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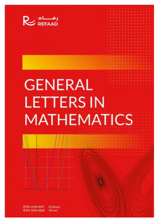

Schultz and Modified Schultz Polynomials of Chain from Alternating Hexagonal and Quadruple Rings

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Abstract

Many topological indices are closely related to chemical and physical properties, especially types of chemical structures that are characterized by the forms of chains of special chemical structures including hexacyclic, pentagonal, and tetracyclic structures. In 1947, the first chemist to find a relationship between topological index is called the Wiener index which was named after the chemical scientist Harold Wiener. He introduced the Wiener index to find a relationship between physic and chemical properties of chemical structures of molecular graphs. Then, the Hosoya polynomial in chemistry was found by Haruo Hosoya in 1988, through which the Wiener index was found, by finding the derivative of this polynomial and then substituting for the value of the variable with one. Therefore, our aim in this paper was to talk about other topological indices called Schultz and modified Schultz indices with mentioning their polynomials and to find general formulas for each of them for an alternating chain of quaternary and hexagonal rings, which have some applications in chemistry. Also, a program was made using the Mathematica program to find the polynomials, indices, and sketches of them with respect to the Schultz distance. The first researcher to talk about the Schultz index was Harry Schultz in 1989 and the first to talk about the modified Schultz index were Sandi Klavžar and Ivan Gutman in 1997. Finally, many types of research are found Schultz and modified Schultz to Lots of graphs and operations defined on it.

Keywords: Schultz, modified Schultz, polynomials, indices, chain of structure chemical.
2010 MSC: MSC 11S05, MSC 06E10, .

1. Introduction

A simple graph that does not contain loops or and define the connected is graph G_p it is the graph that has a path between any two vertices $u,v \in V(G_p)$ and has $V(G_p)$ at least $p-1$ of vertices, the null graph which consists from p of vertices without any edges which are denoted by N_p. In this paper all the graphs are simple, connected, and not null. The number of vertices in graph G is called order a graph G, and the size of graph G is number of edges in graph G [1]. The distance between any two vertices u,v in a connected graph G_p is defined as the shortest path between them, which is denoted by $d(u,v)$ The diameter in a connected graph G_p is a length of the longest path which joins between u and v in G_p , we denoted to the diameter by diam G_p, the path graph has the largest diameter among graphs and the

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complete graph has the smallest diameter in graphs. The number of all unordered pairs in a connected graph is G_p is 1/2 p(p+1) by symbol, we can write $|d_{G_p}(u,v)| = \frac{1}{2p(p+1)}$ .We denoted by degv to the vertex degree which is referred to the number of edges that lies on vertex v [1].

Harold Wiener introduced topological index biology and chemistry in 1947, the Wiener index is defined as [2]:

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

The Japanese scientist Hosoya introduced his polynomial in 1988 and defied it as follows [3]:

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

Also, he defined Hosoya polynomial by Wiener polynomial.
Now, we will define Shultz and modified Shultz polynomials. Shultz introduced his index in 1989 and defined it as follows [4]:

$$Sc(G_p) = \sum_{\{u,v\}\subseteq V(G_p)} (degu + degv)d(u,v),$$

where degu and degv are degrees of vertices u and v.
After that in 1997, for all Klavžar and Gutman together, the modified Shultz index was introduced and defined as follows [5]:

$$Sc^*(G_p) = \sum_{\{u,v\}\subseteq V(G_p)} (degu.degv)d(u,v),$$

We can write the definition of two Shultz and modified Shultz polynomials respectively as:

$$Sc(G_p;x) = \sum_{\{u,v\}\subseteq V(G_p;x)} (degu + degv)x^{d(u,v)},$$

$$Sc^*(G_p;x) = \sum_{\{u,v\}\subseteq V(G_p;x)} (degu.degv)x^{d(u,v)},$$

In addition to that we can conclude that the Schultz and modified Schultz indices are from Schultz and modified Schultz polynomials by the derivative$Sc(G;x)$ and $Sc^*(G;x)$ respectively with respect to x at $x = 1$, that is:

$$Sc(G;x) = \frac{d}{dx}(Sc(G;x))|_{x=1} \text{ and } Sc^*(G;x) = \frac{d}{dx}(Sc^*(G;x))|_{x=1}.$$

We focus in this paper on Shultz and modified Shultz polynomials for hexagonal – quadruple alternating chain graphs. It is of necessity to mention that there are many studies on polynomials and indices furthermore the Schultz and modified Schultz, ([6-10]) and also, there are studies on the application of it ([11-16]).

2. Schultz and Modified Schultz Polynomials for CHQ, CHQH and CQHQ Graphs

In this section, we give three types of different chemical structures in chemical see Figure 1. Some properties have studied Schultz and modified Schultz polynomials that are presented and the Schultz and modified Schultz found.

