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PI index for some special graphs

Li Yan[1], YingfangLi[1], Wei Gao[2] and Junsheng Li[1*]

[1]*School of Engineer, Honghe University, Mengzi, P. R. China*
[2]*School of Information Science and Technology, Yunnan Normal University, Kunming, P. R. China*

ABSTRACT

The Padmakar-Ivan (PI) index is a Wiener-Szeged-like topological index which reflects certain structural features of organic molecules. Each structural feature of such organic molecule can be expressed as a graph. In this paper, we study the PI indices for some special graphs, such as $I_r(F_n)$, $I_r(W_n)$, $\tilde{F}_n$, $\tilde{W}_n$, $I_r(\tilde{F}_n)$ *and* $I_r(\tilde{W}_n)$.

Keywords: PI indices, organic molecules, fan graph, wheel graph, gear fan graph, gear wheel graph, *r*-corona graph

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INTRODUCTION

Wiener index (W) and Szeged index (Sz) are introduced to reflect certain structural features of organic molecules [1, 2]. Khadikar et al. [3, 4] introduced another index called Padmaker-Ivan (PI) index. For the previous results on PI index, can refer [5-8].

In this paper, we study the PI index of several simple connected graphs. The PI index of a graph G is defined as follows:

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

where $e=uv$, $n_{eu}(e|G)$ 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 the 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. In what follows, we write n_{eu} instead of $n_{eu}(e|G)$ for short. The readers can refer to [9] for standard graph theoretic concepts and terms used but undefined in this paper.

In this paper, we determine the PI index for some special graphs. The organization of rest paper is as follows. First, we give some necessary definition in the next section. Then, the main result in this article is given in the third section.

Preliminaries

For each edge $e=uv$, let $n_e=n_{uv}$ be the number of edges with different distance to u and v.

Definition 1. The graph $F_n=\{v\}\vee P_n$ is called a fan graph and the graph $W_n=\{v\}\vee C_n$ is called a wheel graph, where P_n is a path with n vertices and C_n is a cycle with n vertices.

Definition 2. Graph $I_r(G)$ is called r- crown graph of G which splicing r hang edges for every vertex in G. The vertex set of hang edges that splicing of vertex v is called r-hang vertices, note v^*.

Definition 3. By adding one vertex in every two adjacent vertices of the fan path P_n of fan graph F_n, the resulting graph is a subdivision graph called gear fan graph, denote as $\tilde{F}_n$.

Definition 4. By adding one vertex in every two adjacent vertices of the wheel cycle C_n of wheel graph W_n, The resulting graph is a subdivision graph, called gear wheel graph, denoted as $\tilde{W}_n$.

Main results and Proof

Theorem 1. For $n \geq 3$, $PI(I_r(F_n))= (2n^2+2n-8)+r(r(n+1)^2+3n^2+3n-6)$.

Proof. It is trivial for n=3 and n=4. In the following text, we consider $n \geq 5$. Let $P_n=v_1v_2\ldots v_n$ and the r hanging vertices of v_i be v_i^1, v_i^2 ,…, v_i^r $(1 \leq i \leq n)$. Let v be a vertex in F_n beside P_n, and the r hanging vertices of v be v^1, v^2, …, v^r.

By the definition of PI index, we have

$n_{vv_1}=2n+nr-3$, $n_{vv_2}=2n+(n-1)r-3$, $n_{vv_3}=2n+(n-1)r-4$, …, $n_{vv_{\lceil \frac{n}{2}\rceil}}=2n+(n-1)r-4$.

$n_{v_1v_2}=3r+4$, $n_{v_2v_3}=4r+5$, $n_{v_3v_4}=4r+6$, …, $n_{v_{\lceil \frac{n}{2}\rceil -1}v_{\lceil \frac{n}{2}\rceil}}=4r+6$.

$n_{vv^1}=n_{vv^2}=\ldots=n_{vv^r}=r(n+1)+2n-2$.

$n_{v_iv_i^1}=n_{v_iv_i^2}=\ldots=n_{v_iv_i^r}=r(n+1)+2n-2$ for all $1 \leq i \leq n$.

