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苯的萨格勒布指数和萨格勒布多项式

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摘要：拓扑指数是与化合物的分子结构图相关联的数值，其作用是有助于确定有关化合物的性质．如同拓扑索引一样，代数多项式在这个研究领域上也起着至关重要的作用．因此，专门介绍一些苯类的计算结果，给出一些萨格勒布指数的具体形式，这些指数描述了这些分子链的物理化学活性．同时还给出了这些苯结构的萨格勒布多项式的具体形式．

关键词：化学图论；苯；萨格勒布指数；萨格勒布多项式
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Zagreb Indices and Zagreb Polynomials of Benzenoid

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Abstract：Topological indices are numbers associated with the molecular graph of chemical compound and are helpful to determine properties of concerned compound. Like topological indices，algebraic polynomials also play vital role in this direction. This article is devoted to the computational facts of some families of Benzenoids to give closed formulas of some Zagreb Indices which depict physiochemical activists of these molecular chains and closed forms of Zagreb polynomials of these Benzenoid structures.
Key words：chemical graph theory；Benzenoid；Zagreb index；Zagreb polynomial

1　Background Knowledge

In the last decade，discrete geometry and graph theory played a synergic role in the area of research of nanomaterials and nanosciences. It conferred chemists with a variety of useful tools like polynomials，eigenvalues and topological indices to predict some properties of latest synthesized nanomaterials theoretically. To engineer a nanomaterial endowed with a proposed properties，one can control structural sensitive properties like fracture toughness，yield stress etc. through Cheminformatics. It combines mathematics，chemistry and information science to analyze quantitative structure activities that are used to anticipate the biological properties of compounds，see［1—2］.

Here，our main task is to compute first multiple Zagreb index $PM_1(G)$，second multiple Zagreb index $M_2(G)$，hyper-Zagreb index，Zagreb Polynomials $M_1(G,x)$，$M_2(G,x)$ for some families of Benzenoids. A topological index is a numeric graph invariant which characterizes the topology of the graph. Some topological indicesare distance based while others are degree based. These indices and counting related polynomials are of great

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importance and play a vital role in chemical graph theory and particularly in chemistry. In more precise way, a topological index $Top(G)$ of a graph G, is a number with the property that for every graph H isomorphic to G, $Top(H) = Top(G)$. Wiener in [3] introduced the idea of topological index in the realm of paraffin. It is the first and most studied topological index in every respect defined as the sum of distances between all pairs of vertices in G, for more details see [3]. Later Gutman and Trinajstic introduced first Zagreb index in 1972[4]. The first and second Zagreb indices of a graph G are defined as:

$$M_1(G) = \sum_{uv \in E(G)} [\deg(u) + \deg(v)]; \tag{1}$$

$$M_2(G) = \sum_{uv \in E(G)} [\deg(u) \times \deg(v)]. \tag{2}$$

In 2013, Shirdel et al. in [5] proposed "hyper-Zagreb index" which is also degree based given as:

$$HM(G) = \sum_{uv \in E(G)} [\deg(u) + \deg(v)]^2. \tag{3}$$

In 2012 Azimi and Ghorbani[6] proposed two new variants of Zagreb indices, The first multiple Zagreb index as $PM_1(G)$ and second multiple Zagreb index $PM_2(G)$ of a graph G is defined as:

$$PM_1(G) = \prod_{uv \in E(G)} [\deg(u) + \deg(v)]; \tag{4}$$

$$PM_2(G) = \prod_{uv \in E(G)} [\deg(u) \times \deg(v)]. \tag{5}$$

The first Zagreb polynomial $M_1(G, x)$ and second Zagreb polynomial $M_2(G, x)$ are defined as:

$$M_1(G,x) = \sum_{uv \in E(G)} x^{[\deg(u) + \deg(v)]}; \tag{6}$$

$$M_2(G,x) = \sum_{uv \in E(G)} x^{[\deg(u) \times \deg(v)]}. \tag{7}$$

Nowadays there is an extensive research activity on these indices and on these polynomials are available.

