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COMPUTING FIRST AND SECOND ZAGREB INDEX, FIRST AND SECOND ZAGREB POLYNOMIAL OF CAPRA-DESIGNED PLANAR BENZENOID SERIES $Ca_n(C_6)$

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ABSTRACT. In graph theory, various polynomials and topological indices are known, as invariants under graph automorphism. In this paper, we focus on the structure of *Capra*-designed planar benzenoid series $Ca_k(C_6)$, $k \geq 0$ and compute on it several topological indices and polynomials: first and second Zagreb polynomials and their corresponding indices.

Keywords: *Capra Operation, benzenoid series, First Zagreb index, second Zagreb index, First Zagreb polynomial, second Zagreb polynomial.*

INTRODUCTION

Let *G=(V,E)* be a molecular graph with the vertex set *V(G)* and the edge set *E(G).* $|V(G)|=n$, $|E(G)|=e$ are the number of vertices and edges. A molecular graph is a simple finite graph such that its vertices correspond to the atoms and the edges to the chemical bonds. The distance *d(u,v)* in the graph *G* is the number of edges in a shortest path between two vertices *u* and *v*. The number of vertex pairs at unit distance equals the number of edges. A topological index of a graph is a number related to that graph and is invariant under graph automorphism.

Wiener index W(G) is the oldest topological index [1-5], which has found many chemical applications. It is defined as:

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

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Hyper-Wiener index is a more recently introduced distance-based molecular descriptor [6]:

$$WW(G)=\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}\left(d(u,v)+d(u,v)^2\right)=\frac{1}{2}W(G)+\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}d(u,v)^2.$$

Denote by *d(G,k)* the number of vertex pairs of *G* lying at distance k to each other and by *d(G)* the topological diameter (i.e, the longest topological distance in *G)*. Then Wiener and hyper-Wiener indices of *G* can be expressed as [7, 8]:

$$W(G)=\frac{1}{2}\sum_{i=1}^{d(G)} i.d(G,i)$$

$$WW(G)=\frac{1}{2}\sum_{i=1}^{d(G)} i(i+1)d(G,i).$$

Other oldest graph invariant is the *First Zagreb index*, which was formally introduced by *Gutman* and *Trinajstić* [9, 10]. It is denoted by $M_1(G)$ and is defined as the sum of squares of the vertex degrees:

$$M_1(G)=\sum_{v\in V(G)} d(v)^2=\sum_{e=uv\in E(G)}\left[d(u)+d(v)\right]$$

where d_v is the degree of vertex *v*. Next, *Gutman* introduced the *Second Zagreb index* $M_2(G)$ as:

$$M_2(G)=\sum_{e=uv\in E(G)}\left[d(u)\times d(v)\right]$$

Some basic properties of $M_1(G)$ can be found in ref. [9]. For a survey on theory and applications of Zagreb indices see ref. [10]. Related to the two above topological indices, we have the first Zagreb Polynomial $M_1(G,x)$ and second Zagreb Polynomial $M_2(G,x)$, respectively. They are defined as:

$$M_1(G,x)=\sum_{e=uv\in E(G)} x^{d(u)+d(v)}$$

$$M_2(G,x)=\sum_{e=uv\in E(G)} x^{d(u)d(v)}$$

There was a vast research concerning Zagreb indices and Wiener index with its modifications [6] and relations between Wiener, hyper-Wiener and Zagreb indices [9-26].

WHAT IT IS THE CAPRA OPERATION?

A mapping is a new drawing of an arbitrary planar graph *G* on the plane. In graph theory, there are many different mappings (or drawing); one of them is *Capra operation*. This method enables one to build a new structure of a planar graph *G.*

Let *G* be a cyclic planar graph. Capra map operation is achieved as follows:

(i) insert two vertices on every edge of G;
(ii) add pendant vertices to the above inserted ones and
(iii) **c**onnect the pendant vertices in order (-1,+3) around the boundary of a face of G. By runing these steps for every face/cycle of *G,* one obtains the Capra-transform of *G Ca(G)*, see Figure 1.

