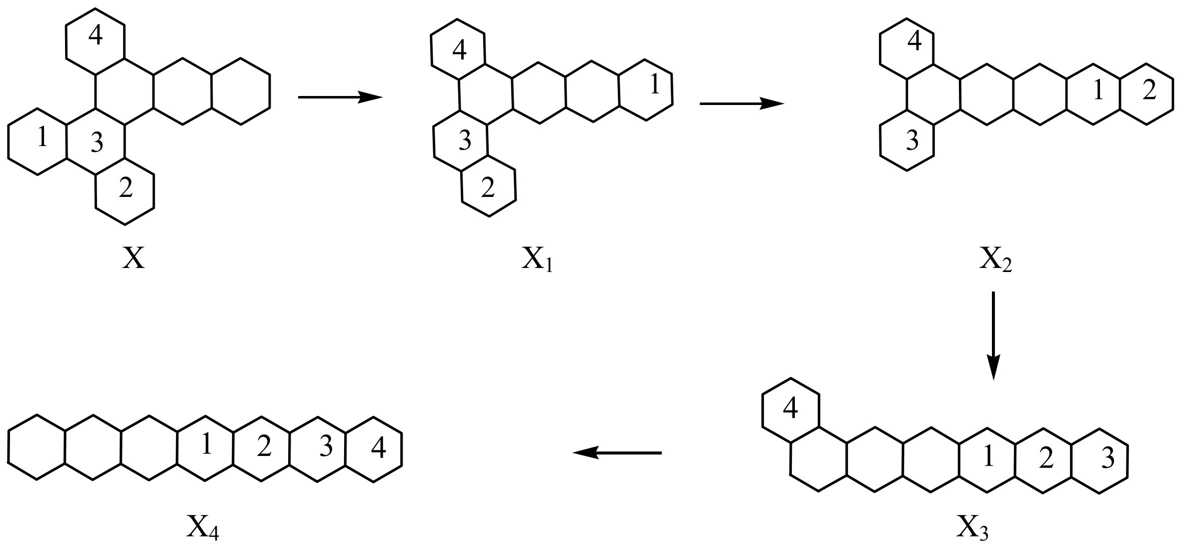

Figure 5. Four transformations of type 1 of X.

Theorem 3. Let X be a catacondensed hexagonal system with h hexagons such that $X \neq L_h$ and let X_1 be a hexagonal system which is instructed by a transformation of type 1. Then, $PI(X_1) < PI(X)$.

Proof. Let $E_1, \ldots, E_k$ and $F_1, \ldots, F_k$ be PI- partitions of X and X_1, respectively. By Lemma 2, $PI(X) = (5h+1)^2 - \sum_{i=1}^{k} |E_i|^2$ and $PI(X_1) = (5h+1)^2 - \sum_{j=1}^{k} |F_j|^2$. Let S be a segment of maximum length t with at least one terminal hexagon. Then there exists $1 \leq i', i'', j' j'' \leq k$ such that $|E_{i'}| = t+1$,$|E_{i''}| = r$, $|F_{j'}| = t+2$ and $|F_{j''}| = r-1$, $r \leq t$, and, for each $1 \leq i, j \leq k$ such that, $i \neq i', i'', j \neq j', j''$ $|E_i| = |F_j|$. Therefore

$$PI(X) = (5h+1)^2 - \sum_{\substack{i=1 \\ i \neq i', i''}}^{k} |E_i|^2 - (t+1)^2 - r^2$$

and

$$PI(X_1) = (5h+1)^2 - \sum_{\substack{j=1 \\ j \neq j', j''}}^{k} |F_j|^2 - (t+2)^2 - (r-1)^2.$$

Since $\sum_{\substack{i=1 \\ i \neq i', i''}}^{k} |E_i|^2 = \sum_{\substack{j=1 \\ j \neq j', j''}}^{k} |F_j|^2$ and $(t+1)^2 + r^2 < (t+2)^2 + (r-1)^2$, one can see that $PI(X_1) < PI(X)$. ∎

Corollary 4. Let X be a catacondensed hexagonal system with h hexagons and $X \neq L_h$. Then $PI(L_h) < PI(X)$.

