PI Index of Extremal Simple Pericondensed Hexagonal Systems

Jianxiu Hao, LiLi He, Min Huang
College of Mathematics, Physics and Information Sciences,
Zhejiang Normal University, P. O. Box: 321004,
Jinhua, Zhejiang, P.R. China;E-mail: sx35@zjnu.cn

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 PI index with respect to the extremal simple pericondensed hexagonal systems and we solve it completely.

Keywords: PI index, Wiener index, 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 [8-14]. 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 see [15, 16, 17, 21].

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 [16]. In the following we write n_{eu} instead of $n_{eu}(e|G)$.

2. Preliminaries

For further details, please see [18, 19].

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 [20].

A 6-cycle will be referred to as *a hexagon.* A *hexagonal system* H 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[20].

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 [20].

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 ($n_i > 0$) [20].

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* [20].

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* [20].

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 [20].

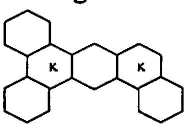

Figure 1

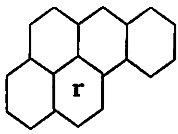

Figure 2.

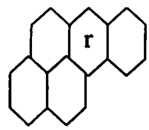

Figure 3.

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) [20].

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 h(S). For any segment S of H $\in CHS_h$, $2 \leq h(S) \leq h$. We say that H consists of the set of segments $S_1, S_2, \ldots, S_s$ with length $h(S_i) = h_i$ for some $s \geq 1$ [20]. For example, in Figure 1 there are one segment with length 3 and three segments with lengths 2, respectively.

In this paper we generalize the definition of segment to simple pericondensed hexagonal system with $n_i = 2$.

Let r be a hexagon of H. *Deletion r from H* means we delete the edges of r which are not shared by other hexagons of H.

Let H be a simple pericondensed hexagonal system with $n_i = 2$. We say a hexagon r is a *special hexagon* of H if r is deleted from H, in the remaining hexagonal systems there is no internal vertex or the number of internal vertices is 1. Hence, we say hexagons r_1 and r_2 are *special hexagons* of H if r_1 and r_2 are deleted from H, there is no internal vertex in the remaining hexagonal systems. However, if any one of r_1 and r_2 is deleted from H, there is one internal vertex in the remaining hexagonal systems. Note that the special hexagon of H may not be unique. However, in the following when we say *spcial hexagon* r of H we mean r is a fixed special hexagon of H.

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

We say that H consists of the set of segments $S_1, S_2, \ldots, S_s$ with lengths $h(S_1) = h_1, h(S_2) = h_2, \ldots, h(S_s) = h_s$, respectively, $s \ge 4$.

We define GL_h as follows: GL_h consists of L_{h-2} and two new hexagons r_1, r_2. Let r_1 be adjacent to both *i*th and *(i + 1)*th hexagons of L_{h-2}, let r_2 be adjacent to jth and (j + 1)th hexagons of L_{h-2}, $1 \le i \le j < h-2$. At last, let r_1 and r_2 share the same segment of GL_h, where $h \ge 5$, $i \in \{1, 2, \ldots, h-4\}$. In GL_h there are four segments: one segment with length h – 2, two segments with lengths 2 and one segment with length 3, respectively.

Define SF as follows: Let H be a simple pericondensed hexagonal system with $n_i = 2$ and h hexagons. If the length of one segment is 3 and the lengths of remaining segments are 2, G is called SF, where $h \ge 5$.

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 $e\# \in C(e)$ 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 [16].

3. Main Results

Lemma 3.1[16].
$$PI(G) = m^2 - \sum_{j=1}^{k} m_j^2,$$

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

Lemma 3.2[20]. (1). Every hexagonal system with h hexagons and n_i internal vertices has $m = 5h + 1 - n_i$ edges.

(2). Let H be a catacondensed hexagonal system, h be the number of hexagons in H, $S_1, S_2, \ldots, S_s$ be the segments of H, h_i be the number of hexagons of S_i, i = 1, 2, …, s, we have $h = h_1 + h_2 + \ldots + h_s - s + 1$.

