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Shultz polynomial and modified shultz polynomial of certain special molecular graphs

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ABSTRACT

Chemical compounds and drugs are often modeled as graphs where each vertex represents an atom of molecule, and covalent bounds between atoms are represented by edges between the corresponding vertices. This graph derived from a chemical compounds is often called its molecular graph, and can be different structures. In this paper, we determine the Shultz polynomial and modified Shultz polynomial of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their r-corona molecular graphs.
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KEYWORDS

Chemical graph theory;
Shultz polynomial;
Modified shultz polynomial;
r-Corona molecular graph.

INTRODUCTION

Wiener index, Gutman index, Shultz 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 or degree-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].

Then the Shultz index of molecular graph G is defined as

$$Sc(G)=\sum_{\{u,v\}\subseteq V(G)}(d(u)+d(v))d(u,v).$$

The Shultz polynomial is denoted as

$$Sc(G,x)=\sum_{\{u,v\}\subseteq V(G)}(d(u)+d(v))x^{d(u,v)}.$$

The graphs considered in this paper are simple and connected. Then the Gutman index (or modified Shultz index) of G is defined by Gutman[9] as

$$Gut(G)=\sum_{\{u,v\}\subseteq V(G)}d(u)d(v)d(u,v).$$

Similarly, the modified Shultz polynomial is defined as

$$Sc^{*}(G,x)=\sum_{\{u,v\}\subseteq V(G)}(d(u)d(v))x^{d(u,v)}.$$

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 Shultz polynomial and modified Shultz polynomial of $I_r(F_n)$, $I_r(W_n)$, $I_r(\tilde{F}_n)$ and $I_r(\tilde{W}_n)$.

SHULTZ POLYNOMIAL

Theorem 1. $Sc(I_r(F_n),x) = (r^2(2n+1)+r(13n-5)+2n^2+5n-7)x+(r^2(9n-3)+r(2n^2+5n-15)$
$+\frac{5n^2-18n+35}{2})x^2+(r^2(n^2-n+1)+r(4n^2-11n+17))x^3+r^2(n^2-3n+2)x^4$.

Proof. Let $P_n=v_1v_2\ldots v_n$ and the r hanging vertices of v_i be v_i^1, $v_i^2,\ldots,$ v_i^r $(1\leq in)$. 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 Shultz polynomial, we have

$$Sc(I_r(F_n),x)=\sum_{i=1}^{r-1}\sum_{j=i+1}^{r}(d(v^i)+d(v^j))x^{d(v^i,v^j)}+\sum_{i=1}^{r}(d(v)+d(v^i))x^{d(v,v^i)}$$

$$+\sum_{i=1}^{n}(d(v)+d(v_i))x^{d(v,v_i)}+\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v)+d(v_i^j))x^{d(v,v_i^j)}+\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)+d(v^j))x^{d(v_i,v^j)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r}(d(v_i^j)+d(v^k))x^{d(v_i^j,v^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}(d(v_i)+d(v_j))x^{d(v_i,v_j)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)+d(v_i^j))x^{d(v_i,v_i^j)}+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r}(d(v_i)+d(v_j^k))x^{d(v_i,v_j^k)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}(d(v_i^j)+d(v_i^k))x^{d(v_i^j,v_i^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_i^k)+d(v_j^t))x^{d(v_i^k,v_j^t)}$$

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

$$+2nr^2x^3+(r(2n-2)+n^2+2n-5)x+(r(n^2-3n+6)+\frac{5n^2-18n+35}{2})x^2+(2nr^2+r(8n-4))x$$

$$+ \quad r((r(2n-4)+4n-18)x^2+(r(n^2-3n+3)+4n^2-11n+17)x^3) \quad + \quad nr(r-1)x^2 \quad +$$
$$r^2((2n-2)x^3+(n^2-3n+2)x^4)$$

$$=(r^2(2n+1)+r(13n-5)+2n^2+5n-7)x+(r^2(9n-3)+r(2n^2+5n-15)+\frac{5n^2-18n+35}{2})x^2$$

$$+(r^2(n^2-n+1)+r(4n^2-11n+17))x^3+r^2(n^2-3n+2)x^4.$$

Corollary 1. $Sc(F_n,x)=(2n^2+5n-7)x+(\frac{5n^2-18n+35}{2})x^2$.

