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VERTEX VERSION OF Co-PI INDEX OF THE POLYCYCLIC AROMATIC HYDROCARBON SYSTEMS PAH_k

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ABSTRACT

Let G be a simple connected graph having vertex set V and edge set E. The length of the smallest path between vertices $u,v \in V(G)$ is called the *distance*, $d(u,v)$, between the vertices u,v. Mathematical chemistry is the area of research engaged in new application of mathematics in chemistry. In mathematics chemistry, we have many topological indices for any molecular graph, that they are invariant on the graph automorphism. The length of the smallest path between vertices $u,v \in V(G)$ is called the *distance*, $d(u,v)$, between the vertices u,v. For an edge $e=uv \in E(G)$, $n_u(e|G)$ represents the number of vertices of G whose distance to u is less than the distance to v in G and $n_v(e|G)$ represents the number of vertices of G whose distance to v is less than the distance to u in G.

In 2010, A Iranmanesh *et.al* introduced the new topological indices. The $Co\text{-}PI_v$ index is the vertex version of Co-PI topological index and is defined as

$Co-PI_v(G)=\sum_{e\in E(G)}|n_u(e|G)-n_v(e|G)|$. In this present study, we introduce a closed formula of this new index of the Polycyclic Aromatic Hydrocarbon systems PAH_k

Keywords: Molecular graphs, chemical structures *Polycyclic Aromatic Hydrocarbon (PAH_k),* Circumcoronene series of Benzenoid; Padmakar-Ivan index; Co-PI index; Cut Method; Orthogonal Cut.

INTRODUCTION

Mathematical chemistry is the area of research engaged in new application of mathematics in chemistry. Major areas of research in mathematical chemistry include chemical graph theory. Chemical graph theory applies graph theory to mathematical modelling of chemical phenomena. Polycyclic aromatic hydrocarbons (PAH_k) are a group of over 200 different chemicals formed when wood, coal, oil, gasoline or other organic materials are burned. They can also be formed in food when fish or meats are charbroiled. "Polycyclic aromatic hydrocarbon" is just a mouthful for an organic molecule in space—not just any organic molecule, but one with a structure sturdy enough to survive the harsh environment between stars. Usually called "PAHs," this class of molecule is almost certainly the culprit responsible for the unidentified infrared emission (UIR) bands discovered in the early 1970s. The UIR bands are seen in many different kinds of objects from starburst galaxies to comets, so understanding their origin is very important. Because the UIR bands are so common, the PAHs which produce them must account for a sizeable fraction of all interstellar carbon in our galaxy and others. Estimates run as high as 15% or more!

What is a polycyclic aromatic hydrocarbon?

The place to start is with the simplest PAH: benzene. It's a *hydrocarbon* because it consists entirely of hydrogen and carbon (C_6H_6). The carbon atoms are arranged in a hexagonal structure with one hydrogen atom attached to each carbon atom. Because benzene has only one ring, it's not really *polycyclic* (does this make it monocyclic—a MAH?).

Each carbon atom has four electrons to share. One goes to the hydrogen atom, and one each to the two neighboring carbons. This leaves one to share with one of its two neighboring carbon atoms, which is why the benzene molecule is drawn with alternating single and double bonds around the hexagon. But at any

time, there's no way to know which bonds are single and which are double. Many chemists just draw a circle around the inside of the ring to show that there are six electrons floating around. Hydrocarbons with this structure are called *aromatic* (because they generally stink—no kidding!) The electrons float above and below the ring, and the electromagnetic fields they generate keep the ring flat.

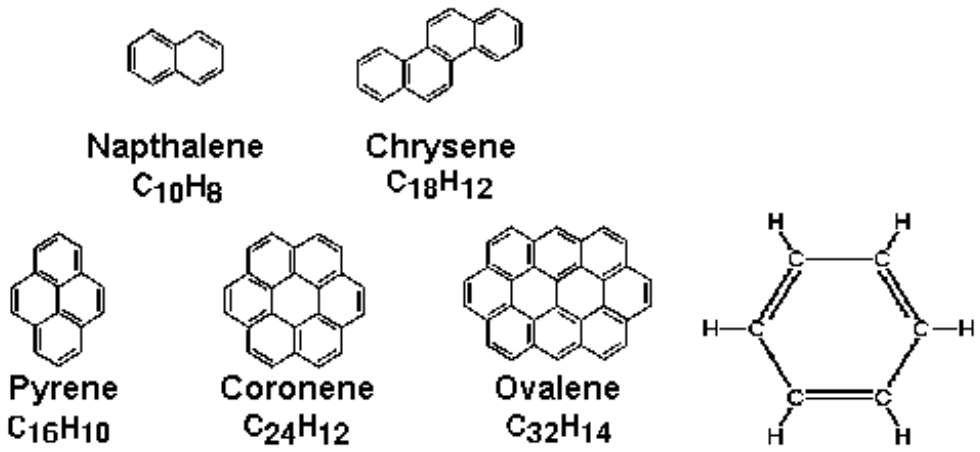

Figure 1: [14] Some example of Polycyclic Aromatic Hydrocarbon PAH_k.

