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Vertex PI Index and Szeged Index of Certain Special Molecular Graphs

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Abstract: The vertex PI index and Szeged index are distance-based topological index which reflect certain structural features of organic molecules. Each structural feature of such organic molecule can be expressed as a graph. In this paper, we determine the vertex PI index and Szeged index of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their r-corona molecular graphs.

Keywords: Chemical graph theory, vertex PI index, Szeged index, Fan molecular graph, Wheel molecular graph, Gear fan molecular graph, Gear wheel molecular graph, r-corona molecular graph.

1. INTRODUCTION

Wiener index, PI index, Hyper-wiener index, Geometric-arithmetic index and Zagreb indices are introduced to reflect certain structural features of organic molecules. Several papers contributed to determine the distance-based index of special molecular graphs (See Yan *et al*., [1, 2], Gao and Shi [3] for more detail). Let P_n and C_n be path and cycle with n vertices. The molecular graph $F_n=\{v\} \vee P_n$ is called a fan molecular graph and the molecular graph $W_n=\{v\} \vee C_n$ is called a wheel molecular graph. Molecular graph $I_r(G)$ is called r- crown molecular graph of G which splicing r hang edges for every vertex in G. By adding one vertex in every two adjacent vertices of the fan path P_n of fan molecular graph F_n, the resulting molecular graph is a subdivision molecular graph called gear fan molecular graph, denote as $\tilde{F}_n$. By adding one vertex in every two adjacent vertices of the wheel cycle C_n of wheel molecular graph W_n, The resulting molecular graph is a subdivision molecular graph, called gear wheel molecular graph, denoted as $\tilde{W}_n$.

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 vertex PI index of G is defined as

$$PI_v(G) = \sum_{e=uv}[n_u(e)+n_v(e)].$$

Khalifeh *et al*., [4] presented the vertex PI indices of cartesian product molecular graphs. Ashrafi *et al*., [5] studied the vertex PI index of an infinite family of fullerenes. Khalifeh *et al*., [6] raised a matrix method for computing vertex PI index of molecular graphs. Yousefi-Azari [7] calculated vertex-PI index of single and multi-walled nanotubes. Mansour and Schork [8] determined the vertex PI index of bridge molecular graphs. Nadjafi-Arani *et al*., [9] presented the extremal molecular graphs with respect to the vertex PI index. Das and Gutman [10] obtained the bound for vertex PI index by virtue of simple molecular graph parameters. Li *et al*., [11] computed the vertex PI of chain molecular graphs. Bahrami and Yazdani [12] yielded the vertex PI index of *V*-phenylenic nanotubes and nanotori.

The Szeged index is closely related to the Wiener index and defined as

$$Sz(G) = \sum_{e=uv} n_u(e)n_v(e).$$

Some conclusion for Szeged index can refer to [13].

In this paper, we present the vertex PI index and Szeged index of $I_r(F_n)$, $I_r(W_n)$, and $I_r(\tilde{W}_n)$.

2. VERTEX PI INDEX

Theorem 1:

$$PI_v(I_r(F_n)) = r^2(n^2+2n+1)+r(2n^2+5n-3)+(n^2+3n-4).$$

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 vertex PI index, we have

$$PI_v(I_r(F_n)) = \sum_{i=1}^{r}(n_v(vv^i)+n_{v^i}(vv^i)) +$$

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

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

$$=r^2(n^2+2n+1)+r(2n^2+5n-3)+(n^2+3n-4).$$

Corollary 1. $PI_v(F_n)=n^2+3n-4$.

Theorem 2.

$PI_v(I_r(W_n))=r^2(n^2+2n+1)+r(2n^2+5n+1)+(n^2+3n)$.

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 vertex PI index, we infer

$$PI_v(I_r(W_n))=\sum_{i=1}^{r}(n_v(vv^i)+n_{v^i}(vv^i))+\sum_{i=1}^{n}(n_v(vv_i)+n_{v_i}(vv_i))+\sum_{i=1}^{n}(n_{v_i}(v_iv_{i+1})+n_{v_{i+1}}(v_iv_{i+1}))+\sum_{i=1}^{n}\sum_{j=1}^{r}(n_{v_i}(v_iv_i^j)+n_{v_i^j}(v_iv_i^j))$$

$$=r(n+1)(r+1)+n(n-1)(r+1)+n(4r+4)+nr(n+1)(r+1)$$

$$=r^2(n^2+2n+1)+r(2n^2+5n+1)+(n^2+3n).$$

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

Theorem 3. $PI_v(I_r(\tilde{F}_n))=4n^2r^2+r(10n^2-4n)+(6n^2-4n)$.

