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(RECOMMENDED CITATION)

ON THE SCHULTZ, MODIFIED SCHULTZ AND HOSOYA POLYNOMIALS AND DERIVED INDICES OF CAPRA-DESIGNED PLANAR BEZENOIDS

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ABSTRACT. In this paper, Schultz, Modified Schultz and Hosoya polynomial and their topological indices of a benzenoid molecular graph constructed by Capra-map operation, $Ca(C_6)$, are calculated. Several examples are given.

Keywords: *Schultz polynomial; Modified Schultz polynomial; Hosoya polynomial; Wiener index; Capra-operated benzenoid.*

INTRODUCTION

Let $G=(V,E)$ be a simple connected graph of finite order $n=|V|$, such that it has the vertex set $V=V(G)$ and edge set $E=E(G)$. A general reference for the notation in Graph Theory is [1]. The distance between vertices u and v of G, denoted $d(u,v)$, is the number of edges in a shortest path connecting them. The largest distance in G is called the diameter, $d(G)$. Another invariant in graph is degree of a vertex $v\in V(G)$ that it is the number of edges incident in it and is denoted by δ_v.

In graph theory, several counting polynomials are known: Schultz polynomial $Sc(G,x)$, Modified Schultz polynomial $Sc^*(G,x)$, Hosoya polynomial $H(G,x)$, etc. Their first derivative (in x=1) define, in general, the corresponding topological indices.

Definitions of the above polynomials and indices are as follows:

$$Sc\left(G,x\right)=\frac{1}{2}\sum_{\{u,v\}\in V\ (G)}(\delta_u+\delta_v)x^{d(u,v)}$$

$$Sc^*\left(G,x\right)=\frac{1}{2}\sum_{\{u,v\}\in V\ (G)}(\delta_u\delta_v)x^{d(u,v)}$$

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$$H(G,x)=\sum_{i=0}^{d(G)} d(G,i)x^{d(u,v)}$$

$$Sc(G)=\frac{1}{2}\sum_{\{u,v\}\in V(G)}(\delta_u+\delta_v)d(u,v)$$

$$Sc^*(G)=\frac{1}{2}\sum_{\{u,v\}\in V(G)}(\delta_u\times\delta_v)d(u,v)$$

$$W(G)=\frac{1}{2}\sum_{v\in V(G)}\sum_{u\in V(G)}d(u,v)=\sum_{i=0}^{d(G)}d(G,i)d(u,v)$$

$$WW(G)=H'(1)+(1/2)H''(1)$$

The Schultz index was introduced by *Schultz* in 1989 [2] while the Modified Schultz index was defined by *Klavžar* and *Gutman* in 1997 [3]. The Schultz index, also called molecular topological index, was studied in many papers [2-17]. These indices have been computed in some nanotubes [12-14, 17-21].

Hosoya polynomial was introduced by *H. Hosoya*, in 1988 [16]. The first derivative of Hosoya polynomial is just the Wiener index; a Hyper-Wiener index, denoted *WW(G)* (see above) can be computed from the first and second derivative of Hosoya polynomial. Wiener index had found numerous application and was reported in [8, 16, 21-32].

The coefficients of Hosoya polynomial can be calculated from layer/shell matrices, as shown by Diudea [33-35], who gave a "chemical" generalization in Hosoya-Diudea weighted polynomials.

In chemistry, physics and nanoscience, there are especially symmetric structures. Such molecular graphs are *Capra-designed planar benzenoids.* Capra *Ca* map operation (also called Septupling S_1) is a method of drawing and modifying the covering of a polyhedral structure, introduced by Diudea [36,37]. A detailed example is given in Figure 1.