Theorem 3.1. Let H be a simple pericondensed hexagonal system with $n_i = 2$, h hexagons and consist of s segments $S_1, S_2, \ldots, S_s$ with lengths $h_1, h_2, .., h_s$, respectively, $h \ge 4$. Then $PI(H) = 25h^2 + s + 3 - 20h - \sum_{i=1}^{s} h_i^2$.

Proof. Let m_i be the number of edges of orthogonal cut C_i defined in Lemma 3.1 and h_i be the length of segment S_i. When $h_i \geq 2$, we have $m_i = h_i + 1$. Thus, the number of edges of H which are not contained by orthogonal cuts stemmed from $S_1, \ldots, S_s$ is $(5h-1)-(h_1+\ldots+h_s)-s$. Thus, the number of orthogonal cuts with $m_i = 2$ is $0.5[(5h-1)-(h_1+\ldots+h_s)-s]$. By Lemma 3.1 and Lemma 3.2 we have

$$PI(H) = (5h-1)^2 - \sum_{i=1}^{s}(h_i+1)^2 - 0.5\times[(5h-1)-(h_1+h_2+\ldots+h_s+s)]\times 4.$$

The theorem follows.

Theorem 3.2. Let H be a simple pericondensed hexagonal system with $n_i = 2$ and h hexagons. Then

(i). $PI(H) \geq PI(GL_h)$ with equality if and only if H is GL_h, where GL_h is defined in section 2, $h \geq 5$.

(ii). $PI(H) \leq PI(SF_h)$ with equality if and only if H is SF_h, where SF_h is defined in section 2, $h \geq 5$.

Proof. Claim 1: Let H be a simple pericondensed hexagonal system with $n_i = 2$, h hexagons and consist of s segments $S_1, \ldots, S_s$ with lengths $h_1, \ldots, h_s$, respectively, $s \geq 4$, $h \geq 4$. Then $h = h_1 + \ldots + h_s - s - 1$.

In fact, we can prove Claim 1 as follows.

Case 1. H contains one special hexagon r which is defined in section 2.

Subcase 1.1. When we delete r from H, we obtain one component H'. See Figure 2. Obviously, H' is a catacondensed hexagonal system. Let H' consist of t segments $S_1^{'},\ldots,S_t^{'}$.

Subcase 1.1.1. $t = s$. By Lemma 3.2 we have

$$h_{H'} = h(S_1^{'}) + h(S_2^{'}) + \ldots + h(S_t^{'}) - t + 1$$
$$= h(S_1) + h(S_2) + \ldots + h(S_s) - 3 - s + 1$$
$$= h_1 + h_2 + \ldots + h_s - s - 2.$$

Since $h_H = h_{H'} + 1$, we have $h = h_1 + \ldots + h_s - s - 1$.

Similarly, we can discuss Subcase 1.1.2, Subcase 1.1.3 and Subcase 1.1.4.

Subcase 1.1.2. $t = s - 1$. Subcase 1.1.3. $t = s - 2$. Subcase 1.1.4. $t = s - 3$.

Subcase 1.2. When we delete r from H, we obtain two components H' and H^*. See Figure 3.

Hence, when we add r to H' and H^* respectively, we obtain two hexagonal systems $H^{r'}$ and H^{r^*}. By the definition of special hexagon, one of $H^{r'}$ and H^{r^*} is a pericondensed hexagonal system with $n_i = 2$, one of $H^{r'}$ and H^{r^*} is a catacondensed hexagonal system. Without loss of generality, let $H^{r'}$ be a pericondensed hexagonal system with $n_i = 2$, let H^{r^*} be a catacondensed hexagonal system.

