

Connective Eccentric Index of Circumcoronene Homologous Series of Benzenoid H_k

Mohammad Reza Farahani

Department of Applied Mathematics of Iran University of Science and Technology (IUST),
Narmak, Tehran 16844, Iran

E-mail address: Mr_Farahani@Mathdep.iust.ac.ir , MrFarahani88@Gmail.com

ABSTRACT

Let G be a molecular graph, a topological index is a numeric quantity related to G which is invariant under graph automorphisms. The eccentric connectivity index $\zeta(G)$ is defined as $\zeta(G) = \sum_{v \in V(G)} d_v \times \varepsilon(v)$ where d_v , $\varepsilon(v)$ denote the degree of vertex v in G and the largest distance between v and any other vertex u of G . The connective eccentric index of graph G is defined as $C^\zeta(G) = \sum_{v \in V(G)} \frac{d_v}{\varepsilon(v)}$. In the present paper we compute the connective eccentric index of *Circumcoronene Homologous Series of Benzenoid* H_k ($k \geq 1$).

Keywords: Molecular graphs; Benzenoid; Connective eccentric index; Eccentric connectivity index

1. INTRODUCTION

In theoretical chemistry molecular structure descriptor or topological indices, are used to compute properties of chemical compounds. Throughout this paper, graph means simple connected graph [1-3]. Let G be a molecular graph, the vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. If $x, y \in V(G)$ then the distance $d(x, y)$ between x and y is defined as the length of a minimum path connecting x and y .

In 1997, the *Eccentric Connectivity index* $\zeta(G)$ of the molecular graph G was proposed by *Sharma, Goswami and Madan* and is defined as [4]:

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

where d_v denotes the degree of the vertex v in G and $\varepsilon(v)$ denote the largest distance between v and any other vertex u of G . In other words, $\varepsilon(v) = \text{Max}\{d(v, u) \mid \forall v \in V(G)\}$.

In 2000, the *Connective Eccentric index* $C^\zeta(G)$ was defined by *Gupta, Singh and Madan* [5,6] as follows:

$$C^\zeta(G) = \sum_{v \in V(G)} \frac{d_v}{\varepsilon(v)}$$

where $d_v, \varepsilon(v)$ denote the degree and eccentric of vertex v in G . See [7-26] for more details and other versions of *Eccentric indices* and *Eccentric polynomials*.

The goal in this paper is computing the Connective eccentric index of *Circumcoronene Homologous Series of Benzenoid* H_k ($k \geq 1$).

2. RESULTS AND DISCUSSION

In this section, we compute the Connective eccentric index $C^\xi(G)$ of Circumcoronene Homologous Series of Benzenoid. Three first members of this Benzenoid family ($H_1 = \text{benzene}$, $H_2 = \text{coronene}$ and $H_3 = \text{circumcoronene}$) are shown in Figure 1. Circumcoronene Homologous Series of Benzenoid is generated from famous molecule *Benzene* or cycle C_6 . We encourage reader to references [18-38] to study some properties of this Benzenoid family.

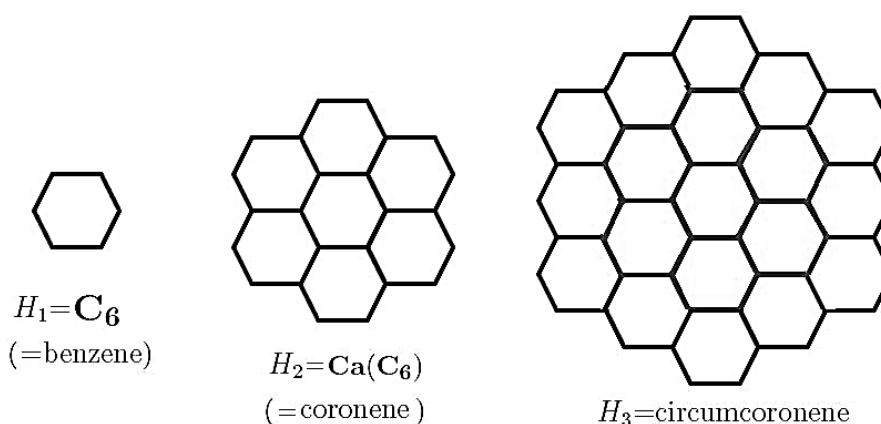


Figure 1. Three first members of Circumcoronene Homologous Series of Benzenoid: $H_1 = \text{benzene}$, $H_2 = \text{coronene}$ and $H_3 = \text{circumcoronene}$ [18-26].

$\forall k \in \mathbb{N}$ Circumcoronene Homologous Series of Benzenoid H_k has $6k^2$ atoms/vertices and $9k^2 - 6k$ bonds/edges (see Figure 2). For further study and more detail of this Benzenoid family, see the paper series [27-35]. Now, we have following theorem for this benzenoid graphs.

