NEW FRONT. CHEM. (**2015**)
Volume 24, Number 2, pp. 137-143
ISSN 2393-2171; ISSN-L 2393-2171

Former: Ann. West Univ. Timisoara – Series Chem.
ISSN: 1224-9513

Research Article

AUGMENTED ECCENTRIC CONNECTIVITY INDEX OF POLYCYCLIC AROMATIC HYDROCARBONS (PAH_K)

Mohammad Reza Farahani(♣)[1], Hafiz Mutee Rehman[2], Muhammad Kamran Jamil[3], Dae-Won Lee[4]

[1]Department of Applied Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran.
[2]Department of Mathematics & Statistics, The University of Lahore, Lahore Pakistan.
[3]Department of Mathematics, Riphah Institute of Computing and Applied Sciences (RICAS), Riphah International University, Lahore, Pakistan.
[4]Independent Scholar, Republic of Korea.

ABSTRACT

Let G be a molecular graph in which the set of vertices represents the atoms and the set of edges corresponds to the bonds. The *Eccentric Connectivity index ξ(G)* is equal to $\xi(G)=\sum_{u\in V(G)} d_u \times \varepsilon(u)$, where $\varepsilon(u)$ referred as the length of a maximal path connecting a vertex u to another vertex of G and d_u referred as the degree of the vertex u. The Augmented eccentric connectivity index of a connected graph G is defined as ${}^{A}\xi(G)=\sum_{v\in V(G)} \frac{M(u)}{\varepsilon(u)}$, where $M(u)$ denotes the product of degrees of all neighborhood of vertex u. In this paper, the augmented eccentric connectivity index for Polycyclic Aromatic hydrocarbons (PAH_k) has been computed.

Keywords: Molecular graph, Eccentric connectivity index, augmented eccentric connectivity index, Polycyclic Aromatic hydrocarbons (PAH_k).

♣ Correspondent author: Tel: +98-919-247-8265, E-mails: Mr_Farahani@Mathdep.iust.ac.ir & MrFarahani88@gmail.com
rehman.mutee@yahoo.com, m.kamran.sms@gmail.com, haverd2001@gmail.com

1. INTRODUCTION

Let G be a molecular graph in which the vertex and the edge sets are represented by V(G) and E(G), respectively, the vertices of the graph represents the atoms of molecules and the edges corresponds to the chemical bond. Let d_u denote the degree of a vertex in G. If $d_u = 1$ then *u* is said to be a pendent vertex. For two vertices *u,v,* $d(u,v)$ defines the length of the shortest path connecting *u* and *v*. The eccentricity of a vertex *u* is defined to be

$$ecc(u) = \max \{ d(v,u) : v \in V(G) \}.$$

A topological index TI is a number that is invariant under the Aut(G). A variety of TIs have been proposed for characterization of chemical structures and used for structure property correlations in QSPR models [1-3]. The eccentric connectivity index of a graph G was proposed by Sharma, Goswami and Madan [4]. A generalization of eccentric connectivity index, known as augmented eccentric connectivity index of a graph G was proposed by Dureja and Madan [5], also the eccentric connectivity index for an infinite family of linear Polycene parallelogram Benzenoid P(n,n) ($\forall$n≥1) was computed in [6] while MEC index for the same structure was computed in [7] and the Ediz eccentric connectivity index of P (n, n) was computed in [9].

