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PI indices of pericondensed benzenoid graphs

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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 a class of pericondensed benzenoid graphs consisting of three rows of hexagonal of various lengths.

KEY WORDS: topological index, PI index, pericondensed benzenoid graph

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. Amongst the topological indices used as descriptors in QSAR, the Wiener index [1] is by far the most popular index, as it has been shown that the Wiener index has a strong correlation with the chemical properties of compounds. Since then, in order to model various molecular properties, many topological indices have been designed [2]. Such a proliferation is still going on and it becoming counter productive.

An overwhelming majority of the chemical applications of Wiener index deal with chemical compounds that have acyclic organic molecules. The molecular graphs of these compounds are trees. Therefore most of the prior work on Wiener indices deals with trees, relating the structure of various trees to Wiener indices. In 1990s, Gutman [3] and coworkers [4] have introduced a generation 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 coincide with the Wiener index. In [5,6], another topological index was

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introduced and it was named Padmakar–Ivan index, abbreviated as PI. This new topological index, PI, does not coincide with the Wiener index. Since PI index is different for acyclic graphs, several applications of PI index are reported in the literatures. Deng [6,7] gave formula for calculating the PI index of catacondensed hexagonal systems and $TUVC_6[2p, q]$, extremal catacondensed hexagonal systems with the minimum or maximum PI index was provided. Chen and Deng [8] investigated the PI index of Phenylenes. Ashrafi and Loghman [9] computed the PI index of zig–zag polyhex and C_4C_8 nanotubes (for other related articles see for [10–12]).

The primary aim of this article is to introduce the method for calculation of PI index for a class of pericondensed benzenoid graphs consisting of three rows of hexagonal of various lengths (in a chemical language, a subclass pericondensed benzenoid) [13,14]. A pericondensed benzenoid graph is a benzenoid graph in which internal vertices appear, that is, belong to three hexagons. Coronene and a number of its derivatives, such as dibenzo $[a, j]$ coronene, dibenzo$[bc, kl]$coronene, naphtho[2,3-a]coronene. They possess interesting mathematical, physical, chemical and biological properties [15]. And the related graph nation and terminology see [16].

2. The definition of 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 edges 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 of E 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 to y and Y is the subset of vertices of $V(G)$ which are closer to y than to 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 $G[Y] = (Y, E_2)$, $n_1(e) = |E_1|$, $n_2(e) = |E_2|$. If G is a bipartite graph, then $n_1(e)$ is the number of edges nearer to x than y and $n_2(e)$ is the number of edges nearer to y than x.

The PI index of a bipartite graph G is defined as

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

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

Let $[X, Y]$ denote the subset of edges between X and Y, $n(e) = |[X, Y]|$ is the number of edges equidistant to the both ends of e, and $n(e) = |E(G)| - (n_1(e) + n_2(e))$ for a bipartite connected graph G. So

$$\mathrm{PI}(G) = |E(G)|^2 - \sum_{e \in E(G)} n(e). \tag{1}$$

Therefore, for computing the PI index of a bipartite graph G, it is enough to calculate $n(e)$ for $e \in E(G)$.

3. Calculation of the PI index of benzenoid graphs from elementary cuts

Let $e = uv \in E(G)$, $e' = u'v' \in E(G)$. If $d(u, u') = d(v, v') = i$ and $d(u, v') = d(v, u') = i + 1$, or vice versa, $i = 0, 1, 2, \ldots$, then e is equidistant to e'. An elementary cuts $C(e)$ with respect to edge e is the set of all edges $e' \in E$ which are equidistant to e: $C(e) = \{e' \in E | e' \text{ is equidistant to } e\}$. Let $C_i = C_i(G)$ denote the elementary cut of length l_i, $i = 1, 2, \ldots, k$. The number of which are $n_1, n_2, \ldots, n_k$, respectively. Then equation (1) is equal to (see [17])

$$\mathrm{PI}(G) = |E(G)|^2 - \sum_{i=1}^{k} n_i l_i^2. \tag{2}$$

Let $a, b, c \in N$. Denote by $G(a, b, c)$ a pericondensed graph [18] as showed in figure 1.

Without loss of the generality, we assume that $c \leqslant a$ in the following.

Theorem 3.1. Let $a, b, c \in N$ and $b < c \leqslant a$, the graph $G(a, b, c)$ be a benzenoid graph depicted in figure 2. Then

$$\mathrm{PI}(G(a, b, c)) = 24a^2 + 24c^2 + 10ab + 50ac + 10bc + 20a - 12b + 20c + 6.$$

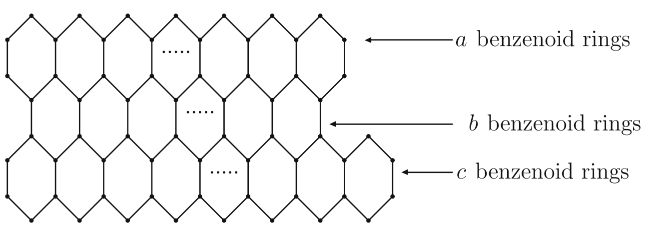

Figure 1. The graph $G(a, b, c)$.