Let the segments of $H^{r'}$ be $S_1^{r'}, S_2^{r'}, \ldots, S_x^{r'}$, let the segments of H^{r^*} be $S_1^{r^*}, S_2^{r^*}, \ldots, S_y^{r^*}$. By Case 1.1 we have

$$h_{H^{r'}} = h(S_1^{r'}) + h(S_2^{r'}) + \ldots + h(S_x^{r'}) - x - 1.$$

By Lemma 3.2 we have $h_{H^{r^*}} = h(S_1^{r^*}) + h(S_2^{r^*}) + \ldots + h(S_y^{r^*}) - y + 1.$

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 H through special hexagon r. 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 H and $h(S_x^{r'}) + h(S_y^{r^*}) - 1$ is the length of one segment of H other than $h(S_1^{r'}), h(S_2^{r'}), \ldots, h(S_{x-1}^{r'})$, $h(S_1^{r^*}), h(S_2^{r^*}), \ldots, h(S_{y-1}^{r^*})$. Hence, we have s = x + y − 1,

$$\begin{aligned}
h_H &= h_{H^{r'}} + h_{H^{r^*}} - 1 \\
&= h(S_1^{r'}) + h(S_2^{r'}) + \ldots + h(S_{x-1}^{r'}) + h(S_1^{r^*}) + h(S_2^{r^*}) + \ldots + h(S_{y-1}^{r^*}) \\
&\quad + [h(S_x^{r'}) + h(S_y^{r^*})] - x - 1 - y + 1 - 1 \\
&= h_1 + h_2 + \ldots + h_{s-1} + h_s - s - 1.
\end{aligned}$$

Case 2. H contains two special hexagons r_1 and r_2 sharing no common segment.

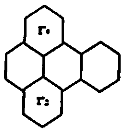

Figure 4.

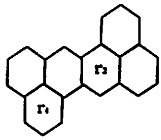

Figure 5.

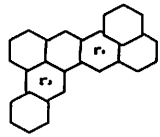

Figure 6.

Subcase 2.1. When we delete r_1 and r_2 from H, we obtain one component H'. See Figure 4.

Obviously, H' is a catacondensed hexagonal system. Let H' consist of t segments $S_1^{'},\ldots,S_t^{'}$.

Subcase 2.1.1. t = s.

Hence, r_1 is adjacent to two segments of H', so is r_2. Similarly, we have

$$\begin{aligned} h_{H'} &= h(S_1^{'})+h(S_2^{'})+\ldots+h(S_s^{'})-s+1 \\ &= h_1+h_2+\ldots+h_s-s-3. \end{aligned}$$

Since $h_H = h_{H'}+2$, we have $h = h_1 + \ldots + h_s - s - 1$.

Similarly, we can discuss Subcase 2.1.2—Subcase 2. 1. 5.

Subcase 2.1.2. t = s – 1, Subcase 2.1.3. t = s – 2, Subcase 2.1.4. t = s – 3,
Subcase 2.1.5. t = s – 4.

Like the proof of Case 1 we can prove Claim 2 as follows:

Claim 2: Let H be a simple pericondensed hexagonal system with $n_i = 1$, h hexagons and consist of s segments $S_1, \ldots, S_s$ with lengths $h_1, \ldots, h_s$, respectively, $s \geq 3$, $h \geq 3$. Then $h = h_1 + \ldots + h_s - s$.

Subcase 2.2. When we delete r_1 and r_2 from H, we obtain two components H' and H^{*}. See Figure 5.

Hence, when we add one of r_1 and r_2 to H' and H^{*} respectively, H' and H^{*} are connected. Without loss of generality, let H_1 be obtained by adding r_1 to connect H' and H^{*}. Let the segments of H_1 be $S_1^{1}, S_2^{1},\ldots,S_t^{1}$. Obviously, H_1 is a pericondensed hexagonal system with $n_i = 1$.

Subcase 2.2.1. t = s – 2.

Hence, when we add r_2 to H_1 we obtain two new segments with lengths 2.

Without loss of generality, let $h_{s-1} = 2$, $h_s = 2$. By Claim 2 we have

$$\begin{aligned} h_{H_1} &= h(S_1^1) + h(S_2^1) + \dots + h(S_{s-2}^1) - (s-2) \\ &= h_1 + h_2 + \dots + h_s - s - 2. \end{aligned}$$

Since $h_H = h_{H_1} + 1$, we have $h = h_1 + \dots + h_s - s - 1$.

Similarly, we can discuss Subcase 2.2.2, Subcase 2.2.3.

