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(G) = ∑

\sum_{e=uv \in E(G)} (n_u(e|G) + n_v(e|G)),

where n_u(e|G) is the number of vertices of G lying closer to u and n_v(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 PAH_k; 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 ∈ 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 ∈ 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_{e=uv \in E(G)} (n_u(e|G) \times n_v(e|G))

SZ_e(G) = ∑

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

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_v(e|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:
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 $PAH_k (\forall k \geq 1)$ as 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.](image)

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 $C_i (\forall i=0,1,2,...,k)$; 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

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

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

$$|V(PAH_k)|=n_u(e|PAH_k)+n_v(e|PAH_k)+n_u(e|PAH_k)+n_v(e|PAH_k)=|V(PAH_k)|-n_e(PAH_k).$$

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:

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

See the paper series for further details [4-9].
\[
= 6 \sum_{e \in v \subset C_k} (k) (n_v(e | PAH_k) + n_u(e | PAH_k)) \\
+ 6 \sum_{e \in v \subset C_k^1} (k + 1) (n_v(e | PAH_k) + n_u(e | PAH_k)) \\
+ \ldots \\
+ 6 \sum_{e \in v \subset C_{k-i+1}} (2k - 1)((n_v(e | PAH_k) + n_u(e | PAH_k)) \\
+ 3 \sum_{e \in v \subset C_j} (2k)((n_v(e | PAH_k) + n_u(e | PAH_k))) \\
= 6k \sum_{v \in \text{C}_k} \nu'(PAH_k) + \sum_{v \in \text{C}_{k-i}} (k+i) \nu'(PAH_k) \\
= 6(6k^2 + 6k) \{ k(9k^2 + 3k) + k^2 + k(k-1) \} \\
= 36k(k+1)[18k^3 + 6k^2 + 3k^2 - k \frac{2}{2}] \\
= 18k(k+1)[18k^3 + 9k^2 - k] \\
= 18k^2(k+1)[18k^2 + 9k - 1]
\]

And this completes the proof of theorem. ■

References


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