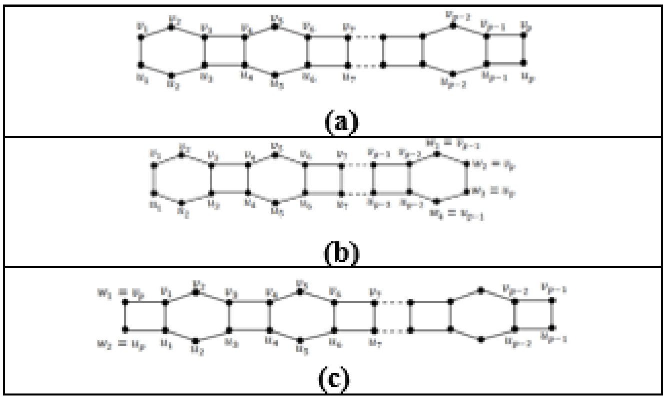


Figure 1: Three types of Different Chemical Structures.

2.1. Some Properties of Three types of Different Chemical Structures

1. Chain hexagonal - quadruple rings CHQ:
   The order is 2p, the size is $\frac{(8p-5)}{3}$, the diameter is p, the number of square rings and hexagonal rings are $\frac{p-1}{3}$, where p=3n+1, $n \in N - \{0\}$.
2. Chain hexagonal - quadruple rings CHQH:
   The order is 2p, the size is $\frac{(8p-6)}{3}$, the diameter is p, the number of $\frac{(p-3)}{3}$ square rings and hexagonal rings are $\frac{p}{3}$, where p=3n, $n \in N - \{0, 1\}$.
3. Chain hexagonal - quadruple rings CQHQ:
   The order is 2p, the size is $\frac{(8p-5)}{3}$, the diameter is p, the number of square rings $\frac{(p+1)}{3}$ and hexagonal rings are $\frac{p-2}{3}$, where p=3n+2, $n \in N - \{0\}$.

We will now present the three proofs for the different types of chemical structures with respect to Schultz and modified Schultz polynomials and then find the indices of it using derivation.

Theorem 2.1. *For all* $p \geqslant 8$, *then we have :*

1.

$$\begin{aligned} Sc(CHQ; x) =& \frac{2}{3}(22p-25)x + \frac{2}{3}(32p-59)x^2 + \frac{2}{3}(34p-91)x^3 + \frac{4}{3}\sum_{i=1}^{\frac{(p-4)}{3}}(16p-48i-13)x^{3i+1} \\ &+ \frac{2}{3}\sum_{i=1}^{\frac{p-4}{3}}(32p-96i-59)x^{3i+2} + \frac{2}{3}\sum_{i=1}^{\frac{p-4}{3}}(32p-96i-89)x^{3i+3} + 8x^p. \end{aligned} \tag{2.1}$$

2.

$$\begin{aligned} Sc^*(CHQ; x) =& (20p-31)x + 4(7p-15)x^2 + 30(p-3)x^3 + \frac{2}{3}\sum_{i=1}^{\frac{(p-4)}{3}}(43p-129i-49)x^{3i+1} \\ &+ 4\sum_{i=1}^{\frac{p-4}{3}}(7p-21i-15)x^{3i+2} + \frac{2}{3}\sum_{i=1}^{\frac{p-7}{3}}(43p-129i-133)x^{3i+3} + 28x^{p-1} + 8x^p. \end{aligned} \tag{2.2}$$

Proof. For all two vertices $u, v \in V(CHQ)$, there is $d(u, v) = k$, $1 \leqslant k \leqslant p$, and obviously $\sum_{i=1}^{p} |D_i| = p(2p-1)$. Then there are seven parts:

A. If d(u,v)=1, then $|D_i| = \frac{8p-5}{3} = q$ and then we have seven subparts of it:

A.1. $|D_1(2,2)| = |\{(u_1, v_1), (u_p, v_p), (u_1, u_2), (v_1, v_2)\}| = 4.$

A.2. $|D_1(2,3)| = |\{(u_{3i-1}, u_{3i}), (v_{3i-1}, v_{3i}) : 1 \leqslant i \leqslant \frac{p-1}{3}\}| = 2(\frac{p-1}{3}).$

A.3. $|D_1(2,3)| = |\{(u_{3i+2}, u_{3i+1}), (v_{3i+2}, v_{3i+1}) : 1 \leqslant i \leqslant \frac{p-1}{3}\}| = 2(\frac{p-4}{3}).$

A.4. $|D_1(2,3)| = |\{(u_p, u_{p-1}), (v_p, v_{p-1})\}| = 2.$

A.5. $|D_1(3,3)| = |\{(u_{3i}, v_{3i}), (u_{3i+1}, v_{3i+1}) : 1 \leqslant i \leqslant \frac{p-4}{3}\}| = 2(\frac{p-4}{3}).$

A.6. $|D_1(3,3)| = |\{(u_{3i}, u_{3i+1}), (v_{3i}, v_{3i+1}) : 1 \leqslant i \leqslant \frac{p-4}{3}\}| = 2(\frac{p-4}{3})$