Theorem 2. $Sc(I_r(W_n),x)=(r^2(n+1)+r(8n+1)+n^2+9n)x+(r^2(n^2+n+1)+r(n^2+4n-1)$
$+3n^2-9n)x^2+(4nr^2+r(n-1)+4n-6)x^3+((n^2-2n)r^2+r(n^2-n)+3n^3+6n+2)x^4$.

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 ($1\le in$). 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 Shultz polynomial, we deduce

$$Sc(I_r(W_n),x)=\sum_{i=1}^{r-1}\sum_{j=i+1}^{r}(d(v^i)+d(v^j))x^{d(v^i,v^j)}+\sum_{i=1}^{r}(d(v)+d(v^i))x^{d(v,v^i)}$$

$$+\sum_{i=1}^{n}(d(v)+d(v_i))x^{d(v,v_i)}+\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v)+d(v_i^j))x^{d(v,v_i^j)}+\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)+d(v^j))x^{d(v_i,v^j)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r}(d(v_i^j)+d(v^k))x^{d(v_i^j,v^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}(d(v_i)+d(v_j))x^{d(v_i,v_j)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)+d(v_i^j))x^{d(v_i,v_i^j)}+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r}(d(v_i)+d(v_j^k))x^{d(v_i,v_j^k)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}(d(v_i^j)+d(v_i^k))x^{d(v_i^j,v_i^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_i^k)+d(v_j^t))x^{d(v_i^k,v_j^t)}$$

$$=r(r-1)x^2+r(n+r+1)x+n(n+2r+3)x+nr(n+r+1)x^2+nr(r+4)x^2+2nr^2x^3$$
$$+(6n+rn)x+(r(n^2-2n)+(3n^2-9n))x^2+nr(r+4)x+(r(n-1)+4n-6)x^3+(r(n^2-n)+3n^3+6n+2)x^4$$
$$+n(r^2-r)x^2+2nr^2x^3+(n^2-2n)r^2x^4$$
$$=(r^2(n+1)+r(8n+1)+n^2+9n)x+(r^2(n^2+n+1)+r(n^2+4n-1)+3n^2-9n)x^2$$
$$+(4nr^2+r(n-1)+4n-6)x^3+((n^2-2n)r^2+r(n^2-n)+3n^3+6n+2)x^4. \square$$

Corollary 2. $Sc(W_n,x)=(n^2+9n)x+(3n^2-9n)x^2+(4n-6)x^3+(3n^3+6n+2)x^4$.

Theorem 3. $Sc(I_r(\tilde{F}_n),x)=(3nr^2+r(14n-6)+n^2+3n-2)x+(4nr^2+r(2n^2+4n-4)$
$+4n^2-4n)x^2+(r^2(n^2+3n-2)+r(7n^2-8n+1)+(3n^2-13n+10))x^3+(r^2(2n^2-n-1)$
$+r(5n^2-12n+8)+6n^2-18n+15)x^4+(r^2(3n^2-9n+5)+r(3n^2-15n+9))x^5+(n-2)(n-2)r^2x^6$.

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 v_i ($1\le i\le n$). 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 Shultz polynomial, we get

$$Sc(I_r(\tilde{F}_n),x)=\sum_{i=1}^{r-1}\sum_{j=i+1}^{r}(d(v^i)+d(v^j))x^{d(v^i,v^j)}+\sum_{i=1}^{r}(d(v)+d(v^i))x^{d(v,v^i)}$$

$$+\sum_{i=1}^{n}(d(v)+d(v_i))x^{d(v,v_i)}+\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v)+d(v_i^j))x^{d(v,v_i^j)}+\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)+d(v^j))x^{d(v_i,v^j)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r}(d(v_i^j)+d(v^k))x^{d(v_i^j,v^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}(d(v_i)+d(v_j))x^{d(v_i,v_j)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)+d(v_i^j))x^{d(v_i,v_i^j)}+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r}(d(v_i)+d(v_j^k))x^{d(v_i,v_j^k)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}(d(v_i^j)+d(v_i^k))x^{d(v_i^j,v_i^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_i^k)+d(v_j^t))x^{d(v_i^k,v_j^t)}$$

