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The PI index of phenylenes

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The Padmakar–Ivan (PI) index is a graph invariant defined as the summation of the sums of $n_{eu}(e|G)$ and $n_{ev}(e|G)$ over all the edges $e = uv$ of a connected graph G, i.e., $\mathrm{PI}(G) = \sum_{e\in E(G)}[n_{eu}(e|G) + n_{ev}(e|G)]$, where $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v and $n_{ev}(e|G)$ is the number of edges of G lying closer to v than to u. An efficient formula for calculating the PI index of phenylenes is given, and a simple relation is established between the PI index of a phenylene and of the corresponding hexagonal squeeze.

KEY WORDS: PI index, phenylene, hexagonal squeeze

1. Introduction

The structure of a molecule could be represented in a variety of ways. The information on the chemical constitution of molecule is conventionally represented by a molecular graph. And graph theory was successfully provided the chemist with a variety of very useful tools, namely, topological index. 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.

In 1990s, Gutman and coworkers [3,4] 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; otherwise, it coincides with the Wiener index. In [5,6], another topological index was introduced and it was named Padmakar–Ivan index, abbreviated as PI. This new topological index, PI, does not coincide with the Wiener index. Deng [7] gave a formula for calculating the PI index of catacondensed hexagonal systems and the extremal catacondensed hexagonal systems with the minimum or maximum

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PI index. Ashrafi and Loghman [8] computed the PI index of zig–zag polyhex nanotubes. Deng [9] computed the PI index of $TUVC_6[2p, q]$.

The primary aim of this article is to introduce the method for calculation of PI index for phenylenes.

2. Phenylenes and their hexagonal squeezes

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. Their respective molecular graphs are also referred to as phenylenes.

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 [10]. 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 PH 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 PH and its HS is shown in figure 1.

For PHs and their HS, some results related to the mathematical properties of Wiener index, Randić index and the second-order Randić index have been reported in the literature [10–12]. In the next section, we will give a formula for calculating the PI index of PHs and establish a simple relation between the PI index of a PH and of the corresponding HS.

3. The PI index of phenylenes

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', i.e., E' is the set of edges between vertices of 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.,

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

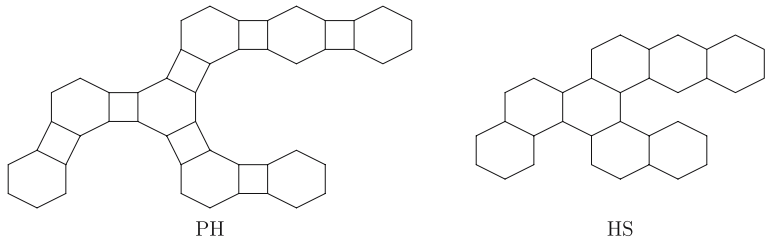

Figure 1. A phenylene (PH) and its hexagonal squeeze (HS).

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

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

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

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

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

For calculating the PI index of a PH, we introduce some conceptions in a PH analogously in a hexagonal system. The linear chain PH is a PH without kinks (see figure 2), where the kinks are the branched or angularly connected hexagons. A segment of a PH is a maximal linear chain in the PH, 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 a PH, $2 \leqslant l(S) \leqslant h$. Particularly, a PH is a full kink one if and only if the lengths of its segment are all equal to 2.

A PH consists of a sequence of segments $S_1, S_2, \ldots, S_n$, $n \geqslant 1$, with lengths $l(S_i) = l_i$, $i = 1, 2, \ldots, n$, 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 PH may be calculated from these structural parameters.

Theorem 1. Let PH be a phenylene with h hexagons and consisting of n segments of lengths $l_1, l_2, \ldots, l_n$, $n \geqslant 1$. Then

$$\mathrm{PI}(\mathrm{PH}) = 64h^2 - 44h + 4n + 4 - 4\sum_{i=1}^{n} l_i^2.$$

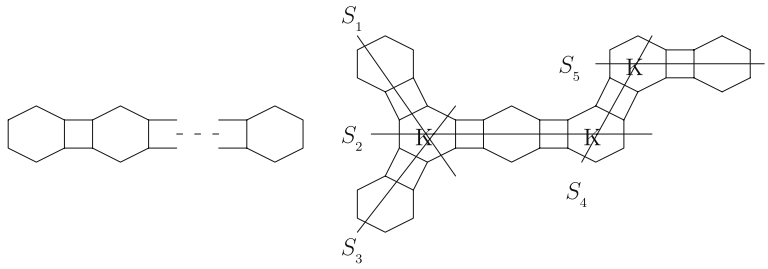

Figure 2. A linear chain phenylene, kinks, and segments of a phenylene.