A.7. $|D_1(3,3)| = |\{(u_{p-1}, v_{p-1})\}| = 1.$

B. If d(u,v)=k, k=3i-1, $i = 1, 2, ..., \frac{p-2}{3}$ then we have five subparts of it:

B.1. $|D_k(2,2)| = |\{(u_{p-k}, u_p), (v_{p-k}, v_p), (u_1, v_k), (v_1, u_k)\}| = 4.$

B.2. $|D_k(2,3)| = |\{(u_{3i-1}, u_{3i+k-1}), (v_{3i-1}, v_{3i+1}), (u_{3i+k}, u_{3i}), (v_{3i+k}, v_{3i}) : 1 \leqslant i \leqslant \frac{p-k-2}{3}\}| = 2(p - k - 2).$

B.3. $|D_k(2,3)| = |\{(u_{3i-1}, u_{3i+k-2}), (v_{3i-1}, v_{3i+k-2}) : 1 \leqslant i \leqslant \frac{p-k+1}{3}\}| = 2(\frac{p-k+1}{3})$

B.4. $|D_k(2,3)| = |\{(u_1, u_{k+1}), (v_1, v_{k+1}), (u_p, v_{p-k+1}), (v_p, u_{p-k+1})\}| = 4.$

B.5. $|D_k(3,3)| = |\{(u_{3i+1}, u_{3i+k+1}), (v_{3i+1}, v_{3i+k+1}), (u_{3i}, v_{3i+k-1}), (v_{3i}, u_{3i+k-1}) : 1 \leqslant i \leqslant \frac{p-k-2}{3}\}| = 4(\frac{p-k-2}{3}).$

Then, $|D_k| = 2(2p - 2k + 1), k = 3i - 1, i = 1, 2, \ldots, \frac{p-2}{3}.$

C. If d(u,v)=k, k=3i, $i = 1, 2, ..., \frac{p-4}{3}$ then we have six subparts of it

C.1. $|D_k(2,2)| = |\{(u_{3i-1}, u_{3i+k-1}), (v_{3i-1}, v_{3i+k-1}) : 1 \leqslant i \leqslant \frac{p-k-1}{3}\}| = 2(\frac{p-k-1}{3})$

C.2. $|D_k(2,3)| = |\{(u_{p-k+1}, v_p), (v_{p-k+1}, u_p)\}| = 2.$

C.3. $|D_k(2,3)| = |\{(u_{3i-1}, v_{3i+k-2}), (v_{3i-1}, u_{3i+k-2}), (v_{3i+k-1}, u_{3i}), (u_{3i+k-1}, v_{3i}) : 1 \leqslant i \leqslant \frac{p-k-1}{3}\}| = 4(\frac{p-k-1}{3})$

C.4. $|D_k(2,3)| = |\{(u_1, u_{1+k}), (v_1, v_{1+k}), (u_p, u_{p-k}), (v_p, v_{p-k}), (u_1, v_k), (v_1, u_k)\}| = 6.$

C.5. $|D_k(3,3)| = |\{(u_{3i}, u_{3i+k}), (v_{3i}, v_{3i+k}), (u_{3i+1}, v_{3i+k}), (v_{3i+1}, u_{3i+k}) : 1 \leqslant i \leqslant \frac{p-k-1}{3}\}| = 4(\frac{p-k-1}{3}).$

C.6. $|D_k(3,3)| = |\{(u_{3i+1}, u_{3i+k+1}), (v_{3i+1}, v_{3i+k+1}) : 1 \leqslant i \leqslant \frac{p-k-4}{3}\}| = 2(\frac{p-k-4}{3}).$
when k=3, we have another case:

C.7. $|D_k(2,2)| = |\{(u_{3i-1}, v_{3i-1}) : 1 \leqslant \frac{p-1}{3}\} = \frac{p-1}{3}$ Then, $|D_k| = 2(2p - 2k + 1), k = 3i - 1, i = 1, 2, \ldots, \frac{p-4}{3}$ and when $|D_3| = \frac{13p-31}{3}$.

D. If d(u,v)=k, k=3i+1, $i = 1, 2, \ldots, \frac{p-4}{3}$ and we have seven subparts of it:

D.1. $|D_k(2,2)| = |\{(u_{3i-1}, v_{3i+k}), (v_{3i-1}, u_{3i+k-2}) : 1 \leqslant i \leqslant \frac{p-k}{3}\}| = 2(\frac{p-k}{3}).$

D.2. $|D_k(2,2)| = |\{(u_1, u_{1+k}), (v_1, v_{1+k})\}| = 2.$

D.3. $|D_k(2,3)| = |\{(u_{3i-1}, u_{3i+k-1}), (v_{3i-1}, v_{3i+k-1}) : 1 \leqslant i \leqslant \frac{p-k}{3}\}| = 2(\frac{p-k}{3}).$