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

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

$$+\sum_{i=1}^{n}\sum_{j=1}^{n-1}(d(v_i)+d(v_{j,j+1}))x^{d(v_i,v_{j,j+1})}+\sum_{i=1}^{n}\sum_{j=1}^{n-1}\sum_{k=1}^{r}(d(v_i)+d(v^k_{j,j+1}))x^{d(v_i,v^k_{j,j+1})}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n-1}(d(v_i^j)+d(v_{k,k+1}))x^{d(v_i^j,v_{k,k+1})}+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n-1}\sum_{t=1}^{r}(d(v_i^j)+d(v^r_{k,k+1}))x^{d(v_i^j,v^r_{k,k+1})}$$

$$+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1}(d(v_{i,i+1})+d(v_{j,j+1}))x^{d(v_{i,i+1},v_{j,j+1})}+\sum_{i=1}^{n-1}\sum_{j=1}^{r}(d(v_{i,i+1})+d(v^j_{i,i+1}))x^{d(v_{i,i+1},v^j_{i,i+1})}$$

$$+\sum_{i=1}^{n-1}\sum_{j\in\{1,2,\cdots,n-1\}-i}\sum_{k=1}^{r}(d(v_{i,i+1})+d(v^k_{j,j+1}))x^{d(v_{i,i+1},v^k_{j,j+1})}+\sum_{i=1}^{n-1}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}(d(v^j_{i,i+1})+d(v^k_{i,i+1}))x^{d(v^j_{i,i+1},v^k_{i,i+1})}$$

$$+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v^k_{i,i+1})+d(v^t_{j,j+1}))x^{d(v^k_{i,i+1},v^t_{j,j+1})}$$

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

$$(r(n^2-n)+(3n^2-5n+2))x^2+(2nr^2+r(8n-4))x+(r^2(n^2-n)+r(4n^2-6n+2))x^3+nr(r-1)x^2$$

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

$$(r(2n^2-5n+3)+(3n^2-13n+10))x^3+(r(n^2-2n+1)+(4n^2-10n+7))x^4+(r^2+3r)(n-1)^2x^4+2r^2(n-1)^2x^5$$

$$+(r+2)(n-2)^2x^4+(r^2+3r)(n-1)x+(r^2+3r)(n^2-5n+3)x^5+r(n-1)(r-1)x^2+(n-2)(n-2)r^2x^6$$

$$=(3nr^2+r(14n-6)+n^2+3n-2)x+(4nr^2+r(2n^2+4n-4)+4n^2-4n)x^2+(r^2(n^2+3n-2)+r(7n^2-8n+1)$$

$$+(3n^2-13n+10))x^3+(r^2(2n^2-n-1)+r(5n^2-12n+8)+6n^2-18n+15)x^4 .$$

$$+(r^2(3n^2-9n+5)+r(3n^2-15n+9))x^5+(n-2)(n-2)r^2x^6 .$$

Corollary 3. $Sc(\tilde{F}_n,x)=(n^2+3n-2)x\ (4n^2-4n)x^2+(3n^2-13n+10)x^3+\ (6n^2-18n+15)x^4$.

Theorem 4. $Sc(I_r(\tilde{W}_n),x)=(r^2(n+1)+r(8n+1)+(n^2+3n))x+(r^2(4n+1)+r(2n^2+4n-1)$

$$+4n^2-n)x^2+(r^2(n^2+3n)+r(7n^2-2n)+5n^2-5n)x^3+(r^2(3n^3-n)+r(8n^2-9n)+2n^2-4n)x^4$$

$+(r^2(3n^2-4n)+r(3n^2-6n))x^5+r^2(n^2-2n)x^6$.