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 vertex PI index, we yield

$$PI_v(I_r(\tilde{F}_n))=\sum_{i=1}^{r}(n_v(vv^i)+n_{v^i}(vv^i))+\sum_{i=1}^{n}(n_v(vv_i)+n_{v_i}(vv_i))+\sum_{i=1}^{n}\sum_{j=1}^{r}(n_{v_i}(v_iv_i^j)+n_{v_i^j}(v_iv_i^j))+\sum_{i=1}^{n-1}(n_{v_i}(v_iv_{i,i+1})+n_{v_{i,i+1}}(v_iv_{i,i+1}))+\sum_{i=1}^{n-1}(n_{v_{i,i+1}}(v_{i,i+1}v_{i+1})+n_{v_{i+1}}(v_{i,i+1}v_{i+1}))+\sum_{i=1}^{n-1}\sum_{j=1}^{r}(n_{v_{i,i+1}}(v_{i,i+1}v_{i,i+1}^j)+n_{v_{i,i+1}^j}(v_{i,i+1}v_{i,i+1}^j))$$

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

$$=4n^2r^2+r(10n^2-4n)+(6n^2-4n).\ \square$$

Corollary 3. $PI_v(\tilde{F}_n)=6n^2-4n$.

Theorem 4.

$PI_v(I_r(\tilde{W}_n))=r^2(4n^2+4n+1)+r(10n^2+7n+1)+(6n^2+3n)$.

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 $v_{i,i+1}^1$, $v_{i,i+1}^2$,…, $v_{i,i+1}^r$ be the *r* hanging vertices of $v_{i,i+1}$ ($1\le i\le n$). Let $v_{n.n+1}=v_{n.1}$, $v_{n+1}=v_1$. In view of the definition of vertex PI index, we deduce

$$PI_v(I_r(\tilde{W}_n))=\sum_{i=1}^{r}(n_v(vv^i)+n_{v^i}(vv^i))+\sum_{i=1}^{n}(n_v(vv_i)+n_{v_i}(vv_i))+\sum_{i=1}^{n}\sum_{j=1}^{r}(n_{v_i}(v_iv_i^j)+n_{v_i^j}(v_iv_i^j))+\sum_{i=1}^{n}(n_{v_i}(v_iv_{i,i+1})+n_{v_{i,i+1}}(v_iv_{i,i+1}))+\sum_{i=1}^{n}(n_{v_{i,i+1}}(v_{i,i+1}v_{i+1})+n_{v_{i+1}}(v_{i,i+1}v_{i+1}))+\sum_{i=1}^{n}\sum_{j=1}^{r}(n_{v_{i,i+1}}(v_{i,i+1}v_{i,i+1}^j)+n_{v_{i,i+1}^j}(v_{i,i+1}v_{i,i+1}^j))=$$

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

$$=r^2(4n^2+4n+1)+r(10n^2+7n+1)+(6n^2+3n).\ \square$$

Corollary 4. $PI_v(\tilde{W}_n)=6n^2+3n$.

3. SZEGED INDEX

The notations for certain special molecular graphs can refer to Theorem 1- Theorem 4.

Theorem 5.

$Sz(I_r(F_n))=r^2(2n^2+4n-5)+r(3n^2+5n-12)+(n^2+2n-6)$.

Proof. Using the definition of Szeged index, we have

$$Sz(I_r(F_n)) = \sum_{i=1}^{r}(n_v(vv^i)n_{v^i}(vv^i)) + \sum_{i=1}^{n}(n_v(vv_i)n_{v_i}(vv_i)) +$$
$$\sum_{i=1}^{n-1}(n_{v_i}(v_iv_{i+1})n_{v_{i+1}}(v_iv_{i+1})) + \sum_{i=1}^{n}\sum_{j=1}^{r}(n_{v_i}(v_iv_i^j)n_{v_i^j}(v_iv_i^j))$$
$$= r(r+n(r+1)) + (2(n-1)(r+1)^2 + (n-2)^2(r+1)^2) +$$
$$4(r+1)^2 + 4(n-3)(r+1)^2 + nr(r+n(r+1))$$
$$= r^2(2n^2+4n-5) + r(3n^2+5n-12) + (n^2+2n-6).$$

Corollary 5. $Sz(F_n) = n^2+2n-6$.