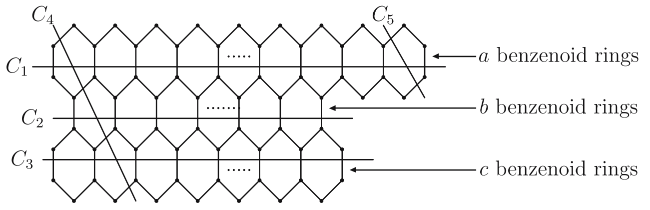

Figure 2. The graph $G(a, b, c)$ with $b < c \leqslant a$.

Proof. There are five types of elementary cuts in $G(a, b, c)$, that's $C = \{C_1, C_2, C_3, C_4, C_5\}$; $l_1 = a + 1, l_2 = b + 1, l_3 = c + 1, l_4 = 4, l_5 = 2$, and $n_1 = 1, n_2 = 1, n_3 = 1, n_4 = 2b, n_5 = 2(a + c - 2b)$, $|E| = 5a + b + 5c + 3$. By equation (2), we have

$$
\begin{aligned}
&\mathrm{PI}(G(a, b, c))\\
&= |E(G)|^2 - \sum_{i=1}^{k} n_i l_i^2\\
&= (5a + b + 5c + 3)^2 - \Big[(a + 1)^2 + (b + 1)^2 + (c + 1)^2 + 16 \times 2b\\
&\quad +4 \times 2(a + c - 2b)\Big]\\
&= 24a^2 + 24c^2 + 10ab + 50ac + 10bc + 20a - 12b + 20c + 6.
\end{aligned}
$$

□

Theorem 3.2. Let $a, b, c \in N$ and $c \leqslant b < a$, the graph $G(a, b, c)$ be a benzenoid graph depicted in figure 3. Then

$$\mathrm{PI}(G(a, b, c)) = 24a^2 + 8b^2 + 8c^2 + 30ab + 30ac + 18bc + 30a + 12b + 8c + 16.$$

Proof. There are six types of elementary cuts in $G(a, b, c)$, that's $C = \{C_1, C_2, C_3, C_4, C_5, C_6\}$; $l_1 = a + 1, l_2 = b + 1, l_3 = c + 1, l_4 = 4, l_5 = 3, l_6 = 2$, and $n_1 = 1, n_2 = 1, n_3 = 1, n_4 = 2c - 1, n_5 = 2(b - c) + 1, n_6 = 2(a - b) + 1$,

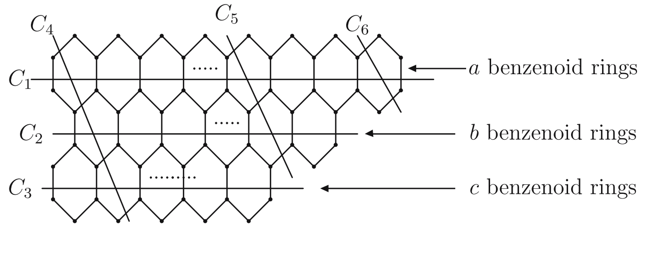

Figure 3. The graph $G(a, b, c)$ with $c \leqslant b < a$.

$|E| = 5a + 3b + 3c + 4$. By equation (2), we have

$$\begin{aligned}
\mathrm{PI}(G(a,b,c)) &= |E(G)|^2 - \sum_{i=1}^{k} n_i l_i^2 \\
&= (5a+3b+3c+4)^2 - ((a+1)^2 + (b+1)^2 + (c+1)^2 \\
&\quad +16 \times (2c-1) + 9 \times (2(b-c)+1)) + 4 \times (2(a-b)+1))) \\
&= 24a^2 + 8b^2 + 8c^2 + 30ab + 30ac + 18bc + 30a + 12b + 8c + 16.
\end{aligned}$$

