

# On Hosoya and Schultz Polynomials of Chain of Pentagonal Graph

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**Abstract:** In order to connect a chain of vertices of rings of a pentagonal graph with a path of length one, we introduce in this work the concepts of Wiener, Schultz, and Modified Schultz indices, as well as Schultz, modified Schultz, and Hosoya polynomials. Along with changing the multiplicities of Schultz and Hosoya, some of Schultz's attributes are also presented.

**Keywords:** Schultz, Schultz modified, Hosoya, pentagonal graph, Schultz indices, Schultz polynomial.

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## 1. Introduction

Let  $G$  be a connected graph. If  $G$  doesn't contain any loops or multiple edges, we said that  $G$  is a simple graph, and we thus assumed that all the graphs in this research were simple. The shortest path between any two vertices in the set vertex  $V(G)$  determines the distance in any connected graph., This was indicated by  $d(u, v)$ , where  $u, v \in V(G)$ . Degree of vertex  $v$  is the quantity of edges connecting each vertex in  $V(G)$  directly with  $v$ , and it is represented as  $degv$  or  $degv$ . The longest path between any two vertices in a connected graph  $G$ , denoted  $diam(G)$ , determines the diameter of the graph  $diam(G) = \max_{u,v \in V(G)} \{d(u, v)\}$ , review the references [1] [2] [3].

A number that may be computed directly from the structural graph of a molecule is called a topological index. The structure and branching pattern of a molecule are quantified by a non-empirical numerical value called its topological index. A molecule's chemical structure needs to be transformed into a unique number (or index) that can be used to describe the molecule under study in order to do a topological analysis on it [4]. Ahmed M. and Mahmood M.A. gave the introduction. [5] Polynomials of Chain of Vertex Connected for Complete Square Graphs: Schultz and Modified Schultz.

Science, Harold Wiener (1947), used these topological indicators for the first time in biology and chemistry. Wiener showed the connections between the physical and chemical properties of organic molecules in graphs [6].

Schultz introduced the Schultz index in 1989 [7], and Klavar and Gutman established the modified Schultz index in 1997 [8]. The Schultz index  $Sc(G)$  and the modified Schultz index  $Sc^*(G)$ , also the Wiener index in 1947 [6]: are each defined as follows:

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

$$Sc^*(G_n) = \sum_{\{u,v\} \subseteq V(G_n)} (dagu \cdot deg v) d(u, v) .$$

$$W(G_n) = \sum_{\{u,v\} \subseteq V(G_n)} d(u, v) .$$

The following are the definitions of the Schultz, modified Schultz Hosoya polynomials, respectively:

$$Sc(G_n; x) = \sum_{\{u,v\} \subseteq V(G_n)} (dagu + deg v) x^{d(u,v)} .$$

$$Sc^*(G_n; x) = \sum_{\{u,v\} \subseteq V(G_n)} (dagu \cdot deg v) x^{d(u,v)}.$$

$$H(G_n; x) = \sum_{\{u,v\} \subseteq V(G_n)} x^{d(u,v)}.$$

Furthermore, we can deduce that the derivatives of  $Sc(G_n; x)$ ,  $Sc^*(G_n; x)$  and  $H(G_n; x)$  with respect to  $x$  when  $x = 1$  correspond to the Schultz, modified Schultz and Wiener indices, respectively, which are derived from Schultz, modified Schultz and Hosoya polynomials.

1 – The Schultz index:  $Sc(G_n) = \frac{d}{dx}(Sc(G_n; x)) \Big|_{x=1}$

2 – The modified Schultz index:  $Sc^*(G_n) = \frac{d}{dx}(Sc^*(G_n; x)) \Big|_{x=1}$

3 –  $w_2$  Wiener index:  $W(G_n) = \frac{d}{dx}(H(G_n; x)) \Big|_{x=1}$

Where  $p(G_n)$  is the order of  $G$  and  $\frac{d}{dx}$  it means derived. References [9] [10] [11] and [12] [13] [14] include a number of current studies on polynomials and indices for Schultz and modified Schultz, as well as applications of Schultz and modified Schultz in chemistry. H. Hosoya created the Wiener polynomial [15], a distance-based polynomial that generates graph distance distributions.