D.4. $|D_k(2,3)| = |\{(u_{3i+k+1}, u_{3i+1}), (v_{3i+k+1}, v_{3i+1}) : 1 \leqslant i \leqslant \frac{p-k-3}{3}\}| = 2(\frac{p-k-3}{3}).$

D.5. $|D_k(2,3)| = |\{(u_1, v_k), (v_p, u_{p-k+1}), (v_1, u_k), (u_p, v_{p-k+1}), (v_p, v_{p-k}), (u_p, u_{p-k})\}| = 6.$

D.6. $|D_k(3,3)| = |\{(u_{3i}, u_{3i+k}), (v_{3i}, v_{3i+k}), (u_{3i+1}, v_{3i+k}), (v_{3i+1}, u_{3i+k}) : 1 \leqslant i \leqslant \frac{p-k-3}{3}\}| = 4(\frac{p-k-3}{3}).$

D.7. $|D_k(3,3)| = |\{(u_{3i}, v_{3i+k-1}), (v_{3i}, v_{3i+k-1}) : 1 \leqslant i \leqslant \frac{p-k}{3}\}| = 2(\frac{p-k}{3})$.

Then, $|D_k| = 2(2p-2k+1)$, k=3i+1, $i = 1, 2, \ldots, (p-4)/3$.

E. If d(u,v)=p-2, and we have two subparts of it:

E.1. $|D_{p-2}(2,2)| = |\{(u_2, u_p), (v_2, v_p), (u_1, v_{p-2}), (v_1, u_{p-2})\}| = 4$.

E.2. $|D_{p-2}(2,3)| = \{(u_1, u_{p-1}), (v_1, v_{p-1}), (u_2, v_{p-1}), (u_p, v_3), (v_2, u_{p-1}), (v_p, u_3)\}| = 6$.

Then,$|D_{p-2}| = 10$.

F. If d(u,v)=p-1, and we have two subparts of it:

F.1. $|D_{p-1}(2,2)| = |\{(u_1, u_p), (v_1, v_p), (u_2, v_p), (v_2, u_p)\}| = 4$.

F.2. $|D_{p-1}(2,3)| = |\{(u_1, v_{p-1}), (v_1, u_{p-1})\}| = 2$.

Then, $|D_{p-1}| = 6$.

G. If d(u,v)=p,and we have one subpart of it: $|D_p(2,2)| = |\{(u_1, v_p), (v_1, u_p)\}| = 2$. Then, $|D_p| = 2$.

From A – G and definitions Schultz and modified Schultz, we obtain (2.1) and (2.2) respectively □

Theorem 2.2. *For all* $p \geqslant 9$, *we have:*

1.

$$Sc(CHQH; x) = \frac{4}{3}(11p-15)x + \frac{8}{3}(8p-15)x^2 + \frac{4}{3}(17p-45)x^3 + \frac{4}{3}\sum_{i=1}^{\frac{p-3}{3}}(16p-48i-15)x^{3i+1} + \frac{8}{3}\sum_{i=1}^{\frac{p-3}{3}}(8p-24i-15)x^{3i+2} + \frac{4}{3}\sum_{i=1}^{\frac{p-6}{3}}(16p-48i-45)x^{3i+3} + 8x^p.$$

2.

$$Sc^*(CHQH; x) = 4(5p-9)x + 2(14p-31)x^2 + 2(15p-46)x^3 + \frac{2}{3}\sum_{i=1}^{\frac{p-3}{3}}(43p-129i-57)x^{3i+1} + 2\sum_{i=1}^{\frac{p-6}{3}}(14p-42i-31)x^{3i+2} + \frac{2}{3}\sum_{i=1}^{\frac{p-6}{3}}(43p-129i-138)x^{3i+3} + 24x^{p-1} + 8x^p.$$

Proof. From Theorem 2.1, we have $Sc(CHQH; x)$ and $Sc^*(CHQH; x)$ by adding the new vertices w_1, w_2, w_3, w_4 and edges $v_pw_1, w_1w_2, w_2w_3, w_3w_4, w_4u_p$ to the graph CHQ and replace all p by p-2. see Figure 1.(b).

