



## Szeged polynomial and edge szeged polynomial of certain special molecular graphs

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### ABSTRACT

The Szeged polynomial and edge Szeged polynomial are distance-based topological parameters 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 Szeged polynomial and edge Szeged polynomial of 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 molecular graph;  
Gear wheel molecular graph;  
 $r$ -corona molecular graph.

### INTRODUCTION

Wiener index, PI index, Shultz index, Szeged 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.,<sup>[1-2]</sup>, Gao et al.,<sup>[3-4]</sup>, Gao and Shi<sup>[5]</sup>, Gao and Wang<sup>[6]</sup>, Xi and Gao<sup>[7-8]</sup>, Xi et al.,<sup>[9]</sup>, Gao et al.,<sup>[10]</sup> for more detail). The notation and terminology used but undefined in this paper can be found in<sup>[11]</sup>.

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  $u$ . The Szeged index is closely related to the Wiener index and de-

finied as

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

Some conclusion for Szeged index can refer to<sup>[12]</sup> and<sup>[13]</sup>. 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 the distance 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 Szeged index 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  $r$  hanging 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  $\tilde{W}_n$ .

In this paper, we present the Szeged polynomial and edge Szeged polynomial of  $\tilde{F}_n$  and  $\tilde{W}_n$ .

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

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

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

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

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

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

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  $P_n = v_1 v_2 \dots v_n$  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  $v_i$  ( $1 \leq i \leq n$ ). Let  $v_{i,i+1}^1, v_{i,i+1}^2, \dots, v_{i,i+1}^r$  be the  $r$  hanging vertices of  $v_{i,i+1}$  ( $1 \leq i \leq n-1$ ). Let  $v$  be a vertex in  $\tilde{F}_n$  beside  $P_n$ , and the  $r$  hanging vertices of  $v$  be  $v^1, v^2, \dots, v^r$ .

By virtue of the definition of Szeged polynomial, we yield

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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  $P_n = v_1 v_2 \dots v_n$  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  $v_i$  ( $1 \leq i \leq n$ ). Let  $v_{i,i+1}^1, v_{i,i+1}^2, \dots, v_{i,i+1}^r$  be the  $r$  hanging vertices of  $(1 \leq i \leq n-1)$ . 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 of the definition of edge Szeged polynomial, we yield

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

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

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

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  $C_n = v_1 v_2 \dots v_n$  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  $v^1, v^2, \dots, v^r$  be the  $r$  hanging vertices of  $v$  and  $v_i^1, v_i^2, \dots, v_i^r$  be the  $r$  hanging vertices of  $v_i$  ( $1 \leq i \leq n$ ). Let  $v_{n,n+1} = v_{1,n}$  and  $v_{i,i+1}^1, v_{i,i+1}^2, \dots, v_{i,i+1}^r$  be the  $r$  hanging vertices of  $(1 \leq i \leq n)$ . Let  $v_{n,n+1} = v_{n,1}$ ,  $v_{n+1} = v_1$ . In view of the definition of edge Szeged polynomial, we deduce

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

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

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

### CONCLUSION

In this paper, we present the Szeged polynomial and edge Szeged 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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