THE SECOND MULTIPLICATIVE ZAGREB ECCENTRICITY INDEX OF CIRCUMCORONENE SERIES OF BENZENOID

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Abstract

Let $G = (V, E)$ be a simple connected graph. The sets of vertices and edges of G are denoted by $V = V(G)$ and $E = E(G)$, respectively. The first and second Zagreb indices are equal to $M_1(G) = \sum_{\nu \in V(G)} d_\nu^2$ and $M_2(G) = \sum_{u\nu \in E(G)} (d_u \times d_\nu)$, respectively. The first and second *multiplicative Zagreb eccentricity* indices of G are defined, respectively, as $\prod E_1(G) = \prod_{\nu \in V(G)} \varepsilon(\nu)^2$ and $\prod E_2(G) = \prod_{u\nu \in E(G)} \varepsilon(\nu) \times \varepsilon(u)$, respectively, where $\varepsilon(\nu)$ is the eccentricity of vertex ν in graph G.

In this paper, we focus on the structure of molecular graph circumcoronene series of benzenoid $H_k(k \geq 1)$ and present a closed formula for the second multiplicative Zagreb eccentricity index of H_k.

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1. Introduction

Let $G = (V, E)$ be a simple connected graph of finite order $n = |V| = |V(G)|$ with the set of vertices and the set of edges $E = E(G)$. A general reference for the notation in graph theory is [1].

For every vertex $\nu \in V(G)$, we denote the degree of ν by d_ν which the degree of any vertex is the number of first neighbour of ν. Let the maximum and minimum degree of all the vertices of G are, respectively, denoted by Δ and δ. The distance $d(u, \nu)$ between the vertices u and ν of the graph G is equal to the length of (number of edges in) the shortest path that connects u and ν. The eccentricity of a vertex is the distance between ν and a vertex farthest from ν and is denoted by $\varepsilon(\nu)$ thus $\varepsilon(\nu) = \mathrm{Max}\{d(u, \nu) \mid \forall u \in V(G)\}$.

Let the maximum and minimum eccentricity over all vertices of G are called the *diameter* and *radius* of G and denoted by $D(G)$ and $R(G)$, respectively.

In other words,

$$D(G) = \mathrm{Max}_{\nu \in V(G)}\{d(u, \nu) \mid \forall u \in V(G)\}, \tag{1}$$

$$R(G) = \mathrm{Min}_{\nu \in V(G)}\{\mathrm{Max}\{d(u, \nu) \mid \forall u \in V(G)\}\}. \tag{2}$$

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena. A molecular graph is a simple finite graph such that its vertices correspond to the

atoms and the edges to the bonds. In chemistry, graph invariants are known as topological indices. In graph theory, we have many different topological indices of arbitrary graph G.

A topological index is a real number related to a molecular graph, it does not rely on the labelling or the pictorial representation of a graph which is invariant under graph automorphisms. Obviously, every topological index defines a counting polynomial and vice versa [1-3].

One of the best known and widely used is the *Zagreb topological index* and was defined about forty years ago by Gutman and Trinajsti in 1972 [4] (or, more precisely, the first Zagreb index, because there exists also a second Zagreb index [3]). The first Zagreb index of G is defined as the sum of the squares of the degrees of all vertices of G [5]. The first and second Zagreb indices of G are denoted by $M_1(G)$ and $M_2(G)$, respectively, and defined as follows:

$$M_1(G) = \sum_{\nu \in V(G)} d_\nu^2, \tag{3}$$

$$M_2(G) = \sum_{u\nu \in E(G)} (d_u \times d_\nu), \tag{4}$$

where d_u and d_ν are the degrees of u and ν, respectively. The *first and second Zagreb indices* M_1 and M_2 are applied to study molecular, chirality in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) analysis, etc.