Let h(k) be the representation the extra degrees of vertices $v_p, w_1, w_2, w_3, w_4, u_p$ with respect to distancing part k, that is $h(k) = (degy + degz)d(y, z)$ such that $d(y, z) = k$, for $1 \leqslant k \leqslant p, y, z \in V(CHQH)$. From Theorem 2.1, we have:

$$\begin{aligned} Coff((Sc(CHQH; x), 1) &= Coff((Sc(CHQ; x), 1) + h(1) \\ &= \frac{2}{3}(22(p-2) - 25) + 26 \\ &= \frac{4}{3}(11p-15). \end{aligned}$$

$$\begin{aligned}
\mathrm{Coff}((Sc(CHQH;x),2) &= \mathrm{Coff}((Sc(CHQ;x),2) + h(2) \\
&= \frac{2}{3}(32(p-2)-59)+42 \\
&= \frac{8}{3}(8p-15).
\end{aligned}$$

$$\begin{aligned}
\mathrm{Coff}((Sc(CHQH;x),3) &= \mathrm{Coff}((Sc(CHQ;x),3) + h(3) \\
&= \frac{2}{3}(34(p-2)-91)+46 \\
&= \frac{4}{3}(17p-45).
\end{aligned}$$

$$\begin{aligned}
\mathrm{Coff}((Sc(CHQH;x),3i+1) &= \mathrm{Coff}((Sc(CHQ;x),3i+1) + h(3i+1) \\
&= \frac{4}{3}(16(p-2)-48i-13)+40 \\
&= \frac{4}{3}(16p-48i-15).
\end{aligned}$$

$$\begin{aligned}
\mathrm{Coff}((Sc(CHQH;x),3i+2) &= \mathrm{Coff}((Sc(CHQ;x),3i+2) + h(3i+2) \\
&= \frac{2}{3}(32(p-2)-96i-59)+42 \\
&= \frac{8}{3}(16p-24i-15).
\end{aligned}$$

$$\begin{aligned}
\mathrm{Coff}((Sc(CHQH;x),3i+3) &= \mathrm{Coff}((Sc(CHQ;x),3i+3) + h(3i+3) \\
&= \frac{2}{3}(32(p-2)-96i-89)+42 \\
&= \frac{4}{3}(16p-48i-45).
\end{aligned}$$

Directly from Figure 1.(b), we have: Coff((Sc(CHQH;x),p)=8.

Now, we find the modified Schultz polynomial of the graph CHQH in the same way find the Schultz polynomial of the graph CHQH from Theorem 2.1.

Let $h^*(k)$ be the representation the extra degrees of vertices $v_p, w_1, w_2, w_3, w_4, u_p$ with respect to distancing part k, that is $h^*(k) = (degy.degz)d(y,z)$ such that d(y,z)=k, for $1 \leqslant k \leqslant p, y, z \in V(CHQH)$. From Theorem 2.1, we have:

$$\begin{aligned}
\mathrm{Coff}(Sc^*(CHSH;x),1) &= \mathrm{Coff}(Sc^*(CHS;x),1) + h^*(1) \\
&= (20(p-2)-31)+35 \\
&= 4(5p-9).
\end{aligned}$$

$$\begin{aligned}
\mathrm{Coff}(Sc^*(CHQH;x),2) &= \mathrm{Coff}(Sc^*(CHQ;x),2) + h^*(2) \\
&= 4(7(p-2)-15)+54 \\
&= 2(14p-31).
\end{aligned}$$

$$\begin{aligned}
\mathrm{Coff}(Sc^*(CHQH;x),3) &= \mathrm{Coff}(Sc^*(CHQ;x),3) + h^*(3) \\
&= 30(p-2-3)+58 \\
&= 2(15p-46).
\end{aligned}$$

$$\begin{aligned}
\mathrm{Coff}(Sc^*(CHQH;x),3i+1) &= \mathrm{Coff}(Sc^*(CHQ;x),3i+1) + h^*(3i+1) \\
&= \frac{2}{3}(43(p-2)-129i-49)+52 \\
&= \frac{2}{3}(43p-129i-57).
\end{aligned}$$

$$\begin{aligned}\mathrm{Coff}(Sc^*(CHQH;x),3i+2) &= \mathrm{Coff}(Sc^*(CHQ;x),3i+2)+h^*(3i+2)\\ &= 4(7(p-2)-21i-15)+54\\ &= 2(14p-42i-31).\end{aligned}$$

$$\begin{aligned}\mathrm{Coff}(Sc^*(CHQH;x),3i+3) &= \mathrm{Coff}(Sc^*(CHQ;x),3i+3)+h^*(k)\\ &= \frac{2}{3}(43(p-2)-129i-133)+54\\ &= \frac{2}{3}(43p-129i-138).\end{aligned}$$

Finally, directly from Figure 1. (b), we have:

$$\mathrm{Coff}(Sc^*(CHQH;x),p-1)=24 \text{ and } \mathrm{Coff}(Sc^*(CHQH;x),p)=8.$$

□

Theorem 2.3. *For all* $p > 8$*, we have:*

1.

$$Sc(CHQH;x) = \frac{4}{3}(11p-1)x+\frac{4}{3}(16p-29)x^2+\frac{2}{3}(43p-101)x^3+\frac{4}{3}\sum_{i=1}^{\frac{p-4}{3}}(16p-48i-11)x^{3i+1} + \frac{2}{3}\sum_{i=1}^{\frac{p-4}{3}}(32p-96i-58)x^{3i+2}+\frac{16}{3}\sum_{i=1}^{\frac{p-4}{3}}(4p-12i-11)x^{3i+3}+8x^p.$$

