COMPUTING EDGE VERSION OF Co-PI INDEX OF POLYCYCLIC AROMATIC HYDROCARBONS (PAHk)

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ABSTRACT

Khadikar and *Ashrafi* proposed the vertex and edge versions of PI index. Recently, *Iranamanesh* and *Farahani* introduced the vertex and edge versions of Co-PI index. The vertex and edge Co-PI index is defined as $Co-PI_v(G) = \sum_{e \in E(G)} |n_u(e|G) - n_v(e|G)|$ and $Co-PI_e(G) = \sum_{e \in E(G)} |m_u(e|G) - m_v(e|G)|$, respectively. In this paper, we compute the edge Co-PI index of *Polycyclic Aromatic Hydrocarbons (PAHk)*.

Keywords: PI indices, Co-PI indices, Polycyclic Aromatic Hydrocarbons.

INTRODUCTION

Let G be a connected graph having vertex set $V(G)$ and edge set $E(G)$. The number of elements in $V(G)$ and $E(G)$ is denoted as $|V(G)|=n$ and $|E(G)|=m|$. The number of vertices attached to a vertex is called its degree. The distance between two vertices is the length of the shortest path connecting them. For an edge $uv \in E(G)$, $n_u(e)$ is the number of vertices closer to the vertex u then the vertex v and $n_v(e)$ is the number of vertices closer to the vertex v then the vertex u. Similarly, $m_u(e)$ is the number of edges closer to the vertex u then the vertex v

and $m_v(e)$ is the number of edges closer to the vertex v then the vertex u.

Chemical graph theory is the topology branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena. In the fields of chemical graph theory, molecular topology and mathematical chemistry, a topological index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound.

In 1947 a chemist *H. Wiener* introduced a distance based topological index known as *Wiener index* [1]. The Wiener index of a graph G is defined as:

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

Where $d(u,v)$ is the distance between the vertices u and v. The Wiener index is one of the oldest and thoroughly studied index, reader can found its history and results in [2-6].

In 2000 *Khadikar* et. al. proposed an important topological index known as the *Padmakar-Ivan* index (PI) [7]. *Ashrafi* et. al. introduced the vertex version of PI index in 2007 [8]. These versions of PI index of a graph G is defined as:

$$PI_e(G) = \sum_{e \in E(G)} \left(m_u(e \mid G) + m_v(e \mid G) \right)$$

$$PI_v(G) = \sum_{e \in E(G)} \left(n_u(e \mid G) + n_v(e \mid G) \right)$$

respectively. Some results on these topological indices are discussed in [9-11]. Recently, two new versions of these indices have been introduced by *A. Iranmanesh et. al.*[12] and *Farahani et. al.* [13]. These new versions are known as *Co-PI$_v$* and *Co-PI$_e$* indices and defined as:

$$Co - PI_v(G) = \sum_{e \in E(G)} \left| n_u(e \mid G) - n_v(e \mid G) \right|$$

$$Co - PI_e(G) = \sum_{e \in E(G)} \left| m_u(e \mid G) - m_v(e \mid G) \right|$$

While computing these indices the edges at equidistance from the vertices u,v are not considered.

Main Results:

Molecule Benzene, *Circumcoronene series(H_k)* and *Polycyclic Aromatic Hydrocarbon (PAH$_k$) (k $\geq$ 1)* is one of the most attracting structures in different fields of sciences especially chemistry, nano sciences and physics. For further results and information of these structures see [14-43]. In this paper, we compute the edge version of co-PI index

of Polycyclic Aromatic Hydrocarbons (PAH$_k$).

In this section, we computed the edge co-PI index of Polycyclic Aromatic Hydrocarbon *(PAH$_k$, k ≥ 1)*. The hydrocarbons molecules "Polycyclic Aromatic Hydrocarbons" is more practical in the chemical and physics and play a role in graphitization of organic materials. Figure 1 shows its first three members. and Figure 2 is its generalization for all appositive integers number *k*. The number of vertices and the number of edges of PAH$_k$ is equal to *$6k^2+6k$* and $9k^2+3k$, respectively.