In 2012, the multiplicative variant of Zagreb indices was introduced by Todeschini et al. [6, 7], Gutman in [8] call these indices as multiplicative Zagreb indices. They are defined as

$$\prod M_1(G) = \prod_{u\nu \in E(G)} d_\nu^2, \tag{5}$$

$$\prod M_2(G) = \prod_{u\nu \in E(G)} (d_u \times d_\nu). \tag{6}$$

The eccentric version of the first Zagreb index was introduced by Ghorbani et al. [9] and Vukicevic et al. [10] in 2012 as follows:

$$M_1^*(G) = \sum_{v \in V(G)} \varepsilon(v)^2, \tag{7}$$

$$M_2^*(G) = \sum_{uv \in E(G)} \varepsilon(v) \times \varepsilon(u), \tag{8}$$

where $\varepsilon(v)$ and $\varepsilon(u)$ is the eccentricity of vertices v and u, respectively [11-13].

Recently in 2012, the *multiplicative Zagreb eccentricity* indices of the connected graph G were introduced by Nilanjan De [14] and are defined, respectively, as follows:

$$\prod E_1(G) = \prod_{uv \in E(G)} \varepsilon(v)^2, \tag{9}$$

$$\prod E_2(G) = \prod_{uv \in E(G)} \varepsilon(v) \times \varepsilon(u). \tag{10}$$

For further results of the Zagreb eccentricity indices, we encourage the reader refer to [15-24].

In this paper, we focus on the structure of famous benzenoid molecular graph "circumcoronene series of benzenoid $H_k (k \geq 1)$" and present a closed formula for the second multiplicative Zagreb eccentricity index of H_k.

2. Main Results and Discussion

The goal of this section is to study the multiplicative Zagreb eccentricity indices of circumcoronene series of benzenoid $H_k (k \geq 1)$. The circumcoronene series of benzenoid is family of benzenoid molecular graph, which consist several copy of C_6 on circumference and are generalizations of benzene molecule and the *benzene* molecule is a usual molecule in chemistry, physics and nano sciences and is very useful to

synthesize aromatic compounds. The general representations and first terms of this benzenoid series are H_1 = benzene, H_2 = coronene, H_3 = circumcoronene, H_4 = circumcircumcoronene are shown Figures 1, 2, and 3. This benzenoid family is presented in many papers; please refer to [24-36].
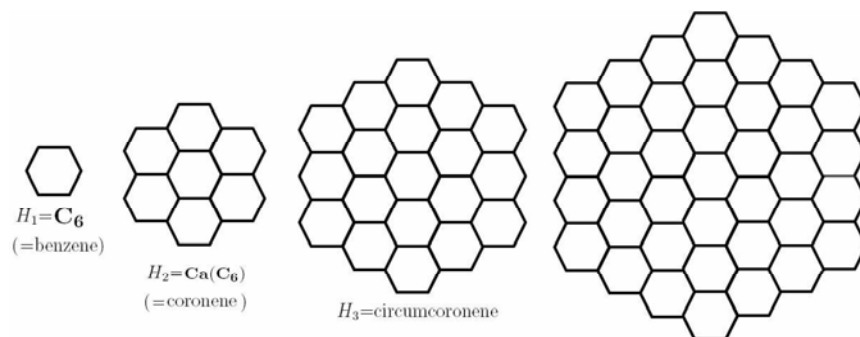

