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Research Article

The Ediz Eccentric Connectivity Index of Polycyclic Aromatic Hydrocarbons PAH_k

Dae-Won Lee[1], Muhammad K. Jamil[2], Mohammad R. Farahani[3]*, Hafiz M. Rehman[4]
[1]Independent Scholar, Republic of Korea.
[2]Department of Mathematics, Riphah Institute of Computing and Applied Sciences (RICAS), Riphah International University, Lahore, Pakistan.
[3]Department of Applied Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran.
[4]Department of Mathematics & Statistics, The University of Lahore, Lahore Pakistan.

***Corresponding author**
Mohammad R. Farahani
Email: mrfarahani88@gmail.com

Abstract: Let $G=(V, E)$ be molecular graph in which the set of vertices and the set of edges of the graph correspond to the atoms of the molecule and chemical bonds, respectively. The *Ediz eccentric connectivity index* $^E\xi^c(G)$ of G is defined as $\sum_{v\in V(G)}\frac{S(v)}{\varepsilon(v)}$, where $S(v)$ is the sum of degrees of all vertices adjacent to vertex v, and $\varepsilon(v)$ is the eccentricity of v. In this paper, we compute the Ediz eccentric connectivity index of Polycyclic Aromatic Hydrocarbons PAH_k.
Keywords: Molecular graph, Eccentricity, Ediz eccentric connectivity Index, Polycyclic Aromatic Hydrocarbons (PAH_k).

INTRODUCTION

Chemical graph theory is a branch of mathematical chemistry which is used to predict the behavior of chemical structure specifically carbon nanostructure have significant attention due to have many applications in chemi-informatics. Recently a new topological index *eccentric connectivity index* has been determined which have high predictability of pharmaceutical properties. One can see [1-4] for some properties and consult [7-11] for some applications.

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. We denote $d(u,v)$ the distance between u and v i. e the length of the shortest path connecting u and v. The eccentricity of a vertex in $V(G)$ is defined to be $ecc(v)=\{\max d(u,v)\ ;\ u\in V(G)\}$.

Different topological indices are introduced so far. The Wiener index is the oldest index defined to be

$$W(G)=\sum_{\{u,v\}\in V(G)} d(u,v)$$

More recently the eccentric connectivity index is defined [9] to be

$$\xi^c(G)=\sum_{v\in V(G)}\deg(v).\ ecc(v)$$

while the modified eccentric connectivity index of G is defined in [12]. The diameter of the graph is maximum eccentricity among vertices of G [13-16].

Also the Ediz eccentric connectivity index is defined to be the summation of the quotient of the sum of the adjacent vertices degrees and eccentricity of the concerned vertex i. e

$$^E\xi^c(G)=\sum_{v\in V(G)}\frac{S(v)}{\varepsilon(v)},$$

PAH_k Considered here is a family of such hydrocarbons containing several copies of benzene on circumference and are ubiquitous products. Poly-aromatic hydrocarbons can be pictured as a small piece of graphene sheets with the free valances of dangling bond saturated by *H*, vice versa which can be interpreted as an infinite *PAH* molecule. These types of molecules have utilization in modeling graphite surface [19-25].

RESULT AND DISCUSSION

In general consider polycyclic Aromatic hydrocarbons PAH_k depicted in Figure 1. This graph has $6n^2$ carbons and $6n$ hydrogen atoms. To compute the Ediz eccentric connectivity index *Ring cut method* for Circumcoronene homologous series of Benzenoid is used.