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 $v_{n,n+1}=v_{1,n}$ and $v_{i,i+1}^1$, $v_{i,i+1}^2$,…, $v_{i,i+1}^r$ be the r hanging vertices of $v_{i,i+1}$ $(1\le in)$. In view of the definition of Shultz polynomial, we yield

$$Sc(I_r(\tilde{W}_n),x)=\sum_{i=1}^{r-1}\sum_{j=i+1}^{r}(d(v^i)+d(v^j))x^{d(v^i,v^j)}+\sum_{i=1}^{r}(d(v)+d(v^i))x^{d(v,v^i)}$$

$$+\sum_{i=1}^{n}(d(v)+d(v_i))x^{d(v,v_i)}+\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v)+d(v_i^j))x^{d(v,v_i^j)}+\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)+d(v^j))x^{d(v_i,v^j)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r}(d(v_i^j)+d(v^k))x^{d(v_i^j,v^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}(d(v_i)+d(v_j))x^{d(v_i,v_j)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)+d(v_i^j))x^{d(v_i,v_i^j)}+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r}(d(v_i)+d(v_j^k))x^{d(v_i,v_j^k)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}(d(v_i^j)+d(v_i^k))x^{d(v_i^j,v_i^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_i^k)+d(v_j^t))x^{d(v_i^k,v_j^t)}$$

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

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

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

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n}(d(v_i^j)+d(v_{k,k+1}))x^{d(v_i^j,v_{k,k+1})}+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n}\sum_{t=1}^{r}(d(v_i^j)+d(v_{k,k+1}^r))x^{d(v_i^j,v_{k,k+1}^r)}$$

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

$$+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r}(d(v_{i,i+1})+d(v_{j,j+1}^k))x^{d(v_{i,i+1},v_{j,j+1}^k)}+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}(d(v_{i,i+1}^j)+d(v_{i,i+1}^k))x^{d(v_{i,i+1}^j,v_{i,i+1}^k)}$$

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

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

$$nr(r+3)x^3+2r^2nx^4+(2r+5)(n^2-n)x^3+(r^2+4r)(n^2-n)x^4+(r^2+3r)(n^2-n)x^4+2r^2(n^2-n)x^5+$$
$$(r+2)(n^2-2n)x^4+nr(r+3)x+(r^2+3r)(n^2-2n)x^5+n(r^2-r)x^2+r^2(n^2-2n)x^6$$
$$=(r^2(n+1)+r(8n+1)+(n^2+3n))x+(r^2(4n+1)+r(2n^2+4n-1)+4n^2-n)x^2+(r^2(n^2+3n)$$
$$+r(7n^2-2n)+5n^2-5n)x^3+(r^2(3n^3-n)+r(8n^2-9n)+2n^2-4n)x^4+(r^2(3n^2-4n)$$
$$+r(3n^2-6n))x^5+r^2(n^2-2n)x^6.$$

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

MODIFIED SHULTZ POLYNOMIAL

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

Theorem 5. $Sc^*(I_r(F_n),x)=(r^2(n^2+n+1)+r(4n^2+2n-2)+(3n^2-2n))x+(r^2(n^2+\frac{3n}{2}+\frac{1}{2})$
$+r(4n^2-\frac{11}{2}n+\frac{3}{2})+4n^2-15n+12)x^2+(nr^2+r(n^2-2n+1)+(n^2-7n+5))x^3+r^2\frac{n(n-1)}{2}x^4$.