We start with a family of Benzenoid molecules, which is called Circumcoronene Series of Benzenoid H_k. The Circumcoronene series of Benzenoid is family of molecular graph, which is constructed by several copies 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.

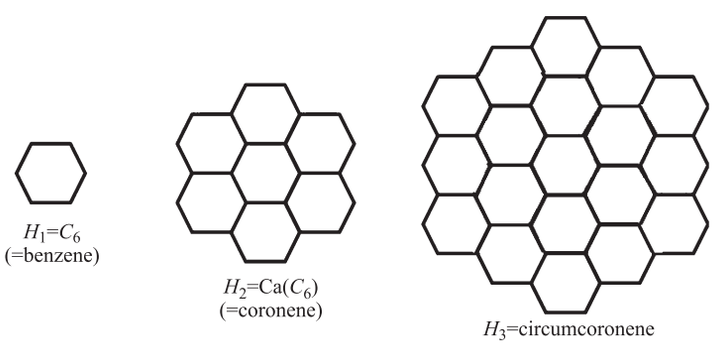

Figure 1　The First Three Graphs H_1, H_2 and H_3 of Circumcoronene Series of Benzenoid H_k

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 (see Figure 2) and used in many papers. In Refs [4, 6] some connectivity topological indices of Capra-designed planar Benzenoids are computed.

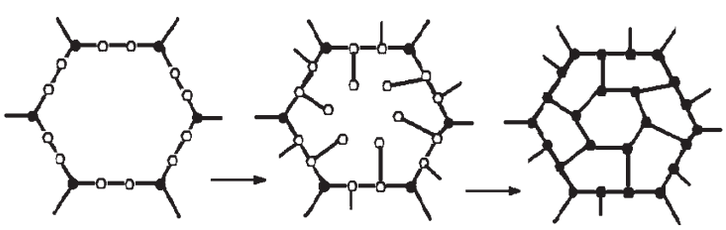

Figure 2　An Example of Capra Map Operation on the Hexagon (Benzene) Face

2 Results

Now we formulate our main results.

Theorem 1 Let H_k be the Circumcoronene series of Benzenoid. Then

Ⅰ. $HM(H_k)=16(6)+25\{12(k-1)\}+36(9k^2-15k+6)$;

Ⅱ. $PM_1(H_k)=4^6\times5^{12(k-1)}\times6^{9k^2-15k+6}$;

Ⅲ. $PM_2(H_k)=4^6\times6^{12(k-1)}\times9^{9k^2-15k+6}$.

Proof Let H_k be the Circumcoronene series of Benzenoid. Edge set of H_k divided into three partitions based on degree of vertices. The first edge partition $E_1(H_k)$ has 6 edges uv, where $\deg(u)=2$, $\deg(v)=2$. The second edge partition $E_2(H_k)$ has $12(k-1)$ edges uv, where $\deg(u)=2$, $\deg(v)=3$. The third edge partition $E_3(H_k)$ has $9k^2-15k+6$ edges uv, where $\deg(u)=3$, $\deg(v)=3$. It is easy to see that $|E_1(H_k)|=d_{22}$, $|E_2(H_k)|=d_{23}$, $|E_3(H_k)|=d_{33}$. Now using definitions given in equations (1), (2), (3) we have

$$\begin{aligned}
\text{Ⅰ. } HM(H_k) &= \sum_{uv\in E(H_k)}[\deg(u)+\deg(v)]^2\\
&= \sum_{uv\in E_1(H_k)}[\deg(u)+\deg(v)]^2+\sum_{uv\in E_2(H_k)}[\deg(u)+\deg(v)]^2+\sum_{uv\in E_3(H_k)}[\deg(u)+\deg(v)]^2\\
&=16|E_1(H_k)|+25|E_2(H_k)|+36|E_3(H_k)|\\
&=16(6)+25\{12(k-1)\}+36(9k^2-15k+6).
\end{aligned}$$

