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Extremal catacondensed hexagonal systems with respect to the PI index

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Abstract

The PI index is a graph invariant defined as the summation of the sums of $n_1(e)$ and $n_2(e)$ over all the edges $e = uv$ of a connected graph G, i.e.,

$$PI(G) = \sum_{e \in E(G)} [n_1(e) + n_2(e)]$$

where $n_1(e)$ is the number of edges of G lying closer to u than to v and $n_2(e)$ is the number of edges of G lying closer to v than to u. A formula for calculating the PI index of catacondensed hexagonal systems is given from the structural parameters. Using the result, the catacondensed hexagonal systems with the minimum and maximum PI index are determined.

1 Induction

The first reported use of a topological index in chemistry was by Wiener [1] in the study of paraffin boiling points. Since then, in order to model various molecular properties, many topological indices have been designed [2]. Such a proliferation is still going on and is becoming counter productive.

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In 1990s, Gutman [3] and coworkers [4] have introduced a generalization of the Wiener index (W) for cyclic graphs called Szeged index (Sz). The main advantage of the Szeged index is that it is a modification of W for cyclic graphs; otherwise, it coincides with the Wiener index. In a attempt to remove this lacuna, [5-6] introduced another topological index PI, recently.

The method for the calculation of PI indices for hexagonal chains was also introduced in [5].

The primary aims of this article are to introduce another method for calculating the PI indices of catacondensed hexagonal systems according to the lengths of their segments, and to determine the catacondensed hexagonal systems with minimum and maximum PI index.

2 Catacondensed hexagonal systems

Hexagonal systems are of great importance for theoretical chemistry because they are the molecular graphs (or, more precisely, the graphs representing the carbon-atom skeleton) of benzenoid hydrocarbons. The mathematical theory of hexagonal systems is nowadays being greatly expanded.

Our standard reference for any terminology of hexagonal systems is [7].

A hexagonal system [7] is a connected plane graph without cut-vertices in which all inner faces are hexagons (and all hexagons are faces), such that two hexagons are either disjoint or have exactly one common edge, and no three hexagons share a common edge.

The hexagonal systems are divided [7] into catacondensed and pericondensed hexagonal systems. In a pericondensed hexagonal system there exist three hexagons share a common vertex; In catacondensed hexagonal systems no three hexagons share a common vertex. The set of all catacondensed hexagonal systems with h hexagons is denoted by CHS_h.

Catacondensed hexagonal systems are further classified into non-branched (in which no hexagon has more than two neighboring hexagons) and branched (in which at least one hexagon has three neighboring hexagons). A catacondensed hexagonal system without branched hexagons is called a hexagonal chain. The set of all hexagonal chains with h hexagons is denoted by HC_h.

The linear chain L_h [7] with h hexagons is the catacondensed hexagonal system without kinks (see Figure 1), where the kinks are the are branched or angularly connected hexagons (see the page 252 in [7]).

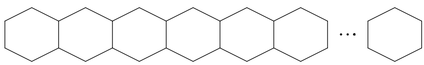

Figure 1. A linear chain L_h.

Fibonacene chains (including helicene chains) [5,7] are the hexagonal chains in which all hexagons, apart from the two terminal ones, are angularly connected, for instance, the graphs G_1, G_2 and G_3 of Figure 2.

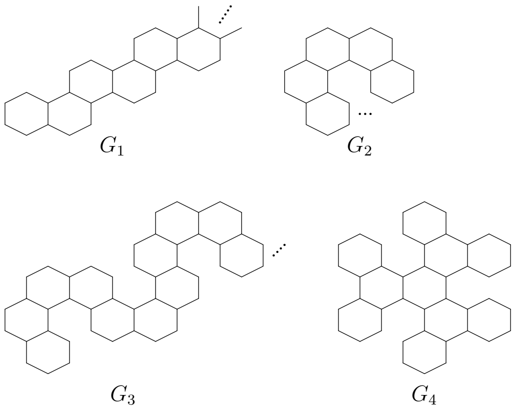

Figure 2. Some full kinks hexagonal systems.

Full kink catacondensed hexagonal systems are the catacondensed hexagonal systems in which all hexagons, apart from the terminal ones, are kinks (angularly connected or branched hexagons), for instance, all the graphs of Figure 2. Clearly, all the Fibonacene chains are full kink catacondensed hexagonal systems.

A segment [7] is a maximal linear chain in a catacondensed hexagonal system, including the kinks and/or terminal hexagons at its end. The number of hexagons in a segment S is called its length and is denoted by $l(S)$. For any segment S of $G \in CHS_h$, $2 \leq l(S) \leq h$. Particularly, a catacondensed hexagonal system is a full kink catacondensed hexagonal system if and only if the lengths of its segment are all equal to 2.