2.

$$Sc^*(CQHQ;x) = 2(10p-3)x+2(14p-29)x^2+2(15p-44)x^3+\frac{2}{3}\sum_{i=1}^{\frac{p-4}{3}}(43p-129i-41)x^{3i+1} + 2\sum_{i=1}^{\frac{p-4}{3}}(14p-42i-29)x^{3i+2}+\frac{2}{3}\sum_{i=1}^{\frac{p-7}{3}}(43p-129i-133)x^{3i+3}+32x^{p-1}+8x^p.$$

Proof. In the same method Theorem 2.2, see Figure 1.(c), we find Schultz and modified Schultz polynomials for the graph CQHQ. □

3. Schultz and Modified Schultz Indices for CHQ, CHQH and CQHQ Graphs

In this section, we find the indices of Schultz and modified Schultz for some chemical structures mentioned earlier

Corollary 3.1. *For all* $p \geqslant 8$*, then we have :*

1. $Sc(CHQ) = \frac{2}{27}(48p^3+27p^2+482p+52)$.
2. $Sc^*(CHQ) = \frac{1}{27}(128p^3-48p^2+72p-125)$.

Proof. 1. From definition Schultz index, we obtain :

$$\begin{aligned}Sc(CHQ) &= \frac{2}{3}(22p-25)+\frac{4}{3}(32p-59)+\frac{6}{3}(34p-91)\\ &+\frac{4}{3}\sum_{i=1}^{\frac{p-4}{3}}(3i+1)(16p-48i-13)+\frac{2}{3}\sum_{i=1}^{\frac{p-4}{3}}(3i+2)(32p-96i-59)\\ &+\frac{2}{3}\sum_{i=1}^{\frac{p-4}{3}}(3i+3)(32p-96i-89)+8p.\end{aligned}$$

$$= \frac{8}{3}(50p-104) + \frac{2}{27}(16p^3+9p^2-363p+384)$$
$$+ \frac{1}{27}(32p^3+15p^2-107p+1996) + \frac{1}{27}(32p^3+21p^2-1803p+4828)$$
$$= \frac{2}{27}(48p^3+27p^2+482p+52).$$

2. From definition modified Schultz index, we obtain :

$$Sc^*(CHQ) = (20p-31) + 8(7p-15) + 90(p-3) + \frac{2}{3}\sum_{i=1}^{\frac{p-4}{3}}(3i+1)(43p-129i-49)$$
$$+4\sum_{i=1}^{\frac{p-4}{3}}(3i+2)(7p-21i-15) + \frac{2}{3}\sum_{i=1}^{\frac{p-7}{3}}(3i+3)(43p-129i-133) + 28(p-1) + 8p.$$
$$= 202p - 449 + \frac{1}{27}(43p^3-18p^2-849p+932)$$
$$+ \frac{2}{9}(7p^3-3p^2-228p+512) + \frac{1}{27}(43p^3-12p^2-3165p+7994)$$
$$= \frac{1}{27}(128p^3-48p^2+72p-125).$$

□

Corollary 3.2. *For all* $p \geqslant 9$*, we have:*

1. $Sc(CHQH) = \frac{4}{9}p^2(8p+3)$.
2. $Sc^*(CHQH) = \frac{4}{27}p(32p^2-24p+27)$.

Proof. 1. From definition Schultz index, we get :

$$Sc(CHQH) = \frac{4}{3}(11p-15) + \frac{16}{3}(8p-15) + \frac{12}{3}(17p-45) + \frac{4}{3}\sum_{i=1}^{\frac{p-3}{3}}(3i+1)(16p-48i-15)$$
$$+ \frac{8}{3}\sum_{i=1}^{\frac{p-3}{3}}(3i+2)(8p-24i-15) + \frac{4}{3}\sum_{i=1}^{\frac{p-6}{3}}(3i+3)(16p-48i-45) + 8p.$$
$$= \frac{40}{3}(10p-21) + \frac{2}{27}(16p^3+3p^2-243p+270)$$
$$+ \frac{4}{27}(8p^3+3p^2-261p+540) + \frac{2}{27}(16p^3+9p^2-1035p+2430)$$
$$= \frac{4}{9}p^2(8p+3).$$

2. From definition modified Schultz index, we get :

$$Sc^*(CHQH) = 4(5p-9) + 4(14p-31) + 6(15p-46) + \frac{2}{3}\sum_{i=1}^{\frac{p-3}{3}}(3i+1)(43p-129i-57)$$
$$+2\sum_{i=1}^{\frac{p-6}{3}}(3i+2)(14p-42i-31) + \frac{2}{3}\sum_{i=1}^{\frac{p-6}{3}}(3i+3)(43p-129i-138) + 24(p-1) + 8p.$$

$$= 2(99p - 230) + \frac{1}{27}(43p^3 - 42p^2 - 603p + 1026)$$
$$+ \frac{1}{9}(14p^3 - 9p^2 - 669p + 1314) + \frac{1}{27}(43p^3 - 27p^2 - 2628p + 7452)$$
$$= \frac{4}{27}p(32p^2 - 24p + 27).$$

□

Corollary 3.3. *For all* $p > 8$, *we have:*

1. $Sc(CQHQ) = \frac{2}{9}(16p^3 + 12p^2 + 75p - 55)$.
2. $Sc^*(CQHQ; x) = \frac{1}{27}(128p^3 - 15p^2 + 99p + 508)$.

