PI Index of Some Simple Pericondensed Hexagonal Systems

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Abstract: The Padmakar-Ivan (PI) index is a Wiener-Szeged-like topological index which reflects certain structural features of organic molecules. In this paper we study the problem of PI index with respect to some simple pericondensed hexagonal systems and we solve it completely.
Keywords: PI index, Organic molecule, Pericondensed hexagonal system.

1. Introduction

Wiener index (W) and Szeged index (Sz) are introduced to reflect certain structural features of organic molecules [1-6]. [7, 8] introduced another index called Padmaker-Ivan (PI) index. PI index is a very useful number in chemistry, as demonstrated in literature [8-16]. In [8] authors studied the applications of PI index to QSRP/QSAR. It turned out that the PI index has a similar discriminating function as Wiener index and Szeged index, sometimes it gave better results. Hence, PI index as a topological index is worth studying. In [9] authors pointed out that PI index is superior to ^0X, ^2X and logP indices for modeling Tadpole narcosis. In [10] the authors reported quantitative structure—toxicity relationship (QSTR) study by using the PI index. They have used 41 monosubstituted nitrobenzene for this purpose. The results have shown that the PI index alone is not an appropriate index for modeling toxicity of nitrobenzene derivatives. Combining PI index with other distance-based topological indices resulted in statistically significant models and excellent results were obtained in pentaparametric models. For the previous results about PI index, please see [17, 18, 19].

Let G be a simple connected graph. The PI index of graph G is defined as follows:

$$PI(G) = \sum[n_{eu}(e|G) + n_{ev}(e|G)],$$

where for edge e = uv $n_{eu}(e|G)$ is the number of edges of G lying closer to u than v, $n_{ev}(e|G)$ is the number of edges of G lying closer to v than u and summation goes over all edges of G. The edges which are equidistant from u and v are not considered for the calculation of PI index [18]. In the following we write n_{eu} instead of $n_{eu}(e|G)$.

2. Preliminaries

For further details, please see [20, 21]. Benzenoid hydrocarbons possess intriguing (and somewhat mysterious) electronic properties and have been attracting the interest of theoretical chemists over 150 years. In addition, they are important raw materials of the chemical industry (used, for instance, for the production of dyes and plastics), but are also dangerous pollutants. Around 1000 distinct benzenoid hydrocarbons are known, some of which consist of more than 100 hexagons. Benzenoid hydrocarbons are hexagonal systems [22].

A 6-cycle will be referred to as *a hexagon.* A *hexagonal system* 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 sets of all hexagonal systems and of all hexagonal systems with h hexagons are denoted by HS and HS_h, respectively [22].

Hexagons sharing a common edge are said to be *adjacent.* Two hexagons of a hexagonal system may have either two common vertices (if they are adjacent) or none (if they are not adjacent). A vertex of a hexagonal system belongs to, at most, three hexagons. A vertex shared by three hexagons is called an *internal vertex* of the respective hexagonal system. The number of internal vertices is denoted by n_i [22].

A hexagonal system is said to be *catacondensed* if it does not possess internal vertices ($n_i = 0$). The sets of all catacondensed hexagonal systems and of all catacondensed hexagonal systems with h hexagons are denoted by CHS and CHS_h, respectively. A hexagonal system is said to be *pericondensed* if it possesses at least one internal vertices ($n_i > 0$) [22].

A hexagonal system is said to be *simple* if it can be embedded into the regular lattice in the plane without overlapping of its vertices. Hexagonal systems that are not simple are called *jammed* [22].

A hexagon r of a catacondensed hexagonal system has either one, two or three neighboring hexagons. If r has one neighboring hexagon, it is said to be *terminal,* and if it has three neighboring hexagons, to be *branched.* Hexagons being adjacent to exactly two other hexagons are classified as angularly or linearly connected (mode A or L). A hexagon r adjacent to exactly two other hexagons possesses two vertices of degree 2. If these two vertices are adjacent, r is *angularly connected,* for short we say that r is *of mode A.* If these two vertices are not adjacent, r is *linearly connected,* and we say that r is *of mode L* [22].