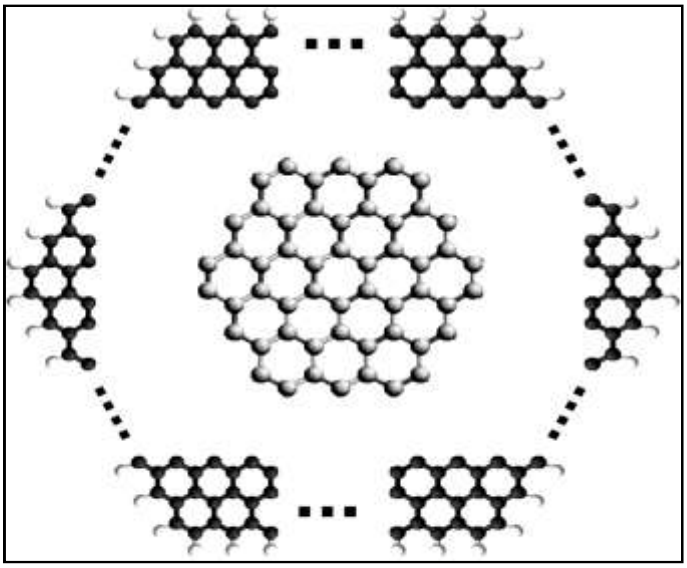

Fig. 1: The general representation of polycyclic aromatic hydrocarbon PAH_k for all integer number *k* [18]

We denote all vertices of degree three of PAH_n by β and γ and all vertices of degree one by α given below (Figure 2):

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

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

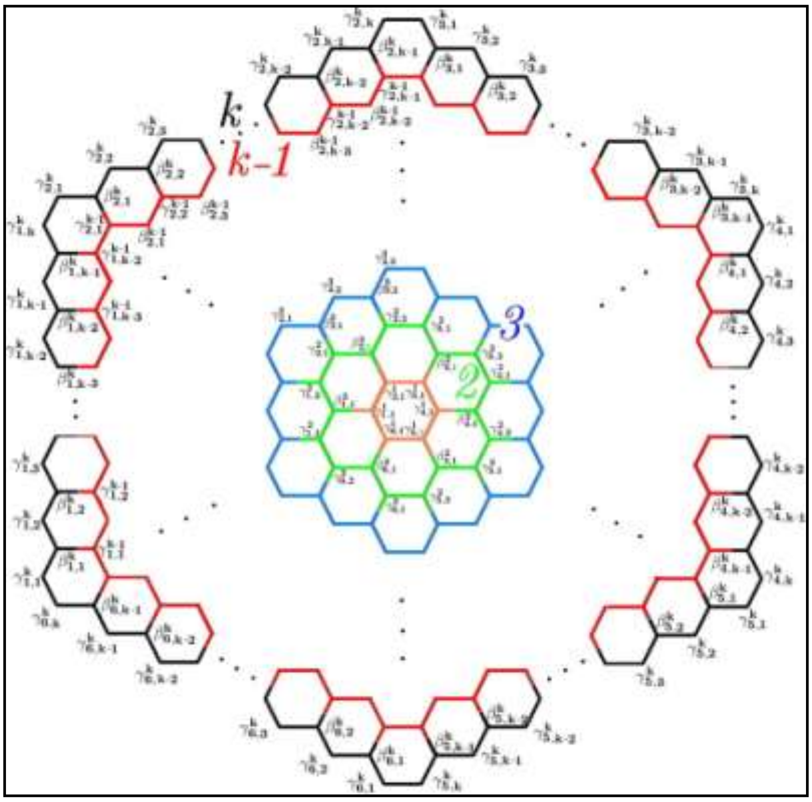

Fig. 2: A general representation of vertices of Circumcoronene Series of Benzenoid H_k with ring cut

We break all the vertices by ring cut such that i^{th} ring-cut consist of vertices $\beta^i_{z,j}\ \gamma^i_{z,j}\ \ (\forall i=1,\dots,k; z\in Z_6\ ,\ j\in Z_i)$ and its size is $6i+6(i-1)$, the common property of a ring cut is their farthest vertices also note that $d(\gamma^i_{z,j}\ ,\ \gamma^k_{z,j})=d(\beta^i_{z,j})=2(k-i).$

From Figure 2, it can be seen that we have two types of $\beta^i_{z,j}$ which is connected inside with $\gamma^i_{z,j}$ as well as $\gamma^k_{z+3,j}$ such that the eccentricity of $\beta^i_{z,j}$ is $2k+2i-1$ and the sum of all degrees of its neighborhood is 9. Also we have $\gamma^i_{z+3,j},\gamma^k_{z+3,j}$ with maximum eccentricity *2(k+i)* and *4k* (respectively) such that the sum of degrees of neighborhood of $\gamma^i_{z+3,j},\gamma^k_{z+3,j}$ are 9 and 7 respectively. The remaining vertex $\alpha_{z+3,j}$ whose degree is one and its neighborhood has degree 3 with eccentricity *4k+1*.