$H_1 = C_6$
(=benzene)
$H_2 = Ca(C_6)$
(=coronene)
H_3=circumcoronene

Figure 1. H_1 = benzene, H_2 = coronene, H_3 = circumcoronene, H_4 = circum-circumcoronene [33-36].
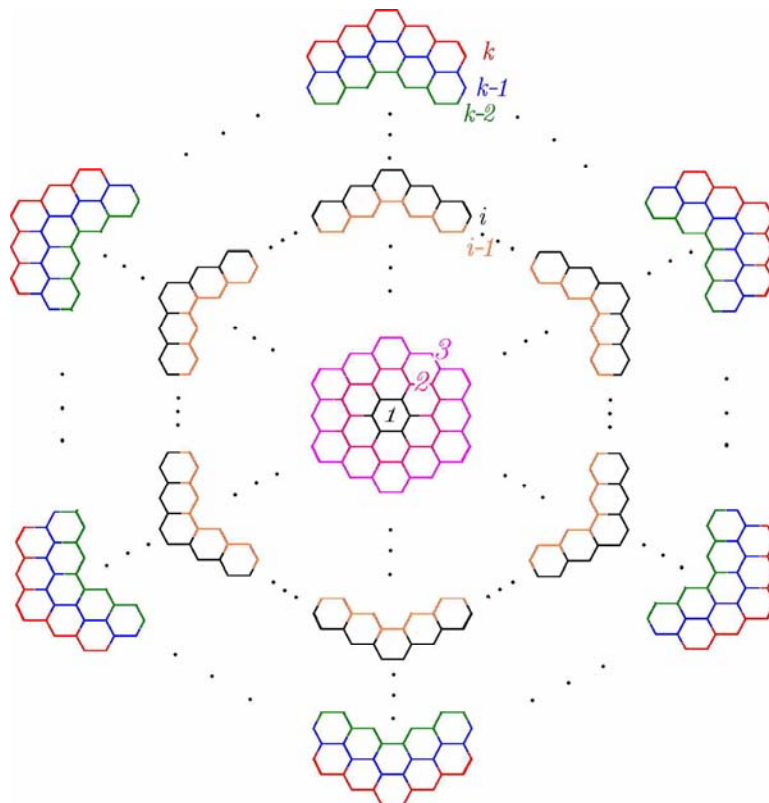
Figure 2. The ring-cuts of circumcoronene series of benzenoid $H_k (k \geq 1)$ [33-36].

Theorem 1. *Let H_k be the benzenoid molecular graph "circumcoronene series of benzenoid H_k" $\forall k \geq 1$. Then the second multiplicative Zagreb eccentricity index of H_k*

$$\prod E_2(H_k) = 2^{6(3i-2)}(2k + 2i - 1)^{6(3i+2k-2)}\left(\prod_{i=1}^{k}\left[(k + i)^{6i}(k + i - 1)^{12(i-1)}\right]\right).$$

(11)

Proof. Consider the circumcoronene series of benzenoid $H_k (k \geq 1)$. Let $V(H_k) = \{\gamma^i{}_{z,j}, \beta^i{}_{z,j} \mid i \in \mathbb{Z}_k \ \& \ j \in \mathbb{Z}_i \ \& \ z \in \mathbb{Z}_6\}$ be a notation for vertices/atoms of H_k and alternatively $E(H_k) = \{\gamma^i{}_{z,j}\beta^i{}_{z,j}, \ \gamma^i{}_{z,j+1}\beta^i{}_{z,j},$ $\gamma^{i-1}{}_{z,j}\beta^i{}_{z,j}$ and $\gamma^i{}_{z,j}\gamma^i{}_{z,j+1} \mid i \in \mathbb{Z}_k \ \& \ j \in \mathbb{Z}_i \ \& \ z \in \mathbb{Z}_6\}$ be a notation for edges/bonds of H_k.

So, from the general structure of H_k in Figures 2 and 3, it is easy to see that the circumcoronene series of benzenoid has $6k^2$ vertices/atoms and there are $9k^2 - 3k$ edges/bonds in general case of this benzenoid graph. Since

$$|V(H_k)| = \sum_{i=1}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}\gamma^i{}_{z,j} + \sum_{i=2}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}\beta^i{}_{z,j} = 6\sum_{i=1}^{k}i + 6\sum_{i=0}^{k-1}i = 6k^2,$$

$$(12)$$

$$|E(H_k)| = \sum_{i=1}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}\left(\gamma^i{}_{z,j}\beta^i{}_{z,j} + \gamma^i{}_{z,j+1}\beta^i{}_{z,j} + \gamma^{i-1}{}_{z,j}\beta^i{}_{z,j} + \gamma^i{}_{z,j}\gamma^i{}_{z,j+1}\right)$$

$$= 6\sum_{i=1}^{k-1}i + 6\sum_{i=1}^{k-1}i + 6\sum_{i=1}^{k-1}i + 6k = 9k^2 - 3k. \qquad (13)$$

Now, to achieve our aims, we should use the *ring-cut method*. The ring-cut method is a modify version of the *cut method* that divide all vertices and edges of a graph G into several partitions (or, more precisely, cuts) with similar mathematical and topological properties. For further study and results of the *cut method* and the *ring-cut method*, we encourage the reader refer to [27, 28, 36].

