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On Topological Indices of Circumcoronene Series of Benzenoid

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ABSTRACT

Let G be a connected graph with vertex and edge sets V (G) and E(G), respectively. The first Zagreb index $M_1(G)$ was originally defined as the sum of the squares of the degrees of all vertices of G. Recently, we know a new version of the first Zagreb index as the Multiplicative Zagreb Eccentricity index that introduced by Nilanjan De and ε(u) is the largest distance between u and any other vertex v of G. In this paper we compute this new topological index of famous molecular graph “Circumcoronene Series of Benzenoid H_k”.

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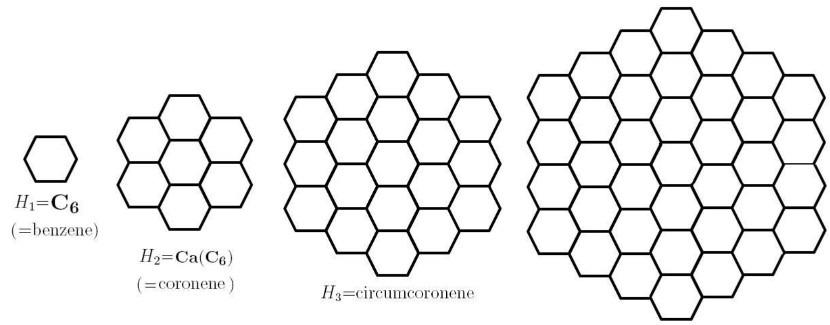
Graphical Abstract



Introduction

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$ and order n and size m, respectively. For every vertex $u \in V(G)$, the edge connecting u and v is denoted by uv and the degree of any vertex is the number of first neighbour of v and is denoted by $d_G(u)$ (or d_u). Let the maximum and minimum degree of all the vertices of G are respectively denoted by Δ and δ. The distance of any two vertices u and v of is defined as the length of the shortest path connecting u and v and is denoted by $d(u,v)$. 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:

$$D(G)=Max_{v\in V(G)}\{d(u,v)|\ \forall u\in V(G)\} \qquad (1)$$

$$R(G)=Min_{v\in V(G)}\{Max\{d(u,v)|\ \forall u\in V(G)\}\} \qquad (2)$$

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 the chemical phenomena [1-3]. This theory had an important effect on the development of the chemical sciences. A topological index of a graph is a number related to a graph which is invariant under graph automorphisms and is a numeric quantity from the structural graph of a molecule. One of the best known and widely used is the *Zagreb topological index* introduced in 1972 by *I. Gutman* and *N. Trinajstić* and is defined as the sum of the squares of the degrees of all vertices of G [4, 5]. The first Zagreb index $M_1(G)$ was originally defined as follows:

$$M_1(G)=\sum_{v\in V(G)}(d_v)^2=\sum_{e=uv\in E(G)}(d_u+d_v). \qquad (3)$$

where d_v denotes the degree of vertex v in G. The multiplicative version of this first Zagreb index was introduced by *Todeschini et. al.* [6, 7] and is defined as:

$$\Pi M_1(G)=\prod_{uv\in E(G)} d_v^{\,2} \qquad (4)$$

The eccentric version of the first Zagreb index was introduced by *M. Ghorbani et al.* [8] and *D. Vukicevic et al.* [9] in 2012 as follows:

$$M^{**}_1(G)=\sum_{v\in V(G)} \varepsilon(v)^2 \qquad (5)$$

The eccentricity of a vertex is the distance between v and a vertex farthest from v and is denoted by $\varepsilon(v)$. In other words, $\varepsilon(v)=Max\{d(u,v)|\ \forall u\in V(G)\}$. The *Eccentric Connectivity index* $\zeta(G)$ of a graph G is defined as [10]:

$$\zeta(G) = \sum_{v\in V(G)} d_v\times\varepsilon(v), \qquad (6)$$

where $\varepsilon(u)$ is the eccentricity of vertex u. This index introduced by *Sharma et al.* in 1997 [10-15]. Recently in 2012, *Nilanjan De* introduced a new version of First Zagreb index [16] as the *Multiplicative Zagreb Eccentricity index* and defined as follows:

