# Fourth Zagreb index of Circumcoronene series of Benzenoid

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**Abstract**

A topological index of a graph is a numeric quantity related to a structure of a molecule which is invariant under graph automorphism. Recently, *Ghorbani* and *Hosseinzadeh* introduced *Fourth Zagreb index* of graphs. In this paper we determine a closed formula of this new topological index of the famous Benzenoid family named Circumcoronene series of Benzenoid $H_k$.

**Keywords**

Molecular graph; Benzenoid graph; Circumcoronene series of benzenoid; Topological index; Eccentricity index; Fourth Zagreb index

## Introduction

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. All graphs in this paper are finite and simple. For terms and concepts not defined here we refer the reader to any of several standard monographs such as e.g. [1-5].

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 [1-5]. This theory had an important effect on the development of the chemical sciences.

A graph invariant is any function on a graph that does not depend on a labelling of its vertices. Such quantities are also called topological indices. One of the best known and widely used is the Zagreb topological index introduced in 1972 by *Gutman* and *Trinajstić* and is defined as the sum of the squares of the degrees of all vertices of $G$ [2, 5]. Let $G$ be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively.

For every vertex $u\in V(G)$, the edge connecting $u$ and $v$ is denoted by $uv$ and $d_G(u)$ (or $d_u$) denotes the degree of $u$ in G (the number of first neighbors of vertex $u$ in $G$).

The Zagreb indices were originally defined as follows:

$$M_1(G)=\sum_{v\in V(G)}(d_v)^2$$
$$M_2(G)=\sum_{e=uv\in E(G)}(d_u\times d_v)$$

here $M_1(G)$ and $M_2(G)$ denote the first and the second Zagreb index, respectively. The first Zagreb index can be also expressed as a sum over edges of $G$,

$$M_1(G)=\sum_{e=uv\in E(G)}(d_u+d_v)$$

The readers interested in more information and some mathematical properties of Zagreb indices for general graphs can be referred to [5-11].

In 2012, *Ghorbani* and *Hosseinzadeh* introduced a new version of Zagreb index [12] as follows:

$$M^{**}_1(G)=\sum_{v\in V(G)}\varepsilon(v)^2$$

In which for a vertex v of $V(G)$ its eccentricity $\varepsilon(v)$ is the largest distance between $v$ and any other vertex $u$ of $G$.

$$\varepsilon(v)=Max\{d(u,v)|\ \forall u\in V(G)\}$$

The maximum eccentricity over all vertices of $G$ is called the diameter of $G$ and denoted by $D(G)$. Also the minimum eccentricity among vertices of $G$ is called the radius and denoted by $r(G)$. In other words,

$$D(G)=Max_{v\in V(G)}\{d(u,v)|\ \forall u\in V(G)\}$$
$$R(G)=Min_{v\in V(G)}\{Max\{d(u,v)|\ \forall u\in V(G)\}\}$$

The eccentric connectivity index $\zeta(G)$ of a graph $G$ is defined as:

$$\zeta(G)=\sum_{v\in V(G)}d_v\times\varepsilon(v)$$

For further study and more details see references [13-17].

The aim of this paper is to investigate a closed formula of new topological Zagreb index for Circumcoronene series of Benzenoid $H_k$ $(k\geq 1)$. In this paper, we call this new Zagreb index by *Fourth Zagreb index* and denote by $M_4(G)$.

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## Material and method

In this section it is presented how to compute this new topological index for Circumcoronene series of Benzenoid $H_k$ $(k\geq 1)$. The Circumcoronene series is part of Benzenoid molecular graph family (consist several copy of benzene $C_6$). The general representation and some first members of this Benzenoid graph family are shown in Figures 1 and 2 (see [14-20]).

