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# A New Version of Zagreb Index of Circumcoronene Series of Benzenoid

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**ABSTRACT.** Among topological indices, Zagreb indices are very important, very old and they have many useful properties in chemistry and specially in mathematics chemistry. First and second Zagreb indices have been introduced by Gutman and Trinajstić as $M_1(G)=\sum_{e=uv\in E(G)}[d_u+d_v]$ and $M_2(G)=\sum_{e=uv\in E(G)}[d_u d_v]$ where $d_u$ denotes the degree of vertex u in G. Recently, we know new versions of Zagreb indices as $M_1^*(G)=\sum_{e=uv\in E(G)}(ecc(v)+ecc(u))$, $M_1^{**}(G)=\sum_{v\in V(G)}ecc(v)^2$ and $M_2^*(G)=\sum_{e=uv\in E(G)}ecc(v)ecc(u)$ where ecc(u) is the largest distance between u and any other vertex v of G. In this paper, we focus one of these new topological indices that we call fifth Zagreb index $M_2^*(G)=M_5(G)$ and we compute this index for a famous molecular graph Circumcoronene series of benzenoid $H_k$ $(k\geq 1)$.

**Keywords:** First Zagreb index, second Zagreb index, Fifth Zagreb index, Circumcoronene series of benzenoid, Cut Method, Ring-cut Method.

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## 1. INTRODUCTION

Let G=(V,E) be a simple connected graph, where V(G) is a non-empty set of vertices and E(G) is a set of edges. A molecular graph in mathematical chemistry is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. 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. A topological index of a molecular graph

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G is a real number related to its structure and is invariant under graph automorphisms.

Among topological indices, Zagreb indices are very important, very old and they have many useful properties in chemistry and especially in mathematical chemistry. First Zagreb index $M_1$ introduced in 1972 by I. Gutman and N. Trinajstic and is de ined as the sum of the squares of the degrees of all vertices of G [1-3].

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

and Second Zagreb index [3,4] is equal to

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

where $d_u$ denotes the degree (number of first neighbors) of vertex u in G. Some mathematical properties of first Zagreb index and second Zagreb index for general graphs can be found in [5-9].

Recently, Ghorbani and Hosseinzadeh introduced new versions of Zagreb indices [10] as follows:

$$M_1^{*}(G) = \sum_{e=uv \in E(G)} \left(\mathrm{ecc}(v) + \mathrm{ecc}(u)\right)$$

$$M_1^{**}(G) = \sum_{v \in V(G)} \mathrm{ecc}(v)^2$$

$$M_2^{*}(G) = \sum_{e=uv \in E(G)} \left(\mathrm{ecc}(v) \times \mathrm{ecc}(u)\right)$$

where ecc(v) denotes the eccentricity of vertex v and is defined as the largest distance between v and any other vertex u of G. Also, if $u,v \in V(G)$ then the distance $d_G(u,v)$ (or $d(u,v)$) between $u$ and $v$ is defined as the length of any shortest path in G connecting $u$ and $v$. So

$$eec(v) = Max_G\{d(u,v) \mid \forall u \in V(G)\}$$

In this paper, we call these indices by Third Zagreb index, Fourth Zagreb index and Fifth Zagreb index as $M_1^{*}(G) = M_3(G)$, $M_1^{**}(G) = M_4(G)$ and $M_2^{*}(G) = M_5(G)$, respectively.

The goal of this paper is computing fifth Zagreb index $M_5(G)$ of a famous molecular graph Circumcoronene series of benzenoid $H_k$, that $k$ is positive integer number. The circumcoronene series of benzenoid is family of molecular graph, which consist several copy of benzene $C_6$ on circumference. Reader can see general representation of this family in Figure 1 and Figure 2.

## 2. Main results and discussion

In this section, we compute fifth Zagreb index $M_5(G)$ for circumcoronene series of benzenoid $H_k$ $\forall k \geq 1$. For achieve to our aims, we use of Ring-cut Method. This method is a modify version of the thoroughbred Cut Method and presented in [11] that dividing all vertices of G into some partitions.

In other words, we insert some vertices of G in a common ring-cut, such that these vertices have similar mathematical properties. For example, reader can see ring-cuts of circumcoronene series of benzenoid in Figure 1.