Proof. From the definition of PI(PH) and figure 2, 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 $2l_i$ in numbers and the contribution of such edges to PI(PH) will be

$$n_1(e) + n_2(e) = (8h - 2) - 2l_i$$

$i = 1, 2, \ldots, n$, where $8h - 2$ is the number of edges in PH. And the other edges will be $(8h - 2) - 2(l_1 + l_2 + \cdots + l_n) = 6h - 2n$ in numbers. Each of them will contribute

$$n_1(e) + n_2(e) = (8h - 2) - 2 = 8h - 4$$

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

$$\begin{aligned} \mathrm{PI(PH)} &= \sum_{i=1}^{n} 2l_i(8h - 2 - 2l_i) + (6h - 2n)(8h - 4) \\ &= 64h^2 - 44h + 4n + 4 - 4\sum_{i=1}^{n} l_i^2. \end{aligned}$$

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

Corollary 2 [5]. For the linear chain phenylene PH with h hexagons,

$$\mathrm{PI(PH)} = 60h^2 - 44h + 8.$$

If $n = h - 1$, $l_1 = l_2 = \cdots = l_n = 2$, then PH is a full kink phenylene.

Corollary 3. For a full kink phenylene PH with h hexagons,

$$\mathrm{PI(PH)} = 64h^2 - 56h + 16.$$

4. Bounds for the PI indices of phenylenes

In this section, we give the bounds of the PI indices of phenylenes.

Theorem 4. For any phenylene PH with h hexagons,

$$60h^2 - 44h + 8 \leqslant \mathrm{PI}(\mathrm{PH}) \leqslant 64h^2 - 56h + 16$$

with the left (right) equality if and only if PH is a linear chain (a full kink) phenylene.

Proof. (i) Let PH be a PH consisting of n segments of lengths $l_1, l_2, \ldots, l_n$, where $l_1 + l_2 + \cdots + l_n = h + n - 1$ and $l_i \geqslant 2$, $i = 1, 2, \ldots, n$. Then

$$\mathrm{PI}(\mathrm{PH}) = 64h^2 - 44h + 4n + 4 - 4\sum_{i=1}^{n} l_i^2$$

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

$$\frac{l_1^2 + l_2^2 + \cdots + l_n^2}{n} \geqslant \left(\frac{l_1 + l_2 + \cdots + l_n}{n}\right)^2$$

then

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

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

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

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

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

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

$$\begin{aligned}\mathrm{PI}(\mathrm{PH}) &= 64h^2 - 44h + 4n + 4 - 4\sum_{i=1}^{n} l_i^2 \\ &\leqslant 64h^2 - 44h + 4n + 4 - 16(h-1) \\ &\leqslant 64h^2 - 56h + 16 \qquad (\text{since } n \leqslant h-1)\end{aligned}$$

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

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

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

and

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

$$\begin{aligned}\mathrm{PI(PH)} &= 64h^2 - 44h + 4n + 4 - 4\sum_{i=1}^{n} l_i^2 \\ &\geqslant 64h^2 - 44h + 4n + 4 - 4h^2 \qquad (\text{since } n \geqslant 1) \\ &\geqslant 60h^2 - 44h + 8\end{aligned}$$

with the equality if and only if $n = 1$, i.e., PH is a linear chain PH.

This result shows that the linear chain PH is the unique PH with the minimum PI index, and the full kink PH are the PHs with the maximum PI index among all the PHs.

5. A relation of the PI index between PH and HS

In the following, we establish a relation between the PI index of a PH and of the corresponding HS.

Let G be a catacondensed hexagonal system with h hexagons and consisting of n segments of lengths $l_1, l_2, \ldots, l_n$, $n \geqslant 1$, Deng [7] proved that

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

For the HS of a PH, HS may be jammed (which possesses lagoons), it is easy to see that the equation above also holds for HS.

Comparing with theorem 1, we have

Theorem 5. Let PH be a phenylene with h hexagons and HS its hexagonal squeeze. Then

$$\mathrm{PI(PH)} = 4\mathrm{PI(HS)} - 36h^2 - 44h + 8.$$

Acknowledgments

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