COMPUTING THE M-POLYNOMIAL OF BENZENOID MOLECULAR GRAPHS

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ABSTRACT. *Let G=(V; E) be a simple connected graph with the vertices and edges sets V=V(G) and E=E(G), respectively. In such a simple molecular graph, vertices represent atoms and edges represent bonds. In graph theory, we have many invariant polynomials and topological indices for a graph. The M-polynomial of G was introduced by S. Klavzar and E. Deutsch as* $M(G,x,y)=\sum_{\delta\le i\le j\le\Delta} m_{ij}(G)x^i y^i$ *, where* $m_{ij}(G)$ *be the be the number of edges e=uv of G such that* $\{d_u,d_v\}=\{i,j\}$ *and* d_u,d_v *are the degree of vertices* $u,v\in V(G)$ *(Obviously* $1\le\delta\le d_v\le\Delta\le|V(G)|-1$*, such that* $\delta=Min\{d_v\,|v\in V(G)\}$ *and* $\Delta=Max\{d_v\,|v\in V(G)\}$*).*

In this paper, we focus on the structure of some families of Benzenoid molecular graphs as "Circumcoronene series of Benzenoid H_k*, Capra-designed planar Benzenoid series* $Ca_k(C_6)$ $(\forall k\ge1)$*" and compute their M-polynomials.*

Keywords: *Molecular graph; Benzenoid; M-polynomials.*

INTRODUCTION

Let *G=(V,E)* be a molecular graph with the vertex set *V=V(G)* and the edge set *E=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. A general reference for the notation in graph theory is [1].

Numerous graph polynomials were introduced in the literature, several of them turned out to be applicable in mathematical chemistry. *Graph polynomials* are invariants of graphs (i.e. functions of graphs that are invariant with respect to graph isomorphism); they are usually polynomials in one or two variables with integer coefficients. Graph polynomials can be interpreted as ordinary generating functions for the coefficient sequences which count in most cases certain subgraphs.

For instance, the Hosoya polynomial [2], see also [3-5], is the key polynomial in the area of distance-based topological indices. In particular, the Wiener index can be computed as the first derivative of the Hosoya polynomial, evaluated at 1.

Important examples of graph polynomials are the domination Polynomial, chromatic polynomial, independence polynomial, matching polynomial, Tutte polynomial, reliability polynomial, characteristic polynomial, subgraph polynomial, clique polynomial, forest polynomial, Padmakar-Ivan polynomial, Omega polynomial. For definition of these polynomials see [6-14].

Recently in 2015 [15], *S. Klavzar* and *E. Deutsch* introduce a degree-based invariants polynomial called the *M*-polynomial, and they show that its role for degree-based invariants is parallel to the role of the Hosoya polynomial for distance-based invariants.

The distance *d(u,v)* between the vertices u and v of the graph G is equal to the length of (number of edges in) the shortest path that connects u and v. An edge *e=uv* of graph G is joined between two vertices u and *v (d(u,v)=1).*

The Hosoya polynomial was introduced by *H. Hosoya* in 1989 [16] and define as follow:

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

The Wiener index *W(G)* [17] is the oldest topological indices (based structure descriptors) that introduced by *H. Wiener* in 1947, which have very chemical applications, mathematical properties and defined as follow [18-22]:

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

where d_u and d_v are the degrees of the vertices *u* and *v* of a graph G, respectively.

Definition 1. [23] Let *G* be a simple connected molecular graph and d_v $(1\le d_v\le n-1)$ be the degrees of vertices/atom *v* in *G*. We divide the vertex set *V(G)* and edge set *E(G)* of *G* into several partitions as follows ($\forall$ *i,j* and *k:* $\delta\le i,j,k\le\Delta$*):*

$V_{\{k\}}=\{v\in V(G)|\ d_v=k\}$

$E_{\{i,j\}}=\{e=uv\in E(G)|d_u=j\ \&\ d_v=i\}$

where δ and Δ are the minimum and maximum of d_v for all $v\in V(G)$ and $\delta=Min\{d_v\,|v\in V(G)\}$ and $\Delta=Max\{d_v\,|v\in V(G)\}$, respectively.

Now, let *G=(V,E)* is a graph and let $m_{ij}(G)$ be the number of edges *e=uv* of *G* such that $\{dv(G),du(G)\}=\{i, j\}$, then the *M-polynomial* of *G* define as follow:

$$M(G,x,y)=\sum_{\delta\le i\le j\le\Delta}m_{ij}(G)x^i y^i$$

where d_u,d_v $(1\le\delta\le d_u,d_v\le\Delta\le|V(G)|-1)$ are the degree of vertices $u,v\in V(G)$. By Definition 1, one can see that $m_{ij}(G)=E_{\{i,j\}}$.