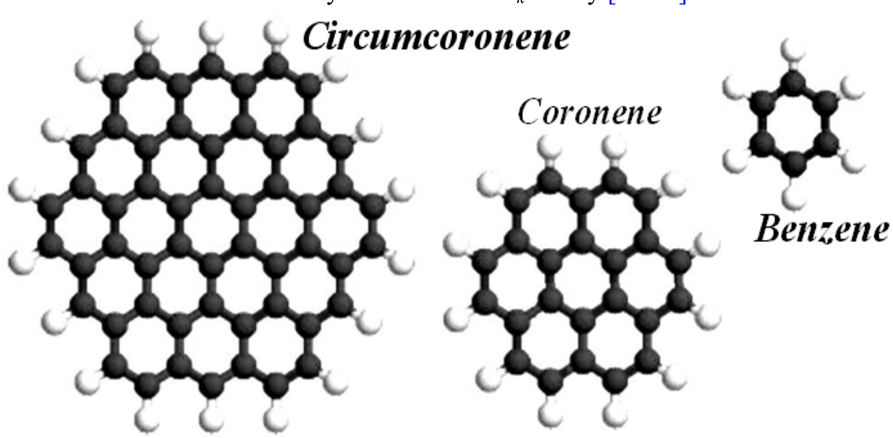
Polycyclic Aromatic hydrocarbons considered here is a family of hydrocarbons which contains several copies of benzene C_6 and play an important role in graphitization of organic materials [10]. For structural detail and tuning of molecular properties toward specific application one can consult [11-17]. See some properties and some useful information about this family readers are encourage to see [18-27].

The first famous members of this hydrocarbon family (PAH family) are denoted and shown as follow

PAHk is structured as:

- For *k=1* we have *Benzene* with six carbon (C) and six hydrogen (H) atoms,
- For *k=2*, *Coronene* with 24 carbon and twelve hydrogen atoms,
- For *k=3 Circumcoronene* with 54 carbon and eighteen hydrogen atoms.

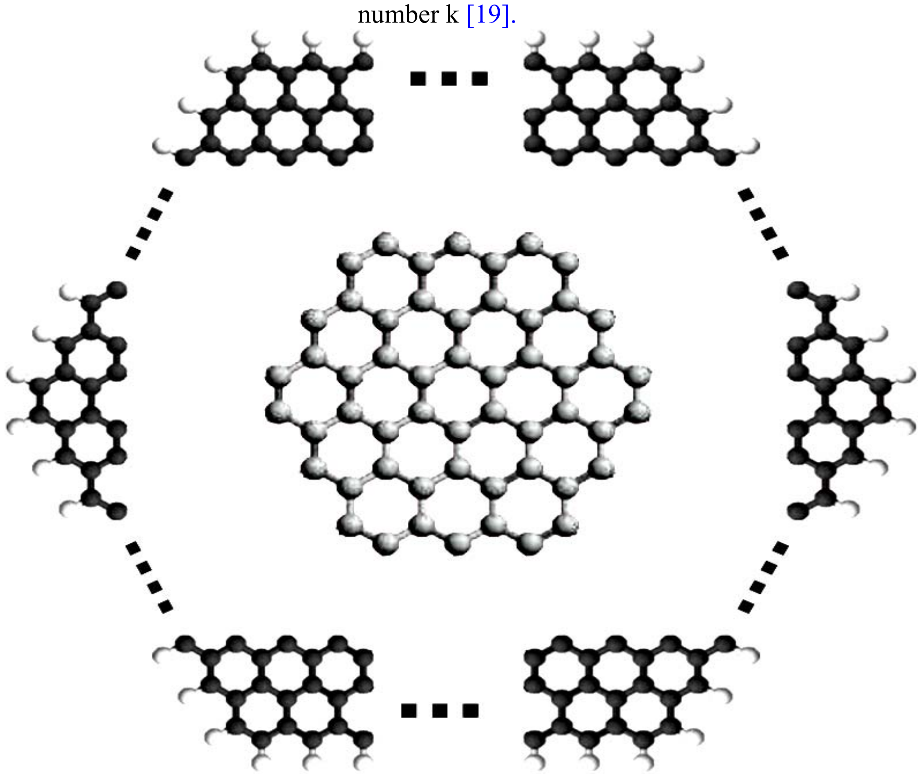
Figure 1: The some first members Benzene, Coronene, Circumcoronene of the Polycyclic Aromatic Hydrocarbons PAH_k family [18-27].