$$\Pi E_1(G)=\prod_{uv\in E(G)} \varepsilon(v)^2, \qquad (7)$$

where $\varepsilon(u)$ is the largest distance between u and any other vertex v of G. The readers interested in more information and some mathematical properties of Zagreb indices for general graphs can be referred to [18-30]. The aim of this paper is to investigate a closed formula of this new topological index "Multiplicative Zagreb Eccentricity index" for famous Benzenoid molecular graph "Circumcoronene series of Benzenoid H_k $(k\geq1)$".

Results and Discussion

The Circumcoronene series of Benzenoid is a famous family of Benzenoid molecular graph, which this family built solely from benzene C_6 (or hexagons) on circumference. For more detail of Benzenoid molecular graphs, see the paper series [29-38]. The general representations and first members of this family are shown in Figures 1 and 2.

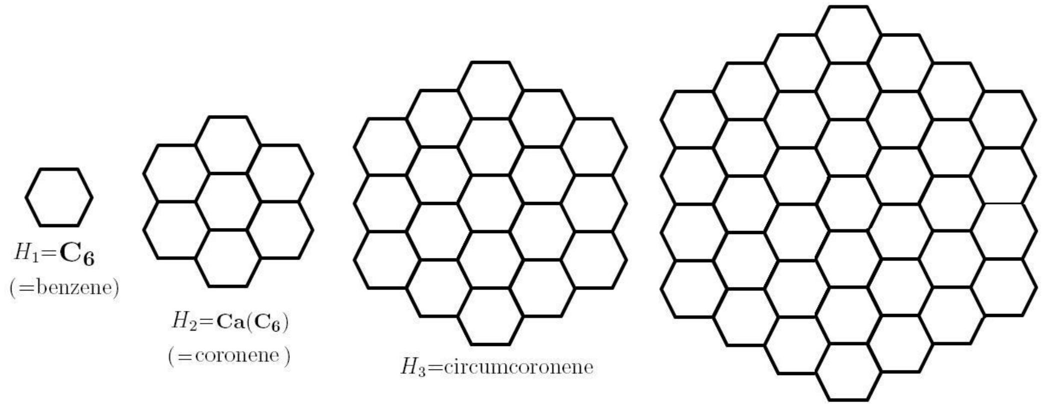


Figure 1. Some first members of *Circumcoronene Series of Benzenoid* H_k ($\forall k\geq1$) [29-33].

Theorem 1. [30] Let H_k be the Circumcoronene Series of Benzenoid, $\forall k\geq1$. Then the First Zagreb index of H_k is equal to $M_1(H_k)=54k^2-30k$.

Theorem 2. [15] Consider the Circumcoronene series of Benzenoid H_k, $\forall k\geq1$. Then the Eccentric Connectivity index of H_k is equal to $\zeta(H_k)= 60k^3-24k^2-18k+18$.

Theorem 3. [29]The first eccentric Zagreb index of the Circumcoronene series of Benzenoid H_k, $\forall k\geq1$ is equal to $M^{**}_1(H_k)=68k^4+4k^3-65k^2+71k-24$.

Theorem 4. Let G be the Circumcoronene series of Benzenoid H_k ($k\geq1$). Then the Multiplicative Zagreb Eccentricity index of H_k is equal to:

$$\Pi E_1(H_k)= \prod_{i=1}^{k}\left(\left(2k+2i-1\right)^{12i}\right)\left(\left(2k+2i-2\right)^{12(i-1)}\right) \qquad (8)$$

Proof. Consider the Circumcoronene series of Benzenoid H_k ($k\geq1$) as shown in Figure2. And let the vertex/atom and edge/bond sets of H_k, $\forall k\geq1$ are equal to:

$V(H_k)=\{\gamma^i_{z,j},\beta^i_{z,j} \mid i\in\mathbb{Z}_k \ \&\ j\in\mathbb{Z}_i \ \&\ z\in\mathbb{Z}_6\}$