Subcase 2.2.2. $t = s - 1$, Subcase 2.2.3. $t = s$.

Subcase 2.3. When we delete r_1 and r_2 from H, we obtain three components H', H'' and H'''. See Figure 6.

Then, we add r_1 to H', H'' and H'''. Without loss of generality, let r_1 connect H' and H''. We denote the new graph H_1. Similarly, we add r_2 to H''' and we obtain a new graph H_2. When H_1 is a pericondensed hexagonal system with $n_i = 1$, H_2 is a catacondensed hexagonal system. Let the segments of H_1 be $S_1^1, S_2^1, \dots, S_x^1$, and the segments of H_2 be $S_1^2, S_2^2, \dots, S_y^2$. When both H_1 and H_2 are pericondensed hexagonal system with $n_i = 1$, we can discuss similarly.

Subcase 2.3.1. H_1 contains exactly one segment which is adjacent to r_2.

Without loss of generality, let the segment be S_x^1 which is adjacent to r_2. Let S_y^2 contain r_2.

Subcase 2.3.1.1. S_x^1 and S_y^2 do not share a common segment in H.

We have $s = x + y + 1$. Hence, $h_i = h(S_x^1)$, $h_j = h(S_y^2) + 1$, $h_p = 2$.

Without loss of generality, let $h_{s-2} = h(S_x^1)$, $h_{s-1} = h(S_y^2) + 1$, $h_s = 2$. By Claim 2 we have

$$\begin{aligned} h_{H_1} &= h(S_1^1) + h(S_2^1) + \dots + h(S_x^1) - x, \\ h_{H_2} &= h(S_1^2) + h(S_2^2) + \dots + h(S_y^2) - y + 1. \end{aligned}$$

$$\begin{aligned} h_H &= h_{H_1} + h_{H_2} \\ &= h(S_1^1) + h(S_2^1) + \dots + h(S_x^1) - x + h(S_1^2) + h(S_2^2) + \dots + h(S_y^2) - y + 1 \\ &= h_1 + h_2 + \dots + h_s - s - 1. \end{aligned}$$

Subcase 2.3.1.2. S_x^1 and S_y^2 share a common segment in H.

In fact, this case can not occur. Otherwise, both H_1 and H_2 are pericondensed hexagonal system with $n_i = 1$.

Similarly, we can discuss Subcase 2.3.2.

Subcase 2.3.2. H_1 contains two segments which are adjacent to r_2.

Case 3. H contains two special hexagons r_1 and r_2 which share a common segment.

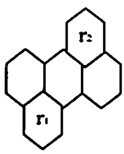

Figure 7.

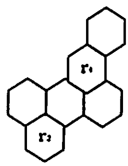

Figure 8.

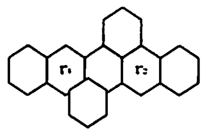

Figure 9.

Subcase 3.1. When we delete r_1 and r_2 from H, we obtain one component H'. See Figue 7.

Obviously, H' is a catacondensed hexagonal system. Let H' consist of t segments $S_1^{'}, \ldots, S_t^{'}$. Since $n_i = 2$ in H, r_1 and r_2 share a common segment, we have $t \geq s-3$. Otherwise, $n_i \geq 3$.

Subcase 3.1.1. $t = s - 3$.

Hence, there must be some $h_i = 2$, $h_j = 2$, $h_k = 3$. Without loss of generality, let $h_{s-2} = 2$, $h_{s-1} = 2$, $h_s = 3$. By Lemma 3.2 we have

$$\begin{aligned} h_{H'} &= h(S_1^{'}) + h(S_2^{'}) + \ldots + h(S_t^{'}) - t + 1 \\ &= h(S_1) + h(S_2) + \ldots + h(S_{s-3}) + (h(S_{s-2}) - 2) + (h(S_{s-1}) - 2) + (h(S_s) - 3) - s + 4 \\ &= h_1 + h_2 + \ldots + h_s - s - 3. \end{aligned}$$

Since $h_H = h_{H'} + 2$, we have $h = h_1 + h_2 + \ldots + h_s - s - 1$.

