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ECCENTRICITY ATOM-BOND CONNECTIVITY INDEX OF POLYCYCLIC AROMATIC HYDROCARBON PAH_k

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ABSTRACT: Let *G=(V,E)* be molecular graph with vertex set V (G) and edge set E(G) 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. 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 $\varepsilon(v)=\{\max d(u,v)\,;\,u\in V(G)\}$. Recently, we proposed the fifth atom-bond connectivity index of a simple connected graph G as $ABC_5(G)=\sum_{uv\in E(G)}\sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)\varepsilon(v)}}$. In this paper, we present more study of the fifth atom-bond connectivity index and compute this new index of polycyclic aromatic hydrocarbons.

INTRODUCTION: Mathematical chemistry focuses on mathematically new ideas and concepts developed or adapted for chemistry. Mathematics may be from any of many diverse mathematical areas. The combination of graph theory and chemistry is called *chemical graph theory*. Graph theory is used to mathematically model molecules in order to gain insight into the physical properties of these chemical compounds. Some physical properties, such as the boiling point, are related to the geometric structure of the compound.

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Polycyclic Aromatic Hydrocarbons *(PAH_k)* are organic compounds containing only carbon and hydrogen that are composed of multiple aromatic rings. PAH_k are neutral, nopolar molecules, they are found in fossil fuels, in tar deposits and are produced when insufficient oxygen or other factors result in incomplete combustion of organic matter. Let *G(V,E)* be a graph, where *V* and *E* represent the set of vertices and the set of edges of graph *G*. For vertices $u, v\in V(G)$, the distance between *u* and *v* is the length of the shortest path connecting them and denoted as *d(u,v).*

The eccentricity of the vertex $v, \varepsilon(v)$, is the maximum distance between *v* and any other vertex of the graph. The maximum and minimum eccentricity in the graph is called its diameter and radius, respectively. The degree of the vertex *v*, *d(v)*, is the number of adjacent vertices to *v*. We used the standard notation from chemical graph theory for further details see [1, 2].

In the field of chemical graph theory, a topological index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are used in the development of quantitative structure activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure.

One of the well-known topological indexes is atom bond connectivity (ABC) index, proposed by Estrada [3]. The *ABC* index of a graph *G* is defined as:

$$ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$$

In 2010, Graovac et al. defined a new version of the atom bond connectivity index [4], it is defined as

$$ABC_2(G)=\sum_{uv\in E(G)}\sqrt{\frac{n_u+n_v-2}{n_u n_v}}$$

where n_u is the number of vertices of graph *G* whose distance to the vertex *u* is smaller than the distance to the vertex *v*.

Farahani introduced the third version of atom bond connectivity index [5] and defined as

$$ABC_3(G)=\sum_{e=uv\in E(G)}\sqrt{\frac{m_v+m_u-2}{m_v.m_u}}$$

where m_u is the number of edges of graph *G* whose distance to the vertex *u* is smaller than the distance to the vertex *v*.

In 2010, Ghorbani [6] defined the fourth version of atom-connectivity index and defined it as

$$ABC_4=\sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_u S_v}}$$

where S_u is the sum of degrees of all neighbor of vertex *u* in graph *G*.

Recently, Farahani [7] proposed the eccentric version of atom-bond connectivity index as:

$$ABC_5(G)=\sum_{uv\in E(G)}\sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)\varepsilon(v)}}$$

A lot of research have been done on this family of topological indices, for further history and results we refer [8-22]. In this paper, we computed the fifth version of atom-bond connectivity index of Polycyclic Aromatic Hydrocarbons *(*PAH_k*)*.

Main Result: Polycyclic Aromatic Hydrocarbons (PAH_k) are a group of more than 100 chemicals. First three member of this group are called Benzene, Coronene and Circumcoronene and shown in **Fig. 1**.

