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Research Article

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Vertex version of pi index of polycyclic aromatic hydrocarbons PAH_K

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Abstract Let *G=(V,E)* be a simple connected molecular graph. *Khadikar et.al*. introduced the *PI* index defined by $PI_v(G) = \sum_{e=uv\in E(G)} (n_v(e|G) + n_u(e|G))$, where $n_u(e|G)$ is the number of vertices of *G* lying closer to *u* and $n_u(e|G)$ is the number of vertices of *G* lying closer to *v*. In this paper, we compute a closed formula of vertex PI index for Polycyclic Aromatic hydrocarbons.

Keywords Poly Aromatic Hydrocarbons *PAHk* ; PI index; Cut Method; Orthogonal Cut.

Introduction

Let *G* be a simple molecular graph such that its vertices set *V(G)* and edge set *E(G)* corresponds to the atoms and bonds respectively. In graph theory, d_v is the degree of a vertex $v \in V(G)$, the number of adjacent vertices with *v* or the size of first neighborhood of vertex *v*. An edge *e=uv* of graph *G* is attached between two vertices *u* and *v*. The distance between two vertices $u, v \in V(G)$ is equal to the number of edges on shortest path between them and it is denoted by *d*(*u*,*v*).

A topological index is a numerical quantity associated with graph *G*. In mathematical chemistry, many topological indices are introduced so far. For any molecular graph G they are invariant on the graph automorphism.

H. Wiener [1] defined the notion of the *Wiener index* and defined as:

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

I. Gutman et. al. [2,3] defined the vertex and edge versions of *Szeged index,* which are defined as

$$Sz_v(G) = \sum [n_u \ (e|G) \times n_v \ (e|G)]$$

$$Sz_e(G) = \sum_{e=uv\in E(G)} \left(m_u(e|G) + m_v(e|G)\right)$$

where $n_u(e|G)$ and $m_u(e|G)$ represents the number of vertices of *G* lying closer to *u* than to *v* and $m_u(e|G)$is the number of edges of *G* lying closer to *u* than to *v*, respectively, analogously $n_v(e|G)$ and $m_u(w|G)$.

Khadikar [4] and *Ashrafi* [8] proposed the edge and vertex versions of *Padmakar-Ivan* index (PI). These versions of PI index of a graph *G* is defined as:

$$PI_e(G)=\sum_{e\in E(G)}\left(m_u(e|G)+m_v(e|G)\right)$$
$$PI_v(G)=\sum_{e\in E(G)}\left(n_u(e|G)+n_v(e|G)\right)$$

See the paper series for further details [4-9].

Polycyclic Aromatic Hydrocarbons

PAH_k considered here is a family of such hydrocarbons containing several copies of benzene on circumference and is ubiquitous products. Polyaromatic 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 type of molecules has utilization in modeling graphite surface [10-16].

Main Result:

Let PAH_k be the *Polycyclic Aromatic Hydrocarbons* ($\forall k\geq 1$). Then the *PI* index of PAH_k is equal to:

$$PI_v(PAH_k)=18k^2(k+1)[18k^2+9k-1]$$

Proof. Consider the general representation of the Polycyclic Aromatic Hydrocarbons PAH_k ($\forall k\geq 1$) *a*s shown in Figure 1, we see that PAH_k has $6k^2+6k$ vertices/atoms and $9k^2+3k$ edge/bonds ($|E(PAH_k)|$), such that $6k^2$ of its verities are Carbon atoms with three bonds and $6k$ of its verities are Hydrogen atoms with one bond.