Also, for example, reader can see the vertex/edge notations and ring-cuts of circumcoronene series of benzenoid in Figures 2 and 3.

Now, by according to Figures 2 and 3 and using the results from [36], we can calculate the eccentric ε of all vertices of circumcoronene series of benzenoid H_k, $\forall k \geq 1$, such that $\forall i = 1, \ldots, k$ and $\forall j \in \mathbb{Z}_i \ \& \ \forall z \in \mathbb{Z}_6$ as follows:

$$\forall i = 1, \ldots, k; \ j \in \mathbb{Z}_{i-1} \ \& \ z \in \mathbb{Z}_6 \ : \ \varepsilon(\beta^i z, j) = \underbrace{d(\beta^i_{z,j}, \beta^i_{z+3,j})}_{4i-3}$$

$$+ \underbrace{d(\beta^i_{z+3,j}, \gamma^k_{z+3,j})}_{2(k-i)+1} = 2(k+1) - 2, \qquad (14)$$

$$\forall i = 1, \ldots, k; \ j \in \mathbb{Z}_i \ \& \ z \in \mathbb{Z}_6 \ : \ \varepsilon(\gamma^i z, j) = \underbrace{d(\gamma^i_{z,j}, \gamma^i_{z+3,j})}_{4i-1}$$

$$+ \underbrace{d(\gamma^i_{z+3,j}, \gamma^k_{z+3,j})}_{2(k-i)} = 2(k+i) - 1. \qquad (15)$$
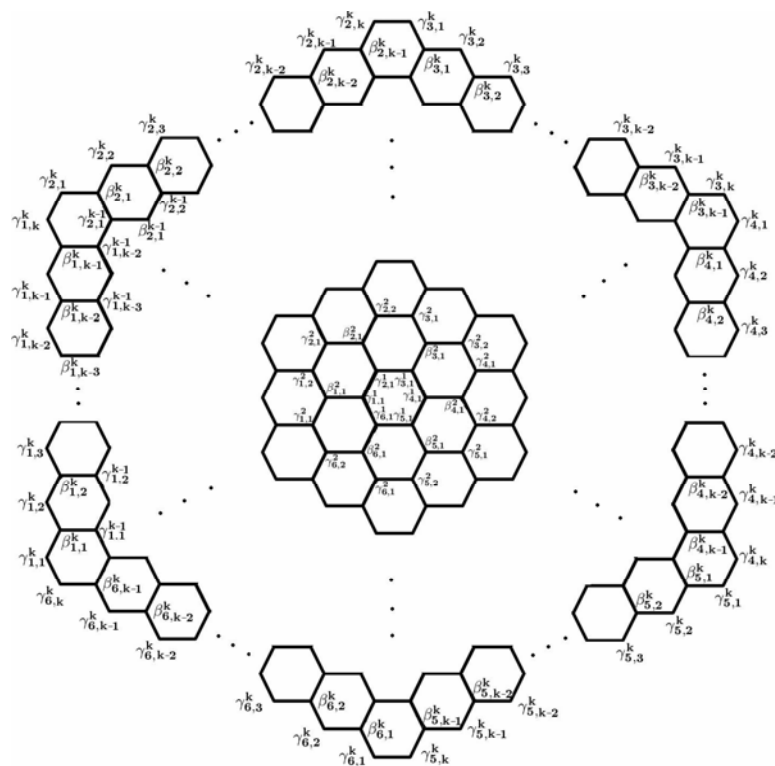

Figure 3. The general representation of circumcoronene series of benzenoid $H_k (\forall k \geq 1)$ [33-36].