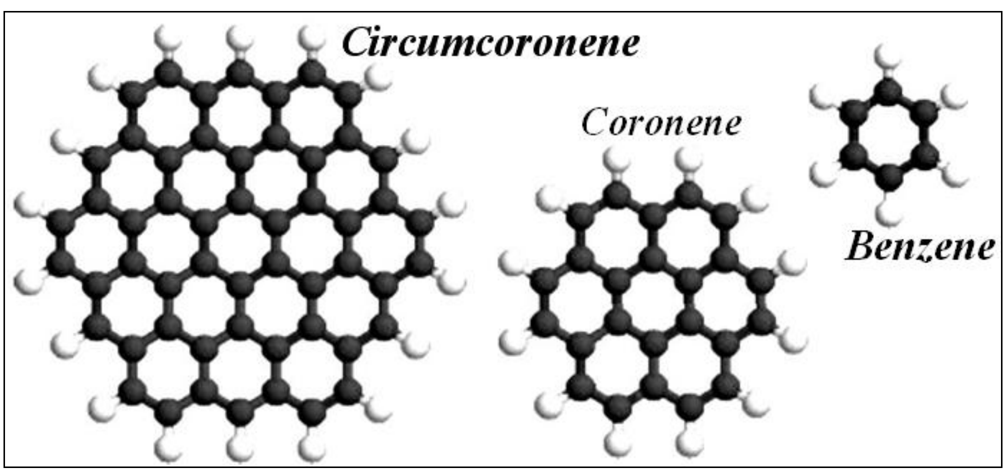

FIG. 1: FIRST THREE MEMBERS OF POLYCYCLIC AROMATIC HYDROCARBONS (PAH_k).

The 2-dimensional lattice of PAH_k has shown in **Fig. 2**. It contains $6k^2+6k$ vertices and $9k^2+3k$ edges. There are many research papers on polycyclic aromatic [23-57].

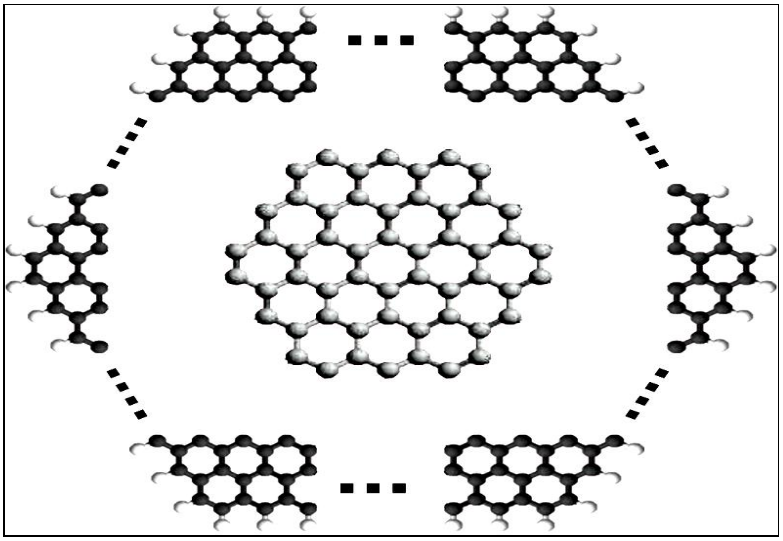

FIG.2: A 2-DIMENSIONAL LATTICE OF POLYCYCLIC AROMATIC HYDROCARBONS (PAH_k).

Theorem: The fifth atom-bond connectivity index of Polycyclic Aromatic Hydrocarbons *(PAH_k)* is equal to:

$$ABC_5(PAH_k)=12(i-1)\sum_{i=2}^{k}\sqrt{\frac{4k+4i-5}{(2k+2i-1)(2k+2i-2)}}+6i\sum_{i=1}^{k}\sqrt{\frac{4k+4i-3}{(2k+2i-1)(2k+2i)}}$$

$$+6\sum_{i=1}^{k}\sqrt{\frac{2(2k+2i-2)}{(2k+2i-1)^2}}+6\sum_{i=1}^{k}\sqrt{\frac{6k+2i-1}{(4k+1)(2k+2i)}}$$

Proof: To obtain our result, we use the Ring cut method [49]. In **Fig. 3**, we apply the ring cuts to the Circumcoroneneseries of Benzenoid.

Clearly, the vertex set is $V(PAH_k)=\{\alpha_{z,l}\ ,\ \beta^i_{z,l}\ ,\ \gamma^i_{z,j}\ : l=1,...,k,\ j\in Z_i,\ l\in Z_{i-1}\ \&\ z\in Z_6\}$, where Z_i = {1,2,…,i}. Also, the edge set is $E(H_k)=\{\gamma^i_{z,j}\beta^i_{z,j},\ \gamma^i_{z,j+1}\beta^i_{z,j},\ \gamma^{i-1}_{z,j}\beta^i_{z,j}$ and $\gamma^i_{z,j}\gamma^i_{z,j+1} | i\in\mathbb{Z}_k\ \&\ j\in\mathbb{Z}_i\ \&\ z\in\mathbb{Z}_6\}$.