2. RESULTS AND DISCUSSION

In this section, we computed the augmented eccentric connectivity index of polycyclic aromatic hydrocarbons (PAH_k). The PAH_k can be thought as small pieces of graphene sheets with the free valences of the dangling bonds saturated by *H.* A graphene sheet can be interpreted as an infinite PAH molecule. Successful utilization of PAH molecules in modeling graphite surfaces has been reported earlier. Figure 2 represent the general representation of polycyclic aromatic hydrocarbons (PAH_k).

Figure 2: The general representation of polycyclic aromatic hydrocarbon PAH_k for all integer number k [19].



Theorem 1: The Augmented Eccentric Connectivity index of PAH_k is

$$^{A}\xi(G) = \frac{1980k^2 + 261k - 27}{(4k-1)(8k+2)} + \sum_{i=1}^{k-1} \frac{162i\,(4k+4i-1)}{4i^2 + (4i+1)2k - 2i}$$

***Proof**:* Consider the general representation of PAHs having $6n^2$ carbons and $6n$ hydrogen atoms We use *Ring cut method* for Circumcoronene homologous series of Benzenoid and denote all vertices of degree three of PAH_n by β and γ and all vertices of degree one by α are:

$$V(PAH_n) = \{\alpha_{z,l}\ ,\ \beta^{i}_{z,l}\ ,\ \gamma^{i}_{z,j}\ : l = 1,\dots,k,\ j \in Z_i\ ,\ l \in Z_{i-1}\ \&\ z \in Z_6\}$$

See Figure 3, where $Z_i = \{1, 2, ..., i\}$ is the cyclic finite group of order *i*.

We divide the all the vertices such that i^{th} ring-cut consist of vertices $\beta^i_{z,j}\ \gamma^i_{z,j}\ (\forall i = 1, ..., k; z \in Z_6\ ,\ j \in Z_i)$ and size of the ring cut is $6i + 6(i-1)$, the common property of a ring cut is their farthest vertices also $d(\gamma^i_{z,j}, \gamma^k_{z,j}) = d(\beta^i_{z,j}) = 2(k-i)$. By ring cuts of PAH_n we have the following eccentricities [27-30] of the corresponding vertices i.e

i. $\varepsilon(\beta^i_{z,j}) = d(\beta^i_{z,j}, \beta^i_{z+3,j}) + d(\beta^i_{z+3,j}, \gamma^k_{z+3,j}) + d(\gamma^k_{z+3,j}, \alpha_{z+3,j}) = 2k + 2i - 1$

For all vertices $\beta^i_{z,j}$ of PAH_k $(\forall i = 1,...,k;\ z \in Z_6;\ \ j \in Z_{i-1})$

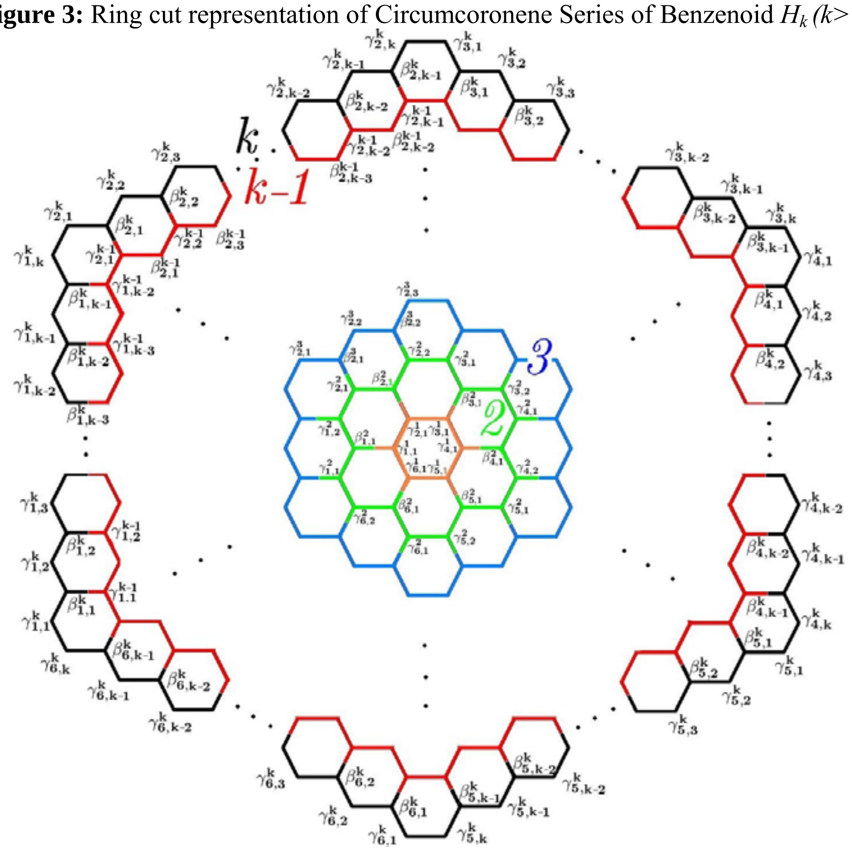
ii. $\varepsilon(\gamma^i_{z,j}) = d(\gamma^i_{z,j}, \gamma^i_{z+3,j}) + d(\gamma^i_{z+3,j}, \gamma^k_{z+3,j}) + d(\gamma^k_{z+3,j}, \alpha_{z+3,j}) = 2(k+i)$