Each branched and angularly connected hexagon in a catacondensed hexagonal system is said to be a *kink,* in contrast to the terminal and linearly connected hexagons. In Figure 1 the kinks are marked by K [22].

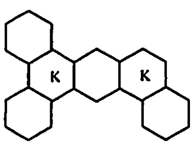

Figure 1

The *linear chain* L_h with h hexagons is the catacondensed system without kinks. (Thus, for $h \geq 2$, L_h possesses two terminal and $h-2$ L-mode hexagons) [22].

Let GL_h be the hexagonal system contains L_h and the *h*th hexagon is adjacent to both *i*th and *(i + 1)*th hexagons of L_{h-1}, where $h \geq 3$, $i \in \{1, 2, \ldots, h-2\}$.

A *segment* is a maximal linear chain in a catacondensed hexagonal system, including the kinks and/or terminal hexagons at its end. A segment including a terminal hexagon is a *terminal segment.* The number of hexagons in a segment S is called *its length* and is denoted by l(S). For any segment S of $G \in CHS_h$, $2 \leq l(S) \leq h$. We say that G consists of the set of segments $S_1, S_2, \ldots, S_h$ with length $l(S_i) = l_i$ for some $n \geq 1$ [22]. For example, in Figure 1 there are one segment with length 3 and three segments with lengths 2, respectively.

We generalize the definitions of segment and kink to simple pericondensed hexagonal system with $n_i = 1$.

Let r be a hexagon of G. *Deletion r from G* means we delete the edges of r which are not shared by other hexagons of G. Let G be a simple pericondensed hexagonal system with $n_i = 1$. We say a hexagon r is a *special hexagon* of G if r is deleted from G, there is no internal vertex in the remaining hexagonal systems.

Thus, we obtain some catacondensed hexagonal systems. Since $n_i = 1$, when we delete r from G, we obtain at most two catacondensed hexagonal systems $G^{'}$ and $G^{''}$. Otherwise, $n_i \geq 2$, which is a contradiction. Note that the special hexagon of G may not be unique. However, in the following when we say *spcial hexagon* r of G we mean r is a fixed special hexagon.

A *segment* is a maximal linear chain in a pericondensed hexagonal system with $n_i = 1$. The number of hexagons in a segment S is called its *length* and is denoted by l(S). For any segment S of G, $2 \leq l(S) \leq h - 1$.

We say that G consists of the set of segments S_1, S_2, ..., S_n with lengths $l(S_1) = l_1$, $l(S_2) = l_2$, ..., $l(S_n) = l_n$, respectively, $n \geq 3$. For example, in GL_h there are one segment with length $h - 1$ and two segments with lengths 2 respectively.

A catacondensed hexagonal system is *a full kink catacondensed hexagonal system* if and only if the lengths of its segments are all equal to 2 [23].

Let G be a full kink catacondensed hexagonal system with at least three hexagons. Adding a new hexagon r to G, if we obtain a simple pericondensed hexagonal system with a unique segment with length 3, the lengths of the remaining segments are all equal to 2 and $n_i = 1$, *SF* denotes the new simple pericondensed hexagonal system with $n_i = 1$.

Graph G is called a *strongly codistance graph* (briefly, *sco graph)* if and only if the edge relation "*sco*" is an equivalence relation for subset C = C(e) of E = E(G). In such a graph G if e# ∈ C(e) we have C(e#) = C(e). The set C(e) is called an *orthogonal cut* with respect to edge e of G. For an sco graph G the edge set E = E(G) is the union of pairwise disjoint equivalence classes of orthogonal cuts $C_j = C_j(G)$, j = 1, 2, ..., k, of graph G. Let $m_j = |C_j|$ the number of edges of orthogonal cut C_j [18].

