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Schultz index, Modified Schultz index, Schultz polynomial and Modified Schultz polynomial of alkanes

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Abstract

The topology of molecule in chemistry can be graphically represented through demonstrating the atoms connection. Using a graph, the atoms are represented by points, while their corresponding covalent bonds are denoted by the edges. A topological index of such graphical modeling is studied to give rise to the numerically graphical parameters. In the current analysis, general formulas are established depending upon some topological indices of alkanes for particular sorts of chemical trees. These indices are Schultz index, Modified Schultz index, Schultz polynomial and Modified Schultz polynomial.

1. INTRODUCTION:

Let G =(V,E) be a simple finite molecular graph having a vertex set V(G) and edge set E(G). If e ∈ G and connecting the vertices u and v, then e = uv.

Moreover, if G is a connected graph, while u and v are two of its vertices, then the distance d(u, v) between the vertices equals to the length of the shortest path connecting them in G. Also the number of adjacent vertices v indicates its degree, which is denoted by dv. In chemical graph theory, invariant polynomials for any graphs have usually integer coefficients. A topological index of G is a numeric quantity derived according to certain rules in chemistry, which can be used to characterize the property of molecule [8].

Topological indices in biology and chemistry was used for the first time in 1947 when chemist Harold Wiener [2] introduced Wiener index to demonstrate correlations between physico-chemical properties of organic compounds of molecular graphs.

Another based structure descriptors is the “molecular topological index” (Schultz index) was introduced by Harry P. Schultz in 1989 [1], while the Modified Schultz index was defined by S. Klavžar and I. Gutman in 1997 [5].

The Schultz index is defined as:

$$Sc(G) = \frac{1}{2} \sum_{\{u,v\} \subset V(G)} (\mathrm{du} + \mathrm{dv})\mathrm{d}\,(\mathrm{u}\,,\mathrm{v})$$

Where du and dv are the degrees of vertices u and v.

And the Modified Schultz index of G is defined as:

$$Sc^{*}(G) = \frac{1}{2} \sum_{\{u,v\} \subset V(G)} (\mathrm{du} + \mathrm{dv})\mathrm{d}\,(\mathrm{u}\,,\mathrm{v})$$

Two important polynomials are distinguished, which are “Schultz polynomial” and “Modified Schultz polynomial”. Schultz and Modified Schultz polynomials of G are respectively defined as:

$$Sc(G,x) = \frac{1}{2} \sum_{\{u,v\} \subset V(G)} (\mathrm{du} + \mathrm{dv})x^{\mathrm{d}\,(\mathrm{u}\,,\mathrm{v})}$$

$$Sc^{*}(G,x) = \frac{1}{2} \sum_{\{u,v\} \subset V(G)} (\mathrm{du.\,dv})x^{\mathrm{d}\,(\mathrm{u}\,,\mathrm{v})}$$

These based structure descriptors and their polynomials were extensively studied and computed before [1],[3],[4],[6] and [7].

2. RESULTS AND DISCUSSION

In this section, the general formulas are constructed for the Schultz index, Modified Schultz index, Schultz polynomial and Modified Schultz polynomial of some classes of chemical trees (alkanes).

Alkanes are hydrocarbons with only single bonds between the atoms, and they have a general formula C_nH_{2n+2} [8], where n is the number of carbon atoms (see Figure 1).

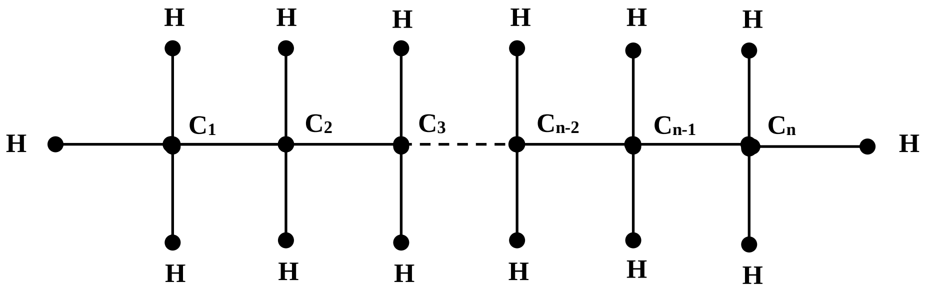

Figure 1: Class of C_nH_{2n+2}

Theorem 2.1. Let n be a positive integer, then the Schultz index (Sc) of a graph G denoted by G = C_nH_{2n+2} is as follows:

1. if n = 1 then G = CH_4 (see Figure 2) and Sc (CH_4) = 22

2. if n = 2 then G = C_2H_6 (see Figure 3) and Sc (C_2H_6) = 88

3. if n ≥ 3 then G = C_nH_{2n+2} and

$$Sc\,(CnH_{2n+2}) = 16n + 22 + 4\sum_{\substack{r=n\\ s=3}}^{\substack{n\\ 3}} rs + \frac{5}{2}\sum_{\substack{f=n\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} ft + 4\sum_{\substack{a=n-1\\ b=1}}^{\substack{n-1\\ 1}} ab \text{ , or}$$

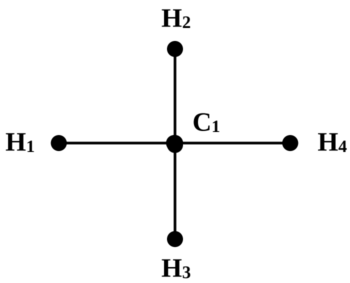

Figure 2: CH_4

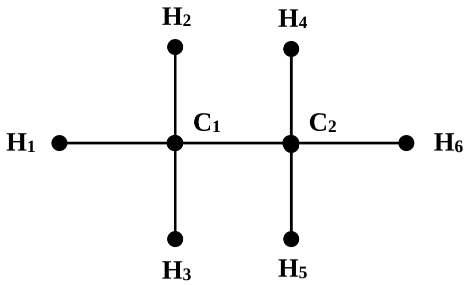

Figure 3: C_2H_6

$$Sc\,(CnH_{2n+2}) = \frac{1}{2}\left[32n + 44 + 2\sum_{\substack{r=4n\\ s=3}}^{\substack{n\\ 12}} rs + 5\sum_{\substack{f=n\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} ft + 8\sum_{\substack{a=n-1\\ b=1}}^{\substack{n-1\\ 1}} ab\right] \text{ where}$$

t is an odd number,

Proof :

1. Sc (CH_4) = $\frac{1}{2}\sum d\,(u+v)d\,(u\,,v)$

$$= \frac{1}{2}\,[4(1+4) + 6\,(1+1)2] \;= \frac{1}{2}\;44 = 22$$

2. Sc (C_2H_6) = $\frac{1}{2}[6(1+4) + 6(1+1).2 + 9(1+1).3 + 6(1+4).2 + (4+4).1]$

$= \frac{1}{2}\ [176] = 88$

3. We will prove by mathematical induction:

when n = 3, then G = C_3H_8 (see Figure 4)

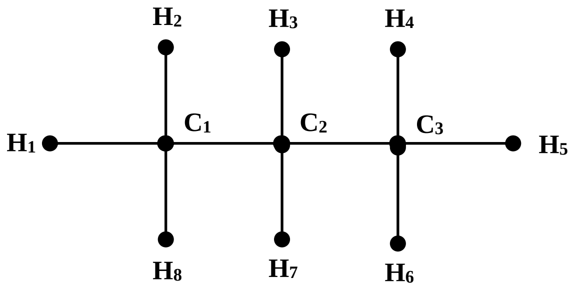

Figure 4: C_3H_8

Hence, by definition of Schultz index

Sc (G) = $\frac{1}{2}\sum(du + dv)\ d\ (u\ ,v)$

$=\frac{1}{2}[8(1+4) + 9(1+1).4 + 10(1+4).2 + 2(4+4).1 + 12(1+1).3 + (4+4).2 + 6(1+4).3 + 7(1+1).2] = \frac{1}{2}\ [434] = 217$

So, it is true that, with

Sc (C_3H_8) = 16 . 3 + 22 + $4\sum_{r=3,\ s=3}^{3,\ 3} rs + \frac{5}{2}\sum_{f=3,\ t=2m+4}^{\text{when } f=2,\ 2} ft + 4\sum_{a=2,\ b=1}^{2,\ 1} ab$

= 48 + 22 + 4 $[3\ .\ 3]$ + $\frac{5}{2}\ [3\ .\ 6 + 2\ .\ 10]$ + 4 $[2\ .\ 1 + 1\ .\ 2]$ = 217 , when n = 3

Let n = k and $G_k = C_kH_{2k+2}$, assuming that it is true for $k \geq 3$;

Sc (G_k) = 16 k + 22 + $4\sum_{r=k,\ s=3}^{k,\ 3} rs + \frac{5}{2}\sum_{f=k,\ t=2m+4}^{\text{when } f=2,\ 2} ft + 4\sum_{a=k-1,\ b=1}^{k-1,\ 1} ab$, or

$= \frac{1}{2}[32\ k + 44 + 2\sum_{r=4k,\ s=3}^{k,\ 12} rs + 5\sum_{f=k,\ t=2m+4}^{\text{when } f=2,\ 2} ft + 8\sum_{a=k-1,\ b=1}^{k-1,\ 1} ab]$

Constructing the graph $G_{k+1} = C_{k+1}H_{2k+4}$ can be done as:

Then, the graph G_k has the form (see Figure 5):

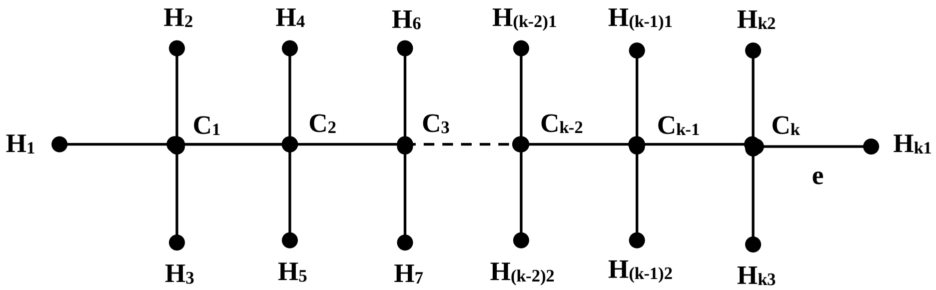

Figure 5: G_k

Thus, the position of the carbon vertex at the i^{th} position is denoted by C_i, the edge e is connecting the end hydrogen vertex H_{k1} in graph G_k with the vertex C_k.