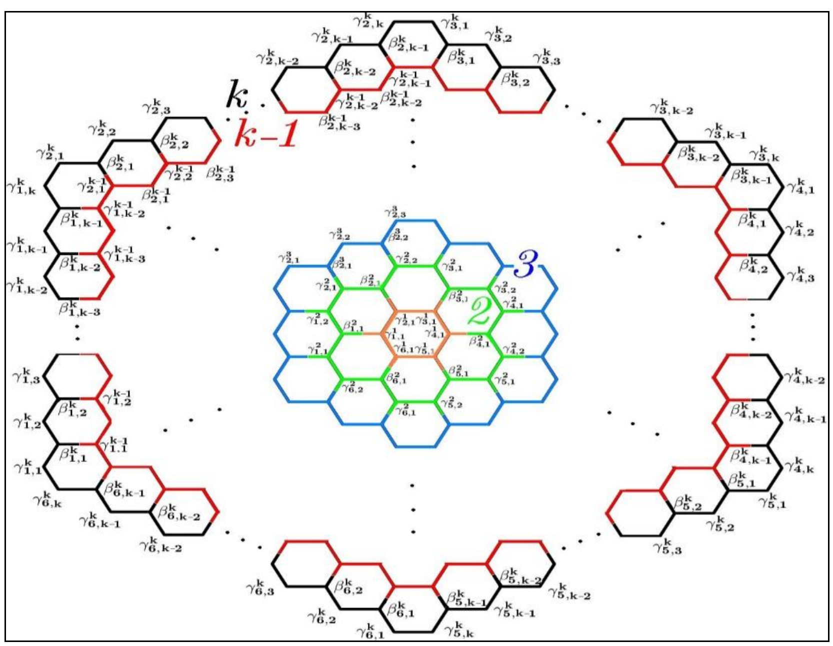

FIG. 3: RING CUT METHOD REPRESENTATION OF POLYCYCLIC AROMATIC HYDROCARBONS (PAH_k).

To obtain the final result we partitions the vertex set and edge set the help of ring cut for illustration see **Fig. 2** [58], we have

- For all vertices $\alpha_{z,j}$ of PAH_k $\left(j \in Z_k, z \in Z_6 \right)$

$$\varepsilon(\alpha_{z,j}) = \underbrace{d(\alpha_{z,j}, \gamma^k_{z,j})}_{1} + \underbrace{d(\gamma^k_{z,j}, \gamma^k_{z',j'})}_{4k-1} + \underbrace{d(\gamma^k_{z',j'}, \alpha_{z',j'})}_{1} = 4k+1$$

- For all vertices $\beta^i_{z,j}$ of PAH_k ($\forall i=1,..,k;\ z \in \mathbb{Z}_6,\ j \in \mathbb{Z}_{i-1}$

$$\varepsilon(\beta^i_{z,j}) = \underbrace{d(\beta^i_{z,j}, \beta^i_{z+3,j})}_{4i-3} + \underbrace{d(\beta^i_{z+3,j}, \gamma^k_{z+3,j})}_{2(k-i)+1} + \underbrace{d(\gamma^k_{z+3,j}, \alpha_{z+3,j})}_{1} = 2k+2i-1$$

- For all vertices $\gamma^i_{z,j}$ of PAH_k ($\forall i=1,..,k;\ z \in \mathbb{Z}_6,\ j \in \mathbb{Z}_i$)

$$\varepsilon(\gamma^i_{z,j}) = \underbrace{d(\gamma^i_{z,j}, \gamma^i_{z+3,j})}_{4i-1} + \underbrace{d(\gamma^i_{z+3,j}, \gamma^k_{z+3,j})}_{2(k-i)} + \underbrace{d(\gamma^k_{z+3,j}, \alpha_{z+3,j})}_{1} = 2(k+i)$$

From above calculation we have the following:

$$ABC_5(G) = \sum_{uv \in E(G)} \sqrt{\frac{\varepsilon(u) + \varepsilon(v) - 2}{\varepsilon(u)\varepsilon(v)}}$$

$$= \left(\sum_{\beta^i_{z,j}\gamma^i_{z,j} \in \mathrm{E}(PAH_k)} \sqrt{\frac{\varepsilon(\beta^i_{z,j}) + \varepsilon(\gamma^i_{z,j}) - 2}{\varepsilon(\beta^i_{z,j})\varepsilon(\gamma^i_{z,j})}} \right) + \left(\sum_{\beta^i_{z,j}\gamma^i_{z,j+1} \in \mathrm{E}(PAH_k)} \sqrt{\frac{\varepsilon(\beta^i_{z,j}) + \varepsilon(\gamma^i_{z,j+1}) - 2}{\varepsilon(\beta^i_{z,j})\varepsilon(\gamma^i_{z,j+1})}} \right)$$