Similarly, we can discuss Subcase 3.1.2, Subcase 3.1.3.

Subcase 3.1.2. $t = s - 2$, Subcase 3.1.3. $t = s - 1$.

Subcase 3.2. When we delete r_1 and r_2 from H, we obtain two components H' and H^{*}. See Figure 8.

Then, we add one of r_1 and r_2 to H' and H^{*} respectively. Without loss of generality, let H_1 be obtained by adding r_1 to connect H' and H^{*}. Let the segments of H_1 be $S_1^1,\ldots,S_t^1$. Obviously, H_1 is a pericondensed hexagonal system with $n_i = 1$.

Subcase 3.2.1. $t = s - 1$.

Hence, when we add r_2 to H_1 we obtain a new segment with length 2. Without loss of generality, let $h_s = 2$. By Claim 2 we have

$$h_{H_1} = h(S_1^1) + h(S_2^1) + \ldots + h(S_{s-1}^1) - (s-1)$$
$$= h_1 + h_2 + \ldots + h_s - s - 2.$$

Since $h_H = h_{H_1} + 1$, we have $h = h_1 + h_2 + \ldots + h_s - s - 1$.

Similarly, we can discuss Subcase 3.2.2.

Subcase 3.2.2. $t = s$.

Subcase 3.3. When we delete r_1 and r_2 from H, we obtain three components H', H'' and H'''. See Figure 9.

Then, we add r_1 to H', H'' and H'''. Without loss of generality, let r_1 connect H' and H''. We denote the new graph H_1 obtained by connecting H' and H'' through r_1. Similarly, we add r_2 to H''' and we obtain a new graph H_2. Obviously, H_1 is a pericondensed hexagonal system with $n_i = 1$, H_2 is a catacondensed hexagonal system. Let the segments of H_1 be $S_1^1,\ldots,S_x^1$, and the segments of H_2 be $S_1^2,\ldots,S_y^2$.

Subcase 3.3.1. There exist S_i^1 and S_j^2 sharing a common segment of H.

Without loss of generality, let the two segments be S_x^1 and S_y^2, and

$h_{s-1} = h(S_x^1) + h(S_y^2)$.

Subcase 3.3.1.1. S_x^1 contains r_1.

Clearly, there is a new segment with length 2 in H through r_2. Without loss of generality, let $h_s = 2$. Then, we have $s = x + y$. By Claim 2 we have

$$h_{H_1} = h(S_1^1) + h(S_2^1) + \ldots + h(S_x^1) - x,$$

$$h_{H_2} = h(S_1^2) + h(S_2^2) + \ldots + h(S_y^2) - y + 1.$$

$$h_H = h_{H_1} + h_{H_2}$$
$$= h_1 + h_2 + \ldots + h_s - s - 1.$$

Subcase 3.3.1.2. S_x^1 does not contain r_1.

We can discuss Subcase 3.3.1.2 similarly, Claim 1 follows.

By Theorem 3.1 Claim 3 is obvious:

Claim 3: $PI(GL_h) = 24h^2 - 16h - 14$.

Claim 4: When $s \geq 5$, we have $PI(H) > PI(GL_h)$.

Obviously, when $s \geq 5$ we have $s^2 + 7s + 22 > \frac{s(s+3)^2}{s-1}$. In the following let $i \neq j$, $h_i \geq 2$, $h_j \geq 2$. Since $s \geq 5$ we have

$$sh_i - \frac{s(s+3)}{s-1} \geq 0,$$
$$(s-1)h_j - (s+3) \geq 0.$$

Hence, we have $[sh_i - \frac{s(s+3)}{s-1}][(s-1)h_j - (s+3)] \geq 0$. Thus, we have

$$s(s-1)h_i h_j + s^2 + 7s + 22 > s(s+3)(h_i + h_j).$$

That is, $h_i h_j + \frac{0.5(s^2+7s+22)}{0.5s(s-1)} > \frac{s+3}{s-1}(h_i + h_j)$. Hence, we have

$$\sum_{1 \leq i < j \leq s} h_i h_j + 0.5(s^2 + 7s + 22) > (s+3)(h_1 + h_2 + \ldots + h_s).$$

