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Connective Eccentric Index of Circumcoronene Homologous Series of Benzenoid H_k

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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 $\xi(G)$ 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. The connective eccentric index of graph G is defined as $C^{\xi}(G) = \sum_{v\in V(G)} {}^{d_v}\!/_{\varepsilon(v)}$. 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* $\xi(G)$ of the molecular graph G was proposed by *Sharma, Goswami and Madan* and is defined as [4]:

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

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

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

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

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 = *benzene*, H_2 = *coronene* and H_3 = *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.

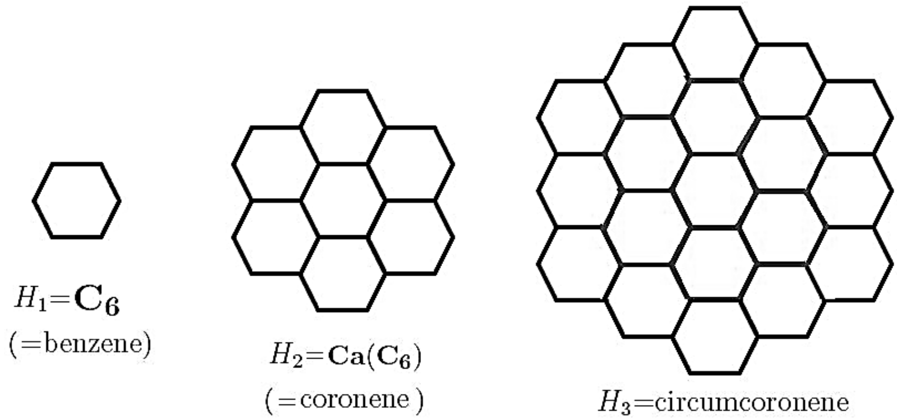

Figure 1. Three first members of Circumcoronene Homologous Series of Benzenoid: H_1 = *benzene*, H_2 = *coronene* and H_3 = *circumcoronene* [18-26].

$\forall k\in\mathbb{N}$ 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 adn is shown in Figure 2, (Z_i, is the cycle finite group):

$$V(H_k) = \{\, \gamma^i_{z,j}, \beta^i_{z,l} \mid i = 1, \ldots, k, j \in Z_i, l \in Z_{i-1}, z \in Z_6 \,\}$$

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].