Now, graph G* can be obtained by removing both the vertex H_{k1} and the edge e from graph G_k (see Figure 6):

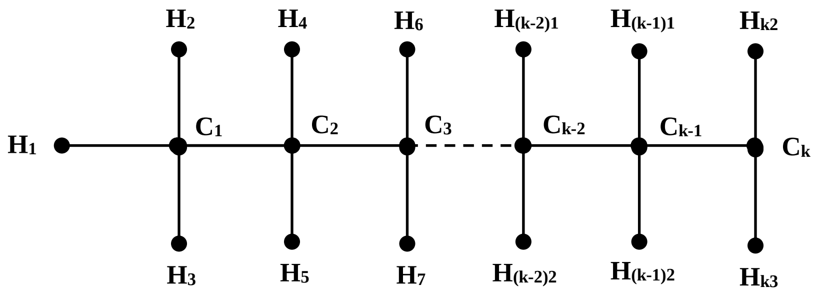

Figure 6: G^*

By removing $\frac{1}{2}\,[(1+4).1]$, which is the relationship of the vertex H_k with C_k according to the rule $\frac{1}{2}\sum(du+dv)d\,(u\,,v)$, and also removing $\frac{1}{2}\,[(1+1).2]$ twice, i.e. $\frac{1}{2}\,[2(1+1).2]$, which is relationship of the vertex H_{k1} with the two vertices H_{k2}, H_{k3}. Also, $\frac{1}{2}\,[3(1+1)(k+1)]$ is removed, which is the relationship of the vertex H_{k1} with the three vertex H_1, H_2 and H_3 that are away about (k + 1) from the removed vertex H_{k1}.

Also, $\frac{1}{2}\,[2(1+1)k]$ is removed, which is the relationship of the vertex H_{k1} with the two vertices H_4 and H_5, and remove $\frac{1}{2}\,[2(1+1)(k-1)]$ which is the relationship of the vertex H_{k1} with the two vertices H_6 and H_7. This procedure is followed until removing $\frac{1}{2}\,[2(1+1).3]$, which is the relationship of the vertex H_{k1} with the two vertices $H_{(k-1)1}$ and $H_{(k-1)2}$. This means that the series $2\sum_{\substack{r=4k\\ s=3}}^{\substack{k\\ 12}} rs$ after removing becomes $2\sum_{\substack{r=4k-2\\s=3}}^{\substack{k\\10}} rs$.

Later, $\frac{1}{2}\,[1(1+4).2]$ is removed, which is the relationship of the vertex H_{k1} with the vertex C_{k-1} and remove $\frac{1}{2}\,[(1+4).3]$,which is the relationship of the vertex H_{k1} with the vertex C_{k-2}. This procedure is followed until removing $\frac{1}{2}\,[(1+4).k]$, which is the relationship of the vertex H_{k1} with the vertex C_1. This means that the series $\sum_{\substack{f=k\\t=2m+4}}^{\substack{\text{when } f=2\\2}} 5ft$ becomes after the subsequent removing $\sum_{\substack{f=k\\t=2m+3}}^{\substack{\text{when } f=2\\2}} 5ft$, that is

$$Sc(G_k) = \frac{1}{2}[32k + 44 - 5 - 2.4 - 3(1+1)(k+1) + 2\sum_{\substack{r=(4k-2)\\s=3}}^{\substack{k\\10}} rs \; + \; 5\sum_{\substack{f=k\\t=2m+3}}^{\substack{\text{when } f=2\\2}} ft \; + \; 8\sum_{\substack{a=k-1\\b=1}}^{\substack{k-1\\1}} ab]$$

Connect the graph G* with the graph U (see Figure 7):

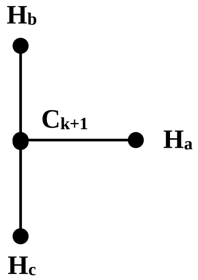

Figure 7**: U**

The graph G_{k+1} is obtained (see Figure 8):

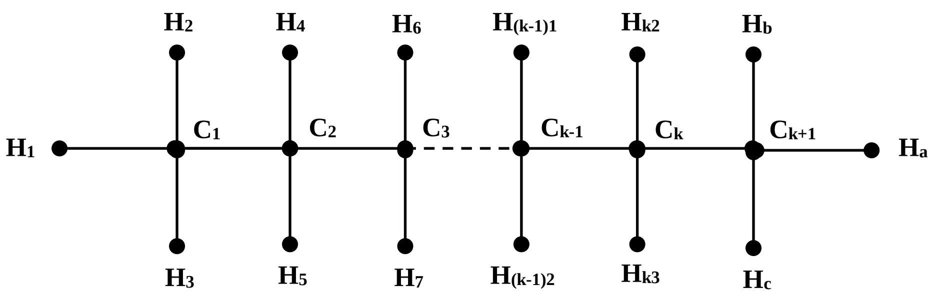

Figure 8**:** G_{k+1}

By adding the graph U to graph G*, $\frac{1}{2}$ $[3(1+4).1]$ is added, which is the relationship of the vertex C_{k+1} with the vertices H_a, H_b and H_c, and adding $\frac{1}{2}$ $[3(1+1).2]$, which is the relationship of the vertices H_a, H_b and H_c with each other. Later, $\frac{1}{2}$ $[9(1+1)(k+2)]$ is added, which is the relationship of the vertices H_a, H_b and H_c with the vertices H_1, H_2 and H_3. Then, $\frac{1}{2}$ $[6(1+1)(k+1)]$ is added as well, which is the relationship of the vertices H_a, H_b and H_c with the two vertices H_4 and H_5. This procedure is followed until adding $\frac{1}{2}$ $[6(1+1).3]$, which is the relationship of the vertices H_a, H_b and H_c with the two vertices H_{k2} and H_{k3}. This means that series $\sum_{L=3}^{k+1} 6(1+1)L$ will be added to series $2\sum_{\substack{r=4k-2\\s=3}}^{\substack{k\\10}} rs$;

$\sum_{\substack{r=4k-2\\s=3}}^{\substack{k\\10}} 2rs \ + \ 2\sum_{L=3}^{k+1} 6L$, where r =10, which means that it should be stopped when k=3

$$= 2\sum_{\substack{r=4k-2\\s=3}}^{\substack{k\\\text{when } k=3}} rs \ + 2\sum_{L=3}^{k} 6L + 12(k+1) \text{ , since } s = L$$

$$=2\sum_{\substack{r=4k-2\\s=3}}^{\substack{k\\\text{when } k=3}} S[r+6] + 12(k+1) = 2\sum_{\substack{r\\s=3}}^{\substack{k\\\text{when } k=3}} S[4k-2+6] + 12(k+1)$$

$$= 2\sum_{\substack{r\\s=3}}^{\substack{k\\\text{when } k=3}} S[4k+4] + 12(k+1) = 2\sum_{\substack{r\\s=3}}^{\substack{k\\\text{when } k=3}} 4.S[k+1] + 12(k+1)$$

$$= 2\sum_{\substack{r=k+1\\s=3}}^{\substack{k\\\text{when } k=4}} 4.Sr + 12(k+1)\ .$$

Now, $\frac{1}{2}$ $[3(1+4).2]$ is added, which is the relationship of the vertices H_a, H_b and H_c with vertex C_k, with adding $\frac{1}{2}$ $[3(1+4).3]$, which is the relationship of the vertices H_a, H_b and H_c with vertex C_{k-1}. This procedure should be followed until adding $\frac{1}{2}$ $[3(1+4)(k+1)]$, which is the relationship of the same vertices with the vertex C_1. Also, $\frac{1}{2}$ $[3(1+4)(k+1)]$ is added, which is the relationship of the vertices H_1, H_2 and H_3 with the vertex C_{k+1}, and adding $\frac{1}{2}$ $[3(1+4)k]$, which is the relationship of the vertices H_4 and H_5 with the vertex C_{k+1}, with adding $\frac{1}{2}$ $[2(1+4)(k-1)]$, which is the relationship of the two vertices H_6 and H_7 with the vertex C_{k+1} .The process is kept until adding $\frac{1}{2}$ $[2(1+4).2]$, which is the relationship of the two vertices H_{k2} and H_{k3} with the vertex C_{k+1}, that means adding $5\sum_{L=k}^{2} 5L + 5.6$ (k+1) to the series