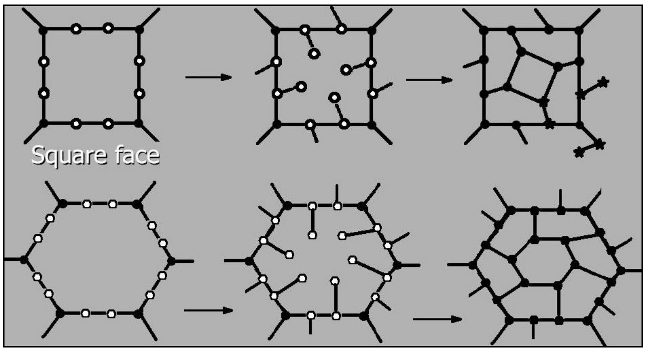

Figure 1. Examples of Capra operation on the square face (top row) and mapping Capra of planar hexagon (bottom row).

By iterating the Capra-operation on the hexagon (i.e. benzene graph C_6) and its Ca-transforms, a benzenoid series (Figures 2 and 3) can be designed. We will use the Capra-designed benzene series to calculate some connectivity indices (see below).

This method was introduced by *M.V. Diudea* and used in many papers [27-36]. Since Capra of planar benzenoid series has a very remarkable structure, we lionize it.

We denote Capra operation by *Ca*, in this paper, as originally *Diudea* did*.* Thus, Capra operation of arbitrary graph *G* is *Ca(G),* iteration of Capra will be denoted by *CaCa(G)* (or we denote $Ca_2(G)$) (Figures 2 and 3).

The benzene molecule is a usual molecule in chemistry, physics and nano sciences. This molecule is very useful to synthesize aromatic compounds. We use the Capra operation to generate new structures of molecular graph benzene series.

Theorem 1. Let $Ca(C_6)$ be the first member of Capra of benzenoid series. Then, *Hosoya polynomial* of $Ca(C_6)$ is equal to:

$$H(Ca(C_6),x)=24+30x^1+48x^2+57x^3+x54x^4+45x^5+30x^6+12x^7$$

and the Wiener index of $Ca(C_6)$ is equal to 1002.

Hosoya polynomial H(G) is equal to $\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} x^{d(u,v)}$. It is easy to see that Wiener index is obtained from Hosoya polynomial as the first derivative, in *x=1*.

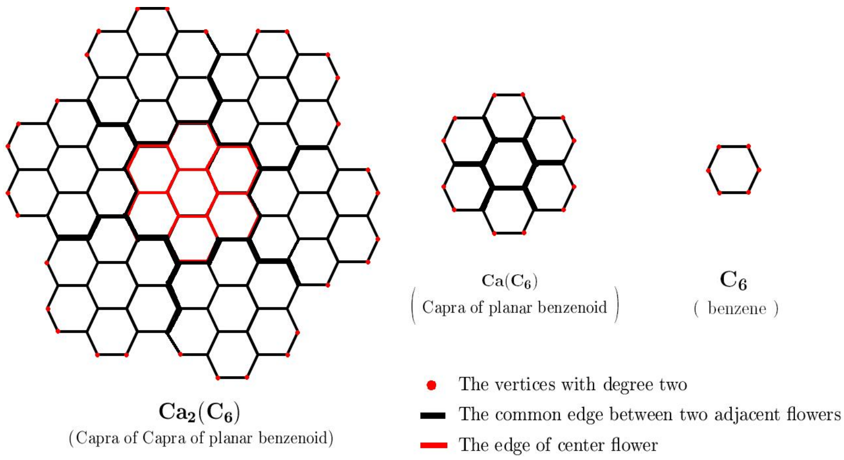

Figure 2. The first two graphs $Ca(C_6)$ and $Ca_2(C_6)$ from the Capra of planar benzenoid series, together with the molecular graph of benzene (denoted here $Ca_0(C_6)$)

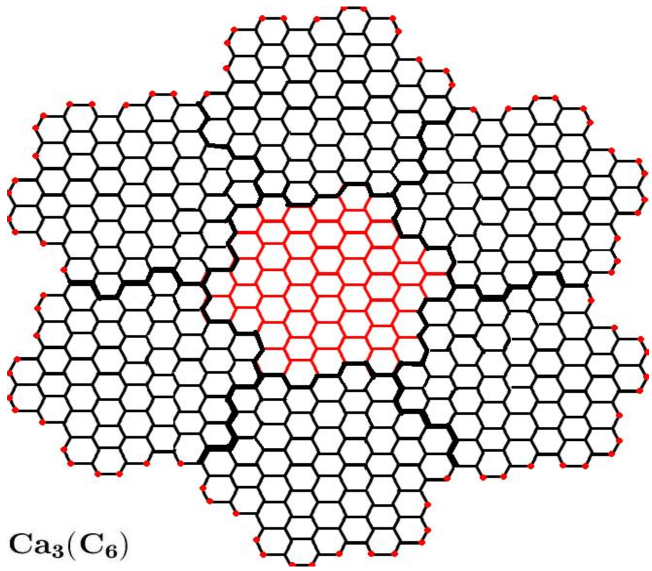

Figure 3. Graph $Ca_3(C_6)$ is the third member of Capra planar benzenoid series.