From above calculation we now find the AECI of PAH_k is

$$
\begin{aligned}
{}^{A}\xi(PAH_k) &= \sum_{u\in V(PAH_k)}\frac{S(u)}{\varepsilon(u)}, \\
&= \sum_{\gamma^k_{z,j}}\frac{S(\gamma^k_{z,j})}{\varepsilon(\gamma^k_{z,j})}+\sum_{\beta^i_{z,j}}\frac{S(\beta^i_{z,j})}{\varepsilon(\beta^i_{z,j})}+\sum_{\gamma^{ik}_{z,j}\in(PAH_{k-1})}\frac{S(\gamma^i_{z,j})}{\varepsilon(\gamma^i_{z,j})}+\sum_{\alpha_{z,j}}\frac{S(\alpha_{z,j})}{\varepsilon(\alpha_{z,j})} \\
&= \sum_{\gamma^k_{z,j}}\frac{7}{4k}+\sum_{i=1}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6}\frac{9}{2k+2i-1}+\sum_{i=1}^{k-1}\sum_{j=1}^{i}\sum_{z=1}^{6}\frac{9}{2(k+i)}+\sum_{\alpha_{z,j}}\frac{3}{4k+1} \\
&= \frac{523k^2+72k-21}{(4k-1)(8k+2)}+\sum_{i=1}^{k-1}\frac{54i(4k+4i-1)}{4i^2+(8i+2)k-2i}\ .\blacksquare
\end{aligned}
$$

Now we obtain the following theorem:

Theorem 1: The Ediz Eccentric Connectivity index of PAH_k is

$$^{A}\xi(G)=\frac{523k^2+72k-21}{(4k-1)(8k+2)}+\sum_{i=1}^{k-1}\frac{54i(4k+4i-1)}{4i^2+(8i+2)k-2i}$$

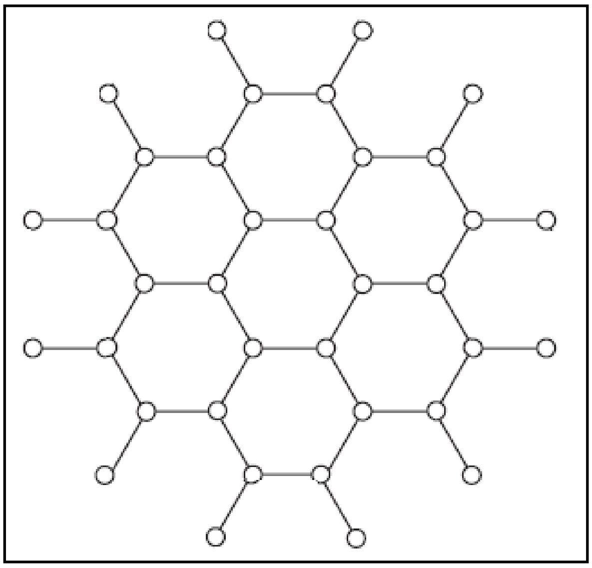

Fig. 3: The polycyclic aromatic hydrocarbon PAH_2

Example 1:

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

$$^{A}\xi(PAH_2)=\sum_{u\in V(PAH_2)}\frac{S(u)}{\varepsilon(u)},$$

$$=\sum_{\gamma_{z,j}^{k}}\frac{S(\gamma_{z,j}^{2})}{\varepsilon(\gamma_{z,j}^{2})}+\sum_{\beta_{z,j}^{i}}\frac{S(\beta_{z,1}^{2})}{\varepsilon(\beta_{z,1}^{2})}+\sum_{\gamma_{z,j}^{ik}\in(PAH_{k-1})}\frac{S(\gamma_{z,j}^{2})}{\varepsilon(\gamma_{z,j}^{2})}+\sum_{\alpha_{z,j}}\frac{S(\alpha_{z,j})}{\varepsilon(\alpha_{z,j})}$$

$$=12\left(\frac{7}{8}\right)+6\left(\frac{27}{5}\right)+6\left(\frac{27}{6}\right)+12\left(\frac{3}{9}\right)$$

$$=73.9\ .\blacksquare$$

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