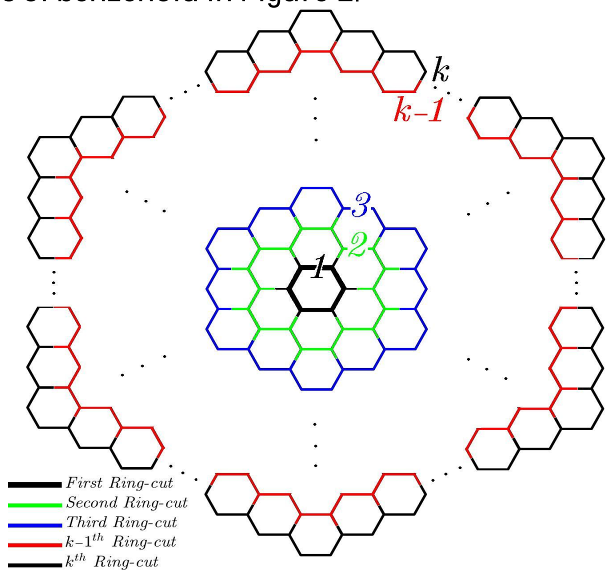


**Figure 1.** The Ring-cuts of general case of circumcoronene series of benzenoid.

Now, we present the closed formula of first Zagreb index $M_1(H_k)$, second Zagreb index $M_2(H_k)$ and fifth Zagreb index $M_5(H_k)$ in following theorems.

**Theorem 1. ([3])** Let G be the circumcoronene series of benzenoid $H_k$ $(\forall k \geq 1)$. Then the first and second Zagreb index of $H_k$ respectively are equal to

$$M_1(H_k) = 54k^2 - 30k$$

and

$$M_2(H_k) = 81k^2 - 63k + 6.$$

**Theorem 2.** The fifth Zagreb index of $H_k$ is equal to

2. $$M_5(H_k) = 102k^4 - 22k^3 - 48k^2 + 22k.$$

After proving Theorem 2, we introduce following denotation that is useful to achieve our aims.

**Notation 1.** Consider general case of circumcoronene series of benzenoid and suppose $\mathbb{Z}_6$ is the cycle inite group of order 6 and parameter i coming from $\mathbb{Z}_k$ $(k \in \mathbb{N})$. We rename all vertices of $H_k$ as follow:

1.2- Consider Benzene $C_6$ (or sub-graph $H_1$ of $H_k$) and call vertices by $\gamma^1_{z,1}$ for every

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$z\in\mathbb{Z}_6$, respectively.

2.1- Name all $\gamma^1_{z,j}$'s adjacent vertices (without name) by $\beta^2_{z,j}$, such that j is constant (=1) and $z\in\mathbb{Z}_6$.

2.2- Name two remaining $\beta^2_{z,j}$'s adjacent vertices by $\gamma^2_{z,j},\gamma^2_{z,j+1}$ $\forall z\in\mathbb{Z}_6$ and j=1 such that edges $\beta^2_{z,j}\gamma^2_{z,j},\beta^2_{z,j}\gamma^2_{z,j+1}$ is in $\mathrm{E}(H_k)$. See Figure 2.

I.1- Name all $\gamma^i_{z,j}$'s adjacent vertices (without name) by $\beta^i_{z,j}$, such that $j=1,\dots,i$ (or $j\in\mathbb{Z}_i$) and $z\in\mathbb{Z}_6$.

I.2- $\forall \mathrm{I}=3,\dots,\mathrm{k}$, name two remaining $\beta^i_{z,j}$'s adjacent vertices by $\gamma^i_{z,j},\gamma^i_{z,j+1}$ such that $j\in\mathbb{Z}_{i-1}$, $z\in\mathbb{Z}_6$ and insert two edges $\beta^i_{z,j}\gamma^i_{z,j}$, $\beta^i_{z,j}\gamma^i_{z,j+1}$ into $\mathrm{E}(H_k)$. See Figure 2.