Hence, if n is odd, then

$$PI(I_r(F_n))=[(2n+nr-3)+(2n+(n-1)r-3)+(2n+(n-1)r-4)\times\frac{(n-1)-4}{2}+(3r+4)+(4r+5)+(4r+6)\times\frac{(n-1)-4}{2}]\times 2+(2n+(n-1)r-4)+(n+1)r(r(n+1)+2n-2)$$

$$=(2n^2+2n-8)+r(n^2+3n-4)+(n+1)r(r(n+1)+2n-2)$$

$$=(2n^2+2n-8)+r(r(n+1)^2+3n^2+3n-6).$$

If n is even, then

$$PI(I_r(F_n))=[(2n+nr-3)+(2n+(n-1)r-3)+(2n+(n-1)r-4)\times\frac{(n-1-4)+1}{2}+(3r+4)+(4r+5)+(4r+6)\times\frac{(n-1-4)-1}{2}]\times 2+(4r+6)+(n+1)r(r(n+1)+2n-2)$$

$$=(2n^2+2n-8)+ r(n^2+3n-4)+(n+1)r(r(n+1)+2n-2)$$

$$=(2n^2+2n-8)+r(r(n+1)^2+3n^2+3n-6).$$

Thus, we get the desire result.

Theorem 2. For $n \geq 6$, $PI(I_r(W_n))=2n^2+3n+r(r(n+1)^2+3n^2+4n-1)$.

Proof. Let $C_n=v_1v_2\ldots v_n$ and v_i^1, v_i^2 ,…, v_i^r be the r hanging vertices of v_i $(1 \leq i \leq n)$. Let v be a vertex in W_n beside C_n, and v^1, v^2, …, v^r be the r hanging vertices of v.

By the definition of PI index, we have

$n_{vv_1}=n_{vv_2}=\ldots=n_{vv_n}=2n+(n-1)r-3$.

$n_{v_1v_2} = n_{v_2v_3} = \ldots = n_{v_{n-1}v_n} = n_{v_nv_1} = 4r+6$.

$n_{vv^1} = n_{vv^2} = \ldots = n_{vv^r} = r(n+1)+2n-1$.

$n_{v_iv_i^1} = n_{v_iv_i^2} = \ldots = n_{v_iv_i^r} = r(n+1)+2n-1$ for all $1 \le i \le n$.

Therefore,

$\mathrm{PI}(I_r(W_n))=(2n+(n-1)r-3)n+(4r+6)n+(r(n+1)+2n-1)r(n+1)=2n^2+3n+r(r(n+1)^2+3n^2+4n-1)$.

Hence, we derive the desire conclusion. □

Theorem 3. For $n \ge 3$, $\mathrm{PI}(\tilde{F}_n)=9n^2-21n+14$.

Proof. It is trivial for n=3 and n=4. In the following text, we consider $n \ge 5$. Let $P_n=v_1v_2\ldots v_n$ and $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1}. Let v be a vertex in F_n beside P_n. By virtue of the definition of PI index, we get

$n_{vv_1} = 3n-4$, $n_{vv_2} = 3n-5$, $n_{vv_3} = 3n-5$, …, $n_{vv_{\lceil \frac{n}{2} \rceil}} = 3n-5$.

$n_{v_1v_{1,2}} = 3n-5$, $n_{v_{1,2}v_2} = 3n-4$, $n_{v_2v_{2,3}} = 3n-5$, $n_{v_{2,3}v_3} = 3n-5$,…, $n_{v_{\lceil \frac{n}{2} \rceil -1, \lceil \frac{n}{2} \rceil} v_{\lceil \frac{n}{2} \rceil}} = 3n-5$.

Thus, if n is odd, then

$$\mathrm{PI}(\tilde{F}_n)=[(3n-4)+(3n-4)+(3n-5) \times \frac{(n-1)-2}{2} + (3n-5) \times (n-2)] \times 2+(3n-5)$$

$=9n^2-21n+14$.

If n is even, then

$\mathrm{PI}(I_r(F_n))=2(3n-4)+(n-2)(3n-5)+2(3n-4)+(2n-4)(3n-5)= =9n^2-21n+14$.

Then, the desire result is given.

Theorem 4. For $n \ge 3$, $\mathrm{PI}(\tilde{W}_n)=3n(2n-3)$.

Proof. Let $C_n=v_1v_2\ldots v_n$ and v be a vertex in W_n beside C_n. $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1}. In view of the definition of PI index, we deduce

$n_{vv_1} = n_{vv_2} = \ldots = n_{vv_n} = 3n-3$.

$n_{v_1v_{1,2}} = n_{v_{1,2}v_2} = n_{v_2v_{2,3}} \ldots = n_{v_{n-1,n}v_n} = n_{v_nv_{n,1}} = n_{v_{n,1}v_1} = 3n-3$.

Therefore,

$\mathrm{PI}(\tilde{W}_n)=3n(2n-3)$.

Hence, we get the desire conclusion.