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

And the size of vertex and edge sets of H_k are equal to

$$n_k=|V(H_k)|=6\sum_{i=1}^{k} i+6\sum_{i=0}^{k-1} i=6k^2$$

$$\text{and } m_k=|E(H_k)|=6\sum_{i=1}^{k-1} i+6\sum_{i=1}^{k-1} i+6\sum_{i=1}^{k-1} i+6k=9k^2-3k. \qquad (9)$$

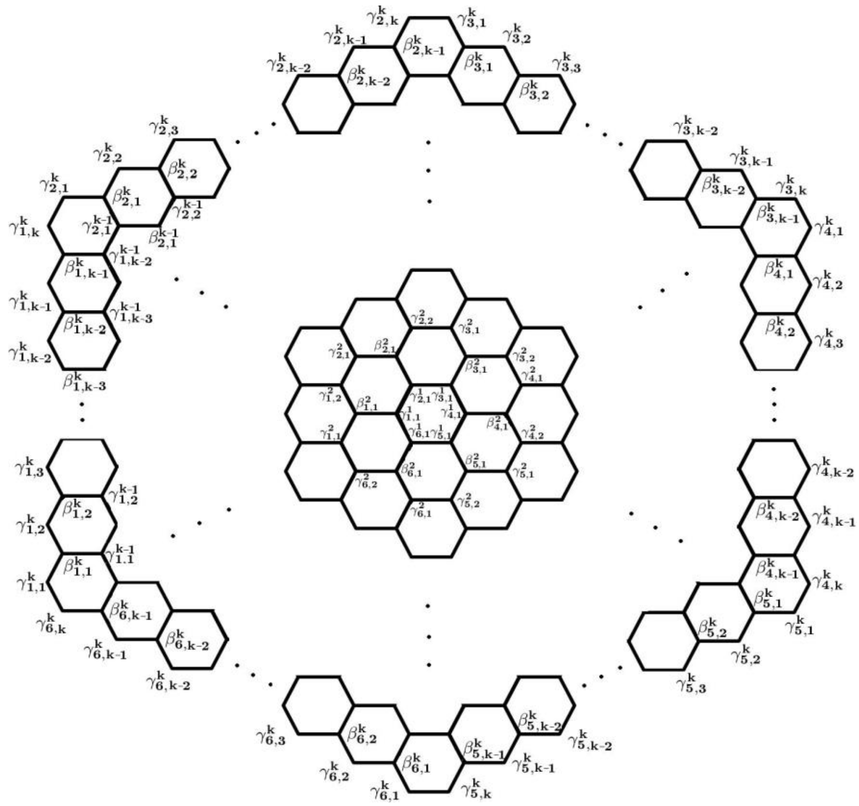


Figure 2. The Circumcoronene series of Benzenoid H_k *(k≥1)* [29-33].

To compute the Multiplicative Zagreb Eccentricity index of H_k, we used the *Cut Method* and the *Ring-cut Method*. The readers can consult [15, 29-33, 37, 38] for more information about the Cut Method and it modify version *Ring-cut Method.* The Ring-cut Method divides all vertices of a graph G into some partitions with similar mathematical and topological properties. We encourage readers see the ring-cuts of Circumcoronene series of Benzenoid in Figure 3, such that $\forall i=1,\dots,k$ and $\forall j\in\mathbb{Z}_i$ & $\forall z\in\mathbb{Z}_6$; all vertices $\beta^i_{z,j}, \gamma^i_{z,j}$ are from I^{th} ring cut R_i of H_k.

