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Research Article

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The Pi polynomial and the Pi index of a family hydrocarbons molecules

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ABSTRACT

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of *which are represented by V(G) and E(G), respectively. A topological index of a graph G is a numeric quantity related to G which is invariant under automorphisms of G. A new counting polynomial, called the Omega polynomial, was recently proposed by Diudea on the ground of quasi-orthogonal cut "qoc" edge strips in a polycyclic graph. Another new counting polynomial called the Pi polynomial. The Omega and Pi polynomials are equal to* $\Omega(G,x)=\sum_c m(G,c)\,x^c$ *and* $\Pi(G,x)=\sum_c m(G,c).c.x^{|E(G)|-c}$ *, respectively. In this paper, the Pi polynomial and the Pi Index of Polycyclic Aromatic Hydrocarbons* PAH_k *are computed.*

Keywords: Counting Polynomial Omega polynomial, qoc strip, Cut Method, Polycyclic Aromatic Hydrocarbons.

INTRODUCTION

Let G be a simple graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by *V(G)* and *E(G)*, respectively. And for a connected molecular graph *G* and $x,y\in V(G)$, t he distance *d(x,y)* between x and y is defined as the length of a minimum path between x and y.

In chemical graph theory and mathematical chemistry, *Topological Indices* are numerical parameters of a graph which characterize its topology and are usually graph invariant.

Mathematical calculations are absolutely necessary to explore important concepts in chemistry. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is an important tool for studying molecular structures. [1-4].

Suppose *G* is an arbitrary simple connected molecular graph. Two edges $e=uv$ and $f=xy$ of G are called co-distant, "*e* co *f*", if and only if $d(u,x)=d(v,y)=k$ and $d(u,y)=d(v,x)=k+1$ or vice versa ($\forall k\geq 1$). It is easy to see that the relation "co" is reflexive and symmetric but it is not necessary to be transitive

If *co* is an equivalence relation: [5-7].

$$e \ co \ e$$
$$e \ co \ f \Leftrightarrow f \ co \ e$$
$$e \ co \ f \ \& \ f \ co \ h \Rightarrow e \ co \ h$$

Set $C(e):=\{f\in E(G) \mid f \ co \ e\}$. If the relation "co" is transitive on *C(e)* then *C(e)* is called an orthogonal cut "oc" of the graph *G*. The graph *G* is called co-graph if and only if the edge set *E(G)* a union of disjoint orthogonal cuts. If any two consecutive edges of an edge-cut sequence are *topologically parallel* within the same face of the covering, such a sequence is called a *quasi-orthogonal cut qoc* strip.

The Omega polynomial $\Omega(G,x)$ for counting qoc strips in G was defined by *M.V. Diudea* in 2006, as [8]

$$\Omega(G,x)=\sum_{c} m\left(\mathrm{G},c\right)\mathrm{x}^{c}$$

where $m(G,c)$ is the number of opposite edge strips of length c and this summation runs up to the maximum length of *qoc* strips in G.

Also, the Pi polynomial $\Pi(G,x)$, for counting *qoc* strips in G was defined as

$$\Pi(G,x)=\sum_{c} m\left(G,c\right).\mathrm{c}.\mathrm{x}^{|E(G)|-c}$$

$\Omega(G,x)$ count equidistant edges in G while $\Pi(G,x)$, count non-equidistant edges. For more study and historical details about the counting polynomials and the counting indices, see papers [9-23]. The Pi index $\Pi(G)$ is equal to first derivative of the Pi polynomial (in $x=1$)

$$\Pi(G)=\sum_{c} m\left(G,c\right)\left(\left|E\left(G\right)\right|-c\right)\times c$$

In this paper, the Pi polynomial and the Pi Index of *Polycyclic Aromatic Hydrocarbons* PAH_k are computed.

RESULTS AND DISCUSSION

In this present section, we compute the Pi polynomial $\Pi(G,x)$ and its index of molecular graph *Polycyclic Aromatic Hydrocarbons* PAH_k, for all positive integer number **k**. The *Polycyclic Aromatic Hydrocarbons* PAH_k for all positive integer number k is ubiquitous combustion products. They have been implicated as carcinogens and play a role in graphitization of organic materials [24]. In addition, they are of interest as molecular analogues of graphite [25] as candidates for interstellar species [26] and as building blocks of functional materials for device applications [25-27]. Synthetic routes to Polycyclic Aromatic Hydrocarbons PAH_k are available [28] and a detailed knowledge of all these features would therefore be necessary for the tuning of molecular properties towards specific applications

For more study and some properties about the hydrocarbon molecules and especially “Polycyclic Aromatic Hydrocarbons PAH_k”, see papers [24-36]. Some examples of hydrocarbon molecules are shown in Figure 1.