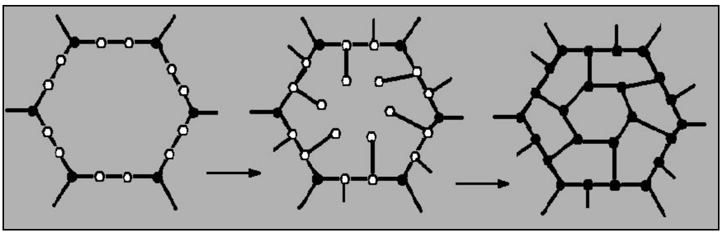

Figure 1. An example of Capra map operation on the hexagon face.

In this paper, we applied Capra operation on the benzene molecular graph C_6 to design planar benzenoid structures; the *k*-iterated benzenoids are denoted $Ca_k(C_6)$). The two first members of this series are shown in Figure 2.

Also, $Ca(C_6)$ is called Coronene H_2 and is the second member of the circumcoronene series of benzenoids H_k, $k \geq 1$. The first three members of circumcoronene series are shown in Figure 3.

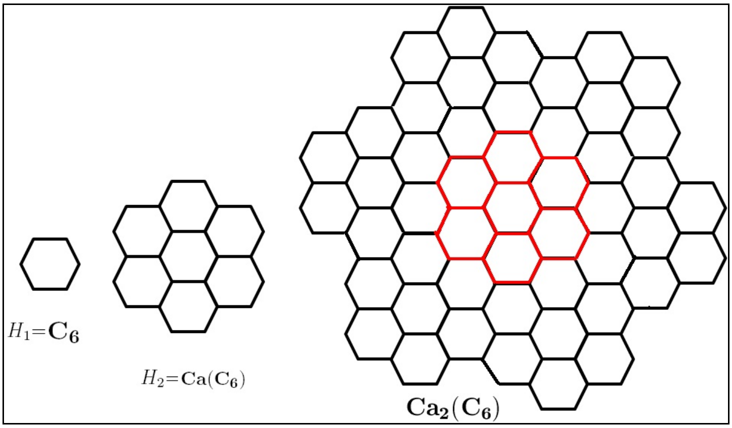

Figure 2. Benzenoid molecular graphs $H_2=Ca(C_6)$ and $Ca_2(C_6)$, representing the first two members of Capra-designed planar benzenoids.

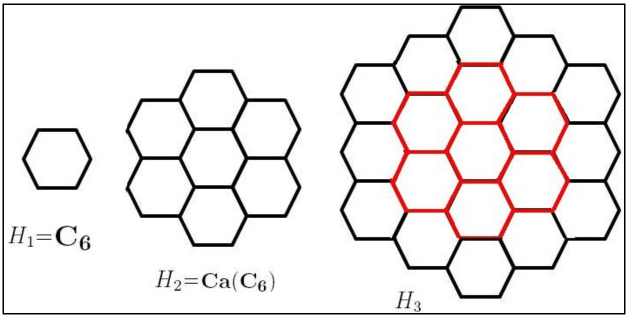

Figure 3. The first three graphs H_1, H_2 and H_3 of the Circumcoronene series.

Within this paper, we focused on the Schultz, Modified Schultz and Hosoya polynomials and their topological indices of the Coronene $Ca(C_6)$ planar benzenoid structure.

Theorem 1. Let $G=Ca(C_6)$ be a Capra-designed planar benzenoid. Then the Schultz polynomial of G is equal to:

$$Sc(G,x)=156x+252x^2+294x^3+276x^4+222x^5+132x^6+48x^7$$

and the Schultz index *Sc(G)=4884*.
The Modified Schultz polynomial of *G* is equal to:

$$Sc^*(G,x)=204x+330x^2+381x^3+348x^4+267x^5+144x^6+48x^7$$

and the Modified Schultz index *Sc*(G)*=5934.

Theorem 2. Let $G=Ca(C_6)$ be a Capra-designed planar benzenoid. Then, the Hosoya polynomial of *G* is equal to:

$$H(G,x)=24+30x^1+48x^2+57x^3+54x^4+45x^5+30x^6+12x^7$$

Also, the Wiener index is *W(G)*=1002, and Hyper Wiener index *WW(G)*=2697.