Theorem: The edge version of co-PI index of Polycyclic Aromatic Hydrocarbons (PAH$_k$, k>0) is equal to
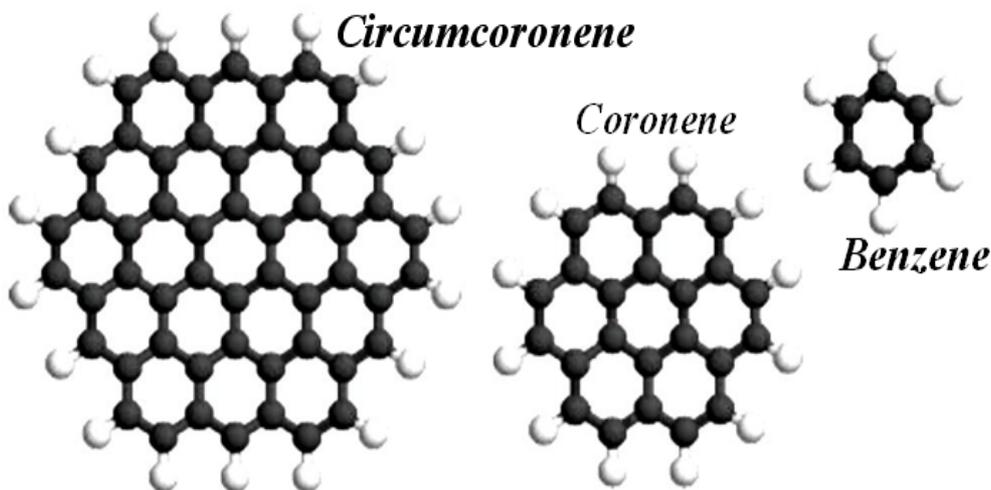
$$PI_e(PAH_k) = \frac{k}{2}\left(63k^3 + 32k^2 - 3k + 4\right)$$

Figure 1: First three members of Polycyclic Aromatic Hydrocarbons (PAH$_k$) for *k=1,2,3*.

Proof: To compute the edge co-PI$_e$ of Polycyclic Aromatic Hydrocarbons PAH$_k$ we just need to find the $m_u(e)$ and $m_v(e)$ for each edge *e=uv* of PAH$_k$. From Figure 2, we notice that any edge cut C_i(*i=0,...,k*), cut *k+i* edge of *PAH$_k$*. Also for C_i, we have

$$m_u(e/PAH_k)=2(k+i)+ (k+(i\text{-}1))+2(k+(i\text{-}1))+ (k+(i\text{-}2))+...+2(k+1)+k$$
$$= \sum\nolimits_{s=i}^{1} 2(k+(i+1)\text{-}s)+ \sum\nolimits_{s=1}^{i} (k+(i\text{-}s))= \sum\nolimits_{s=1}^{i}\left(\left(3k+3i+2\right)-3s\right)$$
$$=(3k+3i+2)i\text{-}\tfrac{3}{2}i(i+1)= \tfrac{3}{2}i^2+\left(3k+\tfrac{1}{2}\right)i \cdot$$

Also, ∀*i=0,...,k* ; *|E(PAH$_k$)|=m_v(e/PAH$_k$)+m_u(e/PAH$_k$)+|C_i|*, where *|C_i|=k+i*, thus

$$m_v(e/PAH_k)= 9k^2+3k\text{-}(k+i)\text{-}\left(\tfrac{3}{2}i^2+\left(3k+\tfrac{1}{2}\right)i\right)= 9k^2+2k-\tfrac{3}{2}i^2-\left(3k+\tfrac{3}{2}\right)i \cdot$$

We the help of these computation we can compute the co-PI$_e$ of PAH$_k$.