2. Main Results

Lemma 3.1[18]. $$PI(G) = m^2 - \sum_{j=1}^{k} m_j^2,$$

where m is the number of edges of G, m_j is the edge number of orthogonal cut C_j.

Theorem 3.2. Let G be a simple pericondensed hexagonal system with $n_i = 1$, h hexagons and consisting of n segments $S_1, S_2, ..., S_n$ with lengths $l_1, l_2, ..., l_n$, respectively, $h \geq 3$. Then

$$PI(G)=25h^2+n-10h-\sum_{i=1}^{n} l_i^2.$$

Proof. Let m_i be the number of edges of orthogonal cut C_i defined in Lemma 3.1 and l_i be the length of segment S_i. When $l_i \geq 2$, we have $m_i = l_i + 1$. Let r be a special hexagon of G defined in section 2.

Case 1. When we delete r from G, we obtain a catacondensed hexagonal system G'. By the definition of catacondensed hexagonal system we have

$$|E(G')| = 5(h-1)+1.$$

Hence, we have

$$|E(G)| = m = 5h.$$

Case 2. When we delete r from G, we obtain two catacondensed hexagonal systems G' and G''.

Similar to Case 1 we have

$$|E(G)| = m = 5h.$$

Thus, the number of edges of G which are not contained by $S_1, S_2, \ldots, S_n$ is

$$5h-(l_1+l_2+\ldots+l_n+n).$$

Thus, the number of orthogonal cuts with $m_i = 2$ is

$$0.5\times[5h-(l_1+l_2+\ldots+l_n+n)].$$

By Lemma 3.1 we have

$$PI(G)=(5h)^2-\sum_{i=1}^{n}(l_i+1)^2-\frac{1}{2}[5h-(l_1+l_2+\ldots+l_n+n)]\times 4$$

$$=25h^2+n-10h-\sum_{i=1}^{n} l_i^2.$$

The theorem follows.

Theorem 3.3. Let G be any simple pericondensed hexagonal system with $n_i = 1$ and h hexagons. Then

(i).$PI(G) \geq PI(GL_h)$ with equality if and only if G is GL_h defined in section 2, $h \geq 3$.

(ii).$PI(G) \leq PI(SF_h)$ with equality if and only if G is SF_h defined in section 2, $h \geq 4$.

Proof. Claim 1: Let G be a simple pericondensed hexagonal system with $n_i = 1$, h hexagons and consisting of n segments $S_1, S_2, \ldots, S_n$ with lengths $l_1, l_2, \ldots, l_n$, $n \geq 3$, $h \geq 3$. Then $h = l_1 + l_2 + \ldots + l_n - n$.

Let r be a special hexagon of G.

Case 1. When we delete r from G, we obtain one catacondensed hexagonal system $G^{'}$. Let $G^{'}$ consist of m segments $S_1^{'}, S_2^{'}, \ldots, S_m^{'}$.

Subcase 1.1. m = n.

From [22] page 253 we have

$$\begin{aligned} h_{G^{'}} &= l(S_1^{'}) + l(S_2^{'}) + \ldots + l(S_m^{'}) - n + 1 \\ &= l(S_1) + l(S_2) + \ldots + l(S_n) - 2 - n + 1 \\ &= l_1 + l_2 + \ldots + l_n - n - 1. \end{aligned}$$

Since $h_G = h_{G^{'}} + 1$, we have

$$h = l_1 + l_2 + \ldots + l_n - n.$$

Similarly, we can prove Subcase 1.2 and Subcase 1.3.

Subcase 1.2. m = n – 1.

Subcase 1.3. m = n – 2.

Case 2. When we delete r from G, we obtain two catacondensed hexagonal systems $G^{'}$ and $G^{''}$.

