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Omega and Cluj-Ilmenau Indices of Hydrocarbon Molecules "Polycyclic Aromatic Hydrocarbons PAH_k"

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Abstract

A topological index is a numerical value associated with chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. In this paper, we computed the Omega and Cluj-Ilumenau indices of a very famous hydrocarbon named as Polycyclic Aromatic Hydrocarbons PAH_k for all integer number *k*.

Keywords

Molecular Graph, Hydrocarbons, Topological Indices

1. Introduction

Let $G=(V,E)$ be a simple finite connected graph, where V and E are the sets of vertices and edges, respectively. The *distance* between two vertices u and v in a graph G is the length of the shortest path connecting them, it is denoted by $d(u,v)$. Two edges $e=uv$ and $f=yz$ in graph G are said to be *codistant* if they satisfy the following condition [1]

$$d(v,y)=d(v,z)+1=d(u,y)+1=d(u,z).$$

If the edges e and f are codistant we write it as *e co f*. Relation *co* is reflexive and symmetric but generally not transitive. If *co* relation is transitive then it is an equivalence relation. A graph G in which *co* is an equivalence relation is called *co-graph*, and the subset of edges $C(e)\{f \in E(G) \mid fcoe\}$ is called an *orthogonal cut* (*oc*) of *G*, also the edge set $E(G)$ can be written as the union of disjoint orthogonal cuts, *i.e.*

$$E(G) = C_1 \cup C_2 \cup \cdots \cup C_l ; C_i \neq C_j \text{ for } i \neq j .$$

Let $e, f \in E(G)$ be two edges of *G* which are opposite or topologically parallel and denote this relation by *e op f*. A set of opposite edges, within the same ring eventually forming a strip of adjacent rings, is called an *opposite edge strip ops*, which is a quasi orthogonal cut (*qoc*). The length of *ops* is maximal irrespective of the starting edge. Let $m(G,c)$ be the number of *ops* strips of length *c*.

The physico-chemical properties of chemical compounds are often modeled by means of molecular graph based structure descriptors, known as *topological indices* [2], [3]. The *Wiener index* is the first distance based topological index [4]. The Wiener index of a graph *G* is defined as

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

M. V. Diudea introduced the *Omega Polynomial* $\Omega(G,x)$ for counting *ops* strips in graph *G* [5]

$$\Omega(G,x) = \sum_c m(G,c) x^c .$$

First derivative of Omega polynomial at $x = 1$ equals the size of the graph *G*, *i.e.*

$$\Omega'(G,1) = \sum_c m(G,c) \times c = |E(G)| .$$

The *Cluj-Ilumenau* index [6] is defined with the help of first and second derivative of Omega polynomial at $x = 1$ as

$$CI(G) = \left[\Omega'(G,x)\right]^2_{x=1} - \left[\Omega'(G,x) + \Omega''(G,x)\right]_{x=1} .$$

The *Omega index* is defined as

$$I_G(G) = \frac{1}{\Omega'(G,x)} \sum_c \sqrt[c]{\Omega^c(G,x)} .$$

2. Discussion and Main Result

Polycylic Aromatic Hydorcarbons (PAH_t) are a group of more than 100 different chemicals, these are formed during the incomplete burning of coal, oil, gas, garbage or other substances. PAH_t are usually found as a mixture containing two or more of these compounds. For further information and results on PAH_t and other molecular graphs and nano-structures, we refer [7]-[22]. In this section, we computed the *Omega* and Cluj-Ilumenau index of Polycyclic aromatic hydrocarbons PAH_t.

Theorem 1. Consider the graph of Polycyclic aromatic hydrocarbons PAH_t, then we have the following

$$Cl(PAH_t) = 81t^4 - 68t^3 + 138t^2 - t$$

$$I_G(PAH_t)=\left(\frac{1}{9t^2+3t}\right)\sum_{c=1}^{2t}\sqrt[c]{6\sum_{i=0}^{t-1}\left(\prod_{j=0}^{c-1}(t+i-j)\right)+3\left(\prod_{j=0}^{c-1}(2t-j)\right)}.$$

Proof Consider the general representation of the Polycyclic aromatic hydrocarbons PAH_t as shown in **Figure 1**. The structure of PAH_t contain $6t^2+6t$ atoms/vertices and $9t^2+3t$ bonds/edges.

To obtain the required result, we used the *Cut Method* [23]-[25]. We calculated the $m(PAH_t,c)$ for all opposite edge strips. From **Figure 2**, it is clear that there are $t+1$ distinct cases of qoc strips for PAH_t and the graph of Polycyclic aromatic hydrocabons's graph is a co-graph. The size of a qoc strip is $|C_i|t+i$ for $i=1,2,\cdots,t-1$ and $|C_0|=t$. Because there are $t+i-1$ co-distant edges with

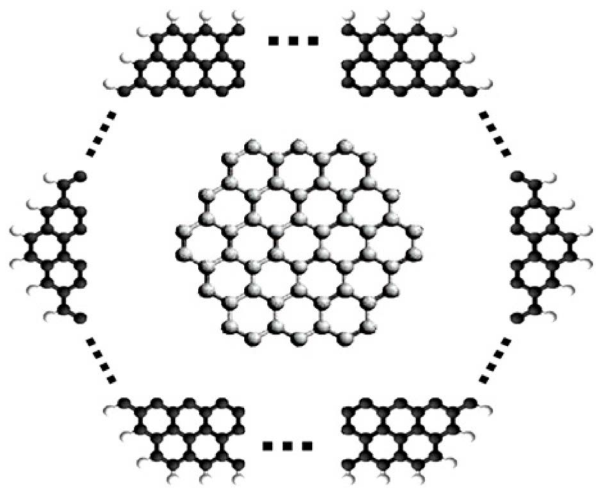

Figure 1. General representation of polycyclic aromatic hydrocarbons PAH_t.