$$+ \left(\sum_{\beta^i_{z,j}\gamma^{i-1}_{z,j} \in \mathrm{E}(PAH_k)} \sqrt{\frac{\varepsilon(\beta^{i+1}_{z,j}) + \varepsilon(\gamma^{i-1}_{z,j}) - 2}{\varepsilon(\beta^{i+1}_{z,j})\varepsilon(\gamma^{i-1}_{z,j})}} \right) + \left(\sum_{\gamma^i_{z,i}\gamma^i_{z+1,1} \in \mathrm{E}(PAH_k)} \sqrt{\frac{\varepsilon(\gamma^i_{z,i}) + \varepsilon(\gamma^i_{z+1,1}) - 2}{\varepsilon(\gamma^i_{z,i})\varepsilon(\gamma^i_{z+1,1})}} \right)$$

$$+ \left(\sum_{\alpha_{z,j}\gamma^k_{z,j} \in E(PAH_k)} \sqrt{\frac{\varepsilon(\alpha_{z,j}) + \varepsilon(\gamma^k_{z,j}) - 2}{\varepsilon(\alpha_{z,j})\varepsilon(\gamma^k_{z,j})}} \right)$$

$$= \sum_{z=1}^{6}\sum_{i=2}^{k}\sum_{j=1}^{i} \sqrt{\frac{\varepsilon(\beta^i_{z,j}) + \varepsilon(\gamma^i_{z,j}) - 2}{\varepsilon(\beta^i_{z,j})\varepsilon(\gamma^i_{z,j})}} + \sum_{z=1}^{6}\sum_{i=2}^{k}\sum_{j=1}^{i} \sqrt{\frac{\varepsilon(\beta^i_{z,j}) + \varepsilon(\gamma^i_{z,j+1}) - 2}{\varepsilon(\beta^i_{z,j})\varepsilon(\gamma^i_{z,j+1})}}$$

$$+ \sum_{z=1}^{6}\sum_{i=1}^{k-1}\sum_{j=1}^{i} \sqrt{\frac{\varepsilon(\beta^{i+1}_{z,j}) + \varepsilon(\gamma^{i-1}_{z,j}) - 2}{\varepsilon(\beta^{i+1}_{z,j})\varepsilon(\gamma^{i-1}_{z,j})}} + \sum_{z=1}^{6}\sum_{i=2}^{k} \sqrt{\frac{\varepsilon(\gamma^i_{z,i}) + \varepsilon(\gamma^i_{z+1,1}) - 2}{\varepsilon(\gamma^i_{z,i})\varepsilon(\gamma^i_{z+1,1})}}$$

$$+ \sum_{z=1}^{6}\sum_{i=1}^{k} \sqrt{\frac{\varepsilon(\alpha_{z,j}) + \varepsilon(\gamma^k_{z,j}) - 2}{\varepsilon(\alpha_{z,j})\varepsilon(\gamma^k_{z,j})}}$$

$$= 6(i-1)\sum_{i=2}^{k} \sqrt{\frac{(2k+2i-1) + (2k+2i-2) - 2}{(2k+2i-1)(2k+2i-2)}} + 6(i-1)\sum_{i=2}^{k} \sqrt{\frac{(2k+2i-1) + (2k+2i-2) - 2}{(2k+2i-1)(2k+2i-2)}}$$

$$+6i\sum_{i=1}^{k}\sqrt{\frac{(2k+2i-1)+(2k+2i)-2}{(2k+2i-1)(2k+2i)}}+6\sum_{i=1}^{k}\sqrt{\frac{2(2k+2i-1)-2}{(2k+2i-1)^2}}$$

$$+6\sum_{i=1}^{k}\sqrt{\frac{(4k+1)+(2k+2i)-2}{(4k+1)(2k+2i)}}$$

$$=12(i-1)\sum_{i=2}^{k}\sqrt{\frac{(2k+2i-1)+(2k+2i-2)-2}{(2k+2i-1)(2k+2i-2)}}+$$

$$+6i\sum_{i=1}^{k}\sqrt{\frac{(2k+2i-1)+(2k+2i)-2}{(2k+2i-1)(2k+2i)}}+6\sum_{i=1}^{k}\sqrt{\frac{2(2k+2i-1)-2}{(2k+2i-1)^2}}$$

$$+6\sum_{i=1}^{k}\sqrt{\frac{(4k+1)+(2k+2i)-2}{(4k+1)(2k+2i)}}$$

$$=12(i-1)\sum_{i=2}^{k}\sqrt{\frac{4k+4i-5}{(2k+2i-1)(2k+2i-2)}}+6i\sum_{i=1}^{k}\sqrt{\frac{4k+4i-3}{(2k+2i-1)(2k+2i)}}$$

$$+6\sum_{i=1}^{k}\sqrt{\frac{2(2k+2i-2)}{(2k+2i-1)^2}}+6\sum_{i=1}^{k}\sqrt{\frac{6k+2i-1}{(4k+1)(2k+2i)}}$$

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