In this paper, we focus on the structure of some famiies of Benzenoid molecular graphs as "*Circumcoronene Series of Benzenoid* H_k*, Capra-designed planar Benzenoid series* $Ca_k(C_6)$ $(\forall k\ge1)$" and compute the *M*-polynomials of these molecular graphs in following sections.

THE *M*-POLYNOMIAL OF CIRCUMCORONENE SERIES OF BENZENOID H_k

In this section, we compute the *M*-polynomial of a family of Benzenoid molecules, which called Circumcoronene Series of Benzenoid H_k. The Circumcoronene series of Benzenoid is family of molecular graph, which consist several copy of benzene C_6 on circumference. The first terms of this series are H_1=benzene, H_2=coronene, H_3=Circumcoronene, see Figure 1, where they are shown. The general representation of Circumcoronene series of Benzenoid is shown in Figure 2. For more study of these molecular graphs see the paper series [24-43].

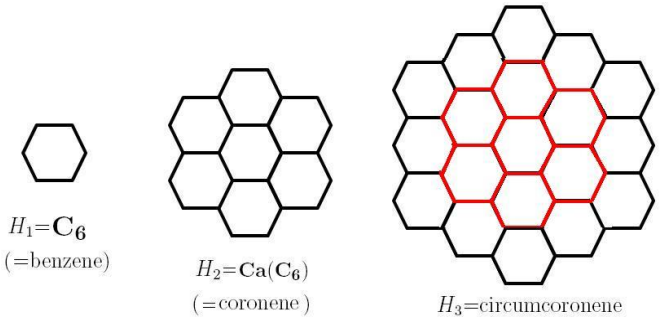

Figure 1. The first three graphs H_1, H_2 and H_3 of Circumcoronene Series of Benzenoid H_k.

Theorem 1. Let H_k be the Circumcoronene series of Benzenoid. Then, the M-polynomial of H_k is equal to:
$M(H_k,x,y)= 6x^2y^2+12(k-1)x^2y^3+(9k^2-15k+6)x^3y^3$.

Proof of Theorem 1. Let H_k $(k\geq 1)$ be the Circumcoronene series of Benzenoid. Such that from Figure 2 and [39-43], we see that this Benzenoid graph has $6k^2$ vertices and $\frac{3\times 6k(k-1)+2\times 6k}{2}=9k_2-3k$ edges. From the structure of H_k, one can see that there are two partitions $V_{\{3\}}=\{v\in V(H_k)|\ d_v=3\}$ and $V_{\{2\}}=\{v\in V(H_k)|\ d_v=2\}$ for the vertexs set $V(H_k)$, with size $6k(k-1)$ and $6k$, respectively. By Definetion 1 and [39-43], we see that the edge set of H_k can be dividing to three partitions as:

$E_{\{2,2\}}=\{e=uv\in E(H_k)|\ d_u=d_v=2\} \rightarrow |E_{\{2,2\}}|=6$
$E_{\{2,3\}}=\{e=uv\in E(H_k)|\ d_u=3\ \&d_v=2\} \rightarrow |E_{\{2,3\}}|=12(k-1)$
$E_{\{3,3\}}=\{e=uv\in E(H_k)|\ d_u=d_v=3\} \rightarrow |E_{\{3,3\}}|=9k^2-15k+6$

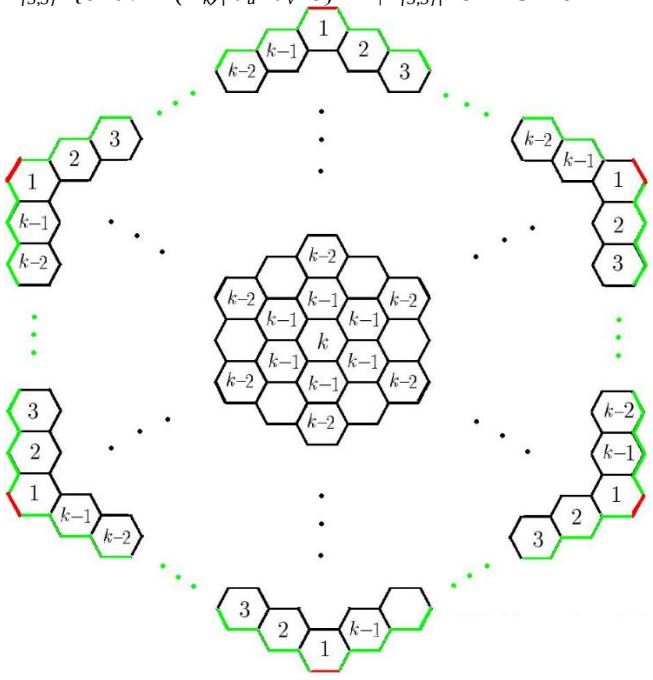

Figure 2. The Circumcoronene series of Benzenoid H_k $(k\geq 1)$ with edges marking.