$5\sum_{\substack{f=k\\ t=2m+3}}^{\substack{\text{when } f=2\\ 2}} ft$; where k is odd, that is

$5\sum_{\substack{f=k\\ t=2m+3}}^{\substack{\text{when } f=2\\ 2}} ft + 5\sum_{L=k}^{2} 5L + 5.6\,(k+1)$, since L = f then

$= 5\sum_{\substack{f=k\\ t=2m+3}}^{\substack{\text{when } f=2\\ 2}} f[t+5] + 5.6\,(k+1) = 5\sum_{\substack{f=k\\ t}}^{\substack{\text{when } f=2\\ 2}} f[2m+3+5] + 5.6\,(k+1)$

$= 5\sum_{\substack{f=k\\ t}}^{\substack{\text{when } f=2\\ 2}} f[2m+8] + 5.6\,(k+1) = 5\sum_{\substack{f=k\\ t=2m+8}}^{\substack{\text{when } f=2\\ 2}} ft + 5.6\,(k+1) = 5\sum_{\substack{f=k+1\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} ft$

Furthermore, $\frac{1}{2}\,[(4+4)k\,]$ needs to be added, which is the relationship of the vertex C_{k+1} with the vertex C_1 and adding $\frac{1}{2}\,[(4+4)(k-1)]$, which is the relationship of the vertex C_{k+1} with the vertex C_2 and keep adding until reaching that vertex $\frac{1}{2}\,[(4+4).1\,]$ is added, which is the relationship of the vertex C_{k+1} with the vertex C_k. This means that the series $\sum_{x=1}^{k} 8x$ is added to the series $8\sum_{\substack{a=k-1\\ b=`1}}^{\substack{(k-1)\\ 1}} ab$

This means $8\sum_{\substack{a=k-1\\ b=1}}^{\substack{(k-1)\\ 1}} ab + 8\sum_{x=1}^{k} x = 8\sum_{\substack{a=k-1\\ b=1}}^{\substack{(k-1)\\ 1}} ab + 8\sum_{x=1}^{k-1} x + 8k$; since x = b

$= 8\sum_{\substack{a=k-1\\ b=1}}^{\substack{(k-1)\\ 1}} b[a+1] + 8k = 8\sum_{\substack{a=k\\ b=1}}^{\substack{k-1\\ a=1}} ba + 8k = 8\sum_{\substack{a=k\\ b=1}}^{\substack{k\\ 1}} ba$

Now, the result is:

$Sc(G_{k+1}) = \frac{1}{2}[32k + 44 - 5 - 2.4 - 3(1+1)(k+1) + 3(1+4) + 3(1+1).2 + 9(1+1)(k+2) + 2\sum_{\substack{r=k+1\\ s=3}}^{\substack{k\\ \text{when } k=4}} 4sr + 12(k+1) + 5\sum_{\substack{f=k+1\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} ft + 8\sum_{\substack{a=k\\ b=1}}^{\substack{k\\ 1}} ab]$

$= \frac{1}{2}\,[44k + 88 + 2\sum_{\substack{r=k+1\\ s=3}}^{\substack{k\\ \text{when } k=4}} 4sr + 12.(k+1) + 5\sum_{\substack{f=k+1\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} ft + 8\sum_{\substack{a=k\\ b=1}}^{\substack{k\\ 1}} ab]$

$= \frac{1}{2}[44(k+1) + 44 + 2\sum_{\substack{r=k+1\\ s=3}}^{\substack{k\\ \text{when } k=4}} 4sr + 12.(k+1) + 5\sum_{\substack{f=k+1\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} ft + 8\sum_{\substack{a=k\\ b=1}}^{\substack{k\\ 1}} ab]$

$= \frac{1}{2}[32(k+1) + 12(k+1) + 44 + 2\sum_{\substack{r=k+1\\ s=3}}^{\substack{k\\ \text{when } k=4}} 4sr + 12(k+1) + 5\sum_{\substack{f=k+1\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} ft + 8\sum_{\substack{a=k\\ b=1}}^{\substack{k\\ 1}} ab] = \frac{1}{2}[32(k+1) + 44 + 2\sum_{\substack{r=k+1\\ s=3}}^{\substack{k\\ \text{when } k=4}} 4sr + 24(k+1) + 5\sum_{\substack{f=k+1\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} ft +$

$$8\ \sum_{\substack{a=k\\b=1}}^{\substack{k\\1}} ab] = \frac{1}{2}[32(k+1) + 44 + [2\sum_{\substack{r=k+1\\s=3}}^{\substack{k\\ \text{when } k=4}} 4sr + 2.4.(k+1).3] +$$

$$5\sum_{\substack{f=k+1\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft\ + 8\ \sum_{\substack{a=k\\b=1}}^{\substack{k\\1}} ab = \frac{1}{2}[32(k+1) + 44 + [2[4.3.(k+1) + 4.4.k +$$

$$4.5.(k-1) + \cdots + 4.k.4 + 4(k+1).3]] + 5\sum_{\substack{f=k+1\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft\ + 8\ \sum_{\substack{a=k\\b=1}}^{\substack{k\\1}} ab$$

$$= \frac{1}{2}[32(k+1) + 44 + 2\sum_{\substack{r=k+1\\s=3}}^{\substack{k+1\\3}} 4sr + 5\sum_{\substack{f=k+1\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft\ + 8\ \sum_{\substack{a=k\\b=1}}^{\substack{k\\1}} ab$$

Since k+1=n, then

$$Sc\ (C_{K+1}H_{2k+4}) = \frac{1}{2}[32n + 44 + 2\sum_{\substack{r=n\\s=3}}^{\substack{n\\3}} 4sr + 5\sum_{\substack{f=n\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft\ + 8\ \sum_{\substack{a=n-1\\b=1}}^{\substack{n-1\\1}} ab]$$

$$Sc\ (C_nH_{2n+2}) = 16n + 22 + 4\sum_{\substack{r=n\\s=3}}^{\substack{n\\3}} sr + \frac{5}{2}\sum_{\substack{f=n\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft\ + 4\ \sum_{\substack{a=n-1\\b=1}}^{\substack{n-1\\1}} ab \quad \blacksquare$$

Theorem 2.2. Let n be appositive integer, then the Modified Schultz index (Sc^*) of a graph G denoted by G = C_nH_{2n+2} is as follows:

1. if n = 1 then G = CH_4 (see Figure 2) and $Sc^*(CH_4) = 14$

2. if n = 2 then G = C_2H_6 (see Figure 3) and $Sc^*(C_2H_6) = \frac{127}{2}$

3. if n ≥ 3 then G = C_nH_{2n+2} and

$$Sc^*(CnH_{2n+2}) = \frac{19}{2}n\ + \frac{25}{2} + 2\ \sum_{\substack{r=n\\s=3}}^{\substack{n\\3}} rs\ \ + 2\ \sum_{\substack{f=n\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft + 8\ \sum_{\substack{a=n-1\\b=1}}^{\substack{n-1\\1}} ab$$

, where t is an odd number, or

$$= \frac{1}{2}\left[19n + 25 + \sum_{\substack{r=4n\\s=3}}^{\substack{n\\12}} rs\ + 4\ \sum_{\substack{f=n\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft + 16\ \sum_{\substack{a=n-1\\b=1}}^{\substack{n-1\\1}} ab\right]$$

Proof :

1. $Sc^*(CH_4) = \frac{1}{2}\sum(du.dv)\ d\ (u\ ,v)$

$$= \frac{1}{2}[4.4 + 6\ (1.1).2]\ \ = \frac{1}{2}[16 + 12]\ \ = \frac{1}{2}\ 28 = 14$$

2. $Sc^*(C_2H_6) = \frac{1}{2}[6(1.4) +\ 6(1.1).2 + 9(1.1).3 + 6(1.4).2 + (4.4).1] = \frac{127}{2}$

3. we will prove by mathematical induction:

when n = 3 than G = C_3H_8 (see Figure 4):

Hence by Definition of Modified Schultz index

$Sc^*(G) = \frac{1}{2}\sum(du.dv)\ d\ (u\ ,v)$

$= \frac{1}{2}[8(1.4) + 9(1.1).4 + 10(1.4).2 + 6(1.4).3 + 2(4.4).1 + (4.4).2 + 7(1.1).2 + 12(1.1).3] = \frac{1}{2}\ [334] = 167$

So it is true that, with

$Sc^*(C_3H_8) = \frac{19}{2}.3 + \frac{25}{2} + 2\sum_{\substack{r=3\\ s=3}}^{3}{}^{3} rs + 2\sum_{\substack{f=3\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} ft + 8\sum_{\substack{a=2\\ b=1}}^{2}{}^{1} ab$

$= 41 + 2\ [3\ .3] + 2\ [3\ .6 + 2\ .10] + 8\ [2\ .1 + 1\ .2] = 167$, when $n = 3$

Let $n = k$ and $G_k = C_kH_{2k+2}$, assuming that it is true for $k \geq 3$;

$Sc^*(G_k) = \frac{19}{2}k + \frac{25}{2} + 2\sum_{\substack{r=k\\ s=3}}^{k}{}^{3} rs + 2\sum_{\substack{f=k\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} ft + 8\sum_{\substack{a=k-1\\ b=1}}^{k-1}{}^{1} ab$, or

$= \frac{1}{2}\ [\ 19k + 25 + \sum_{\substack{r=4k\\ s=3}}^{k}{}^{12} rs + 4\sum_{\substack{f=k\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} ft + 16\sum_{\substack{a=k-1\\ b=1}}^{k-1}{}^{1} ab]$

construct the graph $G_{k+1} = C_{k+1}H_{2k+4}$ can be done as:

Thus, the graph G_k has the form (see Figure 5), the position of the carbon vertex at the i^{th} position is denoted by C_i , the edge e is connecting the end hydrogen vertex H_{k1} in graph G_k with the vertex C_k.

