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Research Article

THE EDGE-SZEGED INDEX OF THE POLYCYCLIC AROMATIC HYDROCARBONS PAH_K

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ABSTRACT
Let $G=(V,E)$, be a simple connected molecular graph with the vertex set $V=V(G)$ and the edge set $E=E(G)$. The PI index of G is defined as $PI_e(G)=\sum_{e=uv\in E(G)}[m_u(e|G)+m_v(e|G)]$. The number of edges of G lying closer to u than to v is denoted by $m_u(e|G)$ and the number of edges of G lying closer to v than to u is denoted by $m_v(e|G)$. In this paper, we compute a closed formula of the PI index of molecular graph "*Polycyclic Aromatic Hydrocarbons* PAH_k", for all positive integer number *k*.

Keywords: *Molecular Graph, Polycyclic Aromatic Hydrocarbons* PAH_k; *PI index* PI_e.

INTRODUCTION
Let $G=(V,E)$, be a simple connected molecular graph with the vertex set $V=V(G)$ and the edge set $E=E(G)$. In molecular graph *G*, vertices are corresponding to the atoms and edges corresponding to the bonds. An edge $e=uv$ ($\in E(G)$) of graph *G* is joined between two vertices *u* and *v* ($\in V(G)$). A general reference for the notation in graph theory is (West, 1996; Todeschini and Consonni, 2000; Trinajstić, 1992; Wiener, 1947).
A topological index is a real number related to a molecular graph. It must be a structural invariant, i.e., it does not depend on the labeling or the pictorial representation of a graph. The Wiener index W is the first topological index proposed to be used in chemistry. It was introduced in 1947 by Wiener for characterization of alkanes. The Wiener is defined as the sum of all distances between distinct vertices as:

$$W(G)=\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}d(u,v)$$

where $d(u,v)$ be the distance (the number of edges in a shortest path) between vertices *u* and *v* of *G*.
The PI index PI_e introduced by Khadikar (2000, 2001, and 2002). It is defined as the sum of $m_u(e|G)+m_v(e|G)$ between all edges $e=uv$ of a graph G, where $m_u(e|G)$ is the number of edges of G lying closer to u than to v and $m_v(e|G)$ is the number of edges of G lying closer to v than to u. In other words, the PI index $PI_e(G)$ is equal to:

$$PI_e(G)=\sum_{e=uv\in E(G)}[m_u(e|G)+m_v(e|G)].$$

Mathematical properties of the PI index for some classes of chemical graphs can be found in recent papers (Ashrafi and Loghman, 2006; Ashrafi and Vakili-Nezhad, 2006; Ashrafi and Loghman, 2006; Ashrafi and Loghman, 2006; Ashrafi and Rezaei, 2007; Deng, 2006; Farahani, 2013; Farahani, 2013; Farahani, 2013; Manoochehrian *et al.*, 2007).
In this paper the PI index PI_e of one of famous hydrocarbon molecules "the *Polycyclic Aromatic Hydrocarbons* PAH_k" are computed.

RESULTS AND DISCUSSIONS
Main Results and Discussions
Let PAH_k be the "Polycyclic Aromatic Hydrocarbons" for all positive integer number *k* and its general representation is shown in Figure 1. The hydrocarbons molecule "Polycyclic Aromatic Hydrocarbons" is more practical in the chemical and physics and play a role in graphitization of organic materials. In Figure

1, the general case of this hydrocarbons molecule are shown. For further study of its properties, see paper series (Wiersum and Jenneskens, 1997; Berresheim *et al.,* 1999; Bauschlicher and Bakes, 2000; Brand *et al.,* 1998; Morgenroth *et al.*, 1998; Dtz *et al.*, 2000; Yoshimura *et al.*, 2001; Stein and Brown, 1987; Dietz *et al.,* 2000; Huber *et al.*, 2003; Jug and Bredow, 2004; Farahani, 2013; Farahani, 2013; Farahani, 2014; Farahani, 2015; Farahani, 2015; Farahani and Schultz, 2013; Farahani and Gao, 2015; Gao and Farahani, 2015). The PI index $PI_e(PAH_k)$ of *Polycyclic Aromatic Hydrocarbons* PAH_k is presented in the following theorem.

Theorem 1: The PI index PI_e of *Polycyclic Aromatic Hydrocarbons* PAH_k $(\forall k\geq 1)$ is equal to $PI_e(PAH_k) = 81k^4+40k^3+6k^2-k$.

Proof: Let PAH_k be the Polycyclic Aromatic Hydrocarbons $(\forall k\geq 1)$. From the general representation of Polycyclic Aromatic Hydrocarbons PAH_k in Figure 1, one can see that there are $6k^2$ Carbon atoms and $6k$ Hydrogen atoms in the structure of PAH_k. Therefore, the number of vertices/atoms of PAH_k is equal to $6k^2+6k$ and alternatively PAH_k have $\frac{1}{2}(1\times 6k+3\times 6k^2)=9k^2+3k$ edge/bonds.

