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Szeged polynomial and edge szeged polynomialof certain special molecular graphs

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ABSTRACT

The Szeged polynomial and edge Szeged polynomial aredistance-based topological parameters which reflect certain structural features of organic molecules. Each structural feature of such organic moleculecan be expressed as a graph. In this paper, we determine theSzeged polynomial and edge Szeged polynomialof fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their *r*-corona molecular graphs. © 2015 Trade Science Inc. - INDIA

KEYWORDS

Chemical graph theory;
Szeged polynomial;
Edge Szeged polynomial;
Fan molecular graph;
Wheel molecular graph;
Gear fan moleculargraph;
Gear wheel moleculargraph;
r-corona moleculargraph.

INTRODUCTION

Wiener index,PI index, Shultz index, Szeged index, Geometric-arithmetic indexand Zagreb indicesare 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 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].

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 thedistance 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*. 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[12] and[13]. The Szeged polynomial is denoted as

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

Let *e*=*uv* be an edge of the molecular graph *G*. The number of edges of *G* whose distance to the vertex *u* is smaller than thedistance to the vertex *v* is denoted by $m_u(e)$. Analogously, $m_v(e)$ is the number of edges of*G* whose distance to the vertex*v* is smaller than the distance to the vertex *u*. Note that edges equidistant to *u* and *v* are not counted. The edge Szegedindex of *G* is defined as

$$Sz_e(G)=\sum_{e=uv} m_u(e)m_v(e).$$

The edge Szeged polynomial is denoted as

$$Sz_e(G,x)=\sum_{e=uv} e^{m_u(e)m_v(e)}.$$

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 $W_n=\{v\}C_n$ 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 . 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 $\tilde{W}_n$.

In this paper, we present the Szeged polynomialand edge Szeged polynomialof,, and .

Szeged Polynomial

Theorem 1. $Sz(I_r(F_n),x)=r(n+1)x^{r+n(r+1)}+2x^{(n-1)(r+1)^2}+(n-2)x^{(n-2)(r+1)^2}+2x^{2(r+1)^2}+(n-3)x^{4(r+1)^2}$.

Proof. Let $P_n=v_1v_2\dots v_n$ and the r hanging vertices of v_i be $v_i^1, v_i^2,\dots, v_i^r$ $(1\le i\le n)$. Let v be a vertex in F_n beside P_n, and the r hanging vertices of v be $v^1, v^2, \dots, v^r$. Using the definition of Szeged polynomial, we have

$$Sz(I_r(F_n),x)=\sum_{i=1}^{r} x^{n_v(vv^i)n_{v^i}(vv^i)}+\sum_{i=1}^{n} x^{n_v(vv_i)n_{v_i}(vv_i)}+\sum_{i=1}^{n-1} x^{n_{v_i}(v_iv_{i+1})n_{v_{i+1}}(v_iv_{i+1})}+\sum_{i=1}^{n}\sum_{j=1}^{r} x^{n_{v_i}(v_iv_i^j)n_{v_i^j}(v_iv_i^j)}$$

$$=rx^{r+n(r+1)}+(2x^{(n-1)(r+1)^2}+(n-2)x^{(n-2)(r+1)^2})+2x^{2(r+1)^2}+(n-3)x^{4(r+1)^2}+nrx^{r+n(r+1)}.\square$$

Corollary 1. $Sz(F_n,x)=2x^{n-1}+(n-2)x^{n-2}+2x^2+(n-3)x^4$.

Theorem 2. $Sz(I_r(W_n),x)=nx^{(n-2)(r+1)^2}+nx^{4(1+r)^2}+(n+1)rx^{r+n(r+1)}$.

Proof. Let $C_n=v_1v_2\dots v_n$ and $v_i^1, v_i^2,\dots, v_i^r$ 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 $v^1, v^2, \dots, v^r$ be the r hanging vertices of v. We denote $v_nv_{n+1}=v_nv_1$. In view of the definition ofSzegedpolynomial, we infer

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

$$=rx^{(r+n(r+1))}+nx^{(n-2)(r+1)^2}+nx^{4(1+r)^2}+nrx^{r+n(r+1)}.$$

Corollary 2. $Sz(W_n,x)=nx^{n-2}+nx^4$.

Theorem 3. $Sz(I_r(\tilde{F}_n),x)=2x^{4(n-1)(r+1)^2}+(3n-4)x^{3(2n-3)(r+1)^2}+2nrx^{2n(r+1)-1}$.

Proof. Let $P_n=v_1v_2\dots v_n$ and $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1}. Let $v_i^1, v_i^2,\dots, v_i^r$ be the r hanging vertices of $v_i(1\le i\le n)$. Let $v_{i,i+1}^1, v_{i,i+1}^2,\dots, v_{i,i+1}^r$ be the r hanging vertices of $(1\le i\le n$-1). Let v be a vertex in F_n beside P_n, and the r hanging vertices of v be $v^1, v^2, \dots, v^r$.