3 PI index

Let G be a connected and undirected graph without multiple edges or loops. By $V(G)$ and $E(G)$ we denote the vertex and edge sets, respectively, of G.

If $G' = (V', E')$ is a subgraph of $G = (V, E)$ and contains all the edges of G that join two vertices in V', then G' is an induced subgraph of G by V' and is denoted by $G[V']$.

Let $e = xy$ be an edge of G, X is the subset of vertices of $V(G)$ which are closer to x than y and Y is the subset of vertices which are closer to y than x, i.e.,

$$X = \{v|v \in V(G), d_G(x,v) < d_G(y,v)\}$$
$$Y = \{v|v \in V(G), d_G(y,v) < d_G(x,v)\}$$

where $d_G(u,v)$ denotes the distance between vertices u and v of G. Let $G[X] = (X, E_1)$ and $G[Y] = (Y, E_2)$,

$$n_1(e) = |E_1|, \qquad\qquad n_2(e) = |E_2|$$

Here, $n_1(e)$ is the number of edges nearer to x than y and $n_2(e)$ is the number of edges nearer to y than x.

Then the PI index of G is defined as

$$PI(G) = \sum_{e \in E(G)} [n_1(e) + n_2(e)]$$

In all case of cyclic graphs, there are edges equidistant to the both ends of the edges. Such edges are not taken into account.

4 A formula for calculating the PI indices of catacondensed hexagonal systems

A catacondensed hexagonal system $G \in CHS_h$ consists of a sequence of segments $S_1, S_2, \cdots, S_n$, $n \geq 1$, with lengths $l(S_i) = l_i$, $i = 1, 2, \cdots, n$, where $l_1 + l_2 + \cdots + l_n = h + n - 1$ since two neighboring segments have always one hexagon in common. Then the PI index of G may be calculated from these structural parameters.

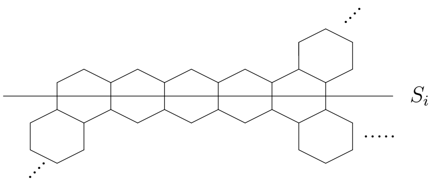

Figure 3.

Theorem 1. Let G be a catacondensed hexagonal system with h hexagons and consisting of n segments of lengths $l_1, l_2, \cdots, l_n$, $n \geq 1$. Then

$$PI(G) = 25h^2 + n - 1 - \sum_{i=1}^{n} l_i^2.$$

Proof. From the definition of $PI(G)$ and the Figure 3, we observe that for any edge e which the straight line S_i cuts across, where the straight line S_i passes through the segment of length l_i. Such edges will be l_i+1 in numbers and the contribution of such edges to $PI(G)$ will be

$$n_1(e)+n_2(e)=(5h+1)-(l_i+1)=5h-l_i$$

$i=1,2,\cdots,n$, where $5h+1$ is the number of edges in G. And the other edges will be $(5h+1)-(l_1+l_2+\cdots+l_n+n)=4h-2n+2$ in numbers. Each of them will contribute

$$n_1(e)+n_2(e)=(5h+1)-2=5h-1$$

to $PI(G)$. Therefore, the sum of the contributions of all the edges will give the PI index for G

$$\begin{aligned} PI(G) &= \sum_{i=1}^{n}(5h-l_i)(l_i+1)+(5h-1)(4h-2n+2) \\ &= 5h\sum_{i=1}^{n}(l_i+1)-\sum_{i=1}^{n}l_i^2-\sum_{i=1}^{n}l_i+(5h-1)(4h-2n+2) \\ &= 5h(h+2n-1)-\sum_{i=1}^{n}l_i^2-(h+n-1)+(5h-1)(4h-2n+2) \\ &= 25h^2+n-1-\sum_{i=1}^{n}l_i^2. \end{aligned}$$

Particularly, if $n=1$ and $l_1=h$, then $G=L_h$ is the linear chain with h hexagons.

Corollary 2([5]). $PI(L_h)=24h^2$.

If $n=h-1$, $l_1=l_2=\cdots=l_n=2$ and G has no branched hexagons, then G is a Fibonacene chain.

Corollary 3([5]). For a Fibonacene chain G with h hexagons,

$$PI(G)=25h^2-3h+2.$$

5 Extremal catacondensed hexagonal systems with respect to the PI index

In this section, we specify the extremal elements in catacondensed hexagonal systems with respect to the PI index.