Now, a graph G* can be obtained by removing both the vertex H_{k1} and the edge e from a graph G_k (see Figure 6): by removing $\frac{1}{2}\ [(1.4).1]$, which is the relationship of the vertex H_k with C_k according to the rule $\frac{1}{2}\sum(du + dv)d\ (u\ ,v)$, and also removing $\frac{1}{2}\ [(1.1).2]$ twice, i.e. $\frac{1}{2}\ [2(1.1).2]$, which is relationship of the vertex H_{k1} with the two vertices H_{k2}, H_{k3}. Also, $\frac{1}{2}\ [3(1.1)(k+1)]$ is removed, which is the relationship of the vertex H_{k1} with the three vertex H_1, H_2 and H_3 that are away about (1 + k) from the removed vertex H_{k1}.

Also, $\frac{1}{2}\ [2(1.1)k]$ is removed, which is the relationship of the vertex H_{k1} with the two vertices H_4 and H_5, and remove $\frac{1}{2}\ [2(1.1)(k-1)]$, which is the relationship of the vertex H_{k1} with the two verticesH_6 and H_7. This procedure is followed until removing $\frac{1}{2}\ [2(1.1).3]$, which is the relationship of the vertex H_{k1} with the two vertices $H_{(k-1)1}$ and $H_{(k-1)2}$. This means that the series $\sum_{\substack{r=4k\\ s=3}}^{k}{}^{12} rs$ after removing becomes $\sum_{\substack{r=4k-2\\ s=3}}^{k}{}^{10} rs$.

Later, $\frac{1}{2}$ $[1(1.4).2]$ is removed, which is the relationship of the vertex H_{k1} with C_{k-1} and remove $\frac{1}{2}$ $[(1.4).3]$, which is the relationship the vertex H_{k1} with the vertex C_{k-2}. This procedure is followed until removing $\frac{1}{2}$ $[(1.4)k]$, which is the relationship of the vertex H_{k1} with the vertex C_1. This, means that the series $4\sum_{\substack{f=k \\ t=2m+4}}^{\substack{\text{when } f=2 \\ 2}} ft$ becomes after the subsequent removing $4\sum_{\substack{f=k \\ t=2m+3}}^{\substack{\text{when } f=2 \\ 2}} ft$, that is

$$Sc*(G_k) = \frac{1}{2}[19k - 25 - 4 - 4 - 3k - 3 + \sum_{\substack{r=(4k-2) \\ s=3}}^{\substack{k \\ 10}} rs \ + \ 4\sum_{\substack{f=k \\ t=2m+3}}^{\substack{\text{when } f=2 \\ 2}} ft \ +$$

$$16\sum_{\substack{a=k-1 \\ b=1}}^{\substack{k-1 \\ 1}} ab] = \frac{1}{2}[16k + 14 + \sum_{\substack{r=(4k-2) \\ s=3}}^{\substack{k \\ 10}} rs \ + \ 4\sum_{\substack{f=k \\ t=2m+3}}^{\substack{\text{when } f=2 \\ 2}} ft \ + \ 16\sum_{\substack{a=k-1 \\ b=1}}^{\substack{k-1 \\ 1}} ab]$$

Connect the graph G* with the graph U (see Figure 7):

The graph G_{k+1} is obtained (see Figure 8):

By adding the graph U to graph G*, $\frac{1}{2}$ $[3(1.4).1]$ is added, which is the relationship of the vertex C_{k+1} with the vertices H_a, H_b and H_c, and adding $\frac{1}{2}$ $[3(1.1).2]$, which is the relationship of the vertices H_a, H_b and H_c with each other. Later $\frac{1}{2}$ $[9(1.1)(k+2)]$ is added, which is the relationship of the vertices H_a, H_b and H_c with the vertices H_1, H_2 and H_3. Then, $\frac{1}{2}$ $[6(1.1)(k+1)]$ is added as well, which is the relationship of the vertices H_a, H_b and H_c with the two vertices H_4 and H_5. This procedure is followed until adding $\frac{1}{2}$ $[6(1.1).3]$, which is the relationship of the vertices H_a, H_b and H_c with the two vertices H_{k2} and H_{k3}, This means that series $\sum_{L}^{k+1} 6(1.1)L$ will be added to series $\sum_{\substack{r=4k-2 \\ s=3}}^{\substack{k \\ 10}} rs$;

$\sum_{\substack{r=4k-2 \\ s=3}}^{\substack{k \\ 10}} rs \ + \ \sum_{L=3}^{k} 6L + 6(k+1)$, where (r =10) which means that it should be stopped when k=3

since s = L

$$= \sum_{\substack{r=4k-2 \\ s=3}}^{\substack{k \\ \text{when } k=3}} S[r+6] + 6(k+1) = \sum_{\substack{r \\ s=3}}^{\substack{k \\ \text{when } k=3}} S[4k-2+6] + 6(k+1)$$

$$= \sum_{\substack{r \\ s=3}}^{\substack{k \\ \text{when } k=3}} S[4k+4] + 6(k+1) = \sum_{\substack{r \\ s=3}}^{\substack{k \\ \text{when } k=3}} 4.S[k+1] + 6(k+1)$$

$= \sum_{\substack{r=k+1 \\ s=3}}^{\substack{k \\ \text{when } k=4}} 4.Sr + 6\ (k+1)$.

Now, $\frac{1}{2}\,[3(1.4).2\,]$ is added, which is the relationship of the vertices H_a, H_b and H_c with vertex C_k, with adding $\frac{1}{2}\,[3(1.4).3\,]$, which is the relationship of the vertices H_a, H_b and H_c with vertex C_{k-1}. This procedure should be followed until adding $\frac{1}{2}$ $[3(1.4)(k+1)\,]$, which is the relationship of the same vertices with the vertex C_1. Also, $\frac{1}{2}\,[3(1.4)(k+1)]$ is added, which is the relationship of the vertices H_1, H_2 and H_3 with the vertex $C_{k+1,}$ and adding $\frac{1}{2}\,[3(1.4)k]$, which is the relationship of the vertices H_4 and H_5 with the vertex C_{k+1}, with adding $\frac{1}{2}\,[2(1.4)(k-1)]$, which is the relationship of the two vertices H_6 and H_7 with the vertex C_{k+1}. The process is kept until adding $\frac{1}{2}\,[2(1.4).2\,]$, which is the relationship of the two vertices H_{k2} and H_{k3} with the vertex $C_{k+}1$, that means adding $4\sum_{L=k}^{2} 5L + 5.6\ (k+1)$ to the series $4\ \sum_{\substack{f=k \\ t=2m+3}}^{\substack{\text{when } f=2 \\ 2}} ft$; where k is odd, that is

$4\ \sum_{\substack{f=k \\ t=2m+3}}^{\substack{\text{when } f=2 \\ 2}} ft + 4\sum_{L=k}^{2} 5L + 5.6\ (k+1)$, since $L = f$ then

$= 4\ \sum_{\substack{f=k \\ t=2m+3}}^{\substack{\text{when } f=2 \\ 2}} f[t+5] + 5.6\ (k+1) = 4\sum_{\substack{f=k \\ t}}^{\substack{\text{when } f=2 \\ 2}} f[2m+3+5] + 5.6\ (k+1)$

$= 5\ \sum_{\substack{f=k \\ t}}^{\substack{\text{when } f=2 \\ 2}} f[2m+8] + 5.6\ (k+1) = 5\ \sum_{\substack{f=k \\ t=2m+8}}^{\substack{\text{when } f=2 \\ 2}} ft + 5.6\ (k+1) = 5\ \sum_{\substack{f=k+1 \\ t=2m+4}}^{\substack{\text{when } f=2 \\ 2}} ft$

Furthermore, $\frac{1}{2}\,[(4.4).k\,]$ needs to be added, which is the relationship of the vertex C_{k+1} with the vertex C_1 and adding $\frac{1}{2}\,[(4.4)(k-1)]$, which is the relationship of the vertex C_{k+1} with the vertex C_2 and keep adding until reaching that vertex $\frac{1}{2}\,[(4.4).1\,]$ is added, which is the relationship of the vertex C_{k+1} with the vertex C_k. This means that the series $16\sum_{x=1}^{k} x$ is added to the series $16\sum_{\substack{a=k-1 \\ b=`1}}^{\substack{(k-1) \\ 1}} ab$