PAHs generally consist of several hexagonal rings. The figure to the left illustrates a few common simple PAHs. Further details on these chemical structures can be seen in [1-36].

Let G be a simple connected graph having vertex set V and edge set E. The length of the smallest path between vertices $u,v \in V(G)$ is called the *distance*, $d(u,v)$, between the vertices u,v. For an edge $e=uv \in E(G)$, $n_u(e|G)$ represents the number of vertices of G whose distance to u is less than the distance to v in G and $n_v(e|G)$ represents the number of vertices of G whose distance to v is less than the distance to u in G. Similarly, $m_u(e|G)$ is the number of edges of G lying closer to u than v and $m_v(e|G)$ is the number of edges of G lying closer to v than u. For a vertex $u \in V(G)$, the number of vertices adjacent to the vertex u is called the *degree* of u, $d(u)$.

H. Wiener [37] defined the first distance based topological index, named as *Wiener index*. The Wiener index of a graph G is defined as

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

Later, *Gutman, Ashrafi and Klavžar* proposed new distance based topological indices the *Szeged index* and the *edge Szeged index* [38, 39]. These indices for a graph G is defined as

$$Sz_v(G) = \sum\left(n_u\ (e \mid G) \times n_v\ (e \mid G)\right)$$

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

For further details see [40-43].

Agarwal and *Ashrafi* [44, 45] defined the *vertex PI index* and *edge PI index* of a graph G 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. For history and recent results we refer [46-48].

Recently, *Hasani* [49] and *Farahani* [50] introduced the *Co* versions of these topological indices as follow:

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

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

In this paper, we computed the vertex Co-PI index of the Polycyclic Aromatic Hydrocarbons molecular structure.

Main Results

The first three members or Polycyclic Aromatic Hydrocarbons (PAH_k) are *Benzene, Coronene* and Circumcoronene as shown in Figure 1. The general representation of Polycyclic Aromatic Hydrocarbon is shown in Figure 2. A general molecular graph of Polycyclic Aromatic Hydrocarbon contains $6k^2+6k$ vertices and $9k^2+3k$ edges.

Theorem 1: Let the graph of *Polycyclic Aromatic Hydrocarbon (PAH_k)*, then the vertex PI index of PAH_k is