Proof. 1. From definition Schultz index, we have:

$$Sc(CQHQ) = \frac{4}{3}(11p - 1) + \frac{8}{3}(16p - 29) + \frac{6}{3}(43p - 101) + \frac{4}{3}\sum_{i=1}^{\frac{p-4}{3}}(3i + 1)(16p - 48i - 11)$$
$$+ \frac{2}{3}\sum_{i=1}^{\frac{p-4}{3}}(3i + 2)(32p - 96i - 58) + \frac{16}{3}\sum_{i=1}^{\frac{p-4}{3}}(3i + 3)(4p - 12i - 11) + 8p$$
$$= \frac{2}{3}(227p - 421) + \frac{2}{27}(16p^3 + 15p^2 - 381p + 260)$$
$$+ \frac{2}{27}(16p^3 + 9p^2 - 537p + 980) + \frac{8}{27}(4p^3 + 3p^2 - 225p + 596)$$
$$= \frac{2}{9}(16p^3 + 12p^2 + 75p - 55).$$

2. From definition modified Schultz index, we have:

$$Sc^*(CQHQ) = 2(10p - 3) + 4(14p - 29) + 6(15p - 44) + \frac{2}{3}\sum_{i=1}^{\frac{p-4}{3}}(3i + 1)(43p - 129i - 41)$$
$$+ 2\sum_{i=1}^{\frac{p-4}{3}}(3i + 2)(14p - 42i - 29) + \frac{2}{3}\sum_{i=1}^{\frac{p-7}{3}}(3i + 3)(43p - 129i - 133) + 32(p - 1) + 8p$$
$$= 2(103p - 209) + \frac{1}{27}(43p^3 + 6p^2 - 921p + 836)$$
$$+ \frac{1}{9}(14p^3 - 3p^2 - 459p + 988) + \frac{1}{27}(43p^3 - 12p^2 - 3165p + 7994)$$
$$= \frac{1}{27}(128p^3 - 15p^2 + 99p + 508).$$

□

4. Applications

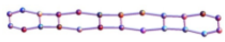
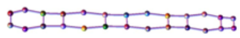
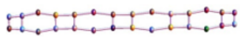
In this section, we obtain the Schultz and modified Schultz for all polynomials and indices for chain hexagonal - quadruple rings(CHQ), chain hexagonal - quadruple - hexagonal rings (CHQH) and chain quadruple - hexagonal - quadruple rings (CQHQ). In the following part, we give algorithm to graphic structures of two dimensions for three types chains: CHQ, CHQH and CQHQ, and then finding the polynomials and indices with respect to Schultz

4.1. *Algorithm*

- Start .
- Enter chain.
- Find adjacent , degree and distance matrices.
- Use two dimension to graphic commands in mathematica programming.
- Determine the diameter of any type of chain.
- Finding the Schultz and modified Schultz polynomial , and then find the indices if them.
- end.

4.2. *Examples*

We take three examples for rings chain: Hexagonal - Quadruple, Hexagonal - Quadruple - Hexagonal and Quadruple - Hexagonal – Quadruple.

CHQH	
$p = 12$	$Sc(CHQH;x) = 156x + 216x^2 + 212x^3 + 172x^4 + 152x^5 + 132x^6 + 108x^7 + 88x^8 + 68x^9 + 44x^{10} + 24x^{11} + 8x^{12}$. $Sc^*(CHQH;x) = 204x + 274x^2 + 268x^3 + 220x^4 + 190x^5 + 166x^6 + 134x^7 + 106x^8 + 80x^9 + 48x^{10} + 24x^{11} + 8x^{12}$. $Sc(CHQH) = 6336$. $Sc^*(CHQH) = 7728$.
CHQ	
$p = 13$	$Sc(CHQ;x) = 174x + 238x^2 + 234x^3 + 196x^4 + 174x^5 + 154x^6 + 132x^7 + 110x^8 + 90x^9 + 68x^{10} + 46x^{11} + 26x^{12} + 8x^{13}$. $Sc^*(CHQ;x) = 229x + 304x^2 + 300x^3 + 254x^4 + 220x^5 + 198x^6 + 168x^7 + 136x^8 + 112x^9 + 82x^{10} + 52x^{11} + 28x^{12} + 8x^{13}$. $Sc(CHQ) = 8146$. $Sc^*(CHQ) = 10145$.
CQHQ	
$p = 14$	$Sc(CQHQ;x) = 192x + 260x^2 + 256x^3 + 220x^4 + 196x^5 + 176x^6 + 156x^7 + 132x^8 + 112x^9 + 92x^{10} + 68x^{11} + 48x^{12} + 28x^{13} + 8x^{14}$. $Sc^*(CQHQ;x) = 254x + 334x^2 + 332x^3 + 288x^4 + 250x^5 + 230x^6 + 202x^7 + 166x^8 + 144x^9 + 116x^{10} + 82x^{11} + 58x^{12} + 32x^{13} + 8x^{14}$. $Sc(CQHQ) = 10272$. $Sc^*(CQHQ) = 13024$.