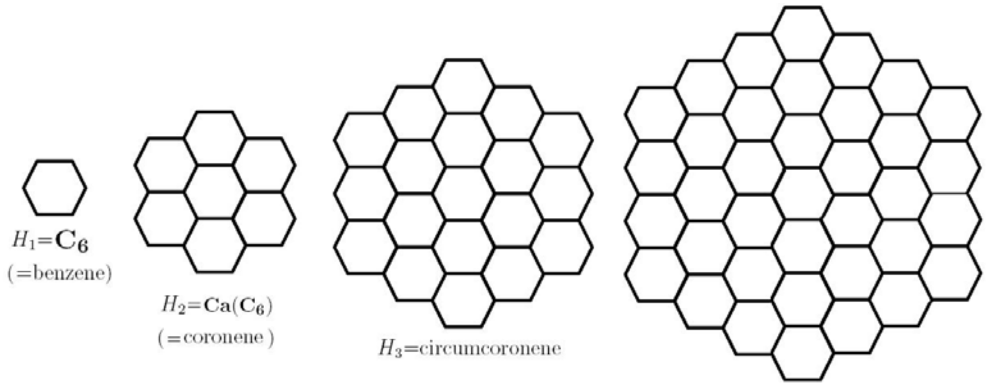


***Figure 1.*** *Some first members of Circumcoronene series of Benzenoid* $H_k$ $(k\geq 1)$ *[14-17]*

In this article we use *Cut method* and *Ring-cut method*. Further studies on *Cut Method* and its modified version *Ring-cut method* can be seen in [19, 20]. Ring-cut method divides all vertices of $G$ into some partitions with similar mathematical and topological properties. For example, readers can see ring-cuts of Circumcoronene series of Benzenoid in Figure 2.

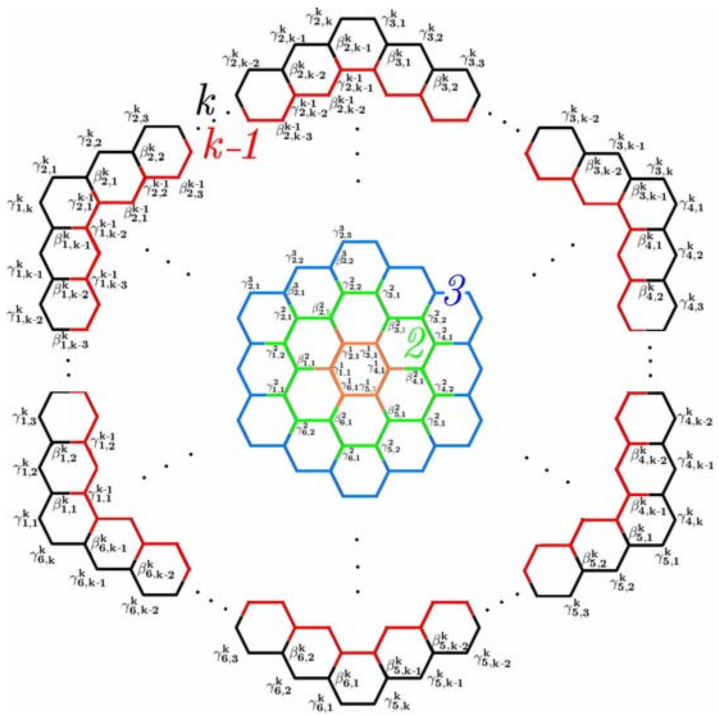


***Figure 2.*** *The Ring-cuts for the general representation of Circumcoronene series of Benzenoid* $H_k$ $(k\geq 1)$ *[14-17]*

Thus, from the general representation of Circumcoronene series of Benzenoid $H_k$ and its ring-cuts in Figure 2, one can see that [14-20]:

I. The vertex/atom set of $H_k$ is $V(H_k)=\{\gamma^i_{z,j}, \beta^i_{z,l} \mid i\in\mathbf{Z}_k \ \&\ j\in\mathbf{Z}_i \ \&\ z\in\mathbf{Z}_6\}$.

II. The edge/bond set of $H_k$ is

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

III. The number of vertices is $n_k=|V(H_k)|=6\sum_{i=1}^{k} i + 6\sum_{i=0}^{k-1} i = 6k^2$ .

IV. The number of edges is $e_k=|E(H_k)|=6\sum_{i=1}^{k-1} i + 6\sum_{i=1}^{k-1} i + 6\sum_{i=1}^{k-1} i + 6k = 9k^2-3k$.

V. $\forall i=1..,k;\ j\in\mathbf{Z}_{i-1}\ \&\ z\in\mathbf{Z}_6$: $\varepsilon(\beta^i_{z,j}) = \underbrace{d(\beta^{\mathbf{i}}_{\mathbf{z},\mathbf{j}}, \beta^{\mathbf{i}}_{\mathbf{z+3},\mathbf{j}})}_{4i-3} + \underbrace{d(\beta^{\mathbf{i}}_{\mathbf{z+3},\mathbf{j}}, \gamma^{\mathbf{k}}_{\mathbf{z+3},\mathbf{j}})}_{2(k-i)+1} = 2(k+i+1)$.