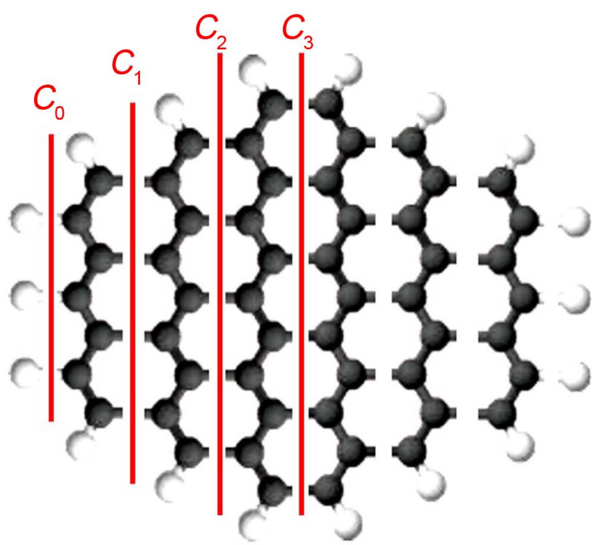

Figure 2. A quasi orthogonal cuts strips on polycyclic aromatic hydrocarbons PAH_t.

$e, \forall e \in C_i$. Also from **Figure 2** one can notice that the number of repetition of these qoc stips C_i is six $\forall i = 0,1,\cdots,t-1$ and the number of repetition of C_t is three times. *i.e.*

- For $i = 0$, $m(PAH_t, c_0) = 6$ and $|C_t| = t$.
- For all $i = 1,2,\cdots,t-1$, $m(PAH_t, c_i) = 6$ and $|C_t| = t+i$.
- For $i = t$, $m(PAH_t, c_t) = 3$ and $|C_t| = 2t$.

From this, we obtain that

$$6|C_0| + 6|C_1| + \cdots + 3|C_t| = 6\sum_{i=0}^{t-1}(t+i) + 6t = 9t^2 + 3t = |E(PAH_t)|.$$

This gives that the Omega polynomial of the Polycyclic aromatic hydrocarbons PAH_t for all non-negative integer number t is equal to

$$\begin{aligned}\Omega(PAH_t, x) &= \sum_c m(PAH_t, c)x^c = \sum_{i=0}^{t} m(PAH_t, c_i)x_i^c \\ &= 6x^{|C_0|} + 6x^{|C_1|} + \cdots + 6x^{|C_{t-1}|} + 3x^{C_t} \\ &= 6x^t + 6x^{t+1} + \cdots + 6x^{2t-1} + 3x^{2t} \\ &= \sum_{i=0}^{t-1}\left(6x^{t+i}\right) + 3x^{2t}\end{aligned}.$$

Now with the help of above polynomial we will investigate the Cluj-Ilmenau and Omega indices of Polycyclic aromatic hydrocarbons PAH_t.

$$\begin{aligned}CI(PAH_t) &= \left[\Omega'(PAH_t, x)\right]^2_{x=1} - \left[\Omega'(PAH_t, x) + \Omega''(PAH_t, x)\right]_{x=1} \\ &= \left[\left(\sum_{i=0}^{t-1}\left(6x^{t+i}\right) + 3x^{2t}\right)'\right]^2_{x=1} - \left[\left(\sum_{i=0}^{t-1}\left(6x^{t+i}\right) + 3x^{2t}\right)' + \left(\sum_{i=0}^{t-1}\left(6x^{t+i}\right) + 3x^{2t}\right)''\right]_{x=1} \\ &= \left[6\sum_{i=0}^{t-1}(t+i)x^{(t+i-1)} + 6tx^{2t-1}\right]^2 - \left[6\sum_{i=0}^{t-1}(t+i)x^{(t+i-1)} + 6tx^{2t-1}\right. \\ &\quad \left. + 6\sum_{i=0}^{t-1}(t+i)(t+i-1)x^{(t+i-2)} + 6t(2t-1)x^{2t-2}\right]_{x=1} \\ &= \left[6\sum_{i=0}^{t-1}(t+i) + 6t\right]^2 - \left[6\sum_{i=0}^{t-1}(t+i) + 6t + 6\sum_{i=0}^{t-1}(t+i)(t+i-1) + 6t(2t-1)\right] \\ &= 81t^4 - 68t^3 + 138t^2 - t\end{aligned}$$

$$I_\Omega(H_k) = \frac{1}{\Omega'(H_k, x)}\sum_c \sqrt[c]{\Omega^c(H_k, x)}\Bigg|_{x=1}$$

As

$$\begin{aligned}\Omega^c(H_t, x) &= 6\sum_{i=0}^{t-1}\left(\prod_{j=0}^{c-1}(t+i-j)\right)x^{(t+i-c)} + 3\left(\prod_{j=0}^{c-1}(2t-j)\right)x^{2t-c} \\ &= \left(\frac{1}{9t^2+3t}\right)\sum_{c=1}^{2t}\sqrt[c]{6\sum_{i=0}^{t-1}\left(\prod_{j=0}^{c-1}(t+i-j)\right) + 3\left(\prod_{j=0}^{c-1}(2t-j)\right)}\end{aligned}$$

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