This means $16\sum_{\substack{a=k-1 \\ b=1}}^{\substack{(k-1) \\ 1}} ab + 16\ \sum_{x=1}^{k} x\ = 16\sum_{\substack{a=k-1 \\ b=1}}^{\substack{(k-1) \\ 1}} ab + 16\ \sum_{x=1}^{k-1} x + 16k$; since $x = b$

$$= 16\sum_{\substack{a=k-1\\b=1}}^{\substack{(k-1)\\1}} b[a+1] + 16k = 16\sum_{\substack{a=k\\b=1}}^{\substack{k-1\\a=1}} ba + 16k = 16\sum_{\substack{a=k\\b=1}}^{\substack{k\\1}} ba$$

Now the result is:

$$Sc^*(G_{k+1}) = \frac{1}{2}\Big[16k + 14 + 3.4 + 3.2 + 9(k+2) + \sum_{\substack{r=k+1\\s=3}}^{\substack{k\\\text{when } k=4}} 4sr + 6(k+1) + 4\sum_{\substack{f=k+1\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft + 16\sum_{\substack{a=k\\b=1}}^{\substack{k\\1}} ab\Big]$$

$$= \frac{1}{2}\Big[25(k+1) + 25 + \sum_{\substack{r=k+1\\s=3}}^{\substack{k\\\text{when } k=4}} 4sr + 6(k+1) + 4\sum_{\substack{f=k+1\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft + 16\sum_{\substack{a=k\\b=1}}^{\substack{k\\1}} ab\Big]$$

$$= \frac{1}{2}\Big[19(k+1) + 6(k+1) + 25 + \sum_{\substack{r=k+1\\s=3}}^{\substack{k\\\text{when } k=4}} 4sr + 6(k+1) + 4\sum_{\substack{f=k+1\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft + 16\sum_{\substack{a=k\\b=1}}^{\substack{k\\1}} ab\Big] = \frac{1}{2}\Big[19(k+1) + 25 + \sum_{\substack{r=k+1\\s=3}}^{\substack{k\\\text{when } k=4}} 4sr + 12.(k+1) + 4\sum_{\substack{f=k+1\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft + 16\sum_{\substack{a=k\\b=1}}^{\substack{k\\1}} ab\Big]$$

$$= \frac{1}{2}\Big[19(k+1) + 25 + \Big[\sum_{\substack{r=k+1\\s=3}}^{\substack{k\\\text{when } k=4}} 4sr + 4.(k+1).3\Big] + 4\sum_{\substack{f=k+1\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft + 16\sum_{\substack{a=k\\b=1}}^{\substack{k\\1}} ab$$

$$= \frac{1}{2}\Big[19(k+1) + 25 + [4.3.(k+1) + 4.4.k + 4.5.(k-1) + \cdots + 4.k.4 + 4(k+1).3] + 4\sum_{\substack{f=k+1\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft + 16\sum_{\substack{a=k\\b=1}}^{\substack{k\\1}} ab$$

$$= \frac{1}{2}\Big[19(k+1) + 25 + \sum_{\substack{r=k+1\\s=3}}^{\substack{k+1\\3}} 4sr + 4\sum_{\substack{f=k+1\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft + 16\sum_{\substack{a=k\\b=1}}^{\substack{k\\1}} ab$$

Since k+1=n, then

$$Sc^*(C_nH_{2n+2}) = \frac{1}{2}\Big[19n + 25 + \sum_{\substack{r=n\\s=3}}^{\substack{n\\3}} 4sr + 4\sum_{\substack{f=n\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft + 16\sum_{\substack{a=n-1\\b=1}}^{\substack{n-1\\1}} ab\Big]$$

$$Sc^*(C_nH_{2n+2}) = \frac{19}{2}n + \frac{25}{2} + 2\sum_{\substack{r=n\\s=3}}^{\substack{n\\3}} sr + 2\sum_{\substack{f=n\\t=2m+4}}^{\substack{\text{when } f=2\\2}} ft + 8\sum_{\substack{a=n-1\\b=1}}^{\substack{n-1\\1}} ab \quad \blacksquare$$

Theorem 3. Let n be appositive integer, then the Schultz polynomial Sc(G, *x*) of a graph G denoted by G = C_nH_{2n+2} is as follows:

1. if n = 1 then G = CH_4 (see Figure 2) and Sc (CH_4, *x*) = $10x + 6x^2$

2. if n = 2 then G = C_2H_6 (see Figure 3) and Sc (C_2H_6, x) = $19x + 21x^2 + 9x^3$

3. if n ≥ 3 then G = C_nH_{2n+2} and

Sc (CnH_{2n+2},x) =

$$\frac{1}{2}\left[10(\mathrm{n}+1)x + 4(\mathrm{n}+4)x^2 + 18x^{(\mathrm{n}+1)} + 2\sum_{\substack{\mathrm{r}=4\mathrm{n}\\ \mathrm{s}=3}}^{\substack{\mathrm{n}\\12}} \mathrm{r}x^{\mathrm{s}} + 5\sum_{\substack{\mathrm{f}=\mathrm{n}\\ \mathrm{t}=2\mathrm{m}+4}}^{\substack{\text{when f=2}\\2}} \mathrm{t}\,x^{f} + 8\sum_{\substack{\mathrm{a}=\mathrm{n}-1\\ \mathrm{b}=1}}^{\substack{\mathrm{n}-1\\1}} \mathrm{a}x^{b}\right],$$

where t is odd number

Proof :

1. Sc (CH_4,x) = $\frac{1}{2}\sum(\mathrm{du}+\mathrm{dv})x^{\mathrm{d(u,v)}}$

$$= \frac{1}{2}[4(1+4)x^1 + 6\,(1+1)x^2] = 10x + 6x^2$$

2. Sc (C_2H_6,x) = $\frac{1}{2}$ $[6(1+4)x^1 + 6(1+1)x^2 + 9(1+1)x^3 + 6(1+4)x^2 + (4+4)x^1]$

$$= 19x + 21x^2 + 9x^3$$

3. we will prove by mathematical induction :

When, n = 3 then, G = C_3H_8 (see Figure 4), Hence by Definition of Schultz polynomial

Sc(G,x)=$\frac{1}{2}[9(1+1)x^4 + 10(1+4)x^2 + 8(1+4)x^1 + 6(1+4)x^3 + 2(4+4)x^1 + 12(1+1)x^3 + 7(1+1)x^2 + (4+4)x^2] = 28x + 36x^2 + 27x^3 + 9x^4$

So, it is true that, with

$$\mathrm{Sc}\ (C_3H_8,\ x) = \frac{1}{2}\left[10(3+1)x + 2(3+4)x^2 + 18x^{(3+1)} + 2\sum_{\substack{\mathrm{r}=4.3\\ \mathrm{s}=3}}^{\substack{3\\12}} \mathrm{r}x^{\mathrm{s}} + 5\sum_{\substack{\mathrm{f}=3\\ \mathrm{t}=2\mathrm{m}+4}}^{\substack{\text{when f=2}\\2}} \mathrm{t}\,x^{f} + 8\sum_{\substack{\mathrm{a}=3-1\\ \mathrm{b}=1}}^{\substack{3-1\\1}} \mathrm{a}x^{b}\right]$$

$$= \frac{1}{2}[40x^1 + 14x^2 + 18x^4 + 2(12x^3) + 5(10x^2 + 6x^3) + 8(2x^1 + x^2)]$$

$$= 28x + 36x^2 + 27x^3 + 9x^4$$

Let n = k and $G_k = C_kH_{2k+2}$, assuming that, it is true for k ≥ 3;

$$\mathrm{Sc}\ (G_k,\ x) = \frac{1}{2}\left[10(\mathrm{k}+1)x + 2(\mathrm{k}+4)x^2 + 18x^{(\mathrm{k}+1)} + 2\sum_{\substack{\mathrm{r}=4\mathrm{k}\\ \mathrm{s}=3}}^{\substack{\mathrm{k}\\12}} \mathrm{r}x^{\mathrm{s}} + 5\sum_{\substack{\mathrm{f}=\mathrm{k}\\ \mathrm{t}=2\mathrm{m}+4}}^{\substack{\text{when f=2}\\2}} \mathrm{t}\,x^{f} + 8\sum_{\substack{\mathrm{a}=\mathrm{k}-1\\ \mathrm{b}=1}}^{\substack{\mathrm{k}-1\\1}} \mathrm{a}x^{b}\right]$$

constructing the graph $G_{k+1} = C_{k+1}H_{2k+4}$ can be done as:

Then, the graph G_k has the form (see Figure 5). Thus, the position of the carbon vertex at the ith position is denoted by C_i, the edge e is connecting the end hydrogen vertex H_{k1} in graph G_k with the vertex C_k.

Now, G* can be obtained by removing both the vertex H_{k1} and the edge e from graph G_k (see Figure 6).

By removing $\frac{1}{2}$ $[(1+4)x^1]$, which is the relationship of the vertex H_k with C_k according to the rule $\frac{1}{2}\sum(\mathrm{d\,u}+\mathrm{dv})x^{\mathrm{d\,(u\,,v)}}$, and also removing $\frac{1}{2}$ $[(1+1)x^2]$ twice, i.e. $\frac{1}{2}$ $[2(1+1)x^2]$, which is relationship of the vertex H_{k1} with the two vertices H_{k2} and H_{k3}. Also, $\frac{1}{2}$ $[3(1+1)x^{k+1}]$ is removed, which is the relationship of the vertex H_{k1} with the three vertex H_1, H_2 and H_3 that are away about (1 + k) from the removed vertex H_{k1}.