MAIN RESULTS

In this section we will prove the two above theorems. At first, we introduce some notations, related to Figure 4.

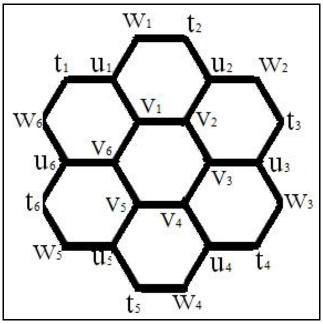

Figure 4. Capra-designed planar molecular graph: Coronene, $Ca(C_6)=H_2$ and the notation used in the text.

Let *V(G)* be the vertex set of $G=Ca(C_6)$ with cardinality 24 and *E(G)* the edge set, of cardinality 30. We describe each vertex of *G* by automorphism *f*, such that:

$$f: V(G) \to \{u_i, v_i, w_i, t_i \mid i \in \mathbb{Z}_6\}.$$

and

$$f: E(G) \to \{v_i v_{i+1}, v_i u_i, u_i w_i, u_i t_i, w_i t_{i+1} \mid i \in \mathbb{Z}_6\}.$$

According to the Figure 4, we have the vertices u_i, v_i of degree 3 and vertices w_i, t_i of degree 2, for all $\mathbb{Z}_6$. $\mathbb{Z}_6 = \{0,1,2,3,4,5\}$ is the cycle finite group of order 6 (or integer number of module 6).

Proof of Theorem 1: Let *G=Ca(C₆)* be the Coronene graph. Since there exists 24 distinct vertices, we have $\binom{n}{2}=276$ distinct shortest paths between vertices u and *v* of *G*. Also, in Coronene there are distances from one to seven, for every vertices $u,v\in V(G)$. In other words,

$$\forall u,v \in V(G), \exists d(u,v) \in \{1,2,...,7\}.$$

So, we will have seven partitions for proof.

I. If *d(u,v)*=1, then $D_1=\{(v_i,v_{i+1}),(v_i,u_i),(u_i,w_i),(u_i,t_i),(w_i,t_{i+1}) \mid i \in \mathbb{Z}_6\}$ and $|D_1|=30$ (that is equal to $|E(G)|$). So, we have three subsets of it.

I-1. $\forall i \in \mathbb{Z}_6$, let $v=v_i$ and $u=u_i=v_{i+1}$. Since $\delta_{v_i}=\delta_{u_i}=3$, hence $\delta_v+\delta_u=6$ and $\delta_v\times\delta_u=9$. Therefore $|\{(u,v) \mid u,v\in V(G), d(u,v)=1 \,\&\, \delta_v+\delta_u=6, \delta_v\times\delta_u=9\}|=6\times 2.$

So, we have two terms $72x^1$, $108x^1$ of the Schultz polynomial and Modified Schultz polynomial, respectively.

I-2. $\forall i \in \mathbb{Z}_6$, let $v=t_i$, w_i and $u=u_i$. Since $\delta_{u_i}=3$ and $\delta_{t_i}=\delta_{w_i}=2$. So, $\delta_v+\delta_u=5$ and $\delta_v\times\delta_u=6$. Therefore $|\{(u,v) \mid u,v\in V(G), d(u,v)=1 \,\&\, \delta_v+\delta_u=5, \delta_v\times\delta_u=6\}|=6\times 2.$ So, we have two sentences $60x^1$, $72x^1$ of the above polynomials.

I-3. $\forall i \in \mathbb{Z}_6$, let $v=w_i$ and $u=t_i$ Since $\delta_{t_i}=\delta_{w_i}=2$. So, $\delta_v+\delta_u=4$ and $\delta_v\times\delta_u=4$. Therefore $|\{(u,v) \mid u,v\in V(G), d(u,v)=1 \,\&\, \delta_v+\delta_u=4, \delta_v\times\delta_u=4\}|=6$.