Proof. By the definition of modified Shultz polynomial, we have

$$Sc^*(I_r(F_n),x)=\sum_{i=1}^{r-1}\sum_{j=i+1}^{r}d(v^i)d(v^j)x^{d(v^i,v^j)}+\sum_{i=1}^{r}d(v)d(v^i)x^{d(v,v^i)}+\sum_{i=1}^{n}d(v)d(v_i)x^{d(v,v_i)}+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v)d(v_i^j)x^{d(v,v_i^j)}$$
$$+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i)d(v^j)x^{d(v_i,v^j)}+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r}d(v_i^j)d(v^k)x^{d(v_i^j,v^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}d(v_i)d(v_j)x^{d(v_i,v_j)}+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i)d(v_i^j)x^{d(v_i,v_i^j)}$$
$$+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r}d(v_i)d(v_j^k)x^{d(v_i,v_j^k)}+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}d(v_i^j)d(v_i^k)x^{d(v_i^j,v_i^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}d(v_i^k)d(v_j^t)x^{d(v_i^k,v_j^t)}$$

$$=\frac{r^2-r}{2}x^2+(r+n)rx+(r^2n+r(n^2+3n-2)+(3n^2-2n))x+nr(r+n)x^2+r(rn+3n-2)x^2+nr^2x^3+$$
$$(r^2(n^2-n)+r(3n^2-8n+4)+(4n^2-15n+12))x^2+nr(rn+3n-2)x+(r(n^2-2n+1)+(n^2-7n+5))x^3+$$
$$\frac{(r^2-r)n}{2}x^2+r^2\frac{n(n-1)}{2}x^4$$
$$=(r^2(n^2+n+1)+r(4n^2+2n-2)+(3n^2-2n))x+(r^2(n^2+\frac{3n}{2}+\frac{1}{2})+r(4n^2-\frac{11}{2}n+\frac{3}{2})$$
$$+4n^2-15n+12)x^2+(nr^2+r(n^2-2n+1)+(n^2-7n+5))x^3+r^2\frac{n(n-1)}{2}x^4.$$

Corollary 5. $Sc^*(F_n,x)=(3n^2-2n)x+(4n^2-15n+12)x^2+(n^2-7n+5)x^3$.

Theorem 6. $Sc^*(I_r(W_n),x)=(r^2(2n+1)+r(n^2+7n)+3n^2)x+(\frac{n^2+4n+1}{2}r^2+r(4n^2-\frac{n}{2}-\frac{1}{2})$
$+\frac{9(n^2-n)}{2})x^2+(r^2(n^2-n)+r(3n^2-6n))x^3+r^2\frac{n(n-1)}{2}x^4$.

Proof. By the definition of modified Shultz polynomial, we have

$$Sc^*(I_r(W_n),x)=\sum_{i=1}^{r-1}\sum_{j=i+1}^{r}d(v^i)d(v^j)x^{d(v^i,v^j)}+\sum_{i=1}^{r}d(v)d(v^i)x^{d(v,v^i)}+\sum_{i=1}^{n}d(v)d(v_i)x^{d(v,v_i)}+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v)d(v_i^j)x^{d(v,v_i^j)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i)d(v^j)x^{d(v_i,v^j)}+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r}d(v_i^j)d(v^k)x^{d(v_i^j,v^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}d(v_i)d(v_j)x^{d(v_i,v_j)}+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i)d(v_i^j)x^{d(v_i,v_i^j)}$$

$$+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r}d(v_i)d(v_j^k)x^{d(v_i,v_j^k)}+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}d(v_i^j)d(v_i^k)x^{d(v_i^j,v_i^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}d(v_i^k)d(v_j^t)x^{d(v_i^k,v_j^t)}$$

$$=\frac{r^2-r}{2}x^2+r(r+n)x+n(r+n)(3+r)x+nr(r+n)x^2+nr(3+r)x^2+nr^2x^3+(3+r)^2\frac{n^2-n}{2}x^2+nr(3+r)x$$

$$+r(n^2-2n)(3+r)x^3+\frac{(r^2-r)n}{2}x^2+r^2\frac{n(n-1)}{2}x^4$$

$$=(r^2(2n+1)+r(n^2+7n)+3n^2)x+(\frac{n^2+4n+1}{2}r^2+r(4n^2-\frac{n}{2}-\frac{1}{2})+\frac{9(n^2-n)}{2})x^2+(r^2(n^2-n)$$

$$+r(3n^2-6n))x^3+r^2\frac{n(n-1)}{2}x^4.$$

Corollary 6. $Sc^*(W_n,x)=3n^2x+(\frac{9(n^2-n)}{2})x^2$.

