Scholars Journal of Engineering and Technology (SJET)
Sch. J. Eng. Tech., 2015; 3(8):679-682
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(An International Publisher for Academic and Scientific Resources)
www.saspublisher.com

ISSN 2321-435X (Online)
ISSN 2347-9523 (Print)

Research Article

Weighted Vertex PI Index for Some Special Graphs

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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. Each structural feature of such organic molecule can be expressed as a graph. In this paper, we study the weighted vertex 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: weighted vertex, PI indices, fan graph, wheel graph, gear fan graph, gear wheel graph, r-corona graph.

Introduction

The studies of topological indices for molecular structures have been conducted for over 35 years. Distance-based topological indices are numerical parameters of molecular structure, and play important roles in physics, chemistry and pharmacology science.

Specifically, let G be a molecular graph, then a topological index can be regarded as a positive real function f: $G \to \mathbb{R}^+$. As numerical descriptors of the molecular structure deduced from the corresponding molecular graph, topological indices have found several applications in theoretical chemistry, like QSPR/QSAR study. For instance, harmonic index, Wiener index, PI index, Randic index and sum connectivity index are introduced to reflect certain structural features and chemical characteristics of organic molecules. Recently, several articles contributed to reporting certain distance-based indices of special molecular graph (See Yan et al., [1-2], Gao et al., [3-4], Gao and Shi [5], Gao and Wang [6], Xi and Gao [7-8], Xi et al., [9], Gao et al., [10] for more detail). The notation and terminology used but undefined in this paper can be found in [11].

In this paper, we study the weighted vertex PI index of several simple connected graphs. Let e=uv be an edge of the molecular graph G. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of G whose distance to the vertex v is smaller than the distance to the vertex u. Note that vertices equidistant to u and v are not counted. The weighted vertexPI index of a graph G was defined by Ilic and Milosavljevic [12] which is stated as follows:

$$PI_w(G)=\sum_{e=uv}(d(u)+d(v))[n_u(e)+n_v(e)].$$

In this paper, we determine the weighted vertexPI 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

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 inG. 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. $PI_w(I_r(F_n)) = r^3(n^2+2n+1)+r^2(8n^2+12n-8)+r(n^3+9n^2+31n-45)$
$+(n^3+2n^2+21n-36)$.

Proof. 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 ($1\le i\le n$). 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 . Using the definition of weighted vertex PI index, we have

$$PI_w(I_r(F_n)) = \sum_{i=1}^{r}(d(v)+d(v^i))(n_v(vv^i)+n_{v^i}(vv^i)) + \sum_{i=1}^{n}(d(v)+d(v_i))(n_v(vv_i)+n_{v_i}(vv_i)) +$$
$$\sum_{i=1}^{n-1}(d(v_i)+d(v_{i+1}))(n_{v_i}(v_iv_{i+1})+n_{v_{i+1}}(v_iv_{i+1})) + \sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)+d(v_i^j))(n_{v_i}(v_iv_i^j)+n_{v_i^j}(v_iv_i^j))$$
$$=(n+r+1)r(n+1)(r+1)+(2n(r+1)(n+2r+2)+(n-2)(n-1)(r+1)(n+2r+3))+2(3r+3)(2r+5)+$$
$$(n-3)(4r+4)(2r+6)+2r(n+1)(r+1)(r+3)+(n-2)r(n+1)(r+1)(r+4)$$
$$=r^3(n^2+2n+1)+r^2(8n^2+12n-8)+r(n^3+9n^2+31n-45)+(n^3+2n^2+21n-36).\square$$

Corollary 1. $PI_w(F_n) = n^3+2n^2+21n-36$.

Theorem 2. $PI_w(I_r(W_n)) = r^3(n^2+2n+1)+r^2(8n^2+14n+2)+r(n^3+8n^2+33n+1)$
$+(n^3+2n^2+29n)$.

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($1\le i\le n$). 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. We denote $v_nv_{n+1}=v_nv_1$. In view of the definition of weighted vertex PI index, we infer

$$PI_w(I_r(W_n)) = \sum_{i=1}^{r}(d(v)+d(v^i))(n_v(vv^i)+n_{v^i}(vv^i)) + \sum_{i=1}^{n}(d(v)+d(v_i))(n_v(vv_i)+n_{v_i}(vv_i)) +$$
$$\sum_{i=1}^{n}(d(v_i)+d(v_{i+1}))(n_{v_i}(v_iv_{i+1})+n_{v_{i+1}}(v_iv_{i+1})) + \sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)+d(v_i^j))(n_{v_i}(v_iv_i^j)+n_{v_i^j}(v_iv_i^j))$$
$$=r(n+1)(r+1)(n+r+1)+n(n-1)(r+1)(n+2r+3)+n(4r+4)(2r+6)+nr(n+1)(r+1)(r+4)$$
$$=r^3(n^2+2n+1)+r^2(8n^2+14n+2)+r(n^3+8n^2+33n+1)+(n^3+2n^2+29n).$$

Corollary 2. $PI_w(W_n) = n^3+2n^2+29n$.

Theorem 3. $PI_w(I_r(\tilde{F}_n)) = 4n^2r^3+r^2(48n^2-32n)+r(2n^3+54n^2-48n)+(2n^3+26n^2-32n)$.