Proof. Let X_1 be a instructed hexagonal system by transformation of type 1, if $X_1 = L_h$ then by Theorem 3, $PI(L_h) = PI(X_1) < PI(X)$ and the proof is completed. Otherwise, we continue this process and obtain X_2 from X_1, by similar way if $X_2 = L_h$, use Theorem 3. Otherwise continue the process. Finally there exists positive integer t such that $X_t = L_h$ and this completes the proof. ■

A semi linear chain $L_h^{'}$ with *h* hexagons is the catacondensed system such that it has a segment of length *h-1* and a segment of length 2 and remained segment have length 1, see Figure 5. In other word, in *PI*-partition E_1, …, E_k of $L_h^{'}$, there exist $1 \leq i', i'' \leq k$, such that $|E_{i'}| = h$,$|E_{i''}| = 3$ and for each $1 \leq i, \leq k$, $i \neq i', i''$, $|E_i| = 2$.

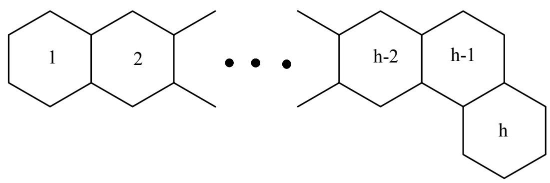

Figure 5. A Semi Linear Chain $L^{'}_{h.}$

Corollary 5. Let X be a catacondensed hexagonal system with *h* hexagons and $X \neq L_h, L'_h$. Then $PI(L'_h) < PI(X)$.

Proof. The proof is straight forward by Theorem 3 and Corollary 4. ■

Define the hexagonal system L''_h with *h* hexagons to be the catacondensed system containing one segment with length *h-2,* two segments of length 2, and remaining segments have length 1, see Figure 6. In other words, in *PI*-partition E_1,…, E_k of L''_h, there exist $1 \leq i', i'', i''' \leq k$, such that $|E_{i'}| = h-1$,$|E_{i''}| = |E_{i'''}| = 3$ and for each $1 \leq i \leq k$, $i \neq i', i'', i'''$, $|E_i| = 2$.

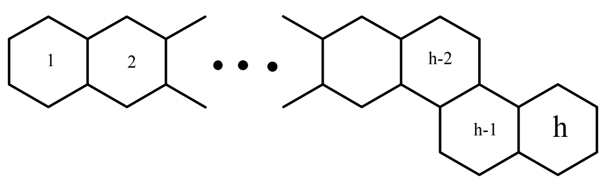

Figure 6. The Hexagonal System $L_h^{''}$.

Corollary 6. Let X be a catacondensed hexagonal system with h hexagons and $X \neq L_h, L'_h, L''_h$. Then $PI(L''_h) \leq PI(X)$.

Proof. The proof is similar to by Theorem 3 and Corollary 4. ■

We now define a transformation of type 2 for hexagonal systems. To do this, we assume that X is a catacondensed hexagonal system with h hexagons. Suppose L is a segment of maximum length which contains at least one terminal hexagon and Z is a zig-zag subgraph of X with the maximum number of hexagons. We omit a terminal hexagon of L and add a hexagon to Z to find a graph Z^1 such that Z^1 is still a zig-zag. The graph constructed from this transformation is denoted by X^1. It is obvious that if X is a zig-zag chain then $X^1 = X$. In Figure 7, this process is explained alternatively to construct graphs X^2, X^3 and X^4 from X.