Now, from the general representation of Circumcoronene series of Benzenoid H_k in Figure 2 and Figure 3 and, we can see that

$$\forall i=1..,k;\ j\in\mathbb{Z}_{i-1}\ \&\ z\in\mathbb{Z}_6:\quad \varepsilon(\beta^i_{z,j}) = \underbrace{d(\beta^i_{z,j}, \beta^i_{z+3,j})}_{4i-3} + \underbrace{d(\beta^i_{z+3,j}, \gamma^k_{z+3,j})}_{2(k-i)+1} = 2(k+i+1) \qquad (10)$$

$$\forall i=1..,k;\ j\in\mathbb{Z}_{i}\ \&\ z\in\mathbb{Z}_6:\quad \varepsilon(\gamma^i_{z,j}) = \underbrace{d(\gamma^i_{z,j}, \gamma^i_{z+3,j})}_{4i-1} + \underbrace{d(\gamma^i_{z+3,j}, \gamma^k_{z+3,j})}_{2(k-i)} = 2(k+i)-1 \qquad (11)$$

By above mansions, it is easy to see that the radius and diameter numbers of H_k are equal to $R(H_k)=2k+1$ and $D(H_k)=4k-1$, respectively. Now by using above mention results, we can compute the

Multiplicative Zagreb Eccentricity index of Circumcoronene series of Benzenoid H_k, $\forall k\in\mathbb{Z}$ as follows:

$$\Pi E_1(H_k)=\prod_{v\in V(H_k)}\varepsilon(v)^2$$

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

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

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

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

$$=\prod_{i=1}^{k}\left(\left(2k+2i-1\right)^{12i}\right)\left(\left(2k+2i-2\right)^{12(i-1)}\right). \qquad (12)$$

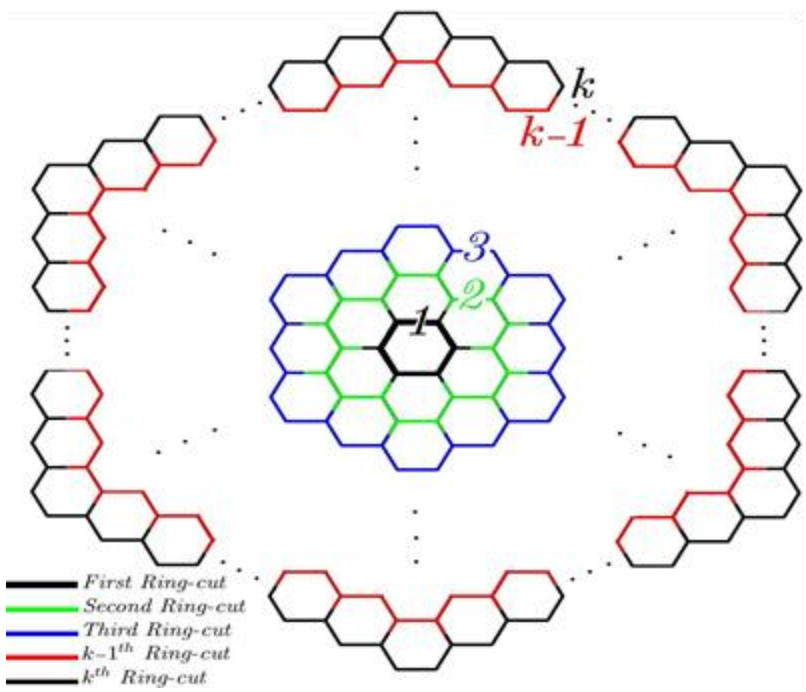


Figure 2. The Ring-cuts of Circumcoronene series of Benzenoid H_k *(k≥1)* [29-33].

Finally, the Multiplicative Zagreb Eccentricity index of H_k $\forall k\in\mathbb{Z}$ is equal to

$$\Pi E_1(H_k)=\prod_{i=1}^{k}\left(\left(2k+2i-1\right)^{12i}\right)\left(\left(2k+2i-2\right)^{12(i-1)}\right) \qquad (13)$$

Conclusion

For a connected graph G, the *Multiplicative Zagreb Eccentricity index* is equal to $\Pi E_1(G)=\prod_{v\in V(G)} \varepsilon(v)^2$, where $\varepsilon(v)$ denotes the eccentricity of a vertex is the distance between v and a vertex farthest from v.

In this paper, we obtained a closed formula of this new index the (Multiplicative Zagreb Eccentricity index) of famous Benzenoid molecular graph for the first time that we called "*Circumcoronene series of benzenoid H_k ($k\geq 1$)*".

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