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The Edge Zagreb indices of Circumcoronene Series of Benzenoid

Research Article

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Abstract: In chemical graph theory, we have many invariant polynomials and topological indices for a molecular graph. One of the best known and widely used is the Zagreb topological index of a graph G $M_1(G)$ introduced in 1972 by I. Gutman and N. Trinajstic and is defined as the sum of the squares of the degrees of all vertices of G, $M_1(G) = \sum_{v\in V(G)} {d_v}^2$ (or $= \sum_{e=uv\in E(G)} d_u + d_v$, where d_u denotes the degree (number of first neighbors) of vertex u in G. Also, the Second Zagreb index $M_2(G)$ is equal to $M_2(G) = \sum_{e=uv\in E(G)} d_u \times d_v$. In this paper, we focus on the structure of molecular graph Circumcoronene Series of Benzenoid H_k $(k > 1)$ and its line graph $L(H_k)$ and counting First Zagreb index and Second Zagreb index of $L(H_k)$.

MSC: 05C05, 92E10.

Keywords: Circumcoronene Series of Benzenoid, Line graph, Degree (of a vertex), Zagreb Topological Index.

1. Introduction

Let G is an arbitrary simple, connected, graph, with the vertex set $V(G)$ and edge set $E(G)$. A general reference for the notation in graph theory is [1-3]. In chemical graphs, the vertices of the graph correspond to the atoms of molecules while the edges represent chemical bonds [4, 5]. Numbers encoding certain structural features of organic molecules and derived from the corresponding molecular graph, are called graph invariants or more commonly topological indices.

A pair of molecular descriptors, known as the First Zagreb index $M_1(G)$ and the Second Zagreb index $M_2(G)$ [1], first appeared in the topological formula for the total-energy of conjugated molecules that has been derived in 1972 [6]. Soon after these indices have been used as branching indices [7].

The Zagreb indices are also used by various researchers in their QSPR and QSAR studies [1,8-10]. The development and use of the Zagreb indices were summarized in [11]. Mathematical properties of the first Zagreb index for general graphs can

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be found in [11-14].

For a simple graph G with the vertex set $V(G)$ and the edge set $E(G)$, the Zagreb indices are given by:

$$M_1(G) = \sum_{v \in V(G)} {d_v}^2 \tag{1}$$

$$M_2(G) = \sum_{e=uv \in E(G)} d_u \times d_v \tag{2}$$

where d_u denotes the degree (number of first neighbors) of vertex u in G. A. Milicevic, S. Nikolic and N. Trinajstic [29] in 2004 reformulated the Zagreb indices in terms of edge-degrees instead of vertex-degrees:

$$EM_1(G) = \sum_{e \in E(G)} {d_e}^2 \tag{3}$$

$$EM_2(G) = \sum_{e \sim f \in E(G)} d_e \times d_f \tag{4}$$

where d_e denotes the degree of the edge $e \in E(G)$, which is defined by $d_e = d_u + d_v - 2$ with $e = uv$, and $\forall e, f \in E(G)$ $e \sim f$ means that the edges e and f are adjacent, i.e., they share a common end-vertex in G.

For a graph G with at least one edge, its line graph L_G is the graph in which $V(L_G) = E(G)$, where two vertices of L_G are adjacent if and only if they are adjacent as edges of G. Then

$$EM_1(G) = M_1(L_G)$$

$$EM_2(G) = M_2(L_G)$$

2. Main Result and Discussion

The circumcoronene homologous 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 $H1 = benzene$, $H_2 = coronene$, $H_3 = circumcoronene$, $H_4 = circumcircumcoronene$, see Figure 1, where they are shown. These molecular graphs are presented in many papers, (see the paper series [30-39]. The goal of this section is to counting First Zagreb index and Second Zagreb index for the line graph of Circumcoronene Series of Benzenoid $L(H_k)$ (For every positive integer number $k > 1$). The general representation of Circumcoronene Series of Benzenoid H_k and its line graph $L(H_k)$ are shown in Figures 2 and 3.