Proof. 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 vi ($1\le i\le n$). Let $v_{i,i+1}^1$, $v_{i,i+1}^2$,…, $v_{i,i+1}^r$ 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 weighted vertex PI index, we yield

$$PI_w(I_r(\tilde{F}_n))=\sum_{i=1}^{r}(d(v)+d(v^i))(n_v(vv^i)+n_{v^i}(vv^i))+\sum_{i=1}^{n}(d(v)+d(v_i))(n_v(vv_i)+n_{v_i}(vv_i))+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)+d(v_i^j))(n_{v_i}(v_iv_i^j)+n_{v_i^j}(v_iv_i^j))+\sum_{i=1}^{n-1}(d(v_i)+d(v_{i,i+1}))(n_{v_i}(v_iv_{i,i+1})+n_{v_{i,i+1}}(v_iv_{i,i+1}))+$$

$$\sum_{i=1}^{n-1}(d(v_{i,i+1})+d(v_{i+1}))(n_{v_{i,i+1}}(v_{i,i+1}v_{i+1})+n_{v_{i+1}}(v_{i,i+1}v_{i+1}))$$

$$+\sum_{i=1}^{n-1}\sum_{j=1}^{r}(d(v_{i,i+1})+d(v^j_{i,i+1}))(n_{v_{i,i+1}}(v_{i,i+1}v^j_{i,i+1})+n_{v^j_{i,i+1}}(v_{i,i+1}v^j_{i,i+1}))$$

$$=r(2n(r+1))(n+r+1)+2\times 2n(r+1)(n+2r+2)+(n-2)2n(r+1)(n+2r+3)+$$

$$2r\times 2n(r+1)(r+3)+(n-2)r\times 2n(r+1)(r+4)+2\times 2n(r+1)(2r+4)+(n-3)2n(r+1)(2r+5)+$$

$$2\times 2n(r+1)(2r+4)+(n-3)2n(r+1)(2r+5)+(n-1)r\times 2n(r+1)(r+3)$$

$$=4n^2r^3+r^2(48n^2-32n)+r(2n^3+54n^2-48n)+(2n^3+26n^2-32n).\qquad \square$$

Corollary3. $PI_w(\tilde{F}_n)=2n^3+26n^2-32n$.

Theorem 4. $PI_w(I_r(\tilde{W}_n))=(4n^2+6n+1)r^3+r^2(28n^2+18n+2)+r(2n^3+52n^2+27n+1)$ $+(2n^3+20n^2+10n)$.

Proof. Let $C_n=v_1v_2\ldots v_n$ and v be a vertex in W_n beside C_n, and $v_{i,i+1}$ 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 $v_{n,n+1}=v_{1,n}$ and $v^1_{i,i+1}$, $v^2_{i,i+1}$,…, $v^r_{i,i+1}$ be the r hanging vertices of $v_{i,i+1}$ ($1\le i\le n$). Let $v_{n.n+1}=v_{n.1}$, $v_{n+1}=v_1$. In view of the definition of weighted vertex PI index, we deduce

$$PI_w(I_r(\tilde{W}_n))=\sum_{i=1}^{r}(d(v)+d(v^i))(n_v(vv^i)+n_{v^i}(vv^i))+\sum_{i=1}^{n}(d(v)+d(v_i))(n_v(vv_i)+n_{v_i}(vv_i))+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)+d(v_i^j))(n_{v_i}(v_iv_i^j)+n_{v_i^j}(v_iv_i^j))+\sum_{i=1}^{n-1}(d(v_i)+d(v_{i,i+1}))(n_{v_i}(v_iv_{i,i+1})+n_{v_{i,i+1}}(v_iv_{i,i+1}))+$$

$$\sum_{i=1}^{n-1}(d(v_{i,i+1})+d(v_{i+1}))(n_{v_{i,i+1}}(v_{i,i+1}v_{i+1})+n_{v_{i+1}}(v_{i,i+1}v_{i+1}))$$

$$+\sum_{i=1}^{n-1}\sum_{j=1}^{r}(d(v_{i,i+1})+d(v^j_{i,i+1}))(n_{v_{i,i+1}}(v_{i,i+1}v^j_{i,i+1})+n_{v^j_{i,i+1}}(v_{i,i+1}v^j_{i,i+1}))$$

$$=r(2n+1)(r+1)(n+r+1)+n(2n+1)(r+1)(n+2r+3)+nr(2n+1)(r+1)(r+4)+n(2n+1)(r+1)(r+5)+$$

$$n(2n+1)(r+1)(r+5)+nr(2n+1)(r+1)(r+3)$$

$$=(4n^2+6n+1)r^3+r^2(28n^2+18n+2)+r(2n^3+52n^2+27n+1)+(2n^3+20n^2+10n).\ \square$$

Corollary 4. $PI_w(\tilde{W}_n)=2n^3+20n^2+10n$.

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 weighted vertex PI index of these special structural features of organic molecules.

Acknowledgment

First we thank the reviewers for their constructive comments in improving the quality of this paper. This work was supported in part by Pecuniary aid of Yunnan Province basic research for application (2013fz127). We also would like to thank the anonymous referees for providing us with constructive comments and suggestions.

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