Conclusion 4.1. It is possible to notice that the results we obtained can be found, some of which depend on other formulas, for example, finding Schultz and modified Schultz polynomials for CHQH and CQHQ structures and its indices dependent on Schultz and modified Schultz polynomials for CHS and its index.

References

[1] G. Chartrand, L. Lesniak, Graphs and Digraphs, 6^{th} ed., Wadsworth and Brooks /Cole. California, (2016).

[2] H. Wiener, Structural Determination of Paraffin Boiling Points, J. Amer. Chem. Soc. 69(1947), pp.17-20. https://doi.org/10.1021/ja01193a005

[3] H. Hosoya, On Some Counting Polynomials in Chemistry, Discrete Appl. (1988), pp.239-157. https://doi.org/10.1016/0166-218x(88)90017-0

[4] H. P. Schultz, Topological Organic Chemistry 1: Graph Theory and Topological Indices of Alkanes, J. Chem. Inf. Comput. Sci. Vol. 29(1989), pp.227–228. https://doi.org/10.1021/ci00063a012

[5] S. Klavžar, I. Gutman, Wiener Number of Vertex-Weighted Graphs and a Chemical Application, Disc. Appl. Math. Vol. 80(1997), pp.73–81. https://doi.org/10.1016/s0166-218x(97)00070-x

[6] M. A. Ahmed, N. M. Haitham, Schultz and Modified Schultz Polynomials of Some Cog-Special Graphs, Open Access Library Journal, Vol.6(2019), pp.1-13. https://doi.org/10.4236/oalib.1105625

[7] M. A. Ahmed, Some Results on Wiener Indices for a Connected Graph G, Italian Journal of Pure and Applied Mathematics, Vol.46(2021), pp.391–399.

[8] Bo. Zhou, Bounds for the Schultz Molecular Topological Index, MATCH Commun. Math Comput. Chem. Vol. 56(2006), pp.189-194.

[9] M. A. Mahmood, M. A. Ahmed, Schultz and Modified Schultz polynomials for Edge –Identification Chain and Ring – for Pentagon and Hexagon Graphs. Journal of Physics: Conference Series, 1818(1)(2021), pp.1-21. https://doi.org/10.1088/1742-6596/1818/1/012063

[10] T. Mansour, M. Schork, Wiener, Hyper-Wiener, Detour and Hyper-Detour Indices of Bridge and Chain Graphs, Journal of Mathematical Chemistry, 47(1)(2013), pp. 72-98. https://doi.org/10.1007/s10910-009-9531-7

[11] M. R. Farahaini, Hosoya, Schultz Modified Schultz Polynomials and their Topological Indices of Benzene Molecules: First Members of polycyclic Aromatic Hydro Carbons (PAHs), International Journal of theoretical chemistry, Vol. 1(2013), No. 2, pp.6-9.

[12] M. R. Farahaini, Schultz and Modified Schultz Polynomials of Coronene Polycyclic Aromatic Hydro Carbons, International Letters of chemistry, Physics and Astronomy, Vol. 32(2014), pp.1-10. https://doi.org/10.18052/www.scipress.com/ilcpa.32.1

[13] K. A. Haneen, Schultz Index, Modified Schultz Index, Schultz Polynomial and Modified Schultz Polynomial of Alkanes, Global Journal of Pure and Applied Mathematics.13(9)(2017), pp.5827-5850.

[14] G. Hassani, A. Iranmanesh, S. Mirzaie, Schultz and Modified Schultz Polynomials of C100 Fullerene, MATCH Commun. Math. Comput. Chem. Vol. 69(2013), pp.87-92.

[15] A. Iranmanesh, Y. A. Zadeh, Computing Szeged and Schultz Indices of HAC3C7C9[p,q] Nanotube by Gap Program, Digest Biostructures, Vol.4(2009), pp.67-72.

[16] P. Saima, U. H. A. Nadeem, M. Mogtaba, B. F. Fozia, I. Nisha, Topological Indices of Novel Drugs Used in Diabetes Treatment and Their QSPR Modeling, Hindawi, Journal of Mathematics,(2022), pp.1-17. https://doi.org/10.1155/2022/5209329