In general, we have two terms $156x^1$, $204x^1$ for the Schultz polynomial and Modified Schultz polynomial, respectively.

II. If d(u, v)=2, then

$D_2=\{(v_i,v_{i+2}),(v_i,u_{i+1}),(v_i,w_i),(v_i,t_i),(v_i,u_{i-1}),(u_i,t_{i+1}),(u_i,w_{i-1}),(w_i,t_i) \mid i \in \mathbb{Z}_6\}$

and $|D_2|=48$. Similarly, we have three subsets of it.

II-1. $\forall i \in \mathbb{Z}_6$, let $v=v_i$ and $u=v_{i+2}$, u_{i+1}, u_{i-1} (or u_{i+5}). Since $\delta_{v_i}=\delta_{u_i}=3$, hence $\delta_v+\delta_u=6$ and $\delta_v\times\delta_u=9$. Therefore $|\{(u,v) \mid u,v\in V(G), d(u,v)=2 \,\&\, \delta_v+\delta_u=6, \delta_v\times\delta_u=9\}|=6\times 3.$

So, we have two terms $108x^2$, $162x^2$ for the Schultz polynomial and Modified Schultz polynomial, respectively.

II-2. $\forall i \in \mathbb{Z}_6$, let ($u=t_i$, w_i & $v=v_i$) or ($v=t_{i+1}$, w_{i-1} & $u=u_i$). Since $\delta_{v_i}=\delta_{u_i}=3$ and $\delta_{t_i}=\delta_{w_i}=2$, therefore $|\{(u,v) \mid u,v\in V(G), d(u,v)=2 \,\&\, \delta_v+\delta_u=5, \delta_v\times\delta_u=6\}|=24$. So, we have two sentences $120x^2$, $144x^2$ of these polynomials.

II-3. $\forall i \in \mathbb{Z}_6$, let $v=w_i$ and $u=t_i$. Since $\delta_{t_i}=\delta_{w_i}=2$, therefore

$$|\{(u,v) \mid u,v\in V(G), d(u,v)=2 \,\&\, \delta_v+\delta_u=4, \delta_v\times\delta_u=4\}|=6.$$

Generally, we have two terms $252x^2$, $330x^2$ for the Schultz polynomial and Modified Schultz polynomial, respectively.

III. If $d(u,v)=3$, then $D_3=\{(v_i,v_{i+3}),(v_i,u_{i+2}),(v_i,u_{i-2}),(v_i,w_{i+1}),$ $(v_i,t_{i+1}),(v_i,w_{i-1}),(v_i,t_{i-1}),(u_i,u_{i+1}),(t_i,t_{i+1}),(w_i,w_{i+1})\mid i\in\mathbb{Z}_6\}$ and $|D_3|=57$. Similarly, we have three subsets of it.

III-1. $\forall i\in\mathbb{Z}_6$, let $v=v_i$ & $u=v_{i+3}, u_{i+2}, u_{i-2}$ or $v=v_{i+1}$ & $u=u_i$. Hence $\delta_v+\delta_u=6$ and $\delta_v\times\delta_u=9$. Therefore $|\{(u,v)\mid u,v\in V(G),d(u,v)=3\&\delta_v+\delta_u=6,\delta_v\times\delta_u=9\}|=6\times3+3=21$

Then, we have $126x^3$ and $189x^3$ in these polynomials.

III-2. $\forall i\in\mathbb{Z}_6$, let $v=v_i$ & $u=t_{i+1},t_{i-1},w_{i+1},w_{i-1}$. Thus $|\{(u,v)\mid u,v\in V(G),d(u,v)=3\&\delta_v+\delta_u=5,\delta_v\delta_u=6\}|=6\times4=24$.

So, we have $120x^3$ and $144x^3$.

