International Letters of Chemistry, Physics and Astronomy
ISSN: 2299-3843, Vol. 32, pp 71-76
doi:10.18052/www.scipress.com/ILCPA.32.71

Online: 2014-04-22

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 $\xi(G)$ 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.

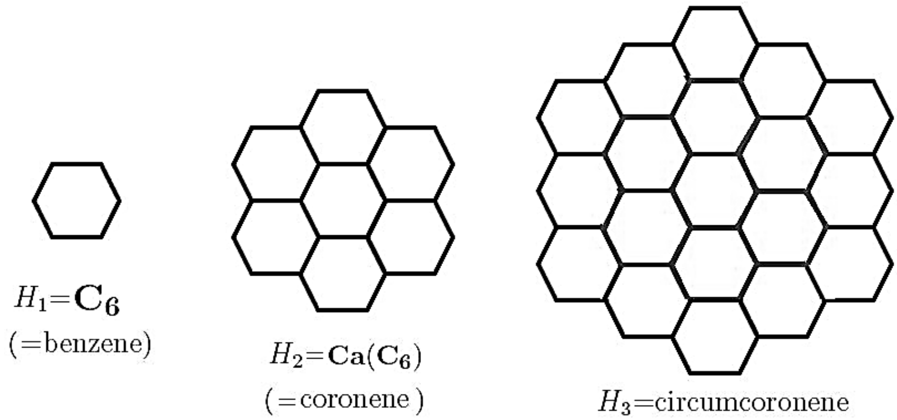

Figure 1. Three first members of Circumcoronene Homologous Series of Benzenoid: H_1 = *benzene*, H_2 = *coronene* and H_3 = *circumcoronene* [18-26].

$\forall k\in\mathrm{N}$ 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].

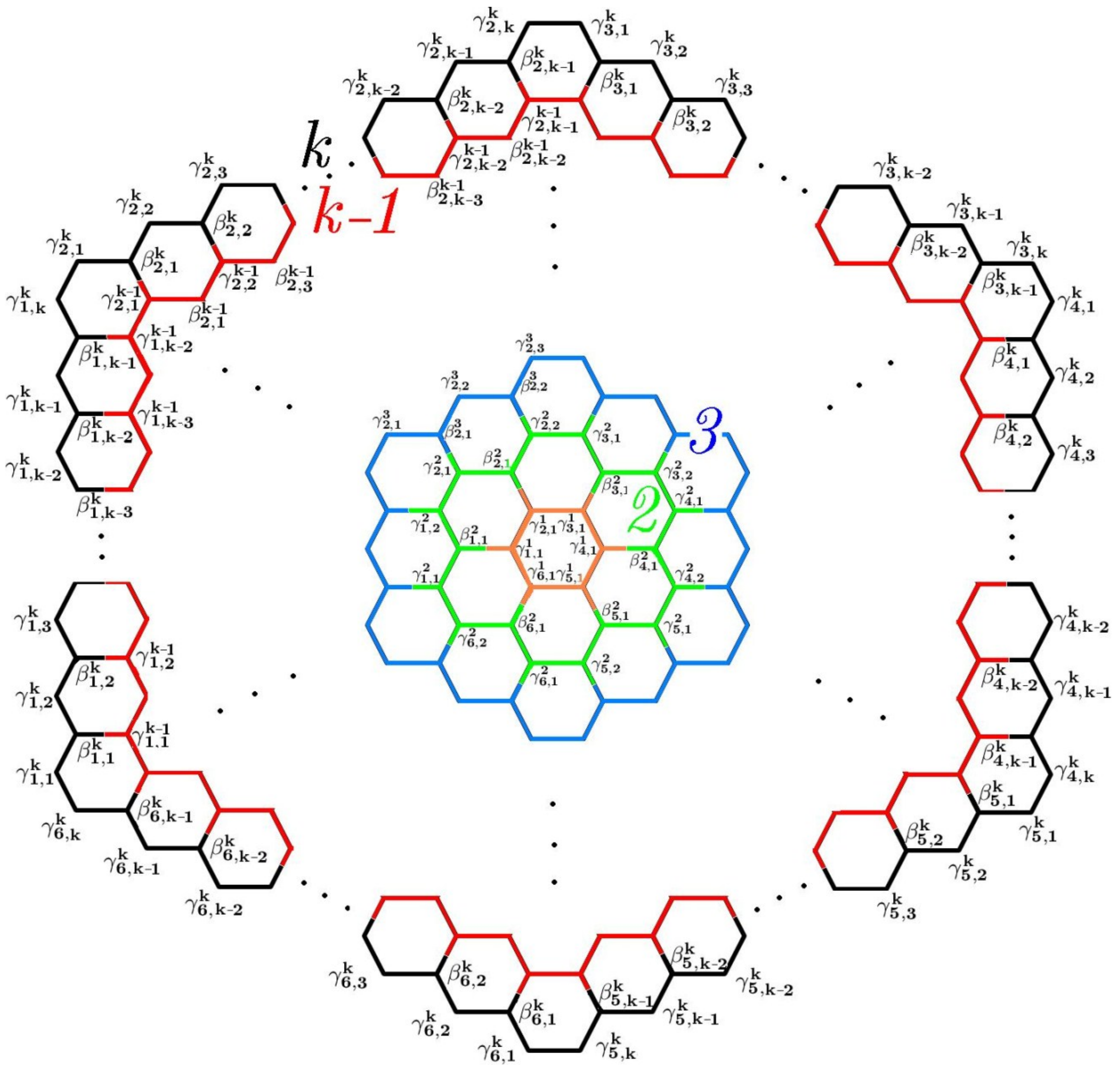

Figure 2. The general representation of Circumcoronene Homologous Series of Benzenoid H_k ($k \geq 1$) [18-26].