$$\begin{aligned}
\text{Ⅱ. } PM_1(H_k) &= \prod_{uv\in E(H_k)}[\deg(u)+\deg(v)]\\
&= \prod_{uv\in E_1(H_k)}[\deg(u)+\deg(v)]\times\prod_{uv\in E_2(H_k)}[\deg(u)+\deg(v)]\times\prod_{uv\in E_3(H_k)}[\deg(u)+\deg(v)]\\
&=4^{|E_1(H_k)|}+5^{|E_2(H_k)|}+6^{|E_3(H_k)|}\\
&=4^6\times5^{12(k-1)}\times6^{9k^2-15k+6}.
\end{aligned}$$

$$\begin{aligned}
\text{Ⅲ. } PM_2(H_k) &= \prod_{uv\in E(H_k)}[\deg(u)\times\deg(v)]\\
&= \prod_{uv\in E_1(H_k)}[\deg(u)\times\deg(v)]\times\prod_{uv\in E_2(H_k)}[\deg(u)\times\deg(v)]\times\prod_{uv\in E_3(H_k)}[\deg(u)\times\deg(v)]\\
&=4^{|E_1(H_k)|}+6^{|E_2(H_k)|}+9^{|E_3(H_k)|}\\
&=4^6\times6^{12(k-1)}\times9^{9k^2-15k+6}.
\end{aligned}$$

Theorem 2 Let $Ca_k(C_6)$ be the capra-designed planner Benzenoids. Then

Ⅰ. $HM(C_{a_k}(C_6))=16(3^k+3)+25(4\times3^k)+36(3(7^k-2\times3^{k-1}-1))$;

Ⅱ. $PM_1(C_{a_k}(C_6))=4^{3^k+3}\times5^{4\times3^k}\times6^{3(7^k-2\times3^{k-1}-1)}$;

Ⅲ. $PM_2(C_{a_k}(C_6))=4^{3^k}\times6^{4\times3^k}\times9^{3(7^k-2\times3^{k-1}-1)}$.

Proof Let $C_{a_k}(C_6)$ be the capra-designed planner Benzenoids. Edge set of divided into three partitions based on degree of vertices. The first edge partition $E_1(C_{a_k}(C_6))$ has 3^k+3 edges uv, where $\deg(u)=\deg(v)=2$. The second edge partition $E_2(C_{a_k}(C_6))$ has 4×3^k edges uv, where $\deg(u)=2,\deg(v)=3$. The third edge partition $E_3(C_{a_k}(C_6))$ has $3(7^k-2\times3^{k-1}-1)$ edges uv, where $\deg(u)=\deg(v)=3$. It is easy to see that $|E_1(C_{a_k}(C_6))|=d_{22}$, $|E_2(C_{a_k}(C_6))|=d_{23}$, $|E_3(C_{a_k}(C_6))|=d_{33}$. Now using definitions given in Equation (1), (2), (3) we have

$$\begin{aligned}
\text{Ⅰ}.\ HM(C_{a_k}(C_6)) &= \sum_{uv\in(C_{a_k}(C_6))}[\deg(u)+\deg(v)]^2\\
&= \sum_{uv\in E_1(C_{a_k}(C_6))}[\deg(u)+\deg(v)]^2+\sum_{uv\in E_2(C_{a_k}(C_6))}[\deg(u)+\deg(v)]^2\\
&+\sum_{uv\in E_3(C_{a_k}(C_6))}[\deg(u)+\deg(v)]^2\\
&=16|E_1(C_{a_k}(C_6))|+25|E_2(C_{a_k}(C_6))|+36|E_3(C_{a_k}(C_6))|\\
&=16(3^k+3)+25(4\times3^k)+36(3(7^k-2\times3^{k-1}-1)).
\end{aligned}$$