Let  $D_k(s, g)$  be the set of all  $(u, v)$  of  $G$  which distance between  $u$  and  $v$  is  $k$  such  $degu = s$  and  $degv = g$  and  $|D_k(G)|$  is the number of pairs  $(u, v)$  of  $G$  that are distance  $k$ ,  $D(G_n, k)$ ". Clearly, from that  $\sum_{k=1}^{diam(G)} |D_k(G)| = \frac{n(G)(n(G)-1)}{2}$ .

## 2. Polynomials for Schultz, Modified Schultz and Hosoya with a one-path of $Ch_{p_2}(W_5)_p$

In this section we compute Hosoya, Schultz and Modified Schultz polynomials, Wiener, Schultz and Modified Schultz indices of connecting the vertices of a chain of pentagonal rings with a one-path.

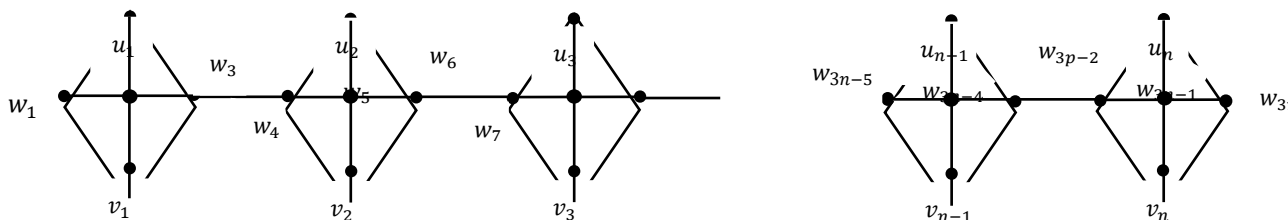


Figure.1. The Graph  $Ch_{p_2}(W_5)_n$

From Fig.1. We not that  $p(Ch_{p_2}(W_5)_n) = 5n$ , for the vertex and  $q(Ch_{p_2}(W_5)_n) = 9 - 1$  and  $diam(Ch_{p_2}(W_5)_n) = 3n - 1$ , for all  $n \geq 3, 1 \leq i, j \leq n, i \neq j, 2 \leq h < 3n$  and  $2 \leq k < 3n, h \neq k$ , then we have:

TABLE 1.  $deg u_i$  and  $deg v_i$

$\times$	$deg u_i = 3$	$deg v_i = 3$	$deg w_1 = 3$	$deg w_h = 4$	$deg w_{3n} = 3$
$+$					
$deg u_j = 3$	9	9	9	12	9
$deg v_j = 3$	9	9	9	12	9
$deg w_1 = 3$	9	9		12	9
$deg w_k = 4$	12	12	12	16	12
$deg w_{3n} = 3$	9	9	9	12	

**Theorem 2.1:** Schultz, Modified Schultz and Hosoya Polynomials with a one-path of  $Ch_{p_2}(W_5)_n$ . Then from p. 1. to p. 8. and  $n \geq 3$ , then we have:

- 1-  $Sc(Ch_{p_2}(W_5)_n; x) = 2(40n - 21)x + 2(29n - 23)x^2 + 2 \sum_{k=3}^{3n-6} \left(38n - \frac{38k}{3} - 1\right)x^k + 2 \sum_{j=4}^{3n-5} \left(26n - \frac{26(j-1)}{3} - 7\right)x^j + 2 \sum_{j=5}^{3n-4} \left(22n - \frac{22(s+1)}{3} + 7\right)x^s + 74x^{3n-3} + 38x^{3n-2} + 6x^{3n-1}$ .
- 2-  $Sc^*(Ch_{p_2}(W_5)_n; x) = 4(36n - 21)x + (105n - 88)x^2 + 4 \sum_{k=3}^{3n-6} \left(33n - \frac{33k}{3} - 2\right)x^k + 12 \sum_{j=4}^{3n-5} \left(8n - \frac{8(j-1)}{3} - 3\right)x^j + 8 \sum_{j=5}^{3n-4} \left(10n - \frac{10(s+1)}{3} + 3\right)x^s + 124x^{3n-3} + 60x^{3n-2} + 9x^{3n-1}$ .
- 3-  $H(Ch_{p_2}(W_5)_n; x) = (11n - 5)x + 2(4n - 3)x^2 + 11 \sum_{k=3}^{3n-6} \left(n - \frac{k}{3}\right)x^k + \sum_{j=4}^{3n-5} \left(7n - \frac{7(j-1)}{3} - 1\right)x^j + 2 \sum_{j=5}^{3n-4} (3n - s + 1)x^s + 11x^{3n-3} + 6x^{3n-2} + x^{3n-1}$ .