Theorem 7. $Sc^*(I_r(\tilde{F}_n),x)=(3nr^2+r(n^2+9n-6)+(3n^2-2n))x+(r^2(\frac{3}{2}n^2+\frac{3}{2}n+\frac{3}{2})$

$$+r(7n^2-7n+\frac{7}{2})+\frac{9n^2-17n+14}{2})x^2+(r^2(2n^2+n-1)+r(8n^2-11n+8)+(6n^2-18n+15))x^3$$

$$+(r^2(\frac{7}{2}n^2-\frac{11}{2}n+3)+r(5n^2-14n+10)+(5n^2-16n+14))x^4+(r^2(n^2-4n+3)$$

$$+r(2n^2-8n+7))x^5+\frac{(n-2)^2}{2}r^2x^6.$$

Proof. By virtue of the definition of modified Shultz polynomial, we get

$$Sc^*(I_r(\tilde{F}_n),x)=\sum_{i=1}^{r-1}\sum_{j=i+1}^{r}d(v^i)d(v^j)x^{d(v^i,v^j)}+\sum_{i=1}^{r}d(v)d(v^i)x^{d(v,v^i)}+\sum_{i=1}^{n}d(v)d(v_i)x^{d(v,v_i)}+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v)d(v_i^j)x^{d(v,v_i^j)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i)d(v^j)x^{d(v_i,v^j)}+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r}d(v_i^j)d(v^k)x^{d(v_i^j,v^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}d(v_i)d(v_j)x^{d(v_i,v_j)}+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i)d(v_i^j)x^{d(v_i,v_i^j)}$$

$$+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r}d(v_i)d(v_j^k)x^{d(v_i,v_j^k)}+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}d(v_i^j)d(v_i^k)x^{d(v_i^j,v_i^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}d(v_i^k)d(v_j^t)x^{d(v_i^k,v_j^t)}$$

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

$$+\sum_{i=1}^{r}\sum_{j=1}^{n-1}\sum_{k=1}^{r} d(v^i)d(v^k_{j,j+1})x^{d(v^i,v^k_{j,j+1})}+\sum_{i=1}^{n}\sum_{j=1}^{n-1} d(v_i)d(v_{j,j+1})x^{d(v_i,v_{j,j+1})}+\sum_{i=1}^{n}\sum_{j=1}^{n-1}\sum_{k=1}^{r} d(v_i)d(v^k_{j,j+1})x^{d(v_i,v^k_{j,j+1})}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n-1} d(v^j_i)d(v_{k,k+1})x^{d(v^j_i,v_{k,k+1})}+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n-1}\sum_{t=1}^{r} d(v^j_i)d(v^r_{k,k+1})x^{d(v^j_i,v^r_{k,k+1})}+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1} d(v_{i,i+1})d(v_{j,j+1})x^{d(v_{i,i+1},v_{j,j+1})}$$

$$+\sum_{i=1}^{n-1}\sum_{j=1}^{r} d(v_{i,i+1})d(v^j_{i,i+1})x^{d(v_{i,i+1},v^j_{i,i+1})}+\sum_{i=1}^{n-1}\sum_{j\in\{1,2,\cdots,n-1\}-i}\sum_{k=1}^{r} d(v_{i,i+1})d(v^k_{j,j+1})x^{d(v_{i,i+1},v^k_{j,j+1})}$$

$$+\sum_{i=1}^{n-1}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v^j_{i,i+1})d(v^k_{i,i+1})x^{d(v^j_{i,i+1},v^k_{i,i+1})}+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v^k_{i,i+1})d(v^t_{j,j+1})x^{d(v^k_{i,i+1},v^t_{j,j+1})}$$