In Figure 2, we mark the members of $E_{\{2,2\}}$ by red color, the members of $E_{\{2,3\}}$by green color and the members of $E_{\{3,3\}}$ by black color and the size of $E_{\{2,2\}}$, $E_{\{2,3\}}$ and $E_{\{3,3\}}$ are equle to 6, $12(k-1)$ and $9k^2-15k+6$, respectively. Thus, the M-polynomial of the Circumcoronene series of Benzenoid H_k is equal to:

$$M(H_k,x,y)= \sum_{i\leq j} m_{ij}(H_k)x^iy^j = \sum_{2\leq 2} m_{22}(H_k)x^2y^2+ \sum_{2\leq 3} m_{23}(H_k)x^2y^3+ \sum_{3\leq 3} m_{33}(H_k)x^3y^3$$

$$= \sum_{uv\in E_{\{2,2\}}} m_{22}(H_k)x^2y^2+ \sum_{uv\in E_{\{2,3\}}} m_{23}(H_k)x^2y^3+ \sum_{uv\in E_{\{3,3\}}} m_{33}(H_k)x^3y^3$$

$$=|E_{\{2,2\}}|\ x^2y^2+|E_{\{2,3\}}|\ x^2y^3+|E_{\{3,3\}}|\ x^3y^3$$
$$=6x^2y^2+12(k-1)x^2y^3+(9k^2-15k+6)x^3y^3.\blacksquare$$

THE *M*-POLYNOMIAL OF CAPRA-ESIGNED PLANAR BENZENOIDS

In this section we compute a closed formula of the *M*-polynomial of *Capra-designed planar Benzenoids*. In chemistry, physics and nanoscience, there are especially symmetric structures. Such molecular graphs are Capra-designed planar Benzenoids. Capra *Ca* map operation is a method of drawing and modifying the covering of a polyhedral structure, introduced by *M.V.Diudea* [44, 45] (see Figure 3) and used in many papers. In Refs [46-58] some connectivity topological indices of Capra-designed planar Benzenoids are computed. The some first members $Ca_0(C_6)$, $Ca(C_6)$, $Ca_2(C_6)$ and $Ca_3(C_6)$ of the Capra of planar Benzenoid *series are shown in Figure 4 and 5.*

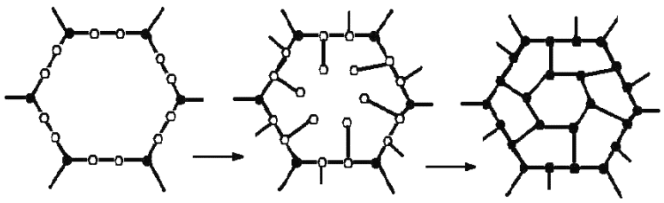

Figure 3. An example of Capra map operation on the hexagon (benzene) face.

Theorem 2. Let $Ca_k(C_6)$ be the Capra-designed planar Benzenoids. Then, the M-polynomial of $Ca_k(C_6)$ is equal to:
$M(Ca_k(C_6),x,y)=(3^k+3)x^2y^2+4(3^k)x^2y^3+3(7^k-2(3^{k-1})-1)x^3y^3$.

Proof of Theorem 2. Consider the molecular graph "Capra-designed planar Benzenoids $Ca_k(C_6)$", where $k\geq 1$ is steps of growth in this type of drawing (Figures 4 and 5). From the structure $Ca_k(C_6)$, we see that the number of vertices/atoms in this Benzenoid molecular graphs is equal to $|V(Ca_k(C_6))|=2\times 7^k+3^{k+1}+1$.