III-3. $\forall i\in\mathbb{Z}_6$, let $v=w_i$ & $u=w_{i+1}$ or $v=t_i$ & $u=t_{i+1}$. Since $\delta_{t_i}=\delta_{w_i}=2$, then $|\{(u,v)\mid u,v\in V(G),d(u,v)=3\&\delta_v+\delta_u=4,\delta_v\times\delta_u=4\}|=12$. Overall, there are the terms $294x^3$, $381x^3$ for the Schultz polynomial and Modified Schultz polynomial, respectively.

IV. If $d(u,v)=4$, then $D_4=\{(v_i,u_{i+3}),(v_i,w_{i+2}),(v_i,w_{i-2}),(v_i,t_{i+2}),$ $(v_i,t_{i-2}),(u_i,w_{i+1}),(u_i,t_{i-1}),(u_i,u_{i+2}),(w_i,t_{i+2})\mid i\in\mathbb{Z}_6\}$ and $|D_4|=54$. Similarly, we have three subsets of D_4.

IV-1. $\forall i\in\mathbb{Z}_6$, since $d(v_i,u_{i+3})=d(u_i,u_{i+2})=4$, thus $|\{(u,v)\in V(G)\mid d(u,v)=4\&$ $\delta_v+\delta_u=6,\delta_v\times\delta_u=9\}|=12$. Thus, we have the term $72x^4$ for the Schultz polynomial and $108x^4$ for the Modified Schultz polynomial.

IV-2. $\forall i\in\mathbb{Z}_6$, let ($u=t_{i+2},t_{i-2},w_{i+2},w_{i-2}$ & $v=v_i$) or ($v=t_{i-1},w_{i-1},w_{i+1}$ & $u=u_i$). Thus, $|\{(u,v)\mid u,v\in V(G),d(u,v)=4\&\delta_v+\delta_u=5,\delta_v\delta_u=6\}|=36$. So, we have the term $180x^4$ for the Schultz polynomial and $216x^4$ for the Modified Schultz polynomial.

IV-3. $\forall i\in\mathbb{Z}_6$, let $v=w_i$ & $u=w_{i+2}$. Thus, $|\{(u,v)\in V(G)\mid u,v\in V(G),d(u,v)=4\&\delta_v+\delta_u=4,\delta_v\delta_u=4\}|=6$.

Generally, the two terms for the Schultz polynomial and Modified Schultz polynomial are $276x^4$, $348x^4$, respectively.

V. If $d(u,v)=5$, then $D_5=\{(v_i,t_{i+3}),(v_i,w_{i+3}),(u_i,w_{i+2}),(u_i,w_{i-2}),(u_i,t_{i+2}),$ $(u_i,t_{i-2}),(u_i,u_{i+2}),(w_i,t_{i-1})\mid i\in\mathbb{Z}_6\}$ and $|D_5|=45$. Again, we have three subsets of D_5 as above.

V-1. We have $|\{(u_i,u_{i+3})\mid\forall i\in\mathbb{Z}_6,d(u_i,u_{i+3})=5\&\delta_v+\delta_u=5,\delta_v\times\delta_u=9\}|=3$. Hence, $18x^5$ and $27x^5$ are the terms for the Schultz polynomial and Modified Schultz polynomial, respectively.

V-2. $\forall i\in\mathbb{Z}_6$, let ($v=t_{i+2},t_{i-2},w_{i+2},w_{i-2}$ & $u=u_i$) or ($u=t_{i+3},w_{i+3}$ & $v=v_i$), therefore $|\{(u,v)\mid u,v\in V(G),d(u,v)=5\&\delta_v+\delta_u=5,\delta_v\delta_u=6\}|=36$. Thus, there is the term $180x^5$ for the Schultz polynomial and $261x^5$ for the Modified Schultz polynomial.

V -3. $\forall i \in \mathbb{Z}_6$ since *d(w$_i$,t$_{i-1}$)=5*, $|\{(u,v)\in V(G)|d(u,v)=5\&\delta_v+\delta_u=\delta_v\delta_u=4\}|=6.$

In general, the terms are $222x^5$, $267x^5$ for these polynomials.