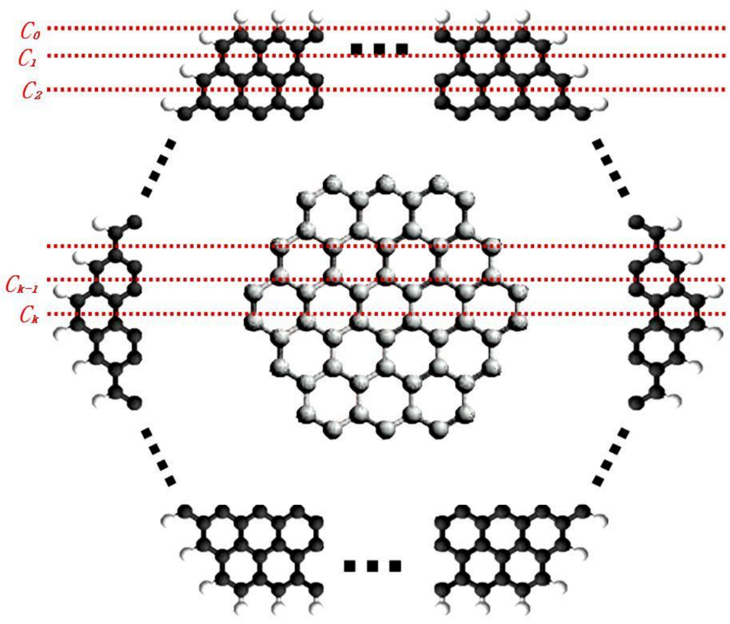

Figure 1: All orthogonal cuts of PAH_k.

Our aims is to compute the *PI* index of the *Polycyclic Aromatic Hydrocarbons* PAH_k. So, we cut PAH_k and see that for an arbitrary edge cut $e=uv$ ($\in E(PAH_k)$), there is an orthogonal cut $C(e)$.

One can see that for i^{th} orthogonal cut C_i ($\forall i=0,1,2,\ldots,k$); there are $k+i$ co-distance edges of PAH_k, and this imply that for all edge $e=uv\in C_i\subset E(PAH_k)$,there are $k+i$ repetitions of the vertex partitions $N_u(e|PAH_k)$ and $N_v(e|PAH_k)$ such that

$$n_v(e|PAH_k)=|\{x|x\in V(PAH_k),d(v,x)<d(x,u)\}=i^2+2(k+1)i+k.$$

From Figure 1, it's easy to see that for all edge $e=uv\in E(PAH_k)$, $N(e|PAH_k)=\emptyset$ and $n(e|PAH_k)=0$. Thus

$$|V(PAH_k)|=n(e|PAH_k)+n_v(e|PAH_k)+n_u(e|PAH_k) \text{ and } n_u(e|PAH_k)=|V(PAH_k)|-n_v(e|PAH_k).$$

Therefore,

$$n_u(e|PAH_k)=\{x/\ x\in V(PAH_k),\ d(u,x)<d(x,v)\}=6k^2+5k-i^2-2(k+1)i$$

Now by using the above calculations, we can compute the *PI* index of the Polycyclic Aromatic Hydrocarbons PAH_k ($\forall k\geq 1$) as follow:

$$PI_v(PAH_k)=\sum_{e=uv\in E(PAH_k)}(n_v(e|PAH_k)+n_u(e|PAH_k))$$

$$= 6 \sum_{e=uv \in C_0} (k)(n_v(e|PAH_k) + n_u(e|PAH_k))$$
$$+ 6 \sum_{e=uv \in C_1} (k+1)(n_v(e|PAH_k) + n_u(e|PAH_k))$$
$$+ \dots$$
$$+ 6 \sum_{e=uv \in C_{k-1}} (2k-1)((n_v(e|PAH_k) + n_u(e|PAH_k))$$
$$+ 3 \sum_{e=uv \in C_k} (2k)((n_v(e|PAH_k) + n_u(e|PAH_k))$$
$$= 6k \sum_{e=uv \in C_k} |V(PAH_k)| + 6 \sum_{\substack{e=uv \in C_i \\ i=0,1,\dots,k-1}} (k+i)|V(PAH_k)|$$
$$= 6|V(PAH_k)|[k \sum_{e=uv \in C_k} + \sum_{\substack{e=uv \in C_i \\ i=0,1,\dots,k-1}} (k+i)]$$
$$= 6(6k^2+6k)[k(9k^2+3k) + k^2 + \frac{k(k-1)}{2}]$$
$$= 36k(k+1)[\frac{18k^3+6k^2+3k^2-k}{2}]$$
$$= 18k(k+1)[18k^3+9k^2-k]$$
$$= 18k^2(k+1)[18k^2+9k-1]$$

And this completes the proof of theorem. ■

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