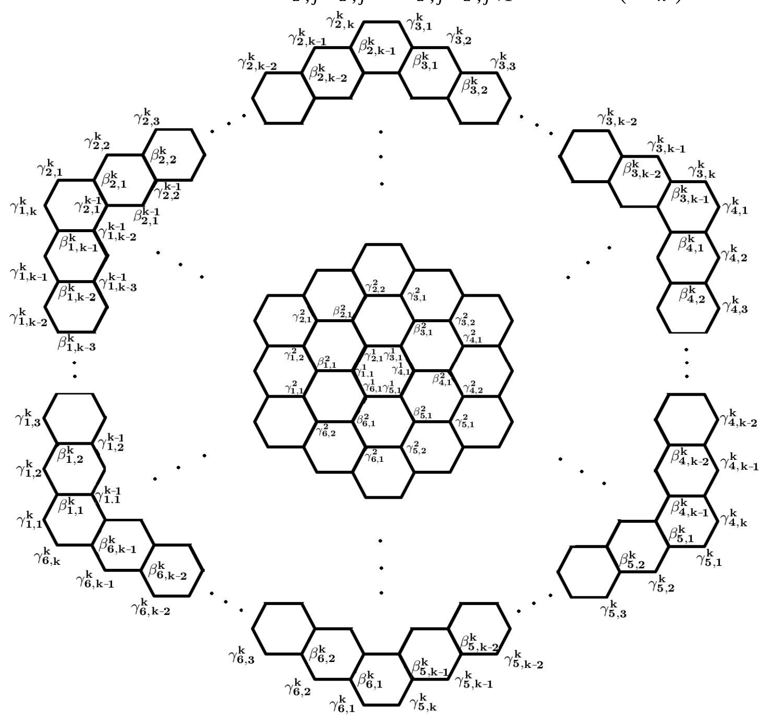

**Figure 2.** The general representation of circumcoronene series, of benzenoid $H_k,(k\geq 1)$.

*Proof.* Consider circumcoronene series of benzenoid $H_k$ $(k\geq 1)$ as shown in Figure 2. At first, we using Notation 1 and name all vertices of $H_k$. So, the vertex set and edge set of circumcoronene series of benzenoid $H_k$ will be

$$V(H_k)=\{\gamma^i_{z,j},\beta^i_{z,l}\mid i=1,\dots,k,\ j\in\mathbb{Z}_i,\ l\in\mathbb{Z}_{i-1} and\ z\in\mathbb{Z}_6\}$$

$$E(H_k)=\{\beta^i_{z,j}\gamma^i_{z,j},\beta^i_{z,j}\gamma^i_{z,j+1},\beta^i_{z,j}\gamma^{i-1}_{z,j}\ and\ \gamma^i_{z,i}\gamma^i_{z+1,1}\mid i\in\mathbb{Z}_k\ j\in\mathbb{Z}_i,z\in\mathbb{Z}_6\}.$$

Obviously, the number of vertices and edges of $H_k$ are equal to $n_k=6\sum_{i=1}^{k}i+6\sum_{i=0}^{k-1}i=6k^2$

and $e_k = 6\sum_{i=1}^{k-1} i + 6\sum_{i=1}^{k-1} i + 6\sum_{i=1}^{k-1} i + 6k = 9k^2 - 3k$.

Here, we attend to properties of Ring-cut method and mixed with above notation of $H_k$. Also, by using of results from [11], we can calculate the important parameter ecc(v) for all $v \in V(H_k)$ as follow:

$\forall i = 1,...,k,\ j \in \mathbb{Z}_{i-1}$ and $z \in \mathbb{Z}_6$; $ecc(\beta_{z,j}^i) = \underbrace{d\left(\beta_{\mathbf{z,j}}^{\mathbf{i}}, \beta_{\mathbf{z+3,j}}^{\mathbf{i}}\right)}_{4i-3} + \underbrace{d\left(\beta_{\mathbf{z+3,j}}^{\mathbf{i}}, \gamma_{\mathbf{z+3,j}}^{\mathbf{k}}\right)}_{2(k-i)+1} = 2(k+i-1)$.

$\forall i = 1,...,k,\ j \in \mathbb{Z}_i$ and $z \in \mathbb{Z}_6$; $ecc(\gamma_{z,j}^i) = \underbrace{d\left(\gamma_{\mathbf{z,j}}^{\mathbf{i}}, \gamma_{\mathbf{z+3,j}}^{\mathbf{i}}\right)}_{4i-1} + \underbrace{d\left(\gamma_{\mathbf{z+3,j}}^{\mathbf{i}}, \gamma_{\mathbf{z+3,j}}^{\mathbf{k}}\right)}_{2(k-i)} = 2(k+i)-1$.

Thus, the fifth Zagreb index $M_5(H_k)$ $(\forall k \geq 1)$ is equal to

$$\mathrm{M}_2^*(H_k) = \sum_{\mathrm{e=uv}\in \mathrm{E}(H_k)} \left(\mathrm{ecc(v)} \times \mathrm{ecc(u)}\right) \Rightarrow$$