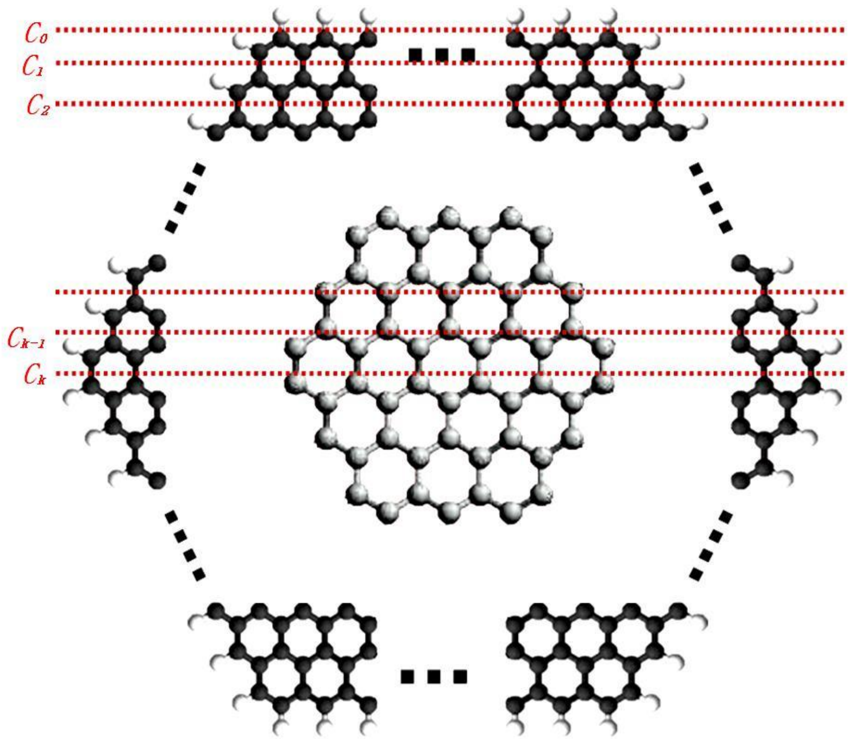

Figure 1: All orthogonal cuts of the Polycyclic Aromatic Hydrocarbons PAH_k.

By definition of the PI index PI_e, it is enough to compute $m_u(e|PAH_k)$ and $m_v(e|PAH_k)$. So, to compute $m_u(e|PAH_k)$ and $m_v(e|PAH_k)$ for all edge $e=uv\in E(PAH_k)$, we attend to Figure 1. By Figure 1, we see that an arbitrary edge cut C_i $(i=0,\dots,k)$, cut $k+i$ edge of PAH_k and also, for i[th] cut C_i;

$$m_v(e|PAH_k)=2(k+i)+(k+(i-1))+2(k+(i-1))+(k+(i-2))+\dots+2(k+1)+k=\sum_{s=i}^{1} 2(k+(i+1)-s)$$
$$+\sum_{s=1}^{i}(k+(i-s))=\sum_{s=1}^{i}\left(\left(3k+3i+2\right)-3s\right)=(3k+3i+2)i-\tfrac{3}{2}i(i+1)=\tfrac{3}{2}i^2+\left(3k+\tfrac{1}{2}\right)i\,.$$

Also, it is easy to see that $\forall i=0,\dots,k$; $|E(PAH_k)|=m_v(e|PAH_k)+m_u(e|PAH_k)+|C_i|$ and $|C_i|=k+i$, thus

$$m_u(e|PAH_k)=9k^2+3k-(k+i)-\left(\tfrac{3}{2}i^2+\left(3k+\tfrac{1}{2}\right)i\right)=9k^2+2k-\tfrac{3}{2}i^2-\left(3k+\tfrac{3}{2}\right)i\,.$$

Now by according to the definition of PI index, we have the following computations of the Polycyclic Aromatic Hydrocarbons $PI_e(PAH_k)$.

$$PI_e(PAH_k)=\sum_{e=uv\in E(PAH_k)} m_v(e|PAH_k)+m_u(e|PAH_k)$$

$$= \sum_{\substack{e=vu\in C(e_i)\\ i=1,\dots,k-1}} 6(k+i)(m_v(e|PAH_k)+m_u(e|PAH_k)) + \sum_{e_k\in C(e_k)} 3(2k)(m_v(e|PAH_k)+m_u(e|PAH_k))$$

$$=6(k)(0+9k^2+2k)+6(k+1)(3k+2+9k^2-k-3)+\dots+6(2k-1)(\tfrac{9}{2}k^2-\tfrac{7}{2}k+1+\tfrac{9}{2}k^2+\tfrac{9}{2}k)$$

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

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

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

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

$$=6k^2(9k^2+11k+2)+3k^2(9k^2+10k+1)-(2k^3+3k^2+k)-6k^2(9k+1)$$

$$=81k^4+40k^3+6k^2-k.$$

Therefore, the proof of Theorem 1 is completed.■

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