By according to Figures 2 and [46-58], we see that the size of two vertex/atom partitions $V_{\{2\}}$ and $V_{\{3\}}$ are equal to $|V_{\{2\}}|=3^{k+1}+3$ and $|V_{\{3\}}|=2(7^k-1)$ and alternatively the number of edges/bonds in this Benzenoid system is equal to

$$|E(Ca_k(C_6))| = \frac{2\left(3^{k+1}+3\right)+3\left(2\left(7^k-1\right)\right)}{2}=3(7^k+3^k).$$

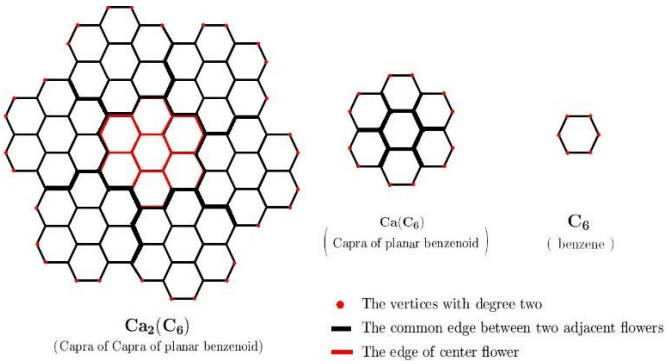

Figure 4. The some first members $Ca_0(C_6)$, $Ca(C_6)$ and $Ca_2(C_6)$ from the Capra-designed operation of planar Benzenoid series.

By according to Figure 4 and 5 and [46-58], one can see that the edge set of $Ca_k(C_6)$ have three edge partitions as:

$E_{\{2,2\}}=\{uv \in E(Ca_k(C_6))|\ d_u=d_v=2\} \rightarrow |E_{\{2,2\}}|=3^k+3$,

$E_{\{2,3\}}=\{uv \in E(Ca_k(C_6))|\ d_u=3\ \&d_v=2\} \rightarrow |E_{\{2,3\}}|=2|V_{\{2\}}|-2|E_{\{2,2\}}|=4(3^k)$,

$E_{\{3,3\}}=\{uv \in E(Ca_k(C_6))|\ d_u=d_v=3\} \rightarrow |E_{\{3,3\}}|=3(7^k-2(3^{k-1})-1)$.

Therefore, we have following computations for the M-polynomial of Capra-designed planar Benzenoids $Ca_k(C_6)$ as follows:

$$M(Ca_k(C_6),x,y)=\sum_{i\le j} m_{ij}(Ca_k(C_6))x^iy^j$$

$$=\sum_{2\le 2} m_{22}(Ca_k(C_6))x^2y^2+\sum_{2\le 3} m_{23}(Ca_k(C_6))x^2y^3+\sum_{3\le 3} m_{33}(Ca_k(C_6))x^3y^3$$

$$=\sum_{E_{\{2,2\}}\subset E(Ca_k(C_6))} m_{22}(Ca_k(C_6))x^2y^2+\sum_{uv\in E_{\{2,3\}}} m_{23}(Ca_k(C_6))x^2y^3+\sum_{uv\in E_{\{3,3\}}} m_{33}(Ca_k(C_6))x^3y^3$$

$$=|E_{\{2,2\}}|\,x^2y^2+|E_{\{2,3\}}|\,x^2y^3+|E_{\{3,3\}}|\,x^3y^3$$

$$=(3^k+3)x^2y^2+4(3^k)x^2y^3+3(7^k-2(3^{k-1})-1)x^3y^3.\blacksquare$$

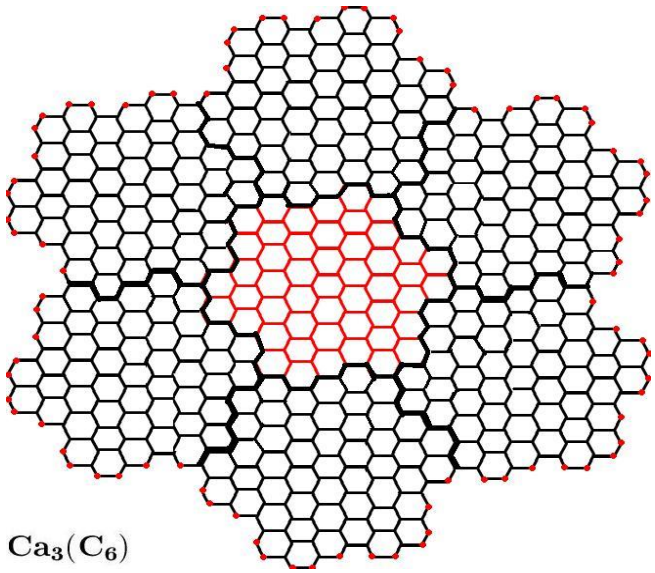

Figure 5.The third member $Ca_3(C_6)$ Capra-designed operation of planar Benzenoid series.

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