**Proof:** Every two vertices  $u, v \in V(Ch_{p_2}(W_5)_n; x)$ , there is  $d(u, v) = k, 1 \leq k \leq n$ , then  $\sum_{i=1}^n |D_i| = \frac{5n(5n-1)}{2}$ . The proof can be divided into five parts:

**P1.** If  $d(u, v) = 1$ , then  $|D_1| = 9n - 1$ , and we have three subsets of it:

**P1.1**  $|D_1(3,3)| = |\{(u_1, w_1), (v_1, w_1), (u_n, w_{3n}), (v_n, w_{3n})\}| = 4$ .

**P1.2**  $|D_1(3,4)| = \left| \left\{ \begin{aligned} &(u_i, w_{3i}), (v_i, w_{3i}), (u_i, w_{3i-1}), (v_i, w_{3i-1}), (u_{i+1}, w_{3i+1}), (v_{i+1}, w_{3i+1}) \\ &, (u_{i+1}, w_{3i+2}), (v_{i+1}, w_{3i+2}): 1 \leq i \leq n - 1 \end{aligned} \right\} \cup \{(w_1, w_2), (w_{3n}, w_{3n-1})\} \right| = 2(4n - 3)$ .

**P1.3**  $|D_1(4,4)| = |\{(w_{3i-1}, w_{3i}), (w_{3i+1}, w_{3i+2}), (w_{3i}, w_{3i+1}): 1 \leq i \leq n - 1\}| = 3(n - 1)$ .

**P2.** If  $d(u, v) = 2$ . Then  $|D_2| = 2(4n - 3)$ , and we have three subsets of it:

**P2.1**  $|D_2(3,3)| = |\{(u_i, v_i), : 1 \leq i \leq n\}| = n$

**P2.2**  $|D_2(3,4)| = |\{(u_i, w_{3i+1}), (v_i, w_{3i+1}), (u_{i+1}, w_{3i}), (v_{i+1}, w_{3i}): 1 \leq i \leq n - 1\} \cup \{(w_1, w_3), (w_{3n}, w_{3n-2})\}| = 2(2n - 1)$ .

**P2.3**  $|D_2(4,4)| = |\{(w_{3i-1}, w_{3i+1}), (w_{3i}, w_{3i+2}): 1 \leq i \leq n - 1\} \cup \{(w_{3i+1}, w_{3i+3}): 1 \leq i \leq n - 2\}| = 3n - 4$ .

**P3.** If  $d(u, v) = k, k = 3r + 3$ , where  $r = 0, 1, 2, \dots, n - 3$ . Then  $|D_k| = \left(11n - \frac{11k}{3}\right)$ , and we have three subsets of it:

**P3.1**  $|D_k(3,3)| = \left| \left\{ \left( u_i, u_{i+\frac{k}{3}} \right), \left( u_i, v_{i+\frac{k}{3}} \right), \left( v_i, v_{i+\frac{k}{3}} \right), \left( v_i, u_{i+\frac{k}{3}} \right) : 1 \leq i \leq n - \frac{k}{3} \right\} \right| = 4 \left( n - \frac{k}{3} \right)$ .

**P3.2**  $|D_k(3,4)| = \left| \left\{ (w_1, w_{k+1}), (w_{3p}, w_{3n-k}) \right\} \cup \left\{ \left( u_i, w_{3i+\frac{2k}{3}} \right), \left( v_i, w_{3i+\frac{2k}{3}} \right), \left( u_{i+\frac{k}{3}}, w_{3i-1} \right), \left( v_{i+\frac{k}{3}}, w_{3i-1} \right) : 1 \leq i \leq n - \frac{k}{3} \right\} \right| = 2 \left( 2n - \frac{2k}{3} + 1 \right)$ .