Theorem 2. For any catacondensed hexagonal system G with h hexagons and any full kink catacondensed hexagonal system F_h with h hexagons,

(i) $PI(G)\le PI(F_h)$ with the equality if and only if G is also a full kink catacondensed hexagonal system;

(ii) $PI(G) \geq PI(L_h)$ with the equality if and only if $G = L_h$.

Proof. (i) Note that F_h consists of $h-1$ segments of length 2, by Theorem 1, we have

$$PI(F_h) = 25h^2 + (h-1) - 1 - 4(h-1)^2 = 25h^2 - 3h + 2.$$

Let G be a catacondensed hexagonal system consisting of n segments of lengths $l_1, l_2, \cdots, l_n$, where $l_1 + l_2 + \cdots + l_n = h + n - 1$ and $l_i \geq 2$, $i = 1, 2, \cdots, n$. Then

$$PI(G) = 25h^2 + n - 1 - \sum_{i=1}^{n} l_i^2$$

by Theorem 1. From Jensen's Inequality with $f(x) = x^2$ (or Root Mean Square-Arithmetic Mean Inequality), we have

$$\frac{l_1^2 + l_2^2 + \cdots + l_n^2}{n} \geq (\frac{l_1 + l_2 + \cdots + l_n}{n})^2,$$

then

$$l_1^2 + l_2^2 + \cdots + l_n^2 \geq \frac{1}{n}(h+n-1)^2 = n + (h-1)^2\frac{1}{n} + 2(h-1).$$

Let $f(n) = n + (h-1)^2\frac{1}{n} + 2(h-1)$, $1 \leq n \leq h-1$, we have

$$f(n) \geq f(h-1) = 4(h-1)$$

since $f'(h-1) = 0$ and $f''(h-1) > 0$. And

$$l_1^2 + l_2^2 + \cdots + l_n^2 \geq 4(h-1)$$

with the equality if and only if $n = h-1$ and $l_1 = l_2 = \cdots = l_n = 2$. So,

$$\begin{aligned} PI(F_h) - PI(G) &= (25h^2 - 3h + 2) - (25h^2 + n - 1 - \sum_{i=1}^{n} l_i^2) \\ &= \sum_{i=1}^{n} l_i^2 - n - 3h + 3 \\ &\geq \sum_{i=1}^{n} l_i^2 - 4(h-1) \qquad \text{(since } n \leq h-1) \\ &\geq 0 \end{aligned}$$

with the equality if and only if $n = h-1$ and $l_1 = l_2 = \cdots = l_n = 2$, i.e., G is a full kink catacondensed hexagonal system.

(ii) For any positive real numbers $x, y \geq 2$, we have $(x-1)(y-1) \geq 1$, i.e., $xy - (x+y) \geq 0$. If $n > 1$, then

$$\begin{aligned} & [l_1^2 + l_2^2 + \cdots + l_n^2] - [l_1^2 + \cdots + l_{n-2}^2 + (l_{n-1} + l_n - 1)^2] \\ = \; & 2(l_{n-1} + l_n) - 2l_{n-1}l_n - 1 < 0 \end{aligned}$$

and

$$\begin{aligned} l_1^2 + l_2^2 + \cdots + l_n^2 &< l_1^2 + \cdots + l_{n-2}^2 + (l_{n-1} + l_n - 1)^2 \\ &< l_1^2 + \cdots + l_{n-3}^2 + (l_{n-2} + l_{n-1} + l_n - 2)^2 \\ &< \cdots \\ &< (l_1 + l_2 + \cdots + l_n - n + 1)^2 = h^2. \end{aligned}$$

$$\begin{aligned} PI(L_h) - PI(G) &= 24h^2 - (25h^2 + n - 1 - \sum_{i=1}^{n} l_i^2) \\ &= \sum_{i=1}^{n} l_i^2 - h^2 - n + 1 \\ &\leq \sum_{i=1}^{n} l_i^2 - h^2 \qquad \text{(since } n \geq 1) \\ &\leq 0 \end{aligned}$$

with the equality if and only if $n = 1$, i.e., $G = L_h$.

This result shows that the linear chain L_h is the unique catacondensed hexagonal system with the minimum PI index, and the full kink catacondensed hexagonal systems F_h are the catacondensed hexagonal systems with the maximum PI index among all the catacondensed hexagonal systems with h hexagons. Since $HC_h \subseteq CHS_h$ and the Fibonacene chains are also the full kink catacondensed hexagonal systems, the linear chain L_h is the unique hexagonal chain with the minimum PI index, and the Fibonacene chains are the hexagonal chains with the maximum PI index among all the hexagonal chains with h hexagons.

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