By these terminologies, we have the following theorem:

Theorem 2. Consider the graph $G=Ca_k(C_6)$ as the iterative Capra of planar benzenoid series. Then:
First Zagreb polynomial of G is equal to

$$M_1(Ca_k(C_6),x)=(3(7^k)-2(3^k)-3)x^6+4(3^k)x^5+(3^k+3)x^4$$

and the First Zagreb index is $M_1(Ca_k(C_6))=18(7^k)+12(3^k)-6$.
Second Zagreb polynomial of G is equal to

$$M_2Ca_k(C_6),x)=(3(7^k)-2(3^k)-3)x^9 4(3^k)x^6(3^k+3)x^4$$

and the Second Zagreb index of G is $M_2(Ca_k(C_6))=27(7^k)+10(3^k)-15$.

RESULTS AND DISCUSSION

Capra transforms of a planar benzenoid series is a family of molecular graphs which are generalizations of benzene molecule C_6.

In other words, we consider the base member of this family is the planar benzene, denoted here $Ca_0(C_6)=C_6=benzene$. It is easy to see that $Ca_k(C_6)=Ca(Ca_{k-1}(C_6))$ (Figures 2 and 3) [27-36]. In addition, we need the following definition.

Definition 3. [21] Let G be a molecular graph and d_v is the degree of vertex $v \in V(G)$. We divide vertex set $V(G)$ and edge set $E(G)$ of graph G to several partitions, as follow:

$$\forall i, \delta < i < \Delta, V_i = \{v \in V(G) \mid d_v = i\},$$

$$\text{and } \forall k, \delta^2 \le k \le \Delta^2, E_k^* = \{e = uv \in E(G) \mid d_v \times d_u = k\}.$$

Obviously, $1 \le \delta \le d_v \le \Delta \le n-1$ such that $\delta = Min\{d_v \mid v \in V(G)\}$ and $\Delta = Max\{d_v \mid v \in V(G)\}$. Now, we start to proof of the above theorem.

Proof of Theorem 2. Let $G=Ca_k(C_6)$ $(k\geq0)$ be the Capra planar benzenoid series. By construction, the structure $Ca_k(C_6)$ collects seven times of structure $Ca_{k-1}(C_6)$ (we call "flower" the substructure $Ca_{k-1}(C_6)$ in the graph $Ca_k(C_6)$). Therefore, by simple induction on k, the vertex set of $Ca_k(C_6)$ will have $7\times|V(Ca_k(C_6))|-6(2\times3^{k-1}+1)$ members. Because, there are $3^{k-1}+1$ and 3^{k-1} common vertices between seven flowers $Ca_{k-1}(C_6)$ in $Ca_k(C_6)$, marked by full black color in the above figures. Similarly, the edge set $E(Ca_k(C_6))$ have $7\times|E(Ca_k(C_6))|-6(2\times3^{k-1}+1)$ members. Since, there are 3^{k-1} and 3^{k-1} common edges (full black color in these figures).

Now, we solve the recursive sequences $|V(Ca_k(C_6))|$ and $|E(Ca_k(C_6))|$. First, suppose $n_k=|V(Ca_k(C_6))|$ and $e_k=|E(Ca_k(C_6))|$ so $n_k = 7n_{k-1} - 4\underbrace{(3^k)}_{\varepsilon_k} - 6$ and $e_k = 7e_{k-1} - 4\underbrace{(3^k)}_{\varepsilon_k}$. Thus, we have