$$=\frac{r^2-r}{2}x^2+r(n+r)x+(r^2n+r(n^2+3n-2)+(3n^2-2n))x+(n^2r+r^2n)x^2+(r^2n^2+r(3n^2-2n))x^2$$

$$+nr^2x^3+(r^2\frac{n^2-n}{2}+r(3n^2-5n+2)+\frac{9n^2-21n+14}{2})x^2+(r^2n+r(3n-2))x+(r^2n^2+r(3n^2-2n))x^3+$$

$$\frac{(r^2-r)n}{2}x^2+r^2\frac{n(n-1)}{2}x^4+(r^2+r(n+2)+2n)x^2+(r^2(n-1)+nr)x^3+(r^2(n-1)+r(2n-2))x^3+$$

$$r^2(n-1)x^4+(r^2(n^2-2n+1)+r(5n^2-12n+10)+(6n^2-18n+15))x^3+(r(n^2-2n+1)+(3n^2-8n+6))x^4$$

$$+(r^2(n^2-2n+1)+r(2n^2-4n+2))x^4+r^2(n-1)^2x^4+(r^2(n^2-2n+2)+r(2n^2-8n+7)+(2n^2-8n+8))x^4$$

$$+(r^2(n-1)+r(2n-2))x+(r^2(n^2-4n+3)+r(2n^2-8n+7))x^5+\frac{(r^2-r)n}{2}x^2+\frac{(n-2)^2}{2}r^2x^6$$

$$=(3nr^2+r(n^2+9n-6)+(3n^2-2n))x+(r^2(\frac{3}{2}n^2+\frac{3}{2}n+\frac{3}{2})+r(7n^2-7n+\frac{7}{2})+\frac{9n^2-17n+14}{2})x^2$$

$$+(r^2(2n^2+n-1)+r(8n^2-11n+8)+(6n^2-18n+15))x^3+(r^2(\frac{7}{2}n^2-\frac{11}{2}n+3)+r(5n^2-14n+10)$$

$$+(5n^2-16n+14))x^4+(r^2(n^2-4n+3)+r(2n^2-8n+7))x^5+\frac{(n-2)^2}{2}r^2x^6.$$

Corollary 7. $Sc^*(\tilde{F}_n,x)=(3n^2-2n)x+(\frac{9n^2-17n+14}{2})x^2+(6n^2-18n+15)x^3+(5n^2-16n+14)x^4$.

Theorem 8. $Sc^*(I_r(\tilde{W}_n),x)=(r^2(3n+1)+r(n^2+9n)+3n^2)x+(r^2(\frac{9}{2}n-\frac{n}{2}+\frac{1}{2})+r(5n^2+n-\frac{1}{2})$

$$+\frac{13}{2}n^2-\frac{9}{2}n)x^2+(r^2(2n^2+n)+r(n^3+5n^2-4n)+2n^3-3n^2)x^3+(r^2(\frac{11}{2}n^2-\frac{13}{2}n)+r(5n^2-5n)$$

$$+2n^2-4n)x^4+(r^2(2n^2-3n)+r(2n^2-4n))x^5+\frac{(n-2)^2}{2}r^2x^6.$$

Proof. In view of the definition of modified Shultz polynomial, we deduce

$$Sc^*(I_r(\tilde{W}_n),x)=\sum_{i=1}^{r-1}\sum_{j=i+1}^{r}d(v^i)d(v^j)x^{d(v^i,v^j)}+\sum_{i=1}^{r}d(v)d(v^i)x^{d(v,v^i)}+\sum_{i=1}^{n}d(v)d(v_i)x^{d(v,v_i)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v)d(v_i^j)x^{d(v,v_i^j)}+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i)d(v^j)x^{d(v_i,v^j)}+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r}d(v_i^j)d(v^k)x^{d(v_i^j,v^k)}+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}d(v_i)d(v_j)x^{d(v_i,v_j)}$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i)d(v_i^j)x^{d(v_i,v_i^j)}+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r}d(v_i)d(v_j^k)x^{d(v_i,v_j^k)}+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}d(v_i^j)d(v_i^k)x^{d(v_i^j,v_i^k)}$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}d(v_i^k)d(v_j^t)x^{d(v_i^k,v_j^t)}+\sum_{i=1}^{n}d(v)d(v_{i,i+1})x^{d(v,v_{i,i+1})}+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v)d(v_{i,i+1}^j)x^{d(v,v_{i,i+1}^j)}$$