Also, $\frac{1}{2}$ $[2(1+1)x^k]$ is removed, which is the relationship of the vertex H_{k1} with the two vertices H_4 and H_5, and remove $\frac{1}{2}$ $[2(1+1)x^{k-1}]$ which is the relationship of the vertex H_{k1} with the two vertices H_6 and H_7. This procedure is followed until removing $\frac{1}{2}$ $[2(1+1)x^3]$, which is the relationship of the vertex H_{k1} with the two vertices $H_{(k-1)1}$ and $H_{(k-1)2}$. This means that the series $2\sum_{\substack{r=4k\\ s=3}}^{\substack{k\\12}} rx^s$ after removing becomes $2\sum_{\substack{r=4k-2\\ s=3}}^{\substack{k\\10}} rx^s$.

Also, $\frac{1}{2}$ $[1(1+4)x^2]$ is removed, which is the relationship of the vertex H_{k1} with C_{k-1}, and remove $\frac{1}{2}$ $[(1+4)x^3]$ which is the relationship of the vertex H_{k1} with the vertex C_{k-2}. This procedure is followed until removing $\frac{1}{2}$ $[(1+4)x^k]$, which is the relationship of the vertex H_{k1} with the vertex C_1. This means that the series $5\sum_{\substack{f=k\\ t=2m+4}}^{\substack{\text{when f=2}\\ 2}} tx^f$ after the sequent removing becomes $5\sum_{\substack{f=k\\ t=2m+3}}^{\substack{\text{when f=2}\\ 2}} tx^f$, that is

$$Sc(G_k,x)=\frac{1}{2}[10(\mathrm{k}+1)x-5x^1+2(\mathrm{k}+4)x^2-4x^2+18x^{k+1}-6x^{k+1}+ 2\sum_{\substack{r=(4k-2)\\ s=3}}^{\substack{k\\10}} rx^s + 5\sum_{\substack{f=k\\ t=2m+3}}^{\substack{\text{when f=2}\\ 2}} tx^f + 8\sum_{\substack{a=k-1\\ b=1}}^{\substack{k-1\\1}} ab]$$

Connect the graph G* with the graph U (see Figure 7). The graph G_{k+1} is obtained (see Figure 8):

By adding the graph U to the graph G*, $\frac{1}{2}$ $[3(1+4)x^1]$ is added which is the relationship of the vertex C_{k+1} with the vertices H_a, H_b and H_c ,and adding $\frac{1}{2}$ $[3(1+1)x^2]$, which is the relationship of the vertices H_a, H_b and H_c with each other. Later $\frac{1}{2}$ $[9(1+1)x^{k+2}]$ is added, which is the relationship of the vertices H_a, H_b and H_c with the vertices H_1 , H_2 and H_3. Then $\frac{1}{2}$ $[6(1+1)x^{k+1}]$ is added as well, which is the relationship of the vertices Ha, H_b , H_c with the two vertices H_4 and H_5. This procedure is followed until adding $\frac{1}{2}$ $[6(1+1)x^3]$, which is the relationship of the vertices H_a, H_b and H_c with the two vertices H_{k2} and H_{k3}, This means that add series $\sum_{L=3}^{k+1} 6(1+1)x^L$ will be added to series $\sum_{\substack{r=4k-2 \\ s=3}}^{\substack{k \\ 10}} 2rx^s$;

$2\sum_{\substack{r=4k-2 \\ s=3}}^{\substack{k \\ 10}} rx^s + 2\sum_{L=3}^{k+1} 6x^L$, where r =10, which means that it should be stopped when k=3

$$= 2\sum_{\substack{r=4k-2 \\ s=3}}^{\substack{k \\ \text{when } k=3}} rx^s + 2\sum_{L=3}^{k} 6x^L + 12x^{k+1} \text{, since } s = L$$

$$=2\sum_{\substack{r=4k-2 \\ s=3}}^{\substack{k \\ \text{when } k=3}} x^s[r+6] + 12x^{k+1} = 2\sum_{\substack{r \\ s=3}}^{\substack{k \\ \text{when } k=3}} x^s[4k-2+6] + 12x^{k+1}$$

$$= 2\sum_{\substack{r \\ s=3}}^{\substack{k \\ \text{when } k=3}} x^s[4k+4] + 12x^{k+1} = 2\sum_{\substack{r \\ s=3}}^{\substack{k \\ \text{when } k=3}} 4x^s[k+1] + 12x^{k+1}$$

$$= 2\sum_{\substack{r=k+1 \\ s=3}}^{\substack{k \\ \text{when } k=4}} 4x^s r + 12x^{k+1}.$$

Now, $\frac{1}{2}$ $[3(1+4)x^2]$ is added, which is the relationship of the vertices H_a, H_b and H_c with vertex C_k, with adding $\frac{1}{2}$ $[3(1+4)x^3]$, which is the relationship of the vertices H_a, H_b and H_c with vertex C_{k-1}. This procedure should befollowed until adding $\frac{1}{2}$ $[3(1+4)x^{k+1}]$, which is the relationship of the same vertices with the vertex C_1. Also, $\frac{1}{2}$ $[3(1+4)x^{k+1}]$ is added, which is the relationship of the vertices H_1, H_2 and H_3 with the vertex $C_{k+1,}$ and adding $\frac{1}{2}$ $[3(1+4)x^k]$, which is the relationship of the vertices H_4 and H_5 with the vertex C_{k+1}, with adding $\frac{1}{2}$ $[2(1+4)x^{k-1}]$, which is the relationship of the two vertices H_6 and H_7 with the vertex C_{k+1}. The process is kept until adding $\frac{1}{2}$ $[2(1+4)x^2]$, which is the relationship of the two vertices H_{k2} and H_{k3} with the vertex C_{k+1}, that means adding $5\sum_{L=k}^{2} 5x^L + 5.6\,x^{k+1}$ to the series

$5\sum_{\substack{f=k \\ t=2m+3}}^{\substack{\text{when } f=2 \\ 2}} tx^f$; where k is an odd, that is

$5\sum_{\substack{f=k \\ t=2m+3}}^{\substack{\text{when } f=2 \\ 2}} tx^f + 5\sum_{L=k}^{2} 5x^L + 5.6\, x^{k+1}$, since L = f then

$= 5\sum_{\substack{f=k \\ t=2m+3}}^{\substack{\text{when } f=2 \\ 2}} x^f[t+5] + 5.6\, x^{k+1} = 5\sum_{\substack{f=k \\ t}}^{\substack{\text{when } f=2 \\ 2}} x^f[2m+3+5] + 5.6\, x^{k+1}$

$= 5\sum_{\substack{f=k \\ t}}^{\substack{\text{when } f=2 \\ 2}} x^f[2m+8] + 5.6\quad x^{k+1} = 5\sum_{\substack{f=k \\ t=2m+8}}^{\substack{\text{when } f=2 \\ 2}} x^f t + 5.6\quad x^{k+1} =$

$5\sum_{\substack{f=k+1 \\ t=2m+4}}^{\substack{\text{when } f=2 \\ 2}} x^f t$

Furthermore, $\frac{1}{2}[(4+4)x^k]$ needs to be added, which is the relationship of the vertex C_{k+1} with the vertex C_1 and adding $\frac{1}{2}[(4+4)x^{k-1}]$, which is the relationship of the vertex C_{k+1} the vertex C_2 and keep adding until reaching that vertex $\frac{1}{2}[(4+4)x^1]$ is added, which is the relationship of the vertex C_{k+1} with the vertex C_k. This means that the series $8\sum_{p=1}^{k} x^p$ is added to the series $8\sum_{\substack{a=k-1 \\ b=`1}}^{\substack{(k-1) \\ 1}} ax^b$.