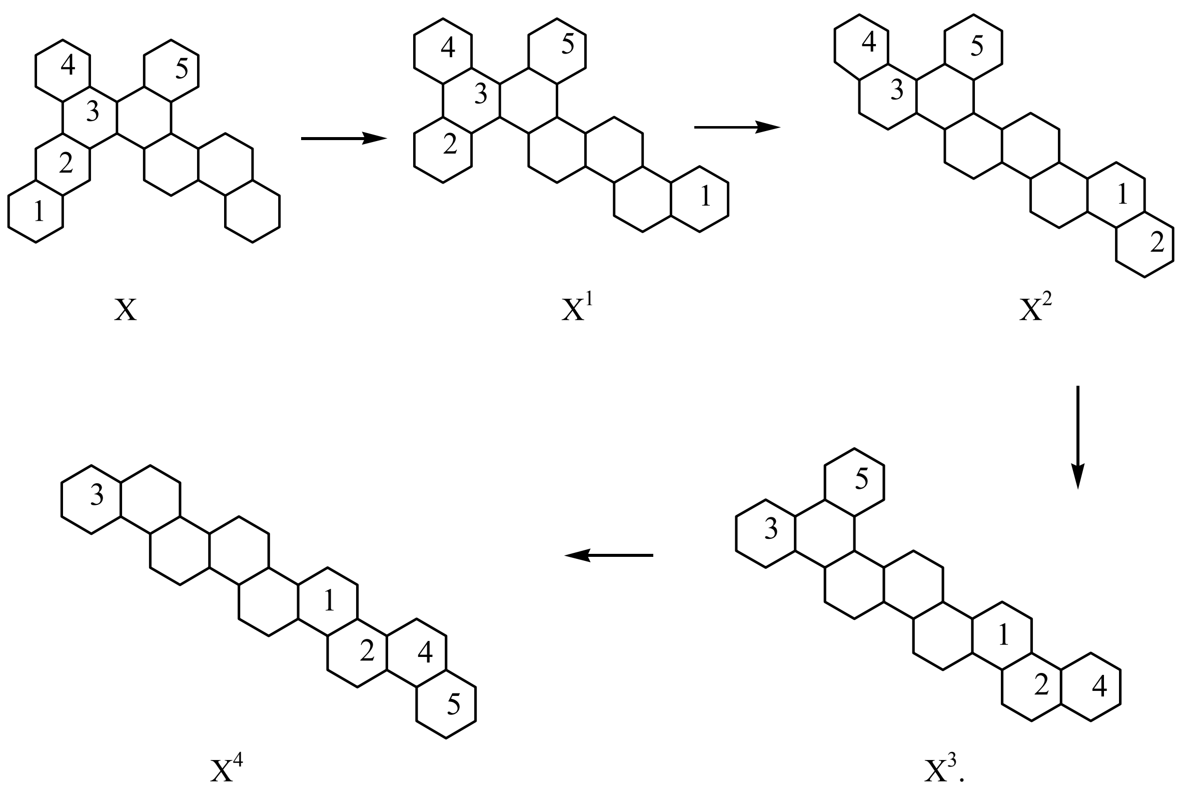

Figure 7. The Action of Transformations of Type 2 on X.

The following theorem and its corollaries are concluded by similar argument as Theorem 3 and its corollaries.

Theorem 6. Let X be a catacondensed hexagonal system with h hexagons and $X \neq Z_h$ and X_1 be a hexagonal system which is instructed by a transformation of type 2. Then, $PI(X) < PI(X^1)$.

Proof. The proof is similar to Theorem 3 and so omitted. ■

Corollary 7. Let *X* be a catacondensed hexagonal system with *h* hexagons and $X \neq Z_h$. Then $PI(X) < PI(Z_h)$.

Suppose h is an odd positive integer. A semi zig-zag chain $Z_h^{'}$ with *h* hexagons is a catacondensed system with exactly one segment of length 3 other segments have length 1 or 2. For even h, a semi zig-zag chain is assumed to be a catacondensed system with exactly two segments of length 3 and other segments have length 1 or 2. We denote the family of semi zig-zag chains, by $\hat{Z}_h$.

Corollary 8. Let $X \neq Z_h$ be a catacondensed hexagonal system containing *h* hexagons. Then $PI(X) < PI(Z_h^{'})$, with equality if and only if *X* is an element of $\hat{Z}_h$.

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