$$
\begin{aligned}
n_k &= 7n_{k-1} - 4\varepsilon_k - 6 \\
&= 7(7n_{k-2} - 4\varepsilon_{k-1} - 6) - 4\varepsilon_k - 6 \\
&= 7^2 n_{k-2} - 7(4\varepsilon_{k-1} + 6) - (4\varepsilon_k + 6) \\
&= 7^3 n_{k-3} - 7^2(4\varepsilon_{k-2} + 6) - 7(4\varepsilon_{k-1} + 6) - (4\varepsilon_k + 6) \\
&\quad\vdots \\
&= 7^i n_{k-i} - 7^{i-1}(4\varepsilon_{k-(i-1)} + 6) - \ldots - 7(4\varepsilon_{k-1} + 6) - (4\varepsilon_k + 6) \\
&= 7^i n_{k-i} - \sum_{j=0}^{i-1} 7^j (4\varepsilon_{k-j} + 6) \\
&\quad\vdots \\
&= 7^k n_{k-k} - \sum_{i=0}^{k-1} 7^i (4\varepsilon_{k-i} + 6) \\
&= 7^k n_0 - 4\sum_{i=0}^{k-1} 7^i 3^{k-i} - 6\sum_{i=0}^{k-1} 7^i. \qquad (1)
\end{aligned}
$$

where $n_0=6$ is the number of vertices in benzene C_6 (Figure 2) and $6\sum_{i=0}^{k-1} 7^i$ is equal to $\frac{6(7^k-1)}{7-1} = 7^k - 1$. On the other hand, since

$$(\alpha - \beta)\sum_{i=0}^{n} \alpha^i \beta^{n-i} = (\alpha - \beta)(\alpha^0\beta^n + \alpha^1\beta^{n-1} + \ldots + \alpha^{n-1}\beta^1 + \alpha^n\beta^0) = (\alpha^{n+1} - \beta^{n+1}).$$

Hence

$$
\begin{aligned}
\sum_{i=0}^{k-1} 7^i 3^{k-i} &= (7^0 3^k + 7^1 3^{k-1} + \ldots + 7^{k-2}3^2 + 7^{k-1}3^1) + 7^k 3^0 - 7^k 3^0 \\
&= \frac{7^{k+1} - 3^{k+1}}{7^1 - 3^1} - 7^k 3^0 \\
&= \frac{7^{k+1} - 3^{k+1} - 4(7^k)}{4} \\
&= \frac{3(7^k) - 3(3^k)}{4} \\
&= \frac{3}{4}(7^k - 3^k). \qquad (2)
\end{aligned}
$$

Therefore, by using equations (1) and (2), we have
$n_k = 6\times 7^k - \left(4\left(\frac{3}{4}(7^k - 3^k)\right) + (7^k - 1)\right)$ and $\forall\, k \geq 0, n_k=|V(Ca_k(C_6))|=2\times 7^k+3^{k+1}+1$.

By using a similar argument and (1), we can see that

$$e_k = 7e_{k-1} - 4ò_k = 7^2 e_{k-2} - 7(4ò_{k-1}) - 4ò_k$$
$$\vdots$$
$$= 7^k e_{k-k=0} - 4\sum_{i=0}^{k-1} 7^i ò_{k-i} = 7^k e_0 - 4\sum_{i=0}^{k-1} 7^i 3^{k-i}.$$

It is easy to see that, the first member of recursive sequence e_k is $e_0=6$, (Figure 2). Now, by using (2), we have $e_k = 6\times 7^k - 4\left(\frac{3}{4}(7^k - 3^k)\right)$ and the size of edge set $E(Ca_k(C_6))$ is equal to: $e_k=|E(Ca_k(C_6))|=3(7^k+3^k)$, $\forall k \geq 0$.

Also, according to Figures 2 and 3, we see that the number of vertices of degree two in the graph $Ca_k(C_6)$ (we denote by $v_2^{(k)}$) is equal to $6\times 3\left(\frac{v_2^{(k-1)}}{6}\right) - 6$. The six removed vertices are the common ones between the six flowers "$Ca_{k-1}(C_6)$" with degree three. By using a similar argument and simple induction, we have $v_2^{(k-1)}$ the numbers of edges of graph $Ca_k(C_6)$, which are in the set E_4 or E_4^* (denoted by $e_4^{(k)}$).

Now, we solve the recursive sequence $v_2^{(k)} = 6(3\left(\frac{v_2^{(k-1)}}{6}\right) - 1)$ and we conclude $v_2^{(k)} = 3v_2^{(k-1)} - 6 = 3(3v_2^{(k-2)} - 6) - 6 = \ldots = 3^k v_2^{(0)} - 6\sum_{i=0}^{k-1} 3^i$.