This means $8\sum_{\substack{a=k-1 \\ b=1}}^{\substack{(k-1) \\ 1}} ax^b + 8\sum_{p=1}^{k} x^p = 8\sum_{\substack{a=k-1 \\ b=1}}^{\substack{(k-1) \\ 1}} ax^b + 8\sum_{p=1}^{k-1} x^p + 8x^k$; since p = b

$= 8\sum_{\substack{a=k-1 \\ b=1}}^{\substack{(k-1) \\ 1}} x^b[a+1] + 8x^k = 8\sum_{\substack{a=k \\ b=1}}^{\substack{k-1 \\ a=1}} x^b a + 8x^k = 8\sum_{\substack{a=k \\ b=1}}^{\substack{k \\ 1}} x^b a$

Now, the result is:

$$Sc(G_k, x) = \frac{1}{2}[10(k+1)x - 5x^1 + 2(k+4)x^2 - 4x^2 + 18x^{k+1} - 6x^{k+1} + 15x + 6x^2 + 18x^{k+2} + 2\sum_{\substack{r=k+1 \\ s=3}}^{\substack{k \\ \text{when} k=4}} 4rx^s + 12x^{k+1} + 5\sum_{\substack{f=k+1 \\ t=2m+4}}^{\substack{\text{when } f=2 \\ 2}} tx^f + 8\sum_{\substack{a=k \\ b=1}}^{\substack{k \\ 1}} x^b a]$$

$= \frac{1}{2}[20x + 10x^2 + 10kx + 2kx^2 + 12x^{k+1} + 18x^{k+2} + 2\sum_{\substack{r=k+1 \\ s=3}}^{\substack{k \\ \text{when } k=4}} 4rx^s +$

$$12x^{k+1} + 5\sum_{\substack{f=k+1\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} tx^f + 8\sum_{\substack{a=k\\ b=1}}^{\substack{k\\ 1}} x^b a\,]$$

$$= \frac{1}{2}[10(k+2)x + 2(k+5)x^2 + 18x^{k+2} + +2\sum_{\substack{r=k+1\\ s=3}}^{\substack{k\\ \text{when} k=4}} 4rx^s + 24x^{k+1} + 5\sum_{\substack{f=k+1\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} tx^f + 8\sum_{\substack{a=k\\ b=1}}^{\substack{k\\ 1}} x^b a]$$

$$= \frac{1}{2}[10(k+2)x + 2(k+5)x^2 + 18x^{k+2} + 2[\sum_{\substack{r=k+1\\ s=3}}^{\substack{k\\ \text{when} k=4}} 4rx^s + 4x^{k+1}.3] + 5\sum_{\substack{f=k+1\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} tx^f + 8\sum_{\substack{a=k\\ b=1}}^{\substack{k\\ 1}} x^b a]$$

$$= \frac{1}{2}[10(k+2)x + 2(k+5)x^2 + 18x^{k+2} + 2\sum_{\substack{r=k+1\\ s=3}}^{\substack{k+1\\ \text{when} k=3}} 4rx^s + 5\sum_{\substack{f=k+1\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} tx^f + 8\sum_{\substack{a=k\\ b=1}}^{\substack{k\\ 1}} x^b a]$$

Since k+1=n, then

$$Sc(CnH_{2n+2},x)=\frac{1}{2}\left[10(n+1)x + 2(n+4)x^2 + 18x^{(n+1)} + 2\sum_{\substack{r=4n\\ s=3}}^{\substack{n\\ \text{when } k=3}} rx^s + 5\sum_{\substack{f=n\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} tx^f + 8\sum_{\substack{a=n-1\\ b=1}}^{\substack{n-1\\ 1}} ax^b\right] \blacksquare$$

Theorem 2.4. Let n be appositive integer, then the Modified Schultz polynomial (Sc^*, x) of a graph G denoted by G = C_nH_{2n+2} is as follows:

1. if n = 1 then G = CH_4 (see Figure 2) and $Sc^*(CH_4, x) = 8x + 3x^2$

2. if n = 2 then G = C_2H_6 (see Figure 3) and $Sc^*(C_2H_6, x) = 20x + 15x^2 + \frac{9}{2}x^3$

3. if n ≥ 3 then G = C_nH_{2n+2} and

$$Sc^*(CnH_{2n+2},x) = \frac{1}{2}\left[8(n+1)x + (n+4)x^2 + 9x^{n+1} + \sum_{\substack{r=4n\\ s=3}}^{\substack{n\\ \text{when } n=3}} rx^s + 4\sum_{\substack{f=n\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} tx^f + 16\sum_{\substack{a=n-1\\ b=1}}^{\substack{n-1\\ 1}} ax^b\right]$$,where t is an odd number

Proof :

1. $Sc^*(CH_4,x) = \frac{1}{2}\sum(du.dv)\, x^{d(u,v)}$

$= \frac{1}{2}[4(1.4)x + 6\,(1.1)x^2] \;= \frac{1}{2}[16x + 6x^2] \;= 8x + 3x^2$

2. $Sc^*(C_2H_6,x) = \frac{1}{2}[6(1.4)x + 6(1.1)x^2 + 9(1.1)x^3 + 6(1.4)x^2 + (4.4)x]$

$=20x + 15x^2 + \frac{9}{2}x^3$

3. we will prove by mathematical induction:

when n = 3, then G = C_3H_8 (see Figure 4):

Hence, by Definition of Modified Schultz polynomial

$Sc^*(G, x) = \frac{1}{2}[8(1.4)x + 9(1.1)x^4 + 10(1.4)x^2 + 6(1.4)x^3 + 2(4.4)x + 7(1.1)x^2 + 12(1.1)x^3 + (4.4)x^2] = \frac{1}{2}[64x + 63x^2 + 36x^3 + 9x^4]$

So, it is true that, with

$Sc^*(C_3H_8,x)=\frac{1}{2}\left[8(3+1)x + (3+4)x^2 + 9x^{3+1} + \sum_{\substack{r=4.3\\ s=3}}^{\substack{3\\ \text{when } n=3}} r x^s + 4\sum_{\substack{f=3\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} t x^f + 16\sum_{\substack{a=3-1\\ b=1}}^{\substack{3-1\\ 1}} a x^b\right]$

$= \frac{1}{2}[32x + 7x^2 + 9x^4 + 12x^3 + 4[6x^3 + 10x^2] + 16[2x^1 + 1x^2]]$, when n = 3

$=\frac{1}{2}[64x + 63x^2 + 9x^4 + 36x^3]$

Let n = k and $G_k = C_kH_{2k+2}$, assuming that it is true for $k \geq 3$;

$Sc^*(G_k,x)= \frac{1}{2}\left[8(k+1)x + (k+4)x^2 + 9x^{k+1} + \sum_{\substack{r=4k\\ s=3}}^{\substack{k\\ \text{when } k=3}} r x^s + 4\sum_{\substack{f=k\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} t x^f + 16\sum_{\substack{a=k-1\\ b=1}}^{\substack{k-1\\ 1}} a x^b\right]$,where t is an odd number

constructing the graph $G_{k+1} = C_{k+1}H_{2k+4}$ can be done as:

Then, the graph G_k has the form (see Figure 5). Thus, the position of the carbon vertex at the i^{th} position is denoted by C_i, the edge e is connecting the end hydrogen vertex H_{k1} in graph G_k with the vertex C_k.

Now, graph G* can be obtained by removing both the vertex H_{k1} and the edge e from graph G_k (see Figure 6). By removing $\frac{1}{2}[(1.4)x]$, which is the relationship of the vertex H_k with C_k according to the rule $\frac{1}{2}\sum(du.dv)x^{d(u,v)}$, and also removing $\frac{1}{2}[(1.1)x^2]$ twice i.e $\frac{1}{2}[2(1.1)x^2]$, which is relationship of the vertex H_{k1} with the two vertices H_{k2}, H_{k3}. Also $\frac{1}{2}\left[3(1.1)x^{k+1}\right]$ is removed, which is the relationship of the vertex H_{k1} with the three vertex H_1, H_2 and H_3 that are away about (1 + k) from the removed vertex H_{k1}. Also, $\frac{1}{2}\left[2(1.1)x^{k}\right]$ is removed, which is the relationship of the vertex H_{k1} with the two vertices H_4 and H_5, and remove $\frac{1}{2}\left[2(1.1)x^{k-1}\right]$ which is the relationship of the vertex H_{k1} with the two vertices H_6 and H_7. This procedure is followed until removing $\frac{1}{2}\left[2(1.1)x^{3}\right]$, which is the relationship of the vertex H_{k1} with the two vertices $H_{(k-1)1}$ and $H_{(k-1)2}$. This means that the series $\sum_{\substack{r=4k\\ s=3}}^{\substack{k\\12}} rx^{s}$ after removing becomes $\sum_{\substack{r=4k-2\\ s=3}}^{\substack{k\\10}} rx^{s}$.

Later, $\frac{1}{2}\left[1(1.4)x^{2}\right]$ is removed, which is the relationship of the vertex H_{k1} with C_{k-1} and remove $\frac{1}{2}\left[(1.4)x^{3}\right]$, which is the relationship H_{k1} with C_{k-2}. This procedure is followed until removing $\frac{1}{2}\left[(1.4)x^{k}\right]$, which is the relationship of the vertex H_{k1} with the vertex C_1. This means that the series $4\sum_{\substack{f=k\\ t=2m+4}}^{\substack{\text{when } f=2\\ 2}} t\,x^{f}$ becomes after the sequent removing $4\sum_{\substack{f=k\\ t=2m+3}}^{\substack{\text{when } f=2\\ 2}} t\,x^{f}$, that is

$$Sc*(G_k,x)=\frac{1}{2}[8(k+1)x+(k+4)x^2+9x^{k+1}-4x-2x^2-3x^{k+1}+\sum_{\substack{r=(4k-2)\\ s=3}}^{\substack{k\\10}} rx^{s} + 4\sum_{\substack{f=k\\ t=2m+3}}^{\substack{\text{when } f=2\\ 2}} t\,x^{f} + 16\sum_{\substack{a=k-1\\ b=1}}^{\substack{k-1\\1}} ax^{b}]$$

$$=\frac{1}{2}[4x+2x^2+6x^{k+1}+8kx+kx^2+\sum_{\substack{r=(4k-2)\\ s=3}}^{\substack{k\\10}} rx^{s} + 4\sum_{\substack{f=k\\ t=2m+3}}^{\substack{\text{when } f=2\\ 2}} t\,x^{f} + 16\sum_{\substack{a=k-1\\ b=1}}^{\substack{k-1\\1}} ax^{b}]$$