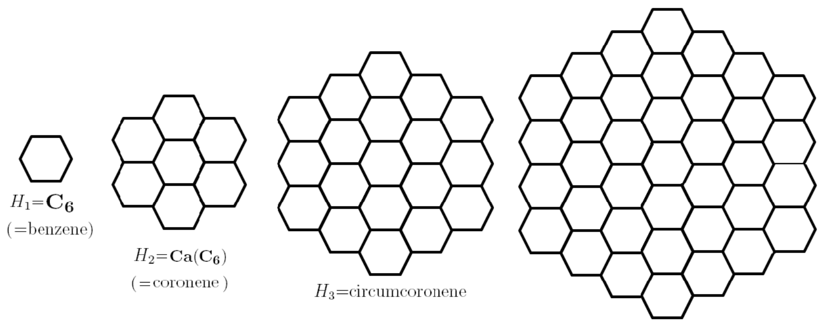

Figure 1. **The first member H_1 (C_6), H_2, H_3 and H_4 from Circumcoronene Series of Benzenoid H_k**

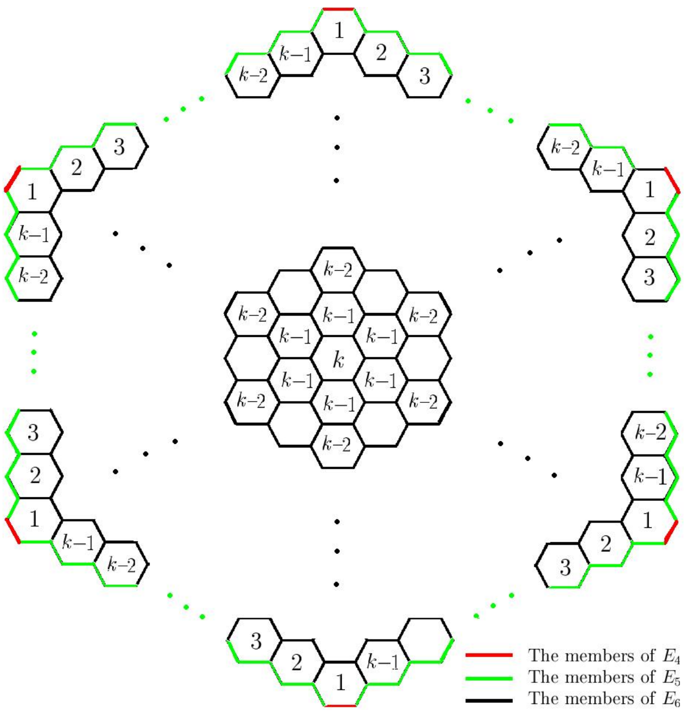

Figure 2. **The general representation of Circumcoronene Series of Benzenoid $H_k (k \geq 1)$ [36-39].**

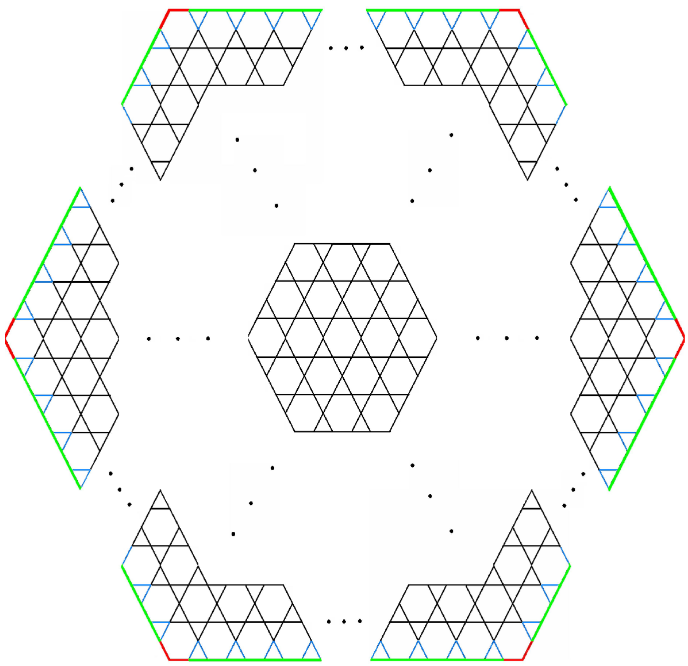

Figure 3. **The line graph of Circumcoronene Series of Benzenoid $L(H_k)$ $(k \geq 1)$ [36-39].**

Theorem 2.1 ([37]). *Let G be the Circumcoronene series of Benzenoid H_k, $\forall k > 1$. Then:*

(1). The First Zagreb index of H_k is equal to $M_1(H_k) = 54k^2 - 30k$

(2). The Second Zagreb index of H_k is equal to $M_2(H_k) = 81k^2 - 63k + 6$

Theorem 2.2. *Let G be the Circumcoronene series of Benzenoid H_k $\forall k \geq 1$, then the First and Second edge Zagreb indices* *of H_k are equal to:*

$$EM_1(H_k) = 12(12k^2 - 11k + 1) \tag{5}$$

$$EM_2(H_k) = 18(16k^2 - 18k + 3) \tag{6}$$

Proof. Consider the Circumcoronene series of Benzenoid H_k, for all positive integer number k, with $6k^2$ vertices and $9k^2 - 3k$ edges. Now, by attention to Figure 2, we see that there are two vertex partitions $V_2 = \{v \in V(H_k)|d_v = 2\}$ and $V_3 = \{v \in V(H_k)|d_v = 3\}$. Obviously, $|V_2| = 6k$ and $|V_3| = 6k(k-1)$. And alternatively, there are three edge partitions/sets E_4, E_5 and E_6 with their size as follow [37-39]:

$$E_4 = \{e = uv \in E(H_k)|d_u = 2\&d_v = 2\} \Rightarrow |E_4| = 6$$

$$E_5 = \{e = uv \in E(H_k)|d_u = 3\&d_v = 2\} \Rightarrow |E_5| = 12(k-1)$$

$$E_6 = \{e = uv \in E(H_k)|d_u = 3\&d_v = 3\} \Rightarrow |E_6| = 9k^2 - 15k + 6$$

Also, from the general representation of line graph of Circumcoronene series of benzenoid in Figure 3, one can see that there are three vertex partitions of $L(H_k)$ with their size as [37-39]:

$$VL_2 = \{e \in E(H_k)|d_e = 2\} \Rightarrow |VL_2| = |E_4| = 6$$

$$VL_3 = \{e \in E(H_k)|d_e = 3\} \Rightarrow |VL_3| = |E_5| = 12(k-1)$$

$$VL_4 = \{e \in V(L(H_k)) \ or \ e \in E(H_k)|d_e = 4\} \Rightarrow |VL_4| = |E_6| = 9k^2 - 15k + 6$$

and Four edge partitions/sets EL_5, EL_6, EL_7 and EL_8 as follow:

$$EL_5 = \{e \sim f \in E(G) \ or \ ef \in E(L(H_k))|d_e = 2, d_f = 3\} \Rightarrow |EL_5| = 2|VL_2| = 12$$

$$EL_6 = \{e \sim f \in E(G) \ or \ ef \in E(L(H_k))|d_e = d_f = 3\} \Rightarrow |EL_6| = |VL_3| - |VL_2| = 6(2k-3)$$

$$EL_7 = \{e \sim f \in E(G) \ or \ ef \in E(L(H_k))|d_e = 3, d_f = 3\} \Rightarrow |EL_7| = |VL_3| - |VL_2| = 12(k-1)$$

$$\begin{aligned} EL_8 = \{e \sim f \in E(G) \ or \ ef \in E(L(H_k))|d_e = d_f = 4\} \Rightarrow |EL_8| &= |E(L(H_k))| - |EL_7| - |EL_6| - |EL_5| \\ &= 18k^2 - 36k + 18 = 18(k-1)^2. \end{aligned}$$

Therefore by these above mentions, the first edge Zagreb index for Circumcoronene series of Benzenoid H_k or the first Zagreb index of line graph $L(H_k)$ is equal to

$$\begin{aligned} EM_1(H_k) &= \sum_{e \in E(H_k)} {d_e}^2 \\ &= \sum_{e \in V(L(H_k))} {d_e}^2 \\ &= \sum_{e_i \in VL_{i-2}, i=2,3,4} {d_{e_i}}^2 \\ &= \sum_{e_4 \in VL_2} {d_{e_4}}^2 + \sum_{e_5 \in VL_3} {d_{e_5}}^2 + \sum_{e_6 \in VL_4} {d_{e_6}}^2 \\ &= \sum_{e_4 \in VL_2} 2^2 + \sum_{e_5 \in VL_3} 3^2 + \sum_{e_6 \in VL_4} 4^2 \\ &= 6 \times 4 + 12(k-1) \times 9 + (9k^2 - 15k + 6) \times 16 \\ &= 144k^2 - 132k + 12 \\ &= 12(12k^2 - 11k + 1) \end{aligned} \tag{7}$$

And it is easy to see that the second edge Zagreb index of H_k or the second Zagreb index of $L(H_k)$ is equal to

$$\begin{aligned}
EM_2(H_k) &= \sum_{e\sim f\in E(H_k)} d_e \times d_f \\
&= \sum_{ef\in E(L(H_k))} d_e \times d_f \\
&= \sum_{ef\in EL_i, i=5,6,7,8} d_e \times d_f \\
&= \sum_{ef\in EL_5} 2\times 3 + \sum_{ef\in EL_6} 3\times 3 + \sum_{ef\in EL_7} 3\times 4 + \sum_{ef\in EL_8} 4\times 4 \\
&= (12\times 6) + (6(2k-3)\times 9) + (12(k-1)\times 12) + (18(k-1)^2\times 16) \\
&= 288k^2 - 324k + 54 \\
&= 18(16k^2 - 18k + 3) \qquad (8)
\end{aligned}$$

And these complete the proof of Theorem 2. □

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