It is obvious that, according to the structure of benzene, $v_2^{(0)} = n_0 = 6$.

Thus, $v_2^{(k)} = 6\times 3^k - 6\left(\frac{3^k - 1}{3-1}\right) = \mathbf{3^{k+1}} + \mathbf{3}$.

Also, $e_4^{(k)} = |E_4| = |E_4^*| = v_2^{(k-1)} = \mathbf{3^k} + \mathbf{3}$ and according to the above definition, it is obvious that, for Capra of planar benzenoid series $G=Ca_k(C_6)$ we have two partitions:
$V_2 = \{v \in V(Ca_k(C_6)) \,|\, d_v = 2\}$ and $V_3 = \{v \in V(Ca_k(C_6)) \,|\, d_v = 3\}$, with the size $3^{k+1} + 3$ and $2(7^k - 1)$, respectively.

On the other hand, according to the structure of Capra planar benzenoid series $Ca_k(C_6)$, there are $2v_2^{(k)}$ edges, such that the first point of them is a vertex with degree two. Among these edges, there exist $v_2^{(k-1)}$ edges, of which the first and end point of them have degree 2 (the members of E_4 or E_4^*).

Thus, $e_5^{(k)} =|E_5|=|E_6^*|= 2v_2^{(k)} - 2e_4^{(k)} = 2v_2^{(k)} - 2v_2^{(k-1)}$. So, the size of edge set E_5 and E_6^* is equal to $e_5^{(k)} = 2(3^{k+1} + 3 - 3^k - 3) = 4(3^k)$

Now, it is obvious that:

$$\begin{aligned} e_6^{(k)} =|E_6|=|E_9^*| &= 3\left(7^k + 3^k\right) - e_5^{(k)} - e_4^{(k)} \\ &= 3\times 7^k + 3^{k+1} - 4\times 3^k - 3^k - 3 \\ &= 3\times 7^k - 2\times 3^k - 3 \\ &= \mathbf{3(7^k - 2(3^{k-1}) - 1)}. \end{aligned}$$

Now, we know the size of all sets $V_2, V_3, E_4, E_4^*, E_5, E_6^*, E_6$ and E_9^*. So, we can calculate the First and Second Zagreb Polynomial of Capra planar benzenoid series $G=Ca_k(C_6)$, as follow:

First Zagreb Polynomial of $G=Ca_k(C_6)$:

$$\begin{aligned} M_1(G,x) &= \sum_{e\in E(G)} x^{d(u)+d(v)} \\ &= \sum_{e\in E_6} x^6 + \sum_{e\in E_5} x^5 + \sum_{e\in E_4} x^4 \\ &= |E_6|x^6 + |E_5|x^5 + |E_4|x^4 \\ &= 3(7^k - 2(3^{k-1}) - 1)x^6 + 4(3^k)x^5 + 3(3^{k-1}+1)x^4 \end{aligned}$$

Second Zagreb Polynomial of $G = Ca_k(C_6)$:

$$\begin{aligned} M_2(G,x) &= \sum_{e\in E(G)} x^{d(u)d(v)} = \sum_{e\in E_9^*} x^9 + \sum_{e\in E_6^*} x^6 + \sum_{e\in E_4^*} x^4 \\ &= 3(7^k - 2(3^{k-1}) - 1)x^9 + 4(3^k)x^6 + 3(3^{k-1}+1)x^4. \end{aligned}$$

Also, according to definition of First and Second Zagreb index, we have:

$$\begin{aligned} M_1(G) = \frac{\partial M_1(G,x)}{\partial x}\Big|_{x=1} &= 18(7^k - 2(3^{k-1}) - 1) + 20(3^k) + 12(3^{k-1}+1) \\ &= 18(7^k) + 12(3^k) - 6 \end{aligned}$$

and $M_2(G)=\frac{\partial M_2(G,x)}{\partial x}|_{x=1}=27(7^k-2(3^{k-1})-1)+24(3^k)+12(3^{k-1}+1)$

$$=27(7^k)+10(3^k)-15$$

Of course, by using $|V_2|$ and$|V_3|$, we have

$$M_1(G)=(3^{k+1}+3)2^2+2(7^k-1)3^2=18(7^k)+12(3^k)-6.$$

Thus, we completed the proof of the theorem 3.

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