**P3.3**  $|D_k(4,4)| = \left| \left\{ (w_{3i-1}, w_{3i+k-1}): 1 \leq i \leq n - \frac{k}{3} \right\} \cup \left\{ (w_{3i}, w_{3i+k}), (w_{3i+1}, w_{3i+k+1}): 1 \leq i \leq n - \frac{k}{3} - 1 \right\} \right| = 3n - k - 2$

**P4.** If  $d(u, v) = j, j = 3r + 4$ , where  $r = 0, 1, 2, \dots, n - 3$ . Then  $|D_j| = 7n - \frac{7(j-1)}{3} - 1$ , and we have three subsets of it:

$$\mathbf{P4.1} \quad |D_j(3,3)| = \left| \left\{ \left( w_1, u_{\frac{j-1}{3}+1} \right), \left( w_1, v_{\frac{j-1}{3}+1} \right), \left( w_{3n}, u_{n-\frac{j-1}{3}} \right), \left( w_{3n}, v_{n-\frac{j-1}{3}} \right) \right\} \right| = 4.$$

$$\mathbf{P4.2} \quad |D_j(3,4)| = \left| \left\{ \left( u_i, w_{3i+j-1} \right), \left( v_i, w_{3i+j-1} \right), \left( u_{i+\frac{(j-1)}{3}+1}, w_{3i+1} \right), \left( v_{i+\frac{(j-1)}{3}+1}, w_{3i+1} \right) \right\} \cup \right. \\ \left. \left\{ (w_1, w_{j+1}), (w_{3n}, w_{3n-j}) \right\} : 1 \leq i \leq n - \frac{j-1}{3} - 1 \right| = 2 \left( 2n - \frac{2(j-1)}{3} - 1 \right).$$

$$\mathbf{P4.3} \quad |D_j(4,4)| = \left| \left\{ (w_{3i-1}, w_{3i+j-1}), (w_{3i}, w_{3i+j}), (w_{3i+1}, w_{3i+j+1}) : 1 \leq i \leq n - \frac{j-1}{3} - 1 \right\} \right| \\ = 3 \left( n - \frac{j-1}{3} - 1 \right)$$

**P5.** If  $d(u, v) = s, s = 3r + 5$ , where  $r = 0, 1, 2, \dots, n - 3$ . Then  $|D_s| = 6 \left( n - \frac{(s+1)}{3} \right) + 2$ , and we have two subsets of it:

$$\mathbf{P5.1} \quad |D_s(3,4)| = \left| \left\{ (u_i, w_{3i+s-1}), (v_i, w_{3i+s-1}), \left( u_{i+\frac{(s+1)}{3}}, w_{3i} \right), \left( v_{i+\frac{(s+1)}{3}}, w_{3i} \right) : 1 \leq i \leq n - \frac{s+1}{3} \right\} \cup \right. \\ \left. \left\{ (w_1, w_{s+1}), (w_{3n}, w_{3n-s}) \right\} \right| = 4 \left( n - \frac{s+1}{3} \right) + 2.$$

$$\mathbf{P5.2} \quad |D_s(4,4)| = \left| \left\{ (w_{3i-1}, w_{3i+s-1}), (w_{3i}, w_{3i+s}) : 1 \leq i \leq n - \frac{s+1}{3} \right\} \right| = 2 \left( n - \frac{s+1}{3} \right)$$

**P6.** If  $d(u, v) = 3n - 3$ . Then  $|D_{3n-3}| = 11$ , and we have three subsets of it:

$$\mathbf{P6.1} \quad |D_{3n-3}(3,3)| = |\{(u_1, u_n), (u_1, v_n), (v_1, v_n), (v_1, u_n)\}| = 4$$

$$\mathbf{P6.2} \quad |D_{3n-3}(3,4)| = |\{(u_1, w_{3n-1}), (v_1, w_{3n-1}), (u_n, w_2), (v_n, w_2)\} \cup \{(w_1, w_{3n-2}), (w_{3n}, w_3)\}| = 6.$$

$$\mathbf{P6.3} \quad |D_{3n-3}(4,4)| = |\{(w_2, w_{3n-1})\}| = 1$$

**P7.** If  $d(u, v) = 3n - 2$ . Then  $|D_{3n-2}| = 6$ , and we have two subsets of it:

$$\mathbf{P7.1} \quad |D_{3n-2}(3,3)| = |\{(u_1, w_{3n}), (v_1, w_{3n}), (w_1, u_n), (w_1, v_n)\}| = 4$$

$$\mathbf{P7.2} \quad |D_{3n-2}(3,4)| = |\{(w_1, w_{3n-1}), (w_{3n}, w_2)\}| = 2.$$