For all vertices $\gamma^i_{z,j}$ of PAH_k $(\forall i = 1,...,k;\ z \in Z_6;\ \ j \in Z_{i-1})$

iii. $\varepsilon(\alpha_{z,j}) = d(\gamma^i_{z,j}, \gamma^i_{z+3,j}) + d(\gamma^i_{z+3,j}, \gamma^k_{z+3,j}) + d(\gamma^k_{z+3,j}, \alpha_{z+3,j}) = 4k + 1$

For all vertices $\alpha_{z,j}$ (hydrogen atoms) of PAH_k $(\forall j = 1,...,k;\ z = 1,...,6$

Figure 3: Ring cut representation of Circumcoronene Series of Benzenoid H_k *(k>1)*.



and compute *M (u)* for every vertex *u* of PAH_n as under:

1. $\forall j \in Z_k, \forall z \in Z_6;\ M(\gamma^k_{z,j}) = 3\times 3\times 1 = 9$; since $\forall \gamma^k_{z,j}; d_{\beta^k_{z,j-1}} = d_{\beta^k_{z,j}} = 3$ and $d_{\alpha_{z,j}} = 1$
2. $\forall j \in Z_{k-1}, \forall z \in Z_6;\ M(\beta^k_{z,j}) = 3\times 3\times 3 = 27$; since $\forall \beta^k_{z,j}; d_{\gamma^k_{z,j+1}} = d_{\gamma^k_{z,j}} = 3$ and $d_{\beta^{k-1}_{z,j}} = 3$
3. $\forall j \in Z_i,, i \in Z_k,\ \forall z \in Z_6;\ M(\beta^i_{z,j}) = M(\gamma^i_{z,j}) = 3\times 3\times 3 = 27$; and $d_u = 3$ since $\forall u \in V(H_k) - \{\gamma^k_{z,j} : j \in Z_i, \forall z \in Z_6\}$
4. $\forall j \in Z_k,\ \forall z \in Z_6;\ M(\alpha_{z,j}) = 3$; since $\forall \gamma^k_{z,j}\ \ d_{\gamma^k_{z,j}} = 3$

It is obvious that all vertices in (1&2) are considered from the i^{th} ring-cut and vertices in (3) are from ring-cuts $1,...,i-1$. Therefore the AECI of PAH_n is