$$+\sum_{i=1}^{r}\sum_{j=1}^{n}d(v^i)d(v_{j,j+1})x^{d(v^i,v_{j,j+1})}+\sum_{i=1}^{r}\sum_{j=1}^{n}\sum_{k=1}^{r}d(v^i)d(v_{j,j+1}^k)x^{d(v^i,v_{j,j+1}^k)}+\sum_{i=1}^{n}\sum_{j=1}^{n}d(v_i)d(v_{j,j+1})x^{d(v_i,v_{j,j+1})}+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r}d(v_i)d(v_{j,j+1}^k)x^{d(v_i,v_{j,j+1}^k)}+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n}d(v_i^j)d(v_{k,k+1})x^{d(v_i^j,v_{k,k+1})}+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n}\sum_{t=1}^{r}d(v_i^j)d(v_{k,k+1}^r)x^{d(v_i^j,v_{k,k+1}^r)}$$

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

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_{i,i+1})d(v_{i,i+1}^j)x^{d(v_{i,i+1},v_{i,i+1}^j)}+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r}d(v_{i,i+1})d(v_{j,j+1}^k)x^{d(v_{i,i+1},v_{j,j+1}^k)}$$

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

$$=\frac{r^2-r}{2}x^2+(r^2+nr)x+(r^2n+r(n^2+3n)+3n^2)x+(r^2n+rn^2)x^2+(r^2n+3rn)x^2+nr^2x^3+$$

$$(r^2\frac{n^2-n}{2}+r(3n^2-3n)+\frac{9n^2-9n}{2})x^2+(r^2n+3rn)x+(r^2(n^2-n)+r(3n^2-3n))x^3+\frac{(r^2-r)n}{2}x^2$$

$$+r^2\frac{n(n-1)}{2}x^4+(r^2n+r(n^2+2n)+2n^2)x^2+(r^2n+rn^2)x^3+(r^2n+2rn)x^3+r^2nx^4+$$

$$(r^2(n^2-n)+r(n^3+n^2-3n)+(2n^3-3n^2))x^3+(r^2(n^2-n)+r(3n^2-3n))x^4+(r^2(n^2-n)+r(2n^2-2n))x^4$$

$$+r^2(n^2-n)x^5+(r^2(n^2-n)+r(2n^2-4n)+(2n^2-4n))x^4+(r^2n+2rn)x+(r^2(n^2-2n)+r(2n^2-4n))x^5$$

$$+\frac{(r^2-r)n}{2}x^2+\frac{(n-2)^2}{2}r^2x^6$$

$$=(r^2(3n+1)+r(n^2+9n)+3n^2)x+(r^2(\frac{9}{2}n-\frac{n}{2}+\frac{1}{2})+r(5n^2+n-\frac{1}{2})+\frac{13}{2}n^2-\frac{9}{2}n)x^2$$

$$+(r^2(2n^2+n)+r(n^3+5n^2-4n)+2n^3-3n^2)x^3+(r^2(\frac{11}{2}n^2-\frac{13}{2}n)+r(5n^2-5n)+2n^2-4n)x^4$$

$$+(r^2(2n^2-3n)+r(2n^2-4n))x^5+\frac{(n-2)^2}{2}r^2x^6.$$

Corollary 8. $Sc^*(\tilde{W}_n,x)=3n^2x+(\frac{13}{2}n^2-\frac{9}{2}n)x^2+(2n^3-3n^2)x^3+(2n^2-4n)x^4$.

CONCLUSION

In this paper, we present the Shultz polynomial and modified Shultz 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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