By virtue ofthe definition ofSzegedpolynomial, we yield

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

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

$$= rx^{r+(r+1)(2n-1)} + 2x^{4(n-1)(r+1)^2} + (n-2)x^{3(2n-3)(r+1)^2} + nrx^{2n(r+1)-1} + (n-1)x^{3(2n-3)(r+1)^2} + (n-1)x^{3(2n-3)(r+1)^2} + (n-1)rx^{2n(r+1)-1}.$$

Corollary3. $Sz(\tilde{F}_n, x) = 2x^{4(n-1)} + (3n-4)x^{3(2n-3)}$.

Theorem 4. $Sz(I_r(\tilde{W}_n), x) = 3nx^{3(2n-2)(r+1)^2} + (2n+1)rx^{(2n+1)(r+1)-1}$.

Proof. Let $C_n = v_1 v_2 \ldots v_n$ 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 $v^1, v^2, \ldots, v^r$. be the r hanging vertices of v and $v_i^1, v_i^2, \ldots, v_i^r$ be the r hanging vertices of $v_i (1 \le i \le n)$. Let $v_{n,n+1} = v_{1,n}$ and $v_{i,i+1}^1, v_{i,i+1}^2, \ldots, v_{i,i+1}^r$ be the r hanging vertices of (1*in*). Let $v_{n.n+1} = v_{n.1}$, $v_{n+1} = v_1$. In view of the definition ofSzegedpolynomial, we deduce

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

$$+ \sum_{i=1}^{n} x^{n_{v_{i,i+1}}(v_{i,i+1}v_{i+1})n_{v_{i+1}}(v_{i,i+1}v_{i+1})} + \sum_{i=1}^{n}\sum_{j=1}^{r} x^{n_{v_{i,i+1}}(v_{i,i+1}v_{i,i+1}^{j})n_{v_{i,i+1}^{j}}(v_{i,i+1}v_{i,i+1}^{j})}$$

$$= rx^{r+2n(r+1)} + nx^{3(2n-2)(r+1)^2} + nrx^{(2n+1)(r+1)-1} + nx^{3(2n-2)(r+1)^2} + nx^{3(2n-2)(r+1)^2} + nrx^{(2n+1)(r+1)-1}.$$

Corollary 4. $Sz(\tilde{W}_n, x) = 3nx^{3(2n-2)}$.

Edge szeged polynomial

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

Theorem 5. $Sz_e(I_r(F_n), x) = (n+1)rx^{2n+r+nr-2} + 2x^{(2n+nr-r-4)(r+1)} + 2x^{(2n+nr-2r-4)(r+2)} + (n-4)x^{(2n+nr-2r-5)(r+2)} + 2x^{(r+1)(2r+3)} + 2x^{(2r+2)(2r+3)} + (n-5)x^{(2r+3)(2r+3)}$.

Proof. Let $P_n = v_1 v_2 \ldots v_n$ and the r hanging vertices of v_i be $v_i^1, v_i^2, \ldots, v_i^r$ $(1 \le i \le n)$. Let v be a vertex in F_n beside P_n, and the r hanging vertices of v be $v^1, v^2, \ldots, v^r$. Using the definition ofedge Szeged polynomial, we have

$$Sz_e(I_r(F_n), x) = \sum_{i=1}^{r} x^{m_v(vv^i)m_{v^i}(vv^i)} + \sum_{i=1}^{n} x^{m_v(vv_i)m_{v_i}(vv_i)} + \sum_{i=1}^{n-1} x^{m_{v_i}(v_i v_{i+1})m_{v_{i+1}}(v_i v_{i+1})} + \sum_{i=1}^{n}\sum_{j=1}^{r} x^{m_{v_i}(v_i v_i^j)m_{v_i^j}(v_i v_i^j)}$$

$$= rx^{2n+r+nr-2} + (2x^{(2n+nr-r-4)(r+1)} + 2x^{(2n+nr-2r-4)(r+2)} + (n-4)x^{(2n+nr-2r-5)(r+2)}) + (2x^{(r+1)(2r+3)} + 2x^{(2r+2)(2r+3)} + (n-5)x^{(2r+3)(2r+3)}) + nrx^{(2n+r+nr-2)}.$$

Corollary 5. $Sz_e(F_n, x) = 2x^{2n-4} + 2x^{2(2n-4)} + (n-4)x^{2(2n-5)} + 2x^3 + 2x^6 + (n-5)x^9$.

Theorem 6. $Sz_e(I_r(W_n), x) = r(n+1)x^{2n+r+nr-1} + nx^{(r+2)(2n+nr-2r-5)} + nx^{(2r+3)(2r+3)}$.