$$
\begin{aligned}
{}^A\xi(PAH_n) &= \sum_{u\in V(PAH_n)} \frac{M(u)}{\varepsilon(u)},\\
&= \sum_{\gamma^k_{z,j}} \frac{M(\gamma^k_{z,j})}{\varepsilon(\gamma^k_{z,j})} + \sum_{\beta^i_{z,j}} \frac{M(\beta^i_{z,j})}{\varepsilon(\beta^i_{z,j})} + \sum_{\gamma^{ik}_{z,j}\in(PAH_{k-1})} \frac{M(\gamma^i_{z,j})}{\varepsilon(\gamma^i_{z,j})} + \sum_{\alpha_{z,j}} \frac{M(\alpha_{z,j})}{\varepsilon(\alpha_{z,j})}\\
&= \sum_{\gamma^k_{z,j}} \frac{9}{4k} + \sum_{i=1}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6} \frac{27}{2k+2i-1} + \sum_{i=1}^{k-1}\sum_{j=1}^{i}\sum_{z=1}^{6} \frac{27}{2(k+i)} + \sum_{\alpha_{z,j}} \frac{3}{4k+1}\\
&= 6k.\frac{9}{4k} + 6k.\frac{3}{4k+1} + \left[\sum_{i=1}^{k-1} \frac{162i(4k+4i-1)}{4i^2+(8i+2)k-2i} + \frac{162k}{4k-1}\right]\\
&= \frac{171k+27}{8k+2} + \frac{162k}{4k-1} + \left[\sum_{i=1}^{k-1} \frac{162i(4k+4i-1)}{4i^2+(8i+2)k-2i} + \frac{162k}{4k-1}\right]\\
&= \frac{1980k^2+261k-27}{(4k-1)(8k+2)} + \sum_{i=1}^{k-1} \frac{162i(4k+4i-1)}{4i^2+(8i+2)k-2i}
\end{aligned}
$$

which completes the proof. ■

Example 1: The Augmented eccentric connectivity index ${}^A\xi(PAH_2)$ is

$$
\begin{aligned}
{}^A\xi(PAH_2) &= \sum_{u\in V(PAH_2)} \frac{M(u)}{\varepsilon(u)},\\
&= \sum_{\gamma^k_{z,j}} \frac{M(\gamma^2_{z,j})}{\varepsilon(\gamma^2_{z,j})} + \sum_{\beta^i_{z,j}} \frac{M(\beta^2_{z,1})}{\varepsilon(\beta^2_{z,1})} + \sum_{\gamma^{ik}_{z,j}\in(PAH_{k-1})} \frac{M(\gamma^2_{z,j})}{\varepsilon(\gamma^2_{z,j})} + \sum_{\alpha_{z,j}} \frac{M(\alpha_{z,j})}{\varepsilon(\alpha_{z,j})}\\
&= 12\left(\frac{9}{8}\right) + 6\left(\frac{27}{5}\right) + 6\left(\frac{27}{6}\right) + 12\left(\frac{3}{9}\right) = 76.9 .
\end{aligned}
$$

4. CONCLUSION

In this paper an augmented eccentric connectivity index for polycyclic Aromatic hydrocarbons is computed. These types of graphs are the generalization of C_6 which is frequently used in chemistry physics and Nanoscience and is very useful to synthesize the aromatic compounds.