$$\begin{aligned}
\text{Ⅱ}.\ PM_1(C_{a_k}(C_6)) &= \prod_{uv\in E(C_{a_k}(C_6))}[\deg(u)+\deg(v)]\\
&= \prod_{uv\in E_1(C_{a_k}(C_6))}[\deg(u)+\deg(v)]\times\prod_{uv\in E_2(C_{a_k}(C_6))}[\deg(u)+\deg(v)]\\
&\times\prod_{uv\in E_3(C_{a_k}(C_6))}[\deg(u)+\deg(v)]\\
&=4^{|E_1(C_{a_k}(C_6))|}+5^{|E_2(C_{a_k}(C_6))|}+6^{|E_3(C_{a_k}(C_6))|}\\
&=4^{3^k+3}\times5^{4\times3^k}\times6^{3(7^k-2\times3^{k-1}-1)}.
\end{aligned}$$

$$\begin{aligned}
\text{Ⅲ}.\ PM_2(C_{a_k}(C_6)) &= \prod_{uv\in E(C_{a_k}(C_6))}[\deg(u)\times\deg(v)]\\
&= \prod_{uv\in E_1(C_{a_k}(C_6))}[\deg(u)\times\deg(v)]\times\prod_{uv\in E_2(C_{a_k}(C_6))}[\deg(u)\times\deg(v)]\\
&\times\prod_{uv\in E_3(C_{a_k}(C_6))}[\deg(u)\times\deg(v)]\\
&=4^{|E_1(C_{a_k}(C_6))|}+6^{|E_2(C_{a_k}(C_6))|}+9^{|E_3(C_{a_k}(C_6))|}\\
&=4^{3^k+3}\times6^{4\times3^k}\times9^{3(7^k-2\times3^{k-1}-1)}.
\end{aligned}$$

Theorem 3　Let H_k be the Circumcoronene series of Benzenoid. Then

$$M_1(H_k,x)=6x^4+12(k-1)x^5+(9k^2-15k+6)x^6;$$

$$M_2(H_k,x)=6x^4+12(k-1)x^6+(9k^2-15k+6)x^9.$$

Proof　Let H_k be the Circumcoronene series of Benzenoid. Edge set of H_k divided into three partitions based on degree of vertices. The first edge partition $E_1(H_k)$ has 6 edges uv, where $\deg(u)=2$, $\deg(v)=2$. The second edge partition $E_2(H_k)$ has $12(k-1)$ edges uv, where $\deg(u)=2$, $\deg(v)=3$. The third edge partition $E_3(H_k)$ has $9k^2-15k+6$ edges uv, where $\deg(u)=3$, $\deg(v)=3$. It is easy to see that $|E_1(H_k)|=d_{22}$, $|E_2(H_k)|=d_{23}$, $|E_3(H_k)|=d_{33}$. Now using Equations (4) and (5), we have

$$\begin{aligned}
M_1(H_k,x) &= \sum_{uv\in E(H_k)}x^{[\deg(u)+\deg(v)]}\\
&= \sum_{uv\in E_1(H_k)}x^{[\deg(u)+\deg(v)]}+\sum_{uv\in E_2(H_k)}x^{[\deg(u)+\deg(v)]}+\sum_{uv\in E_3(H_k)}x^{[\deg(u)+\deg(v)]}\\
&=|E_1(H_k)|x^4+|E_2(H_k)|x^5+|E_3(H_k)|x^6\\
&=6x^4+12(k-1)x^5+(9k^2-15k+6)x^6.
\end{aligned}$$

$$\begin{aligned}
M_2(H_k,x) &= \sum_{uv\in E(H_k)}x^{[\deg(u)\times\deg(v)]}\\
&= \sum_{uv\in E_1(H_k)}x^{[\deg(u)\times\deg(v)]}+\sum_{uv\in E_2(H_k)}x^{[\deg(u)\times\deg(v)]}+\sum_{uv\in E_3(H_k)}x^{[\deg(u)\times\deg(v)]}\\
&=|E_1(H_k)|x^4+|E_2(H_k)|x^6+|E_3(H_k)|x^9\\
&=6x^4+12(k-1)x^6+(9k^2-15k+6)x^9.
\end{aligned}$$