Theorem 1. Let G be the Circumcoronene Homologous Series of Benzenoid H_k ($\forall k \geq 1$). Then the Connective Eccentric index $C^\xi(G)$ of H_k is equal to

$$C^\xi(H_k) = \sum_{i=1}^{k-1} \left(\frac{9i(4k+4i-1)}{2i^2 + (4k-1)i + 2k^2 - k} \right) + \frac{12k}{4k-1}$$

Before prove the Theorem 1, we denote all vertices and edges of Circumcoronene Homologous Series of Benzenoid H_k , as follow and is shown in Figure 2, (Z_i , is the cycle finite group):

$$V(H_k) = \{ \gamma_{z,j}^i, \beta_{z,l}^i \mid i = 1, \dots, k, j \in Z_i, l \in Z_{i-1}, z \in Z_6 \}$$

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

Proof. By considering Circumcoronene Homologous Series of Benzenoid $G = H_k (\forall k \geq 1)$ as shown in Figure 2 and refer to [18-26] and using the *Ring-cut Method* for circumcoronene homologous series of Benzenoid, we can compute its connective eccentric index. The *Ring-cut Method* is a modify version of the thoroughbred *Cut Method*. The general form of this method is introduced in [18-26] For more study and detail information of the Cut Method see [28,31,32].

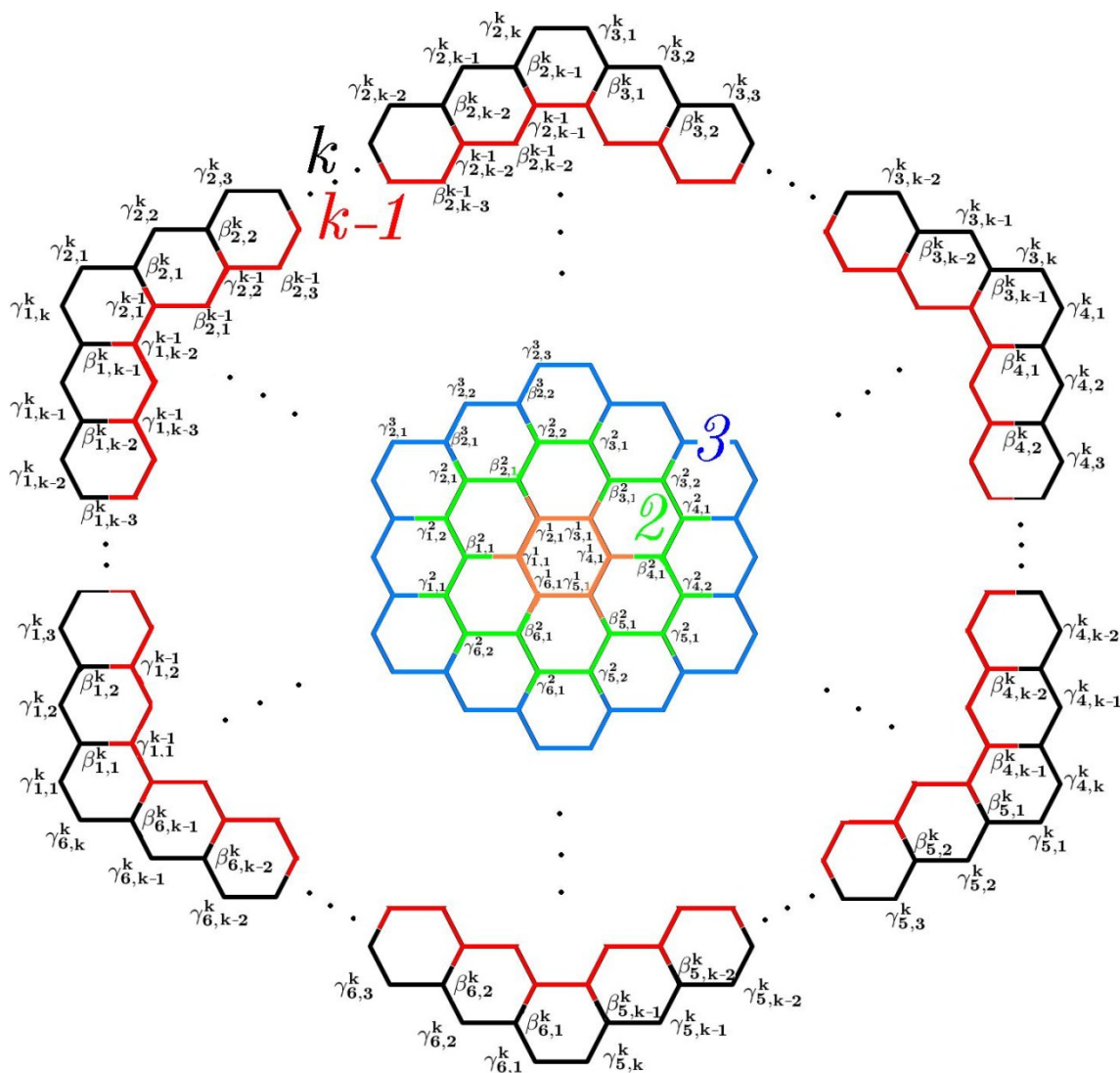


Figure 2. The general representation of Circumcoronene Homologous Series of Benzenoid $H_k (k \geq 1)$ [18-26].