Since $\sum_{i=1}^{s} h_i^2 + 2\sum_{1 \leq i < j \leq s} h_i h_j = (h_1 + h_2 + \ldots + h_s)^2$, we have

$$(h_1 + h_2 + \ldots + h_s)^2 - 2s(h_1 + h_2 + \ldots + h_s) + s^2 + 2s + 1 + s + 17$$
$$> 6(h_1 + h_2 + \ldots + h_s) - 4s - 4 + \sum_{i=1}^{s} h_i^2.$$

Hence, we have

$$(h_1+h_2+...+h_s)^2-2(s+1)(h_1+h_2+...+h_s)+(s+1)^2+s+17$$
$$>4(h_1+h_2+...+h_s)-4s-4+\sum_{i=1}^{s}h_i^2.$$

By Claim 1 we have $h=h_1+...+h_s-s-1$.

Thus, we have $h^2+s+17>4h+\sum_{i=1}^{s}h_i^2$.

Hence, we have $25h^2+s+3-20h-\sum_{i=1}^{s}h_i^2>24h^2-16h-14$.

By Theorem 3.1 and Claim 3 we have PI(H) > PI(GL_h). Claim 4 follows.

Let S_1, ..., S_s be segments of H. Suppose $s = 4$, $h \geq 5$, and there are two special hexagons in H. Because each special hexagon occupies at least two segments. By the definition of segment, at most one segment above is occupied by the two special hexagons of H at the same time. The remaining $h-2$ hexagons occupy at least one segment which is not occupied by one of the two special hexagons of H. Since $s = 4$, H is GL_h.

When $s = 4$, $n_i = 2$, $h \geq 5$ and there is a unique special hexagon in H, H contains subgraph H^* which is defined in Figure 10.

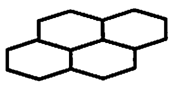

Figure 10. H^*

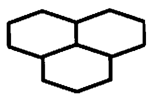

Figure 11. H^{****}

By the definition of segment H^* has 5 segments. Hence, H has at least 5 segments, which contradicts with $s = 4$. Hence, PI(H) = PI(GL_h) if and only if H = GL_h. The first part of Theorem 3.2 follows.

In the following we want to prove the second part of Theorem 3.2: PI(H) $\leq$ PI(SF_h) with equality if and only if H is SF_h, where $h \geq 5$.

By Theorem 3.1 Claim 5 is obvious:

Claim 5: PI(SF_h) $= 25h^2-20h-3s-2$, where SF is defined in section 2, $h \geq 5$.

Claim 6: when $h \geq 5$, $n_i = 2$, there exists $h_j \geq 3$.

In fact, when there is a unique special hexagon r in H, H contains a subgraph H^*, which is defined in Figure 10. Hence, when $h \geq 5$, we have $h_i \geq 3$.

Suppose H contains two special hexagons r_1 and r_2 in H. When r_1 and r_2 share a common segment, the length of the common segment must be at least 3, Claim 6 follows. Otherwise, suppose r_1 and r_2 do not share a common segment in H. We delete r_1 and r_2 from H and obtain H^{**}. If the number of components in H^{**} is at least 2, there must be two components which are connected by r_1 or by r_2, Claim 6 follows. Thus, suppose H^{**} is connected. We add r_1 to H^{**} and obtain H^{***}. H^{***} must contain subgraph H^{****} which is defined in Figure 11. In H^{****} one of the hexagons is r_1. Since $h \geq 5$, there must be at least one hexagon which is adjacent to H^{****} and it is not a special hexagon. Claim 6 follows. By Claim 6 we have $4s+5 \leq \sum_{i=1}^{s} h_i^2$. By Theorem 3.1 and Claim 5 the second part of Theorem 3.2 follows.

Acknowledgements: The project supported by the Natural Science Foundation of Department of Education of Zhejiang Province of China (No. 20070441); National Nature Science Foundation of China (No. 10971198), Zhejiang Provincial Natural Science Foundation of China (No. Y6090699); Zhejiang Innovation Project (No. T200905); Innovation Project of Optimization and Control of Network Systems of Zhejiang Normal University; ZSDZZZZXK03; Z6110786.