Connect the graph G* with the graph U (see Figure 7). The graph G_{k+1} is obtained (see Figure 8). By adding the graph U to the graph G*, $\frac{1}{2}\left[3(1.4)x\right]$ is added, which is the relationship of the vertex C_{k+1} with the vertices H_a, H_b and H_c , and adding $\frac{1}{2}$ $\left[3(1.1)x^{2}\right]$, which is the relationship of the vertices H_a , H_b and H_c with each other. Later $\frac{1}{2}\left[9(1.1)x^{k+2}\right]$ is added, which is the relationship of the vertices H_a , H_b and

H_c with the vertices H_1, H_2 and H_3 . Then $\frac{1}{2}[6(1.1)x^{k+1}]$ is added as well, which is the relationship of the vertices H_a, H_b , H_c with the two vertices H_4 and H_5. This procedure is followed until adding $\frac{1}{2}[6(1.1)x^3]$, which is the relationship of the vertices H_a, H_b and H_c with the two vertices H_{k2} and H_{k3}. This means that series $\sum_{L=3}^{k+1} 6(1.1)x^L$ will be added to series $\sum_{\substack{r=(4k-2)\\ s=3}}^{\substack{k\\ 10}} rx^s$;

$\sum_{\substack{r=(4k-2)\\ s=3}}^{\substack{k\\ 10}} rx^s + \sum_{L=3}^{k} 6x^L + 6x^{k+1}$, where r =10, which means that is should be stoped when k=3

since s = L, so

$$= \sum_{\substack{r=4k-2\\ s=3}}^{\substack{k\\ \text{when } k=3}} x^s[r+6] + 6x^{k+1} = \sum_{\substack{r\\ s=3}}^{\substack{k\\ \text{when } k=3}} x^s[4k-2+6] + 6x^{k+1}$$

$$= \sum_{\substack{r\\ s=3}}^{\substack{k\\ \text{when } k=3}} x^s[4k+4] + 6x^{k+1} = \sum_{\substack{r\\ s=3}}^{\substack{k\\ \text{when } k=3}} 4x^s[k+1] + 6x^{k+1}$$

$$= \sum_{\substack{r=k+1\\ s=3}}^{\substack{k\\ \text{when } k=4}} 4x^s r + 6\, x^{k+1}.$$

Now, $\frac{1}{2}[3(1.4)x^2]$ is added, which is the relationship of the vertices H_a, H_b and H_c with vertex C_k, with adding $\frac{1}{2}[3(1.4)x^3]$, which is the relationship of the vertices H_a, H_b and H_c with vertex C_{k}-1. This procedure should be followed until adding $\frac{1}{2}[3(1.4)x^{k+1}]$, which is the relationship of the same vertices with the vertex C_1. Also, $\frac{1}{2}[3(1.4)x^{k+1}]$ is added, which is the relationship of the vertices H_1, H_2 and H_3 with the vertex C_{k+1}, and adding $\frac{1}{2}[3(1.4)x^k]$, which is the relationship of the vertices H_4 and H_5 with the vertex C_{k+1}, with adding $\frac{1}{2}[2(1.4)x^{k-1}]$, which is the relationship of the two vertices H_6 and H_7 with the vertex C_{k+1}. The process is kept until adding $\frac{1}{2}[2(1.4)x^2]$, which is the relationship of the two vertices H_{k2} and H_{k3} with the vertex C_{k+1} , that means adding $4\sum_{L=k}^{2} 5x^L + 5.6\, x^{k+1}$ to the series $4\sum_{\substack{f=k\\ t=2m+3}}^{\substack{\text{when } f=2\\ 2}} t\,x^f$; where k is odd, that is

$$4\sum_{\substack{f=k\\ t=2m+3}}^{\substack{\text{when } f=2\\ 2}} tx^f + 4\sum_{L=k}^{2} 5x^L + 5.6\, x^{k+1}, \text{ since } L = f \text{ then}$$

$= 4\sum_{\substack{f=k \\ t=2m+3}}^{\substack{\text{when } f=2 \\ 2}} x^f[\mathrm{t}+5] + 5.6\, x^{k+1} = 4\sum_{\substack{f=k \\ t}}^{\substack{\text{when } f=2 \\ 2}} x^f[2\mathrm{m}+3+5] + 5.6\, x^{k+1}$

$= 5\sum_{\substack{f=k \\ t}}^{\substack{\text{when } f=2 \\ 2}} x^f[2\mathrm{m}+8] + 5.6\; x^{k+1} = 5\sum_{\substack{f=k \\ t=2m+8}}^{\substack{\text{when } f=2 \\ 2}} x^f \mathrm{t} + 5.6\; x^{k+1} =$
$5\sum_{\substack{f=k+1 \\ t=2m+4}}^{\substack{\text{when } f=2 \\ 2}} \mathrm{t}\, x^f$

Furthermore $\frac{1}{2}\,[(4.4)x^k\,]$ needs to be added, which is the relationship of the vertex C_{k+1} with the vertex C_1 and adding $\frac{1}{2}\,[(4.4)x^{k-1}]$, which is the relationship of the vertex C_{k+1} with the vertex C_2 and keep adding until reaching that vertex $\frac{1}{2}\,[(4.4)x\,]$is added, which is the relationship of the vertex C_{k+1} with the vertex C_k, which means adding the series $16\sum_{p=1}^{k} x^p$ to the series $16\sum_{\substack{a=k-1 \\ b=`1}}^{\substack{(k-1) \\ 1}} \mathrm{a}x^b$

This means $16\sum_{\substack{a=k-1 \\ b=1}}^{\substack{(k-1) \\ 1}} \mathrm{a}x^b + 16\sum_{p=1}^{k} x^p = 16\sum_{\substack{a=k-1 \\ b=1}}^{\substack{(k-1) \\ 1}} \mathrm{a}x^b + 16\sum_{p=1}^{k-1} x^p + 16x^k$;

Since $p = b$

$= 16\sum_{\substack{a=k-1 \\ b=1}}^{\substack{(k-1) \\ 1}} x^b[\mathrm{a}+1] + 16x^k = 16\sum_{\substack{a=k \\ b=1}}^{\substack{k-1 \\ a=1}} x^b\mathrm{a} + 16x^k = 16\sum_{\substack{a=k \\ b=1}}^{\substack{k \\ 1}} \mathrm{a}x^b$

Now the result is

$$\mathrm{Sc}*(G_{k+1},x) = \frac{1}{2}[4x + 2x^2 + 6x^{k+1} + 8\mathrm{k}x + \mathrm{k}x^2 + 12x + 3x^2 + 9x^{k+2} + \sum_{\substack{r=k+1 \\ s=3}}^{\substack{k \\ \text{when } k=4}} 4x^s\mathrm{r} + 6\,x^{k+1} + 5\sum_{\substack{f=k+1 \\ t=2m+4}}^{\substack{\text{when } f=2 \\ 2}} \mathrm{t}\,x^f + 16\sum_{\substack{a=k \\ b=1}}^{\substack{k \\ 1}} \mathrm{a}x^b\,]$$

$= \frac{1}{2}[8(\mathrm{k}+2)x + (\mathrm{k}+5)x^2 + 9x^{k+2} + [\sum_{\substack{r=k+1 \\ s=3}}^{\substack{k \\ \text{when } k=4}} 4x^s\mathrm{r} + 12\,x^{k+1}] +$
$5\sum_{\substack{f=k+1 \\ t=2m+4}}^{\substack{\text{when } f=2 \\ 2}} \mathrm{t}\,x^f + 16\sum_{\substack{a=k \\ b=1}}^{\substack{k \\ 1}} \mathrm{a}x^b\,]$

$=\frac{1}{2}[8(\mathrm{k}+2)x + (\mathrm{k}+5)x^2 + 9x^{k+2} + [4x^3(\mathrm{k}+1) + 4x^4\mathrm{k} + 4x^5(\mathrm{k}-1) + \cdots +$
$4x^k.4 + 4x^{k+1}.3] + 5\sum_{\substack{f=k+1 \\ t=2m+4}}^{\substack{\text{when } f=2 \\ 2}} \mathrm{t}\,x^f + 16\sum_{\substack{a=k \\ b=1}}^{\substack{k \\ 1}} \mathrm{a}x^b\,]$

$$= \frac{1}{2}[8(k+2)x + (k+5)x^2 + 9x^{k+2} + \sum_{\substack{r=k+1 \\ s=3}}^{\substack{k+1 \\ \text{when } k=3}} 4x^s r + 5 \sum_{\substack{f=k+1 \\ t=2m+4}}^{\substack{\text{when } f=2 \\ 2}} t x^f$$

$$+ 16 \sum_{\substack{a=k \\ b=1}}^{\substack{k \\ 1}} a x^b]$$

Since k+1=n, then

$$Sc^*(C_nH_{2n+2},x) = \frac{1}{2}[8(n+1)x + (n+4)x^2 + 9x^{n+1} + \sum_{\substack{r=n \\ s=3}}^{\substack{n \\ \text{when } k=3}} 4x^s r + 5 \sum_{\substack{f=n \\ t=2m+4}}^{\substack{\text{when } f=2 \\ 2}} t x^f + 16 \sum_{\substack{a=n-1 \\ b=1}}^{\substack{n-1 \\ 1}} a x^b]$$

, where t is an odd number ■

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