$$Co - PI_v(PAH_k) = \left(2k^4 + \frac{32}{3}k^3 - 2k^2 - \frac{2}{3}k\right)$$

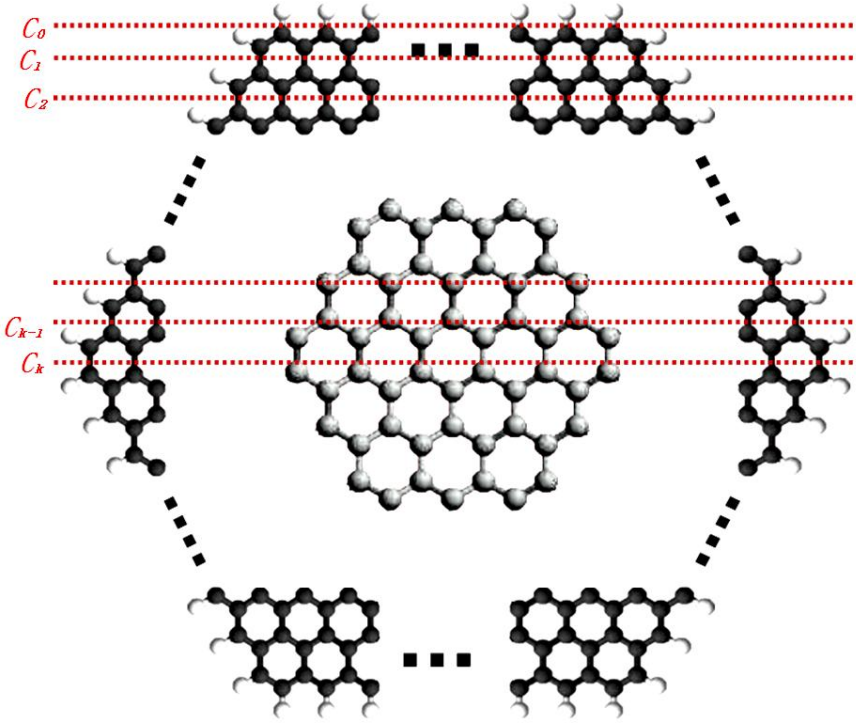

Figure 1. All orthogonal cuts of the Polycyclic Aromatic Hydrocarbons *PAH*

Proof: From Figure 2, it is clear that for each edge of PAH_k there is an orthogonal cut $C(e)$. Also, notice that for orthogonal cut C_i $(i=0,1,2,\ldots,k)$; there are $k+i$ co-distance edges of PAH_k, so we can say 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

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

that for all edge $e=uv \in E(PAH_k)$, $N(e|PAH_k)=\emptyset$ and $n(e|PAH_k)=0$.

Thus

$$|V(PAH_k)|=n(e|PAH_k)+n_v(e|PAH_k)+n_u(e|PAH_k)$$

and

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

Therefore,

$$n_u(e|PAH_k) = \{x / \ x \in V(PAH_k), \ d(u,x) < d(x,v)\}$$

$$= 6k^2 + 5k - i^2 - 2(k+1)i$$

With the help of above calculation, now we compute the vertex Co-PI index of Polycyclic Aromatic Hydrocarbons PAH_k,

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

$$= 6 \sum_{e=uv \in C_0} (k) \left| n_v(e|PAH_k) - n_u(e|PAH_k) \right|$$
$$+ 6 \sum_{e=uv \in C_1} (k+1) \left| n_v(e|PAH_k) - n_u(e|PAH_k) \right|$$
$$+ \ldots + 6 \sum_{e=uv \in C_{k-1}} (2k-1) \left| (n_v(e|PAH_k) - n_u(e|PAH_k) \right|$$
$$+ 3 \sum_{e=uv \in C_k} (2k) \left| (n_v(e|PAH_k) - n_u(e|PAH_k) \right|$$

$$= 6 \sum_{\substack{e_i = u_i v_i \in C_i \\ i=0,\ldots,k-1}} (k+i) \left| n_{u_i}(e_i|PAH_k) - n_{v_i}(e_i|PAH_k) \right|$$
$$+ 3 \sum_{e_k = u_k v_k \in C_k} (2k) \left| (n_{u_k}(e_k|PAH_k) - n_{v_k}(e_k|PAH_k) \right|$$

$$= 6 \sum_{\substack{e_i = u_i v_i \in C_i \\ i=0,\ldots,k-1}} (k+i) \left| \left(6k^2 + 5k - i^2 - 2(k+1)i\right) - \left(i^2 + 2(k+1)i + k\right) \right|$$
$$+ 6k \sum_{e_k = u_k v_k \in C_k} \left| \left(6k^2 + 5k - k^2 - 2(k+1)k\right) - \left(k^2 + 2(k+1)k + k\right) \right|$$

$$= 6 \sum_{\substack{e_i = u_i v_i \in C_i \\ i=0,\ldots,k-1}} (k+i) \left| 6k^2 + 4k - 2i^2 - 4(k+1)i \right| + 6k \sum_{e_k = u_k v_k \in C_k} 0$$

$$= 6 \sum_{i=0,\ldots,k-1} (k+i) \left(6k^2 + 4k - 2i^2 - 4(k+1)i\right)$$

since $n_u(e|PAH_k) \geq n_v(e|PAH_k)$.

$$= 6 \sum_{i=0,\ldots,k-1} \left(-2i^3 - 2(3k+2)i^2 + 2k^2 i + 2k^2(3k+2)\right)$$

$$= -12 \sum_{i=1}^{k-1} i^3 - 2(3k+2) \sum_{i=1}^{k-1} i^2 + 2k^2 \sum_{i=1}^{k-1} i + \sum_{i=1}^{k-1} 2k^2(3k+2)$$

$$= -12\left(\frac{k^4}{4} - \frac{k^3}{2} + \frac{k^2}{4}\right) - 2(3k+2)\left(\frac{k^3}{3} - \frac{k^2}{2} + \frac{k}{6}\right) + 2k^2\left(\frac{k^2}{2} - \frac{k}{2}\right) + 2k^3(3k+2)$$

$$= \left(2k^4 + \frac{32}{3}k^3 - 2k^2 - \frac{2}{3}k\right).$$

And these computations complete the proof. ■

CONFLICT OF INTERESTS

The authors declare that there is no conflict of interests regarding the publication of this paper.

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