Theorem 6.

$$Sz(I_r(W_n)) = r^2(2n^2+4n+1) + r(3n^2+5n) + (n^2+2n).$$

Proof. In view of the definition of Szeged index, we infer

$$Sz(I_r(W_n)) = \sum_{i=1}^{r}(n_v(vv^i)n_{v^i}(vv^i)) + \sum_{i=1}^{n}(n_v(vv_i)n_{v_i}(vv_i)) +$$
$$\sum_{i=1}^{n}(n_{v_i}(v_iv_{i+1})n_{v_{i+1}}(v_iv_{i+1})) + \sum_{i=1}^{n}\sum_{j=1}^{r}(n_{v_i}(v_iv_i^j)n_{v_i^j}(v_iv_i^j))$$
$$= r(r+n(r+1)) + n(n-2)(r+1)^2 + 4n(1+r)^2 +$$
$$nr(r+n(r+1))$$
$$= r^2(2n^2+4n+1) + r(3n^2+5n) + (n^2+2n).$$

Corollary 6. $Sz(W_n) = n^2+2n$.

Theorem 7.

$$Sz(I_r(\tilde{F}_n)) =$$
$$r^2(22n^2-43n+28) + r(40n^2-88n+56) + (18n^2-43n+28).$$

Proof. By virtue of the definition of Szeged index, we yield

$$Sz(I_r(\tilde{F}_n)) = \sum_{i=1}^{r}(n_v(vv^i)n_{v^i}(vv^i)) + \sum_{i=1}^{n}(n_v(vv_i)n_{v_i}(vv_i)) +$$
$$\sum_{i=1}^{n}\sum_{j=1}^{r}(n_{v_i}(v_iv_i^j)n_{v_i^j}(v_iv_i^j))$$
$$+ \sum_{i=1}^{n-1}(n_{v_i}(v_iv_{i,i+1})n_{v_{i,i+1}}(v_iv_{i,i+1})) +$$
$$\sum_{i=1}^{n-1}(n_{v_{i,i+1}}(v_{i,i+1}v_{i+1})n_{v_{i+1}}(v_{i,i+1}v_{i+1}))$$
$$+ \sum_{i=1}^{n-1}\sum_{j=1}^{r}(n_{v_{i,i+1}}(v_{i,i+1}v_{i,i+1}^j)n_{v_{i,i+1}^j}(v_{i,i+1}v_{i,i+1}^j))$$
$$= r(r+(r+1)(2n-1)) + 8(n-1)(r+1)^2 +$$
$$3(n-2)(2n-3)(r+1)^2 + nr(2n(r+1)-1) +$$
$$3(n-1)(2n-3)(r+1)^2 + 3(n-1)(2n-3)(r+1)^2 +$$
$$(n-1)r(2n(r+1)-1)$$
$$=$$
$$r^2(22n^2-43n+28) + r(40n^2-88n+56) + (18n^2-43n+28).$$

Corollary 7. $Sz(\tilde{F}_n) = 18n^2-43n+28$.

Theorem 8.

$$Sz(I_r(\tilde{W}_n)) = r^2(22n^2-14n+1) + r(40n^2-34n) + (18n^2-18n).$$

Proof. In view of the definition of Szeged index, we deduce

$$PI_v(I_r(\tilde{W}_n)) = \sum_{i=1}^{r}(n_v(vv^i)n_{v^i}(vv^i)) + \sum_{i=1}^{n}(n_v(vv_i)n_{v_i}(vv_i)) +$$
$$\sum_{i=1}^{n}\sum_{j=1}^{r}(n_{v_i}(v_iv_i^j)n_{v_i^j}(v_iv_i^j))$$
$$+ \sum_{i=1}^{n}(n_{v_i}(v_iv_{i,i+1})n_{v_{i,i+1}}(v_iv_{i,i+1})) +$$
$$\sum_{i=1}^{n}(n_{v_{i,i+1}}(v_{i,i+1}v_{i+1})n_{v_{i+1}}(v_{i,i+1}v_{i+1}))$$
$$+ \sum_{i=1}^{n}\sum_{j=1}^{r}(n_{v_{i,i+1}}(v_{i,i+1}v_{i,i+1}^j)n_{v_{i,i+1}^j}(v_{i,i+1}v_{i,i+1}^j))$$
$$= r(r+2n(r+1)) + 3n(2n-2)(r+1)^2 + nr((2n+1)(r+1)-1) +$$
$$3n(2n-2)(r+1)^2$$
$$+ 3n(2n-2)(r+1)^2 + nr((2n+1)(r+1)-1)$$
$$= r^2(22n^2-14n+1) + r(40n^2-34n) + (18n^2-18n).\ \square$$

Corollary 8. $Sz(\tilde{W}_n) = 18n^2-18n$.

CONFLICT OF INTEREST

The authors confirm that this article content has no conflict of interest.

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