**P8.** If  $d(u, v) = 3n - 1$ . Then  $|D_{3n-1}| = 1$ , and we have one subset of it:

$$\mathbf{P8.1} \quad |D_{3n-1}(3,3)| = |\{(w_1, w_{3n})\}| = 1$$

Now, from **P1** to **P8** and the **table 3.1** Our produce:

$$1- \quad Sc(Ch_{p_2}(W_5)_n; x) = \{6(4) + 7(2(4n - 3)) + 8(3(n - 1))\} x + \{6(n) + 7(2(2n - 1)) + 8(3n - 4)\} x^2 + \\ \left\{ 6 \left( 4 \left( n - \frac{k}{3} \right) \right) + 7 \left( 2 \left( 2n - \frac{2k}{3} + 1 \right) \right) + 8(3n - k - 2) \right\} x^k + \left\{ 6(4) + 7 \left( 2 \left( 2n - \frac{2(j-1)}{3} - 1 \right) \right) + \right. \\ \left. 8 \left( 3 \left( n - \frac{j-1}{3} - 1 \right) \right) \right\} x^j + \left\{ 7 \left( 4 \left( n - \frac{s+1}{3} \right) + 2 \right) + 8 \left( 2 \left( n - \frac{s+1}{3} \right) \right) \right\} x^s + \{6(4) + 7(6) + 8(1)\} x^{3n-3} + \\ \{6(4) + 7(2)\} x^{3n-2} + \{6(1)\} x^{3n-1} \\ = 2(40n - 21)x + 2(29n - 23)x^2 + 2 \sum_{k=3}^{3n-6} \left( 38n - \frac{38k}{3} - \right. \\ \left. 1 \right) x^k + 2 \sum_{j=4}^{3n-5} \left( 26n - \frac{26(j-1)}{3} - 7 \right) x^j + 2 \sum_{j=5}^{3n-4} \left( 22n - \right. \\ \left. \frac{22(s+1)}{3} + 7 \right) x^s + 74x^{3n-3} + 38x^{3n-2} + 6x^{3n-1}$$

- 2-  $Sc^*(Ch_{p_2}(W_5)_n; x) = \{9(4) + 12(2(4n - 3)) + 16(3(n - 1))\} x + \{9(n) + 12(2(2n - 1)) + 16(3n - 4)\} x^2 + \{9(4(n - \frac{k}{3})) + 12(2(2n - \frac{2k}{3} + 1)) + 16(3n - k - 2)\} x^k + \{9(4) + 12(2(2n - \frac{2(j-1)}{3} - 1)) + 16(3(n - \frac{j-1}{3} - 1))\} x^j + \{12(4(n - \frac{s+1}{3}) + 2) + 16(2(n - \frac{s+1}{3}))\} x^s + \{9(4) + 12(6) + 16(1)\} x^{3p-3} + \{9(4) + 12(2)\} x^{3p-2} + \{9(1)\} x^{3p-1}$
- 3-  $= 4(36n - 21)x + (105n - 88)x^2 + 4 \sum_{k=3}^{3n-6} (33n - \frac{33k}{3} - 2) x^k + 12 \sum_{j=4}^{3n-5} (8n - \frac{8(j-1)}{3} - 3) x^j + 8 \sum_{s=5}^{3n-4} (10n - \frac{10(s+1)}{3} + 3) x^s + 124x^{3n-3} + 60x^{3n-2} + 9x^{3n-1}$ .
- 4-  $H(Ch_{p_2}(W_5)_n; x) = \{4 + 2(4n - 3) + 3(n - 1)\} x + \{n + 2(2n - 1) + (3n - 4)\} x^2 + \{4(n - \frac{k}{3}) + 2(2n - \frac{2k}{3} + 1) + (3n - k - 2)\} x^k + \{4 + 2(2n - \frac{2(j-1)}{3} - 1) + 3(n - \frac{j-1}{3} - 1)\} x^j + \{4(n - \frac{s+1}{3}) + 2 + 2(n - \frac{s+1}{3})\} x^s + \{4 + 6 + 1\} x^{3n-3} + \{4 + 2\} x^{3n-2} + \{1\} x^{3n-1}$   
 $= (11n - 5)x + 2(4n - 3)x^2 + 11 \sum_{k=3}^{3n-6} (n - \frac{k}{3}) x^k + \sum_{j=4}^{3n-5} (7n - \frac{7(j-1)}{3} - 1) x^j + 2 \sum_{s=5}^{3n-4} (3n - s + 1) x^s + 11x^{3n-3} + 6x^{3n-2} + x^{3n-1}$ .