Theorem 4　Let $C_{a_k}(C_6)$ be the capra-designed planner Benzenoids. Then

$$M_1(C_{a_k}(C_6),x)=(3^k+3)x^4+(4\times 3^k)x^5+3(7^k-2\times 3^{k-1}-1)x^6;$$

$$M_2(C_{a_k}(C_6),x)=(3^k+3)x^4+(4\times 3^k)x^6+3(7^k-2\times 3^{k-1}-1)x^9.$$

Proof Let $C_{a_k}(C_6)$ be the capra-designed planner Benzenoids. Edge set $C_{a_k}(C_6)$ of divided into three partitions based on degree of vertices. The first edge partition $E_1(C_{a_k}(C_6))$ has 3^k+3 edges uv, where $\deg(u)=\deg(v)=2$. The second edge partition $E_2(C_{a_k}(C_6))$ has 4×3^k edges uv, where $\deg(u)=2$, $\deg(v)=3$. The third edge partition $E_3(C_{a_k}(C_6))$ has $3(7^k-2\times 3^{k-1}-1)$ edges uv, where $\deg(u)=\deg(v)=3$. It is easy to see that $|E_1(C_{a_k}(C_6))|=d_{22}$, $|E_2(C_{a_k}(C_6))|=d_{23}$, $|E_3(C_{a_k}(C_6))|=d_{33}$. Now using Equations (6) and (7), we have

$$\begin{aligned}
M_1(C_{a_k}(C_6),x) &= \sum_{uv\in E(C_{a_k}(C_6))} x^{[\deg(u)+\deg(v)]}\\
&= \sum_{uv\in E_1(C_{a_k}(C_6))} x^{[\deg(u)+\deg(v)]}+\sum_{uv\in E_2(C_{a_k}(C_6))} x^{[\deg(u)+\deg(v)]}+\sum_{uv\in E_3(C_{a_k}(C_6))} x^{[\deg(u)+\deg(v)]}\\
&= |E_1(C_{a_k}(C_6))|x^4+|E_2(C_{a_k}(C_6))|x^5+|E_3(C_{a_k}(C_6))|x^6\\
&= (3^k+3)x^4+(4\times 3^k)x^5+3(7^k-2\times 3^{k-1}-1)x^6.
\end{aligned}$$

$$\begin{aligned}
M_2(C_{a_k}(C_6),x) &= \sum_{uv\in E(C_{a_k}(C_6))} x^{[\deg(u)\times\deg(v)]}\\
&= \sum_{uv\in E_1(C_{a_k}(C_6))} x^{[\deg(u)\times\deg(v)]}+\sum_{uv\in E_2(C_{a_k}(C_6))} x^{[\deg(u)\times\deg(v)]}+\sum_{uv\in E_3(C_{a_k}(C_6))} x^{[\deg(u)\times\deg(v)]}\\
&= |E_1(C_{a_k}(C_6))|x^4+|E_2(C_{a_k}(C_6))|x^6+|E_3(C_{a_k}(C_6))|x^9\\
&= (3^k+3)x^4+(4\times 3^k)x^6+3(7^k-2\times 3^{k-1}-1)x^9.
\end{aligned}$$

3 Conclusions

In this article we computed Zagreb polynomials and Zagreb indices of two families of benzenoidal chains. These computations are helpful in determining physical properties of these molecules and polymers involving them. These indices can predict properties like heat of formation, and structural properties like fracture toughness without going in to chemical labs. Thus we can save time and cost.

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