$$Co\text{-}PI_e(PAH_k)= \sum_{e=uv\,\in E(PAH_k)} |m_v(e/PAH_k)\text{-}m_u(e/PAH_k)|$$
$$= \sum_{\substack{e=vu\in C(e_i)\\ i=0,1,...,k-1}} 6(k+i)/(m_v(e/PAH_k)\text{-}m_u(e/PAH_k))|$$

$$+ \sum_{e_k \in C(e_k)} 3(2k)/(m_v(e/PAH_k)-m_u(e/PAH_k))/$$

$$=6(k)(9k^2+2k-0)+6(k+1)(9k^2-k-3-3k-2)+\ldots$$

$$+6(2k-1)(\tfrac{9}{2}k^2+\tfrac{9}{2}k-\tfrac{9}{2}k^2+\tfrac{7}{2}k-1)+0$$

$$= \sum_{\substack{e=vu\in C(e_i) \\ i=0,1,\ldots,k-1}} 6(k+i)\left(9k^2+2k-3i^2-i(6k+2)\right)$$

$$= 6k^2\sum_{i=0}^{k-1}(9k+2)-6(9k+2)\sum_{i=0}^{k-1}i^2+18k^2\sum_{i=0}^{k-1}i-18\sum_{i=0}^{k-1}i^3$$

$$= 6k^3(9k+2)-6(9k+2)\frac{(k-1)k(2k-1)}{6}+18k^2 \cdot k-18\frac{k^2(k+1)^2}{4}$$

$$= \frac{k}{2}\left(63k^3+32k^2-3k+4\right)$$
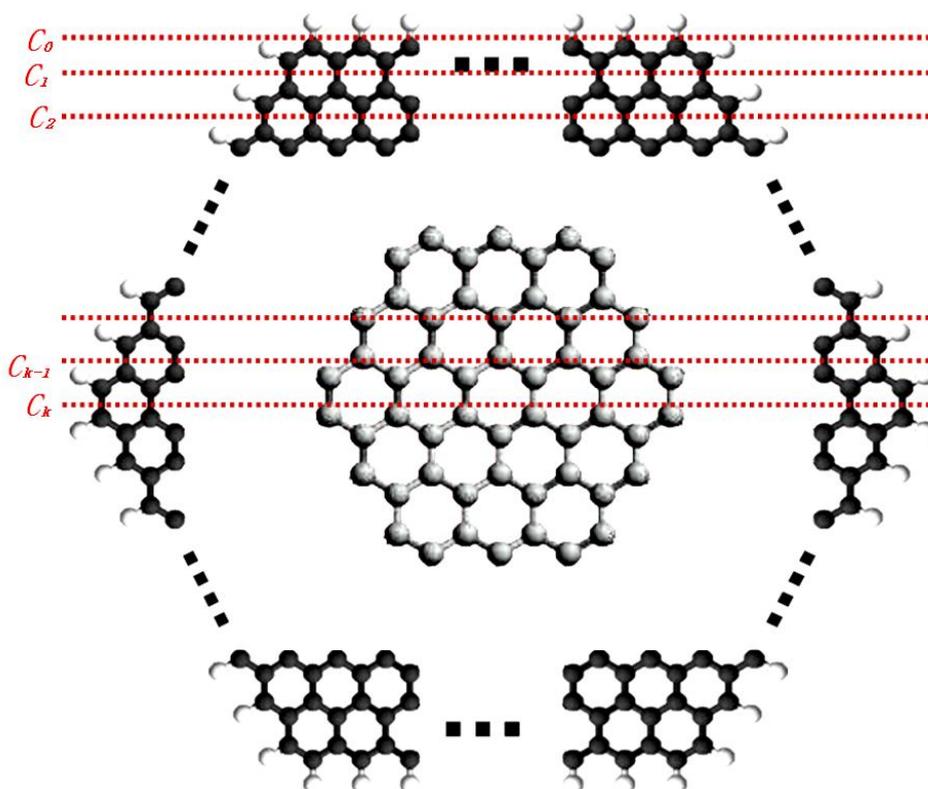
And this completes the proof.

Figure 2: General representation of Polycyclic Aromatic Hydrocarbons with orthogonal cuts

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