To compute the connective eccentric index of H_k , we see that

$$\forall i = 2, \dots, k; j \in \mathbb{Z}_{i-1} \ \& \ z \in \mathbb{Z}_6: \varepsilon(\beta^i_{z,j}) = 2k + 2i - 2$$

$$\forall i = 1, \dots, k; j \in \mathbb{Z}_i \ \& \ z \in \mathbb{Z}_6: \varepsilon(\gamma^i_{z,j}) = 2k + 2i - 1$$

Also, by according to Figure 2, one can see that the vertices in general representation of molecular graph Circumcoronene Homologous Series of Benzenoid H_k have degree two or three, such that

$$V_2(H_k) = \{v \in V(H_k) | d_v = 2\} = \{\gamma_{z,i}^k | \forall i \in \mathbb{Z}_i \ \& \ z \in \mathbb{Z}_6\}$$

and alternatively $V_3(H_k) = V(H_k) - V_2(H_k)$.

$$\begin{aligned} C^\xi(H_k) &= \sum_{v \in V(G)} \frac{d_v}{\varepsilon(v)} \\ &= \sum_{\gamma_{z,j}^k \in V_2(H_k)} \frac{d_{\gamma_{z,j}^k}}{\varepsilon(\gamma_{z,j}^k)} + \sum_{\gamma_{z,j}^i \in V_3(H_k)} \frac{d_{\gamma_{z,j}^i}}{\varepsilon(\gamma_{z,j}^i)} + \sum_{\beta_{z,j}^i \in V_3(H_k)} \frac{d_{\beta_{z,j}^i}}{\varepsilon(\beta_{z,j}^i)} \\ &= \sum_{\substack{\gamma_{z,j}^k \in V_2(H_k) \\ j \in \mathbb{Z}_k; z \in \mathbb{Z}_6}} \frac{2}{4k-1} + \sum_{\substack{\gamma_{z,j}^i \in V_3(H_k); z \in \mathbb{Z}_6 \\ i=1, \dots, k-1; j \in \mathbb{Z}_i}} \frac{3}{2k+2i-1} + \sum_{\substack{\beta_{z,j}^i \in V_3(H_k); z \in \mathbb{Z}_6 \\ i=2, \dots, k; j \in \mathbb{Z}_{i-1}}} \frac{3}{2k+2i-2} \\ &= \sum_{z=1}^6 \sum_{j=1}^k \left(\frac{2}{4k-1} \right) + \sum_{z=1}^6 \sum_{i=1}^{k-1} \sum_{j=1}^i \left(\frac{3}{2k+2i-1} \right) + \sum_{z=1}^6 \sum_{i=2}^k \sum_{j=1}^{i-1} \left(\frac{3}{2k+2i-2} \right) \\ &= 6k \left(\frac{2}{4k-1} \right) + \sum_{i=1}^{k-1} \left(\frac{3 \times 6i}{2k+2i-1} \right) + \sum_{i=2}^k \left(\frac{3 \times 6(i-1)}{2k+2i-2} \right) \\ &= \frac{2 \times 6k}{4k-1} + \sum_{i=1}^{k-1} \left(\frac{3 \times 6i}{2k+2i-1} \right) + \sum_{j=1}^{k-1} \left(\frac{3 \times 6j}{2k+2j} \right) \\ &= \sum_{i=1}^{k-1} \left(\frac{18i(2k+2i-1+2k+2i)}{2(k+i)(2k+2i-1)} \right) + \frac{12k}{4k-1} \end{aligned}$$

Thus $\forall k \geq 1$, the connective eccentric index of H_k is equal to

$$C^\xi(H_k) = \sum_{i=1}^{k-1} \left(\frac{9i(4k+4i-1)}{2i^2 + (4k-1)i + 2k^2 - k} \right) + \frac{12k}{4k-1}$$

and this completed the proof of Theorem 1.

3. CONCLUSION

The eccentric connectivity index $\xi(G)$ is defined as $\xi(G) = \sum_{v \in V(G)} d_v \times \varepsilon(v)$ where d_v , $\varepsilon(v)$ denote the degree of vertex v in G and the largest distance between v and any other vertex u of G . In this paper, we counting the connective eccentric index $C^\xi(G) = \sum_{v \in V(G)} \frac{d_v}{\varepsilon(v)}$ of *Circumcoronene Homologous Series of Benzenoid* H_k ($k \geq 1$).

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