$$\begin{aligned}
\mathrm{M}_5(H_k) = & \sum_{\beta_{z,j}^i \gamma_{z,j}^i \in \mathrm{E}(H_k)} [\mathrm{ecc}(\beta_{z,j}^i)\mathrm{ecc}(\gamma_{z,j}^i)] + \sum_{\beta_{z,j}^i \gamma_{z,j+1}^i \in \mathrm{E}(H_k)} [\mathrm{ecc}(\beta_{z,j}^i)\mathrm{ecc}(\gamma_{z,j+1}^i)] \\
& + \sum_{\beta_{z,j}^i \gamma_{z,j}^{i-1} \in \mathrm{E}(H_k)} [\mathrm{ecc}(\beta_{z,j}^i)\mathrm{ecc}(\gamma_{z,j}^{i-1})] + \sum_{\gamma_{z,i}^i \gamma_{z+1,1}^i \in \mathrm{E}(H_k)} [\mathrm{ecc}(\gamma_{z,i}^i)\mathrm{ecc}(\gamma_{z+1,1}^i)] \\
= & \sum_{i=2}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6} [\mathrm{ecc}(\beta_{z,j}^i)\mathrm{ecc}(\gamma_{z,j}^i)] + \sum_{i=2}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6} [\mathrm{ecc}(\beta_{z,j}^i)\mathrm{ecc}(\gamma_{z,j+1}^i)] \\
& + \sum_{i=1}^{k-1}\sum_{j=1}^{i}\sum_{z=1}^{6} [\mathrm{ecc}(\beta_{z,j}^{i+1})\mathrm{ecc}(\gamma_{z,j}^i)] + \sum_{i=1}^{k}\sum_{z=1}^{6} [\mathrm{ecc}(\gamma_{z,i}^i)\mathrm{ecc}(\gamma_{z+1,1}^i)] \\
= & 6\sum_{i=2}^{k}\sum_{j=1}^{i}\left[\mathrm{ecc}(\beta_{1,j}^i)\mathrm{ecc}(\gamma_{1,j}^i)\right] + 6\sum_{i=2}^{k}\sum_{j=1}^{i} [\mathrm{ecc}(\beta_{1,j}^i)\mathrm{ecc}(\gamma_{1,j+1}^i)] \\
& + 6\sum_{i=1}^{k-1}\sum_{j=1}^{i} [\mathrm{ecc}(\beta_{1,j}^{i+1})\mathrm{ecc}(\gamma_{1,j}^i)] + 6\sum_{i=1}^{k} [\mathrm{ecc}(\gamma_{1,i}^i)\mathrm{ecc}(\gamma_{2,1}^i)] \\
= & 2\left(\sum_{i=2}^{k} 6(i-1)\left[(2k+2i-1)(2k+2i-2)\right]\right) \\
& + \sum_{i=2}^{k} 6i\left[(2k+2i-3)(2k+2i-2)\right] + \sum_{i=1}^{k} 6(2k+2i-1)^2 \\
= & 12\sum_{i=1}^{k} (i-1)\left[4k^2 + 4i^2 + 8ki - 6k - 6i + 2\right] \\
& + 6\sum_{i=1}^{k} i\left[4k^2 + 4i^2 + 8ki - 10k - 10i + 6\right] - 6(4k^2 - 2k) + 6\sum_{i=1}^{k}\left[4k^2 + 4i^2 + 8ki - 4i - 4k + 1\right] \\
= & 12\sum_{i=1}^{k}\left[4i^3 + (8k-10)i^2 + (4k^2 - 14k + 8)i - (4k^2 - 6k + 2)\right] \\
& + 6\sum_{i=1}^{k}\left[4i^3 + (8k-10)i^2 + (4k^2 - 10k + 6)i\right] - 6(4k^2 - 2k) + 6\sum_{i=1}^{k}\left[4k^2 + 4i^2 + 8ki - 4i - 4k + 1\right]
\end{aligned}$$

$$=\sum_{i=1}^{k}72i^{3}+\sum_{i=1}^{k}\left(144k-156\right)i^{2}$$

$$+\sum_{i=1}^{k}\left(72k^{2}-218k+108\right)i-\sum_{i=1}^{k}\left(24k^{2}-48k+18\right)-6\left(4k^{2}-2k\right)$$

$$=72\left(\frac{k(k+1)}{2}\right)^{2}+12\left(12k-13\right)\left(\frac{k(k-1)(2k-1)}{6}\right)$$

$$+12\left(6k^{2}-19k+9\right)\left(\frac{k(k+1)}{2}\right)-\left(24k^{3}-24k^{2}+6k\right)$$

$$=\left(18k^{4}+36k^{3}+18k^{2}\right)+\left(48k^{4}+20k^{3}-54k^{2}-26k\right)$$

$$+\left(36k^{4}-54k^{3}-36k^{2}+54k\right)-\left(24k^{3}-24k^{2}+6k\right)$$

Finally, $\forall k\in\mathbb{N}$, the fifth Zagreb index of circumcoronene series of benzenoid is equal to $M_5(H_k)=102k^4-22k^3-48k^2+22k$.

It's clear that for every edge $uv\in E(C_6)$ acc(v)=acc(u)=3, thus $M_5(H_1)=6(3\times3)=54$ and the proof is complete. □

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