Theorem 5. For $n \ge 3$, $\mathrm{PI}(I_r(\tilde{F}_n))=(9n^2-21n+14)+ 2nr(6n+2nr-5)$.

Proof. It is trivial for n=3 and n=4. In the following text, we consider $n \ge 5$. Let $P_n=v_1v_2\ldots v_n$ and $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1}. Let v_i^1, v_i^2 ,…, v_i^r be the r hanging vertices of v_i ($1 \le i \le n$). Let $v_{i,i+1}^1$, $v_{i,i+1}^2$,…,

$v^{r}_{i,i+1}$ be the r hanging vertices of $v_{i,i+1}$ ($1\le i\le n$-1). Let v be a vertex in F_n beside P_n, and the r hanging vertices of $v$be v^1, v^2, …, v^r.

By virtue of the definition of PI index, we get

n_{vv_1} =(3n-4)+2nr, n_{vv_2} =(3n -5)+2nr, n_{vv_3} =(3n -5)+2nr, …, $n_{vv_{\lceil \frac{n}{2}\rceil}}$ =(3n -5)+2nr.

$n_{vv^1}=n_{vv^2}=\ldots=n_{vv^r}$ =3n+2nr-3.

$n_{v_1v_{1,2}}$ =(3n-5)+2nr, $n_{v_{1,2}v_2}$ =(3n-4)+2nr,…, $n_{v_{\lceil \frac{n}{2}\rceil-1,\lceil \frac{n}{2}\rceil}v_{\lceil \frac{n}{2}\rceil}}$ =(3n-5)+2nr.

$n_{v_iv_i^1}=n_{v_iv_i^2}=\ldots=n_{v_iv_i^r}$ =3n+2nr-3 for all $1\le i\le n$.

$n_{v_{i,i+1}v^1_{i,i+1}}=n_{v_{i,i+1}v^2_{i,i+1}}=\ldots=n_{v_{i,i+1}v^r_{i,i+1}}$ =3n+2nr-3 for all $1\le i\le n$-1.

Hence, in terms of Theorem 3, we infer

PI(I_r(F_n))=(9n^2-21n+14)+2nr(3n-2)+2nr(3n+2nr-3)=(9n^2-21n+14)+ 2nr(6n+2nr-5).

Thus, the result is hold.

Theorem 6. For $n\ge 3$, PI(I_r($\tilde{W}_n$))=3n(2n-3)+r(2n+1)(6n+r(2n+1)-1).

Proof. Let $C_n=v_1v_2\ldots v_n$ and v be a vertex in W_n beside C_n. $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1}. Let v^1, v^2, …, v^r be the r hanging vertices of v and v_i^1, v_i^2 ,…, v_i^r be the r hanging vertices of v_i ($1\le i\le n$). Let $v_{n,n+1}=v_{n,1}$, and $v^1_{i,i+1}$, $v^2_{i,i+1}$,…, $v^r_{i,i+1}$ be the r hanging vertices of $v_{i,i+1}$ ($1\le i\le n$). In view of the definition of PI index, we deduce

$n_{vv_1}=n_{vv_2}=\ldots=n_{vv_n}$ =(3n-3)+r(2n+1).
$n_{v_1v_{1,2}}=n_{v_{1,2}v_2}=n_{v_2v_{2,3}}\ldots=n_{v_{n-1,n}v_n}=n_{v_nv_{n,1}}=n_{v_{n,1}v_1}$ =(3n-3)+r(2n+1).
$n_{vv^1}=n_{vv^2}=\ldots=n_{vv^r}$ =3n+r(2n+1)-1.
$n_{v_iv_i^1}=n_{v_iv_i^2}=\ldots=n_{v_iv_i^r}$ =3n+r(2n+1)-1 for all $1\le i\le n$.
$n_{v_{i,i+1}v^1_{i,i+1}}=n_{v_{i,i+1}v^2_{i,i+1}}=\ldots=n_{v_{i,i+1}v^r_{i,i+1}}$ =3n+r(2n+1)-1 for all $1\le i\le n$.

Therefore, using Theorem 4, we get

PI(I_r($\tilde{W}_n$))=3n(2n-3)+3n(r(2n+1))+r(2n+1)(3n+r(2n+1)-1)
=3n(2n-3) +r(2n+1)(6n+r(2n+1)-1).

As conclusion, we obtain the final conclusion.

CONCLUSION

Fan graph, wheel graph, gear fan graph, gear wheel graph and their r-corona graph are common structural features of organic molecules. The contributions of our paper are determining the PI index of these special structural features of organic molecules.

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