Hence, we add r to $G^{'}$ and $G^{''}$ respectively, we obtain two hexagonal systems $G^{r'}$ and $G^{r''}$. By the definition of special hexagon, one of $G^{r'}$ and $G^{r''}$ is a pericondensed hexagonal system with $n_i = 1$, one of $G^{r'}$ and $G^{r''}$ is a catacondensed hexagonal system. Hence, let $G^{r'}$ be a pericondensed hexagonal system with $n_i = 1$ and $G^{r''}$ be a catacondensed hexagonal system.

Let the segments of $G^{r'}$ be $S_1^{r'}, S_2^{r'}, \ldots, S_x^{r'}$, let the segments of $G^{r''}$ be $S_1^{r''}, S_2^{r''}, \ldots, S_y^{r''}$. By Case 1 we have

$$h_{G^{r'}} = l(S_1^{r'}) + l(S_2^{r'}) + \ldots + l(S_x^{r'}) - x.$$

From [20] page 253 we have

$$h_{G^r} = l(S_1^{r''}) + l(S_2^{r''}) + \ldots + l(S_y^{r''}) - y + 1.$$

By the definition of special hexagon there exist i and j such that $S_i^{r'}$ and $S_j^{r''}$ share a common segment of G through special hexagon r. Without loss of generality, let i = x, j = y; By the definition of special hexagon $S_1^{r'}, S_2^{r'}, \ldots, S_{x-1}^{r'}, S_1^{r''}, S_2^{r''}, \ldots, S_{y-1}^{r''}$ are the segments of G and $l(S_x^{r'}) + l(S_y^{r''}) - 1$ is the length of one segment of G other than

$$l(S_1^{r'}), l(S_2^{r'}), \ldots, l(S_{x-1}^{r'}), l(S_1^{r''}), l(S_2^{r''}), \ldots, l(S_{y-1}^{r''}).$$

Hence, we have

$$n = x + y - 1,$$

$$\begin{aligned} h_G &= h_{G^{r'}} + h_{G^{r''}} - 1 \\ &= l(S_1^{r'}) + l(S_2^{r'}) + \ldots + l(S_{x-1}^{r'}) + l(S_1^{r''}) + l(S_2^{r''}) \\ &+ \ldots + l(S_{y-1}^{r''}) + [l(S_x^{r'}) + l(S_y^{r''})] - x - y + 1 - 1 \\ &= l_1 + l_2 + \ldots + l_{n-1} + l_n - n. \end{aligned}$$

Hence, Claim 1 follows. The following claim is obvious:

Claim 2: n = 3 if and only if

$$n^2 + 3n + 6 = \frac{n(n+1)^2}{n-1}.$$

Obviously, when n > 3 we have

$$n^2 + 3n + 6 > \frac{n(n+1)^2}{n-1}.$$

Obviously, when $n \geq 3$, $l_i \geq 2$, $l_j \geq 2$, and $i \neq j$, we have

$$nl_i - \frac{n(n+1)}{n-1} \geq 0,$$

$$(n-1)l_j - (n+1) \geq 0;$$

$$[nl_i - \frac{n(n+1)}{n-1}][(n-1)l_j - (n+1)] \geq 0,$$

$$n(n-1)l_i l_j + \frac{n(n+1)^2}{n-1} \geq n(n+1)(l_i + l_j),$$

$$n(n-1)l_i l_j + n^2 + 3n + 6 \geq n(n+1)(l_i + l_j),$$

$$l_i l_j + \frac{n^2+3n+6}{n(n-1)} \geq \frac{n+1}{n-1}(l_i + l_j),$$

$$l_i l_j + \frac{\frac{n^2+3n+6}{2}}{\frac{n(n-1)}{2}} \geq \frac{n+1}{n-1}(l_i + l_j),$$

$$\sum_{1 \leq i < j \leq n} l_i l_j + \frac{n^2+3n+6}{2} \geq (n+1)(l_1 + l_2 + \ldots + l_n),$$

$$2\sum_{1 \leq i < j \leq n} l_i l_j + n^2 + 3n + 6 \geq 2(n+1)(l_1 + l_2 + \ldots + l_n).$$