Proof. Let $C_n = v_1 v_2 \ldots v_n$ and $v_i^1, v_i^2, \ldots, v_i^r$ 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 $v^1, v^2, \ldots, v^r$ be the r hanging vertices of v. We ddenote $v_n v_{n+1} = v_n v_1$. In view of the definition of edge Szeged polynomial, we infer

$$Sz_e(I_r(W_n),x)=\sum_{i=1}^{r}x^{m_v(vv^i)m_{v^i}(vv^i)}+\sum_{i=1}^{n}x^{m_v(vv_i)m_{v_i}(vv_i)}+\sum_{i=1}^{n}x^{m_{v_i}(v_iv_{i+1})m_{v_{i+1}}(v_iv_{i+1})}+\sum_{i=1}^{n}\sum_{j=1}^{r}x^{m_{v_i}(v_iv_i^j)m_{v_i^j}(v_iv_i^j)}$$

$$=r(n+1)x^{2n+r+nr-1}+nx^{(r+2)(2n+nr-2r-5)}+nx^{(2r+3)(2r+3)}.\square$$

Corollary 6. $Sz_e(W_n,x)=nx^{2(2n-5)}+nx^9$.

Theorem 7. $Sz_e(I_r(\tilde{F}_n),x)=2x^{(2r+1)(2nr+3n-2r-5)}+(3n-4)x^{(3r+2)(2nr+3n-3r-7)}+2nrx^{3n+2nr-3}$.

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, $v_i^2,\ldots$, v_i^r be the r hanging vertices of vi $(1\le i\le n)$. Let $v_{i,i+1}^1$, $v_{i,i+1}^2,\ldots$, $v_{i,i+1}^r$ be the r hanging vertices of $(1\le i\le n\text{-}1)$. 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 ofthe definition of edge Szeged polynomial, we yield

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

$$\sum_{i=1}^{n-1}x^{m_{v_{i,i+1}}(v_{i,i+1}v_{i+1})m_{v_{i+1}}(v_{i,i+1}v_{i+1})}+\sum_{i=1}^{n-1}\sum_{j=1}^{r}x^{m_{v_{i,i+1}}(v_{i,i+1}v_{i,i+1}^j)m_{v_{i,i+1}^j}(v_{i,i+1}v_{i,i+1}^j)}$$

$$=rx^{3n+2nr-3}+(2x^{(2r+1)(2nr+3n-2r-5)}+(n-2)x^{(3r+2)(2nr+3n-3r-7)})+nrx^{3n+2nr-3}+(n-1)x^{(3r+2)(2nr-3r+3n-7)}++.$$

Corollary7. $Sz_e(\tilde{F}_n,x)=2x^{3n-5}+(3n-4)x^{2(3n-7)}$.

Theorem 8. $Sz_e(I_r(\tilde{W}_n),x)=3nx^{(3r+2)(2nr+3n-2r-5)}+(2n+1)rx^{2nr+3n+r-1}$.

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, $v_i^2,\ldots$, 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 $v_{i,i+1}^1$, $v_{i,i+1}^2,\ldots$, $v_{i,i+1}^r$ be the r hanging vertices of $(1\le i\le n)$. Let $v_{n.n+1}=v_{n.1}$, $v_{n+1}=v_1$. In view of the definition of edge Szeged polynomial, we deduce

$$Sz_e(I_r(\tilde{W}_n),x)\ =\ =\ \sum_{i=1}^{r}x^{m_v(vv^i)m_{v^i}(vv^i)}+\sum_{i=1}^{n}x^{m_v(vv_i)m_{v_i}(vv_i)}+\sum_{i=1}^{n}\sum_{j=1}^{r}x^{m_{v_i}(v_iv_i^j)m_{v_i^j}(v_iv_i^j)}+\sum_{i=1}^{n}x^{m_{v_i}(v_iv_{i,i+1})m_{v_{i,i+1}}(v_iv_{i,i+1})}$$

$$+\sum_{i=1}^{n}x^{m_{v_{i,i+1}}(v_{i,i+1}v_{i+1})m_{v_{i+1}}(v_{i,i+1}v_{i+1})}+\sum_{i=1}^{n}\sum_{j=1}^{r}x^{m_{v_{i,i+1}}(v_{i,i+1}v_{i,i+1}^j)m_{v_{i,i+1}^j}(v_{i,i+1}v_{i,i+1}^j)}$$

$$=rx^{2nr+3n+r-1}+nx^{(3r+2)(2nr+3n-2r-5)}+nrx^{2nr+3n+r-1}+nx^{(3r+2)(2nr+3n-2r-5)}+nx^{(3r+2)(2nr+3n-2r-5)}+nrx^{2nr+3n+r-1}.$$

Corollary 8. $Sz_e(\tilde{W}_n,x)=3nx^{2(3n-5)}$.

CONCLUSION

In this paper, we present the Szeged polynomialand edgeSzeged polynomial of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their r-corona molecular graphs. The results obtained in our paper illustrate the promising application prospects for chemistry and pharmacy science.

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