**Example 2.2:** It is possible to calculate polynomials with ease

- 1-  $Sc(Ch_{p_2}(W_5)_3; x) = 198x + 128x^2 + 150x^3 + 90x^4 + 58x^5 + 74x^6 + 38x^7 + 6x^8$   
 $Sc^*(Ch_{p_2}(W_5)_3; x) = 348x + 227x^2 + 256x^3 + 156x^4 + 104x^5 + 124x^6 + 60x^7 + 9x^8$   
 $H(Ch_{p_2}(W_5)_3; x) = 28x + 18x^2 + 22x^3 + 13x^4 + 10x^5 + 11x^6 + 6x^7 + x^8$
- 2-  $Sc(Ch_{p_2}(W_5)_4; x) = 278x + 186x^2 + 226x^3 + 156x^4 + 102x^5 + 150x^6 + 90x^7 + 58x^8 + 74x^9 + 38x^{10} + 6x^{11}$   
 $Sc^*(Ch_{p_2}(W_5)_4; x) = 492x + 332x^2 + 388x^3 + 252x^4 + 184x^5 + 256x^6 + 156x^7 + 104x^8 + 124x^9 + 60x^{10} + 9x^{11}$   
 $H(Ch_{p_2}(W_5)_4; x) = 39x + 26x^2 + 33x^3 + 20x^4 + 14x^5 + 22x^6 + 13x^7 + 10x^8 + 11x^9 + 6x^{10} + x^{11}$

**Corollary 2.3:** For all  $n \geq 3$  then we have:

- 1-  $Sc(Ch_{p_2}(W_5)_n) = 550n - 438 + 2 \sum_{k=3}^{3n-6} (38n - \frac{38k}{3} - 1) k + 2 \sum_{j=4}^{3n-5} (26n - \frac{26(j-1)}{3} - 7) j + 2 \sum_{s=5}^{3n-4} (22n - \frac{22(s+1)}{3} + 7) s$
- 2-  $Sc^*(Ch_{p_2}(W_5)_n) = 933n - 761 + 4 \sum_{k=3}^{3n-6} (33n - \frac{33k}{3} - 2) k + 12 \sum_{j=4}^{3n-5} (8n - \frac{8(j-1)}{3} - 3) j + 8 \sum_{s=5}^{3n-4} (10n - \frac{10(s+1)}{3} + 3) s$
- 3-  $W(Ch_{p_2}(W_5)_n) = 81n - 63 + 11 \sum_{k=3}^{3n-6} (n - \frac{k}{3}) k + \sum_{j=4}^{3n-5} (7n - \frac{7(j-1)}{3} - 1) j + 2 \sum_{s=5}^{3n-4} (3n - s + 01) s$ .

**Proof:** The proof can be obtained directly through the Theorem 2.1.

**Corollary 2.4:** For all  $n \geq 3$  then we have:

- 1-  $Sc(Ch_{p_2}(W_5)_n) = 1444n - 2020$ .
- 2-  $Sc^*(Ch_{p_2}(W_5)_n) = 2481n - 3493$ .

$$3- W(Ch_{P_2}(W_5)_n) = 216n - 300.$$

**Proof:** The proof can be obtained directly through the Theorem 2.1 and Corollary 2.3.

### 3. Some properties of Schultz polynomial coefficients, modified Schultz polynomials, and Hosoya for some chains and rings of graphs:

Some properties polynomial	Property1	Property2	Property3	Property4	Property5	Property6
$Sc(Ch_{P_2}(W_5)_n; x)$	Not j-unimodal	Not monotonically increasing And not monotonically decreasing	Not palindromic	Troubled	Not equality	Positive
$Sc^*(Ch_{P_2}(W_5)_n; x)$	Not j-unimodal	Not monotonically increasing And not monotonically decreasing	Not palindromic	Troubled	Not equality	Positive
$H(Ch_{P_2}(W_5)_n; x)$	Not j-unimodal	Not monotonically increasing And not monotonically decreasing	Not palindromic	Troubled	Not equality	Positive

**Conclusion:** we present the concept of Schultz, modified Schultz and Hosoya Polynomials to connect a chain of vertices of rings of a pentagonal graph, with a path of length one. In addition to some special results.

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