Since

$$\sum_{i=1}^{n} l_i^2 + 2\sum_{1 \leq i < j \leq n} l_i l_j = (l_1 + l_2 + \ldots + l_n)^2,$$

$$(l_1 + l_2 + \ldots + l_n)^2 - 2(n+1)(l_1 + l_2 + \ldots + l_n) + n^2 + 3n + 6 \geq \sum_{i=1}^{n} l_i^2,$$

$$(l_1 + l_2 + \ldots + l_n)^2 - 2n(l_1 + l_2 + \ldots + l_n) + n^2 + n - 2(l_1 + l_2 + \ldots + l_n) + 2n + 6 \geq \sum_{i=1}^{n} l_i^2,$$

$$(l_1 + l_2 + \ldots + l_n - n)^2 + n - 2(l_1 + l_2 + \ldots + l_n - n) + 6 \geq \sum_{i=1}^{n} l_i^2.$$

By Claim 1 we have

$$h^2 + n - 2h + 6 \geq \sum_{i=1}^{n} l_i^2.$$

By Theorem 3.2 we have

$$PI(G) = 25h^2 + n - 10h - \sum_{i=1}^{n} l_i^2,$$

$$PI(GL_h) = 24h^2 - 8h - 6,$$

$$PI(G) \geq PI(GL_h).$$

By Claim 2 $PI(G) = PI(GL_h)$if and only if $G = GL_h$. The first part follows.

Claim 3: $PI(SF_h) = 25h^2 - 13h - 2$.

In fact, By Claim 1 we have $h = 3 + 2(n - 1) - n$. Hence, we have $n = h - 1$.

By Theorem 3.2 we have

$$PI(SF_h) = 25h^2 + (h - 1) - 10h - [9 + 4(h - 2)]$$

$$=25h^2-13h-2.$$

By the definition of segment we have $l_i \geq 2$, where $i = 1, 2, \ldots, n$. Since $h \geq 4$, by the definition of simple pericondensed hexagonal system with $n_i = 1$ we know that there exists some $l_i \geq 3$, without loss of generality, let $l_n \geq 3$. Hence, we have

$$l_i-\frac{3}{2}\geq\frac{1}{2}, l_n-\frac{3}{2}\geq\frac{3}{2},$$

where $i = 1, 2, \ldots, n-1$. Thus, we have

$$(l_1-\frac{3}{2})^2+(l_2-\frac{3}{2})^2+\ldots+(l_n-\frac{3}{2})^2\geq\frac{n}{4}+2.$$

Claim 4: $(l_1-\frac{3}{2})^2+(l_2-\frac{3}{2})^2+\ldots+(l_n-\frac{3}{2})^2=\frac{n}{4}+2$ if and only of $l_1=2, l_2=2, \ldots, l_{n-1}=2, l_n=3$.

Claim 4 is clear. Hence, we have

$$(l_1-\frac{3}{2})^2+(l_2-\frac{3}{2})^2+\ldots+(l_n-\frac{3}{2})^2+2n-2-\frac{9n}{4}\geq 0,$$

$$\sum_{i=1}^{n} l_i^2-3(l_1+l_2+\ldots+l_n)+2n-2\geq 0,$$

$$n+3(l_1+l_2+\ldots+l_n)-3n+2\leq\sum_{i=1}^{n} l_i^2,$$

$$n+3(l_1+l_2+\ldots+l_n-n)+2\leq\sum_{i=1}^{n} l_i^2.$$

By Claim 1 we have

$$n+3h+2\leq\sum_{i=1}^{n} l_i^2,$$

$$25h^2+n-10h-\sum_{i=1}^{n} l_i^2\leq 25h^2-13h-2,$$

$$PI(G)\leq PI(SF_h).$$

By Claim 4 we know that $PI(G) = PI(SF_h)$ if and only if G is SF_h. The theorem follows.

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