VI. If *d(u,v)=6*, then $D_6=\{(u_i,t_{i+3}),(u_i,w_{i+3}),(w_i,w_{i+2}),(w_i,t_{i-2}),(t_i,t_{i+2})\,|\,i\in\mathbb{Z}_6\}$ and $|D_6|=30$. It means that, we have two subsets of D_6.

VI-1. We have $|\{(u_i,w_{i+3}),(u_i,t_{i+3})\,|\,\forall i\in\mathbb{Z}_6, d(u,v)=6\ \&\ \delta_v+\delta_u=5, \delta_v\times\delta_u=6\}|=12$. Then, $60x^6$ and $72x^6$ are the two terms for the Schultz polynomial and Modified Schultz polynomial, respectively.

VI-2. $\forall i\in\mathbb{Z}_6$, since *d(w$_i$,w$_{i+2}$)=d(w$_i$,t$_{i-2}$)=d(t$_i$,t$_{i+2}$)=6*. Therefore, $|\{(u,v)\,|\,u,v\in V(G), d(u,v)=6\ \&\ \delta_v+\delta_u=\delta_v\delta_u=4\}|=18$. In general, we have $132x^6$ for the Schultz polynomial and $144x^6$ for the Modified Schultz polynomial.

VII. If d(u,v)=7, then $|D_7|=|\{\forall i\in\mathbb{Z}_6,(w_i,t_{i+3}),\underline{(w_i,w_{i+3})},\underline{(t_i,t_{i+3})}\,|\ d(u,v)=7\ \&\ \delta_v+\delta_u=\delta_v\delta_u=4\}|=12$. Thus, there is the same term $48x^7$ for the Schultz polynomial and Modified Schultz polynomial. Now, we enumerate all distinct shortest path of any $u,v\in V(G)$. Thus the Schultz polynomial of $Ca(C_6)$ is: $Sc(Ca(C_6),x)=156x+252x^2+294x^3+276x^4+222x^5+132x^6+48x^7$ and the Schultz index is $Sc(Ca(C_6))=4884$.

The Modified Schultz polynomial of $Ca(C_6)$ is:
$Sc^*(Ca(C_6),x)=204x+330x^2+381x^3+348x^4+267x^5+144x^6+48x^7$
and the Modified Schultz index $Sc^*(Ca(C_6))=5934$.

Thus, the *proof* of Theorem 1 is complete.

Proof of Theorem 2. Let $Ca(C_6)$) be the molecular graph of Coronene. Since $D_i=D_i(3,3)\bigcup D_i(3,2)\bigcup D_i(2,2)$, $\forall i\in\{1,2,...,7\}$ therefore the set of distances in *G* is given by the following relation: $d(G,i)=|D_i|=|D_i(3,3)|+|D_i(3,2)|+|D_i(2,2)|$. Keeping in mind the definition of Hosoya polynomial and the data provided in the proof of Theorem 1, the formula of this polynomial in Coronene is:

$$H(G,x)=\sum_{i=0}^{d(G)}d(G,i)x^i=24+30x+48x^2+57x^3+54x^4+45x^5+30x^6+12x^7.$$

Hence, the Wiener and Hyper Wiener indices of Coronene are:

$$W(G)=\sum_{i=0}^{d(G)}i\times d(G,i)=24\times0+30\times1+48\times2+57\times3+54\times4+45\times5+30\times6+12\times7=1002.$$

$WW(G)=1002+(1/2)(48\times2+57\times3\times2+54\times4\times3+45\times5\times4+30\times6\times5+12\times7\times6)=2697$

Thus, the *proof* of Theorem 2 is complete.

CONCLUSIONS

In this paper, Schultz, Modified Schultz and Hosoya polynomials and their topological indices in the molecular graph of Coronene (constructed by Capra-operated benzenoid: $Ca(C_6)$ (or H_2)) are calculated. These polynomials and indices could be useful in the topological investigation of benzenoids molecules.

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