VI. $\forall i=1..,k;\ j\in\mathbf{Z}_i\ \&\ z\in\mathbf{Z}_6$: $\varepsilon(\gamma^i_{z,j}) = \underbrace{d(\gamma^{\mathbf{i}}_{\mathbf{z},\mathbf{j}}, \gamma^{\mathbf{i}}_{\mathbf{z+3},\mathbf{j}})}_{4i-1} + \underbrace{d(\gamma^{\mathbf{i}}_{\mathbf{z+3},\mathbf{j}}, \gamma^{\mathbf{k}}_{\mathbf{z+3},\mathbf{j}})}_{2(k-i)} = 2(k+i)-1$.

VII. The radius number of $H_k$ is equal to $r(H_k)=2k+1$.

VIII. The diameter number of $H_k$ is equal to $D(H_k)=4k-1$.

IX. $\zeta(H_k)=60k^3-24k^2-18k+18$.

where all vertices $\beta^i_{z,j}, \gamma^i_{z,j}$ are from $I^{th}$ ring cut $R_i$ of $H_k$, such that $i=1,\dots,k$ and $j\in\mathbf{Z}_i\ \&\ z\in\mathbf{Z}_6$ ($\mathbf{Z}_n$ is the cycle finite group of order n).

## Results

Now, we can exhibit the closed formula of Fourth Zagreb index $M_4(H_k)$ in following theorem and its proof.

**Theorem 1:** Let $G$ be the Circumcoronene series of Benzenoid $H_k$ $(k\geq 1)$. Then Fourth Zagreb index of $H_k$ is equal to:

$$M^{**}_1(Hk)=M_4(Hk)=68k^4+4k^3-65k^2+71k-24 \qquad (1)$$

**Proof:** Consider Circumcoronene series of Benzenoid $G=H_k$ $(k\geq 1)$ as shown in Figure 2. Thus, we refer to definition of Fourth Zagreb index $M_4(H_k)$ and compute this index for $G=H_k$ in general case $(k\in\mathbf{Z})$ as follows:

$$M^{**}_1(H_k)=\sum_{v\in V(Hk)} \varepsilon(v)^2 \Rightarrow \qquad (2)$$

$$M_4(H_k)=\sum_{\gamma^i_{z,j}\in V(H_k)}\left[\varepsilon(\gamma^i_{z,j})\right]^2+\sum_{\beta^i_{z,j}\in V(H_k)}\left[\varepsilon(\beta^i_{z,j})\right]^2 \quad (3)$$

$$=\sum_{i=1}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}[\varepsilon(\gamma^i_{z,j})]^2+\sum_{i=2}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}[\varepsilon(\beta^i_{z,j})]^2$$

$$=\sum_{z=1}^{6}\sum_{i=1}^{k}\sum_{j=1}^{i}[\varepsilon(\gamma^i_{z,j})]^2+\sum_{z=1}^{6}\sum_{i=2}^{k}\sum_{j=1}^{i}[\varepsilon(\beta^i_{z,j})]^2$$

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

$$=6\sum_{i=1}^{k} i(4k^2+4i^2+8ki-4k-4i+1)+6\sum_{i=1}^{k} (i-1)(4k^2+4i^2+8ki-8k-8i+4)$$

$$=\sum_{i=1}^{k}24i^3+6\sum_{i=1}^{k}(16k-16)i^2+6\sum_{i=1}^{k}\left(8k^2-20k+13\right)i-6\sum_{i=1}^{k}\left(4k^2-8k+4\right)$$

$$=24\left(\frac{k(k-1)}{2}\right)^2+96(k-1)\left(\frac{k(k+1)(2k+1)}{6}\right)+6\left(8k^2-20k+13\right)\left(\frac{k(k-1)}{2}\right)-24(k-1)^2(k)$$

$$=(12k^4+24k^3+12k^2)+(32k^4+16k^3-32k^2-16k)+(24k^4-36k^3-21k^2+39k)$$
$$-(24k^2-48k+24)$$

Finally, $\forall k\in \mathbf{Z}$, the Fourth Zagreb index is equal to:

$$M_4(H_k)=68k^4+4k^3-65k^2+71k-24 \quad (4)$$

Obviously, $M_4(H_1=C_6)=6(3)^2=54$ and the proof is complete.

## Conclusion

In this paper, we have computed closed formula of Fourth Zagreb index for famous Benzenoid molecular graph "Circumcoronene series of Benzenoid $H_k$ ($k\geq1$)".

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