REFERENCES

1. I. Gutman, N. Trinajstić, Chem. Phys. Lett. 17, (1972), 535.
2. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals, Chem. Phys. Lett.17, 535-538 (1972).
3. R. Todeschini, V Consonni, Hand book of Molecular descriptors, Weinheim, Wiley-VCH, (2000)
4. D.E. Needham I.C. Wei and P.G. Seybold, Molecular modeling of the Physical properties of Alkanes. J.Am. Chem. Soc. 110, 4186-4194. (1988)
5. V. Sharma, R. Goswami and A.K. Mada. Eccentric connectivity index: A novel highly discriminating topological descriptor for structure property and structure activity studies, J. Chem. Inf. Comput. Sci., vol. 37, pp.273-282, 1997.
6. H. Dureja and A. K. Madan, Super augmented eccentric connectivity indices; new
7. generation highly discriminating topological descriptors for QSAR/ QSPR Modeling, Med. Chem. Res., vol. 16, pp. 331-341, 2007.
8. M. Alaeiyan, R. Mojarad, J. Asadpour. A new method for computing eccentric connectivity polynomial of an infinite family of linear Polycene parallelogram Benzenoid. Optoelectron. Adv. Mater.-Rapid Commun. 2011, 5(7), 761 -763.
9. M. Alaeiyan and J. Asadpour. Computing the MEC polynomial of an infinite family of the logram P(n,n). Optoelectron. Adv. Mater.-Rapid Commun. 2012, 6(1-2), 191-193.
10. M.R. Farahani. Connective Eccentric Index of Linear Parallelogram P(n,n). Int. Letters of
11. Chemistry, Physics and Astronomy 18, (2014), 57-62.
12. M.R. Farahani, M. K. Jamil, M.R. Rajesh Kanna, S. Hosamani. About the Ediz Eccentric connectivity index of Linear Polycene Parallelogram Benzenoid. International Journal of Scientific & Engineering Research, 7, 2016, In press.
13. U.E. Wiersum, L.W. Jenneskens. Gas Phase Reactions in Organic Synthesis, (Ed.: Y. Valle. e), Gordon and Breach Science Publishers, Amsterdam. The Netherlands, 1997, 143–194.
14. A.J. Berresheim, M. Muller, K.Mullen, Chem. Rev. 1999, 99, 1747–1785.
15. C.W. Bauschlicher, Jr, E.L.O. Bakes, Chem. Phys. 2000, 262, 285-291
16. A.M. Craats, J.M. Warman, K.Mullen, Y. Geerts, J. D. Brand, Adv. Mater. 1998, 10, 36-38.
17. M. Wagner, K. Mullen, Carbon 1998, 36, 833- 837
18. F. Dtz, J.D. Brand, S. Ito, L. Ghergel, K. Mullen, J. Am. Chem. Soc. 2000, 122, 7707-7717
19. K. Yoshimura, L. Przybilla, S. Ito, J.D. Brand, M. Wehmeir, H. J.Rder, K. M. llen, Macromol. Chem. Phys. 2001, 202, 215-222.
20. A. Soncini, E. Steiner, P.W. Fowler, R.W. A. Havenith and L.W. Jenneskens. Manuscript

21. M.R. Farahani. Some Connectivity index of Polycyclic Aromatic Hydrocarbons. Advances in Materials and Corrosion. 1(2) (2013) 65-69.
22. M.R. Farahani. Zagreb Indices and Zagreb Polynomials of Polycyclic Aromatic Hydrocarbons PAHs. Journal of Chemica Acta. 2(1) (2013) 70-72.
23. M.R. Farahani. Computing Theta Polynomial and Theta Index of V-phenylenic Planar, Nanotubes and Nanotori. Int. J. Theoretical Chemistry. 1(2) (2013) 09-16.
24. M.R. Farahani. Schultz and Modified Schultz Polynomials of Coronene Polycyclic Aromatic Hydrocarbons. Letters of Chemistry, Physics and Astronomy. 2014, 13(1), 1-10.
25. M.R. Farahani and W. Gao. On Multiple Zagreb indices of Polycyclic Aromatic Hydrocarbons PAH. Journal of Chemical and Pharmaceutical Research. 2015, 7(10), 535-539.
26. M.R. Farahani and M.R. Rajesh Kanna. The Pi polynomial and the Pi Index of a family Hydrocarbons Molecules. Journal of Chemical and Pharmaceutical Research. 2015, 7(11), 253-257.
27. W. Gao and M.R. Farahani. Theta polynomial Θ(G,x) and Theta index Θ(G) of Polycyclic Aromatic Hydrocarbons PAHk. Journal of Advances in Chemistry. 2015, 12(1), 3934-3939.
28. M.R. Farahani. Eccentricity Version of Atom-Bond Connectivity Index of Benzenoid Family ABC5(Hk). World Applied Sciences Journal, 21(9) (2013) 1260-1265.
29. M.R. Farahani. Computing Eccentricity Connectivity Polynomial of Circumcoronene Series of Benzenoid Hk by Ring-Cut Method. Annals of West University of Timisoara-Mathematics and Computer Science. 51(2) (2013) 29–37.
30. M.R. Farahani. A New Version of Zagreb Index of Circumcoronene Series of Benzenoid. New. Front. Chem. (2014) 23(2) 141-147.