References

[1] H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc. 69(1947) 17-20.

[2] H. Wiener, Correlation: a heat of isomerization and differences in heats of vaporization of isomers, among the paraffin hydrocarbons, J. Am. Chem. Soc. 69(1947) 2636-2638.

[3] H. Wiener, Influence of interatomic forces on paraffin properties, J. Chem. Phys. 15(1947) 766-767.

[4] I. Gutman, Y.N. Yeh, S. Lee , Y.L. Luo, Some recent results in the theory of the Wiener number, Indian J. Chem. 32A (1993) 651-661.

[5] P.V. Khadikar, N.V. Deshpande, P.P. Kale, A.Dabrynin, I. Gutman, G. Domotor, The Szeged index and an analogy with the wiener index, J. Chem. Inf. Comput. Sci. 35(1995) 545-550.

[6] P.V. Khadikar, P.P. Kale, N.V. Deshpande, S. Karmarkar, V.K. Agrawal, Szeged indices of hexagonal chains, MATCH Commun. Math. Comput. Chem. 43 (2001) 7-15.

[7] P.V. Khadikar, On a novel structural descriptor PI, Nat. Acad. Sci. Lett. 23(2000) 113-118.

[8] P.V. Khadikar, S. Karmarkar, V.K. Agrawal, A novel PI index and its applications to QSPR/QSAR studies, J. Chem. Inf. Comput. Sci. 41(2001) 934-949.
[9]. M. Jaiswal, P.V. Khadikar, QSAR study on tadpole narcosis using PI index: a case of hetergenous set of compounds. *Biorg. Med. Chem.* **2004** , 12, 1731-1736.
[10]. P.V. Khadikar, S. Karmarkar, S. Singh, A. Shrivastava, Use of the PI index in predicting toxicity of nitrobenzene derivatives. *Biorg. Med. Chem.* **2002** , 10, 3161-3170.
[11] V.K. Agrawal, P.V. Khadikar, QSAR prediction of toxicity of nitrobenzene, Biorg. Med. Chem. 9(2001) 3035-3040.
[12] S. Singh, S. Joshi, A. Shrivastava, P.V. Khadikar, A novel method for estimating motor octane number (MON) – a structure-property relationship approach, J. Sci. Ind. Res. 61(2002) 961-965.
[13] M. Jaiswal, P.V. Khadikar, Use of distance-based topological indices for the estimation of ^{13}C NMR shifts: a case of benzene derivatives, J. Indian Chem. Soc. 82 (2005) 247-249.
[14] P.V. Khadikar, D. Mandloi, A.V. Bajaj, Novel applications of PI index estimating organic reactivity: CH acidity, s-character and steric energy, Oxid. Commun. 27(2004) 23-28.
[15] P.V. Khadikar, P.P. Kale, N.V. Deshpande, S. Karmarkar, V.K. Agrawal, Novel PI indices of hexagonal chains, J. Math. Chem. 29(2001) 143-150.
[16] P.E. John, P.V. Khadikar, J. Singh, A method of computing the PI index of benzenoid hydrocarbons using orthogonal cuts, J. Math. Chem. 42(2006) 37-45.
[17] J. Hao, Some bounds for PI Indices, MATCH Commun. Math. Comput. Chem. 60(2008) 121-134.
[18] J.A. Bondy, U.S.R. Murty, Graph Theory with Applications, London, Macmillan Press Ltd, 1976.
[19] C.H. Papadimitriou, K. Steiglitz, Combinatorial Optimization: Algorithms and Complexity, Englewood Cliffs, New Jersey, Prentice-Hall,Inc, 1982.
[20] A.A. Dobrynin, I. Gutman, S. Klavzar, P. Zigert, Wiener index of hexagonal systems, Acta Applicandae Mathematicae 72(2002) 247-294.
[21]. Jianxiu Hao, PI index of some simple pericondensed hexagonal systems, ARS Combinatoria, 92.Jul.(2009), 137-147.