□

Theorem 3.3. Let $a, b, c \in N$ and $c = a \leqslant b$, the graph $G(a,b,c)$ be a benzenoid graph depicted in figure 4. Then

$$\mathrm{PI}(G(a,b,c)) = 34a^2 + 24b^2 + 60ab + 32a + 40b + 28.$$

Proof. There are five types of elementary cuts in $G(a,b,c)$, that's $C = \{C_1, C_2, C_3, C_4, C_5\}$; $l_1 = a+1 = c+1, l_2 = b+1, l_3 = 4, l_4 = 3, l_5 = 2$, and $n_1 = 2, n_2 = 1, n_3 = 2(a-1), n_4 = 2, n_5 = 2(b-a+1)$, $|E| = 6a + 5b + 5$. By equation (2), we have

$$\begin{aligned}
\mathrm{PI}(G(a,b,c)) &= |E(G)|^2 - \sum_{i=1}^{k} n_i l_i^2 \\
&= (6a+5b+5)^2 - (2 \times (a+1)^2 + (b+1)^2 \\
&\quad +16 \times 2(a-1) + 9 \times 2 + 4 \times 2(b-a+1)) \\
&= 34a^2 + 24b^2 + 60ab + 32a + 40b + 28.
\end{aligned}$$

□

Theorem 3.4. Let $a, b, c \in N$ and $c < a \leqslant b$, the graph $G(a,b,c)$ be a benzenoid graph depicted in figure 5. Then

$$\mathrm{PI}(G(a,b,c)) = 8a^2 + 24b^2 + 8c^2 + 30ab + 18ac + 30bc + 18a + 40b + 14c + 26.$$

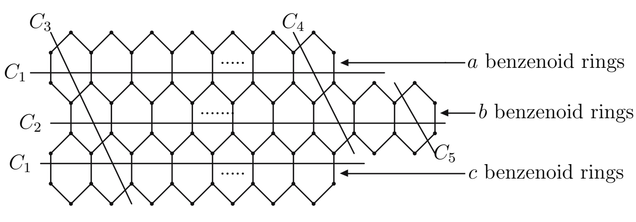

Figure 4. The graph $G(a,b,c)$ with $c = a \leqslant b$.

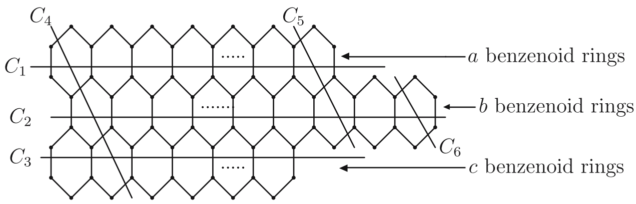

Figure 5. The graph $G(a, b, c)$ with $c < a \leqslant b$.

Proof. There are six types of elementary cuts in $G(a, b, c)$, that's $C = \{C_1, C_2, C_3, C_4, C_5, C_6\}$; $l_1 = a + 1$, $l_2 = b + 1$, $l_3 = c + 1$, $l_4 = 4$, $l_5 = 3$, $l_6 = 2$, and $n_1 = 1, n_2 = 1, n_3 = 1, n_4 = 2c - 1, n_5 = 2(a - c), n_6 = 2(b - a) + 3$, $|E| = 3a + 5b + 3c + 5$. By equation (2), we have

$$\begin{aligned}
\mathrm{PI}(G(a, b, c)) &= |E(G)|^2 - \sum_{i=1}^{k} n_i l_i^2 \\
&= (3a + 5b + 3c + 5)^2 - ((a + 1)^2 + (b + 1)^2 + (c + 1)^2 \\
&\quad +16 \times (2c - 1) + 9 \times 2(a - c) + 4 \times (2(b - a) + 3)) \\
&= 8a^2 + 24b^2 + 8c^2 + 30ab + 18ac + 30bc + 18a + 40b + 14c + 26.
\end{aligned}$$

□

4. The main results

From theorems 3.1–3.4 and the symmetry of a and c, we get the following results about the PI index of the graph $G(a, b, c)$

$$\mathrm{PI}(G(a, b, c))$$
$$= \begin{cases}
24a^2 + 24c^2 + 10ab + 50ac + 10bc + 20a - 12b + 20c + 6, & b < c \leqslant a, \\
24a^2 + 24c^2 + 10ab + 50ac + 10bc + 20a - 12b + 20c + 6, & b < a \leqslant c, \\
24a^2 + 8b^2 + 8c^2 + 30ab + 30ac + 18bc + 30a + 12b + 8c + 16, & c \leqslant b < a, \\
8a^2 + 8b^2 + 24c^2 + 18ab + 30ac + 30bc + 8a + 12b + 30c + 16, & a \leqslant b < c, \\
8a^2 + 24b^2 + 8c^2 + 30ab + 18ac + 30bc + 18a + 40b + 14c + 26, & c < a \leqslant b, \\
8a^2 + 24b^2 + 8c^2 + 30ab + 18ac + 30bc + 14a + 40b + 18c + 26, & a < c \leqslant b, \\
34a^2 + 24b^2 + 60ab + 32a + 40b + 28, & c = a \leqslant b.
\end{cases}$$

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