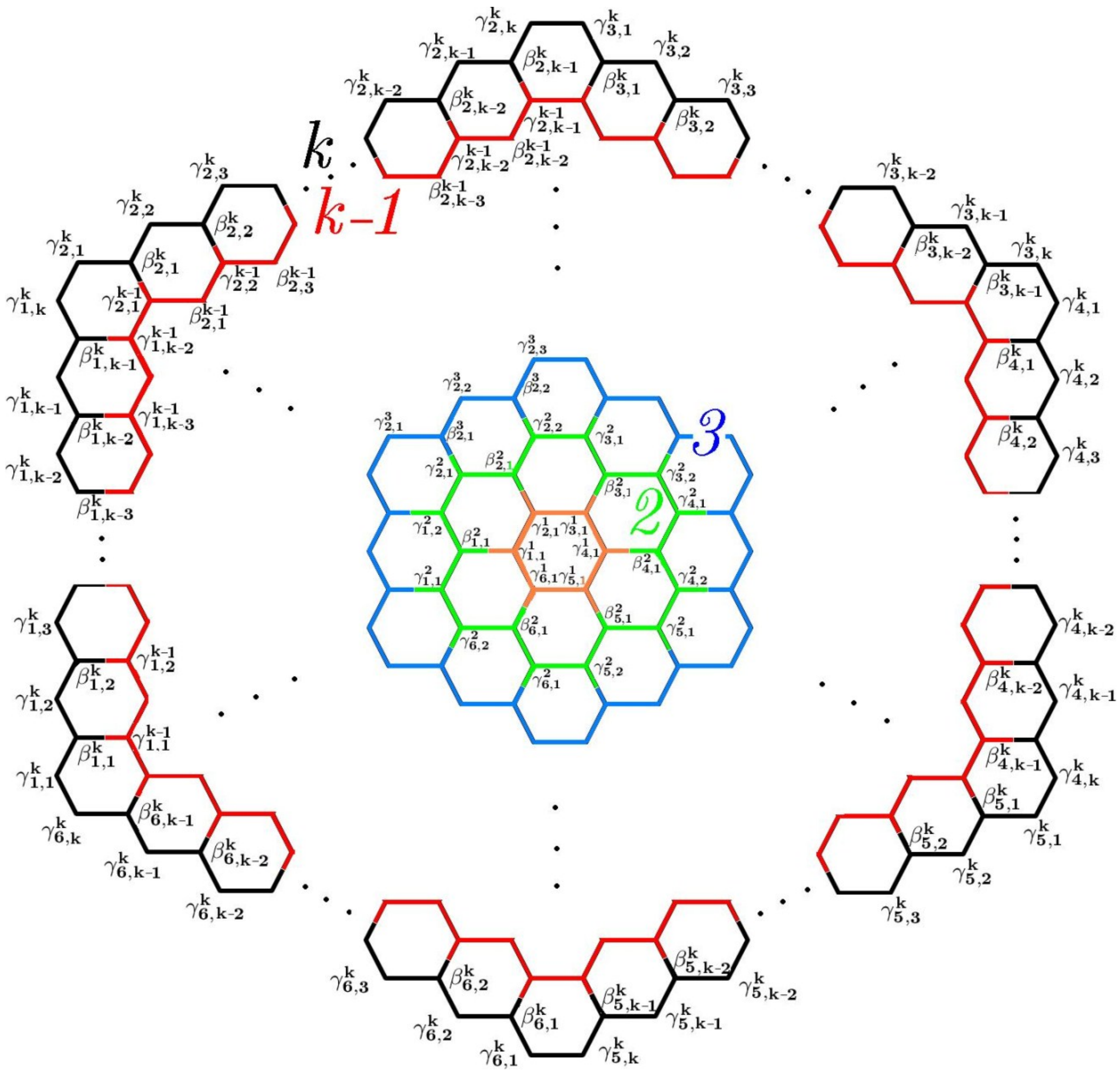

Figure 2. The general representation of Circumcoronene Homologous Series of Benzenoid H_k $(k \geq 1)$ [18-26].

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

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

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

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

$$=\sum_{\gamma^k_{z,j}\in V_2(H_k)}\frac{d_{\gamma^k_{z,j}}}{\varepsilon(\gamma^k_{z,j})}+\sum_{\gamma^i_{z,j}\in V_3(H_k)}\frac{d_{\gamma^i_{z,j}}}{\varepsilon(\gamma^i_{z,j})}+\sum_{\beta^i_{z,j}\in V_3(H_k)}\frac{d_{\beta^i_{z,j}}}{\varepsilon(\beta^i_{z,j})}$$

$$=\sum_{\substack{\gamma^k_{z,j}\in V_2(H_k)\\ j\in\mathbb{Z}_k;z\in\mathbb{Z}_6}}\frac{2}{4k-1}+\sum_{\substack{\gamma^i_{z,j}\in V_3(H_k);z\in\mathbb{Z}_6\\ i=1,\dots,k-1;j\in\mathbb{Z}_i}}\frac{3}{2k+2i-1}+\sum_{\substack{\beta^i_{z,j}\in V_3(H_k);z\in\mathbb{Z}_6\\ i=2,\dots,k;j\in\mathbb{Z}_{i-1}}}\frac{3}{2k+2i-2}$$

$$=\sum_{z=1}^{6}\sum_{j=1}^{k}\left(\frac{2}{4k-1}\right)+\sum_{z=1}^{6}\sum_{i=1}^{k-1}\sum_{j=1}^{i}\left(\frac{3}{2k+2i-1}\right)+\sum_{z=1}^{6}\sum_{i=2}^{k}\sum_{j=1}^{i-1}\left(\frac{3}{2k+2i-2}\right)$$

$$=6k\left(\frac{2}{4k-1}\right)+\sum_{i=1}^{k-1}\left(\frac{3\times 6i}{2k+2i-1}\right)+\sum_{i=2}^{k}\left(\frac{3\times 6(i-1)}{2k+2i-2}\right)$$

$$=\frac{2\times 6k}{4k-1}+\sum_{i=1}^{k-1}\left(\frac{3\times 6i}{2k+2i-1}\right)+\sum_{j=1}^{k-1}\left(\frac{3\times 6j}{2k+2j}\right)$$

$$=\sum_{i=1}^{k-1}\left(\frac{18i(2k+2i-1+2k+2i)}{2(k+i)(2k+2i-1)}\right)+\frac{12k}{4k-1}$$

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 $C^{\xi}(G)=\sum_{v\in V(G)} {d_v}/{\varepsilon(v)}$ of *Circumcoronene Homologous Series of Benzenoid* H_k $(k \geq 1)$.

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