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

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

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

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 ($k \geq 1$).*

References

[1] H. Wiener, *J. Am. Chem. Soc.* 69(1) (1947) 17-20.

[2] I. Gutman, N. Trinajstić, *Chem. Phys. Lett.* 17 (1972) 535-538.

[3] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Weinheim, Wiley-VCH, (2000).

[4] V. Sharma, R. Goswami, A. K. Madan, *J. Chem. Inf. Comput. Sci.* 37 (1997) 273-282.

[5] S. Gupta, M. Singh, A. K. Madan, *J. Mol. Graph. Model.* 18 (2000) 18-25.

[6] S. Gupta, M. Singh, A. K. Madan, *J. Math. Anal. Appl.* 266 (2002) 259-268.

[7] A.R. Ashrafi, M. Ghorbani, M. Hemmasi, *Digest. J. Nanomater. Bios.* 4(3) (2009) 483-486.

[8] S. Alikhani, M. A. Iranmanesh, *Digest. J. Nanomater. Bios.* 6(1) (2011) 253-257.

[9] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, New York, (1986).

[10] M. A. Johnson, G. M. Maggiora, *Concepts and Applications of Molecular Similarity*, Wiley Interscience, New York, (1990).

[11] M. Ghorbani, M. Ghazi, *Digest. J. Nanomater. Bios.* 5(4) (2010) 1107-1111.

[12] V. Kumar, S. Sardana, A. K. Madan, *J. Mol. Model.* 10 (2004) 399-407.

[13] M. Fischermann, A. Homann, D. Rautenbach, L. A. Szekely, L. Volkmann, *Discrete Appl. Math.* 122 (2002) 127-137.

[14] S. Sardana, A. K. Madan, *MATCH Commun. Math. Comput. Chem.* 43 (2001) 85-89.

[15] A. R. Ashrafi, M. Ghorbani, M. Jalali, *Optoelectron. Adv. Mater.-Rapid Comm.* 3 (2009) 823-826.

[16] H. Dureja, A. K. Madan, *Med. Chem. Res.* 16 (2007) 331–341.

[17] Z. Yar Ahmadi, *Iran. J. Math. Chem*, 1(2) (2010) 105-110.

[18] M. R. Farahani. *Annals of West University of Timisoara-Mathematics and Computer Science* 51(2) (2013) 29-37.

[19] M. R. Farahani. *Journal of Advances in Physics* 2(1) (2013) 48-52.

[20] M. R. Farahani. *Int. J. Chem. Model.* 6(1) (2014).

[21] M. R. Farahani, *Journal of Chemica Acta* 2 (2013) 22-25.

[22] M. R. Farahani, *World Applied Sciences Journal* 21(9) (2013) 1260-1265.

[23] M. R. Farahani, Two New Version of Zagreb Index of Circumcoronene Series of Benzenoid. *Int. J. Computational Sciences & Applications.* (2013) In press.

[24] M. R. Farahani, *Chemical Physics Research Journal* 6(1) (2013) 27-33.

[25] M. R. Farahani, *Journal of Chemica Acta* 2 (2013) 26-31.

[26] M. R. Farahani, *Journal of Mathematical Nanoscience* 2(1) (2012) 15-20.

[27] S. Klavžar, I. Gutman, B. Mohar, *J. Chem. Int Comput. Sci.* 35 (1995) 590-593.

[28] V. Chepoi, S. Klavžar, Distances in benzenoid systems: Further developments. *Discrete Mathematics* 192 (1998) 27-39.

[29] P. Zigert, S. Klavžar, I. Gutman, *ACH Models Chem.* 137 (2000) 83-94.

[30] A. Soncini, E. Steiner, P. W. Fowler, R. W. A. Havenith, L. W. Jenneskens, *Chem. Eur. J.* 9 (2003) 2974-2981.

[31] P. E. John, P. V. Khadikar, J. Singh, *J. Math. Chem.* 42(1) (2007) 27-45.

[32] S. Klavžar, *MATCH Commun. Math. Comput. Chem.* 60 (2008) 255-274.

[33] M. R. Farahani, M. P. Vlad, *Studia Univ. Babes-Bolyai, Chemia.* 57(4) (2012).

[34] M. R. Farahani, *J. Applied Mathe. & Informatics.* 31(3) (2013).

[35] M. R. Farahani, *Int. J. Chem. Model.* 6(1) (2014).

[36] M. R. Farahani, *International Letters of Chemistry, Physics and Astronomy* 11(1) (2014) 74-80.

[37] M. R. Farahani, *International Letters of Chemistry, Physics and Astronomy* 12 (2014) 56-62.

[38] M. R. Farahani, *International Letters of Chemistry, Physics and Astronomy* 12 (2014) 63-68.

(Received 04 April 2014; accepted 12 April 2014)