Thus by according to Figures 2 and 3 and above results, we have following computations for the second multiplicative Zagreb eccentricity index of circumcoronene series of benzenoid $H_k(k \geq 1)$ as

$$\Pi E_2(H_k) = \prod_{uv \in E(H_k)} (\varepsilon(\nu) \times \varepsilon(u))$$

$$= \left(\prod_{\beta_{z,j}^i \gamma_{z,j}^i \in E(H_k)} \varepsilon\left(\beta_{z,j}^i\right)\varepsilon\left(\gamma_{z,j}^i\right) \right) \times \left(\prod_{\beta_{z,j}^i \gamma_{z,j+1}^i \in E(H_k)} \varepsilon\left(\beta_{z,j}^i\right)\varepsilon\left(\gamma_{z,j+1}^i\right) \right)$$

$$\times \left(\prod_{\beta_{z,j}^i \gamma_{z,j}^{i-1} \in E(H_k)} \varepsilon\left(\beta_{z,j}^{i+1}\right)\varepsilon\left(\gamma_{z,j}^{i-1}\right) \right) \times \left(\prod_{\gamma_{z,j}^i \gamma_{z+1,1}^i \in E(H_k)} \varepsilon\left(\gamma_{z,i}^i\right)\varepsilon\left(\gamma_{z+1,1}^i\right) \right)$$

$$= \prod_{z=1}^{6}\left(\prod_{i=2}^{k}\prod_{j=1}^{i} \varepsilon\left(\beta_{z,j}^i\right)\varepsilon\left(\gamma_{z,j}^i\right) \right) \times \prod_{z=1}^{6}\left(\prod_{i=2}^{k}\prod_{j=1}^{i} \varepsilon\left(\beta_{z,j}^i\right)\varepsilon\left(\gamma_{z,j+1}^i\right) \right)$$

$$\times \prod_{z=1}^{6}\left(\prod_{i=1}^{k-1}\prod_{j=1}^{i} \varepsilon\left(\beta_{z,j}^{i+1}\right)\varepsilon\left(\gamma_{z,j}^{i-1}\right) \right) \times \prod_{z=1}^{6}\left(\prod_{i=2}^{k} \varepsilon\left(\gamma_{z,i}^i\right)\varepsilon\left(\gamma_{z+1,1}^i\right) \right). \ (16)$$

Now, we can insert the equivalences of eccentric $\varepsilon(\beta^i_{z,j})$ and $\varepsilon(\gamma^i_{z,j})$ $(\forall i = 1, \ldots, k; \ j \in \mathbb{Z}_{i-1} \ \& \ z \in \mathbb{Z}_6)$ by their exact value $2(k+i) - 2$ and $2(k+i) - 1$, respectively.

$$\Pi E_2(H_k) = \prod_{i=2}^{k}[(2k + 2i - 1)(2k + 2i - 2)]^{6(i-1)}$$

$$\times \prod_{i=2}^{k}[(2k + 2i - 1)(2k + 2i - 2)]^{6(i-1)}$$

$$\times \prod_{i=1}^{k}[(2k + 2i - 1)(2k + 2i)]^{6i} \times \prod_{i=1}^{k}\left[(2k + 2i - 1)^2\right]^6$$

$$= \left(\frac{\prod_{i=1}^{k} [(2k + 2i - 1)(2k + 2i - 2)]^{12(i-1)}}{(2k + 1)(2k)^0 = 1} \right)$$

$$\times \prod_{i=1}^{k} [2(2k + 2i - 1)(k + i)]^{6i} \times \prod_{i=1}^{k} [(2k + 2i - 1)]^{12}$$

$$= 2(2k + 2i - 1)^{12(i-1)} \times 2(2k + 2i - 1)^{6i} \times (2k + 2i - 1)^{12k}$$

$$\times \left(\prod_{i=1}^{k} [(k + i - 1)]^{12(i-1)} \times \prod_{i=1}^{k} [(k + i)]^{6i} \right)$$

$$= 2^{6(3i-2)} (2k + 2i - 1)^{6(3i+2k-2)} \left(\prod_{i=1}^{k} \left[(k + i)^{6i} (k + i - 1)^{12(i-1)} \right] \right).$$

(17)

Finally, the second multiplicative Zagreb eccentricity index of H_k, $\forall k \in \mathbb{Z}$ is equal to

$$\prod E_2(H_k) = 2^{6(3i-2)} (2k + 2i - 1)^{6(3i+2k-2)} \left(\prod_{i=1}^{k} \left[(k + i)^{6i} (k + i - 1)^{12(i-1)} \right] \right).$$

(18)

Here, we complete the proof of the Theorem 1.   □

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