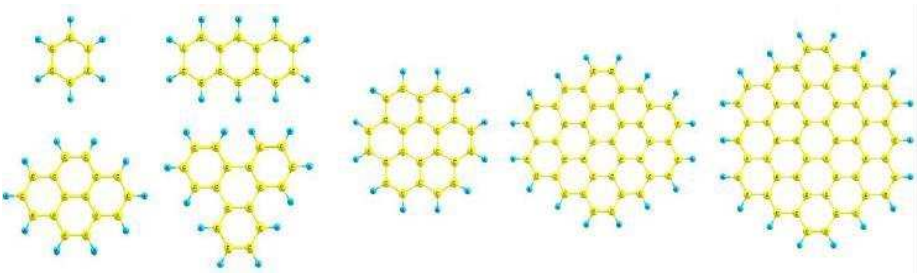

Figure 1. [24-36]: Some examples of hydrocarbon molecules

Theorem 1. Let PAH_k be the Polycyclic Aromatic Hydrocarbons PAH_k The Pi polynomial $\Pi(PAH_k,x)$ and its index $\Pi(PAH_k)$, $\forall k\geq 1$, are equal to

$$\Pi(PAH_k,x)=\sum_{i=0}^{k}\left(6\left(k+i\right)\mathrm{x}^{9k^2+k+i}\right)+6kx^{9k^2+k}$$

$$\Pi(PAH_k)=81k^4+95k^3+15k^2+k.$$

Proof: Consider the general representation of this *Polycyclic Aromatic Hydrocarbons* PAH_k ($\forall k\geq 1$) with $6k^2+6k$ vertices/atoms and $9k^2+3k$ edge/bonds. From the structure of this hydrocarbon molecule, we see that there are $6k^2$ Carbon atoms and $6k$ Hydrogen atoms in its structure.

Now, for counting all *qoc* strips in *Polycyclic Aromatic Hydrocarbons* PAH_k, we using the Cut Method. The general form of Cut Method was introduced by *S. Klavžar* in 2008 and some its properties and result are presented in papers [37-39].
Thus, from Figure 2 for computing the Pi polynomial and Pi index of the Polycyclic Aromatic Hydrocarbons, we have following results (see Figure 2).

1. There are $k+1$ distinct cases of *qoc strips* for PAH_k.
2. The size of ith *qoc strip* C_i $\forall i\in\{1,2,..,k-1\}$ is equal to $k+i$
3. The number of isomorphs of ith *qoc strip* C_i $\forall i\in\{1,2,..,k-1\}$ is equal 6.
4. The size of outer *qoc strip* C_0 is equal to k.
5. There are 6 *qoc strip* isomorphs with C_0.
6. The size of center *qoc strip* C_k is equal to $2k$.
7. There are three of center *qoc strip* C_k.

Now by using above mentions, the Pi polynomial of the Polycyclic Aromatic Hydrocarbons PAH_k ($\forall k\geq 1$) will be

$$
\begin{aligned}
\Pi(PAH_k,x) &= \sum_{c} m\left(PAH_k,c\right).c.x^{|E(PAH_k)|-c}\\
&= \sum_{i=0}^{k}|C_i|\, m\left(PAH_k,c_i\right)x^{|E(PAH_k)|-|C_i|}\\
&= m\left(PAH_k,c_0\right)|C_0|\,x^{|E(PAH_k)|-|C_0|}+\sum_{i=1}^{k-1} m\left(PAH_k,c_i\right)|C_i|\,x^{|E(PAH_k)|-|C_i|}\\
&\quad + m\left(PAH_k,c_k\right)|C_k|\,x^{|E(PAH_k)|-|C_k|}\\
&= 6kx^{|E(PAH_k)|-k}+6(k+1)x^{|E(PAH_k)|-(k+1)}+\ldots+6(2k-1)x^{|E(PAH_k)|-(2k-1)}+3(2k)x^{|E(PAH_k)|-2k}\\
&= 6kx^{9k^2+2k}+6(k+1)x^{9k^2+2k-1}+\ldots+6(2k-1)x^{9k^2+k+1}+6kx^{9k^2+k}\\
&= \sum_{i=0}^{k}\left(6(k+i)x^{9k^2+k+i}\right)+6kx^{9k^2+k}.
\end{aligned}
$$

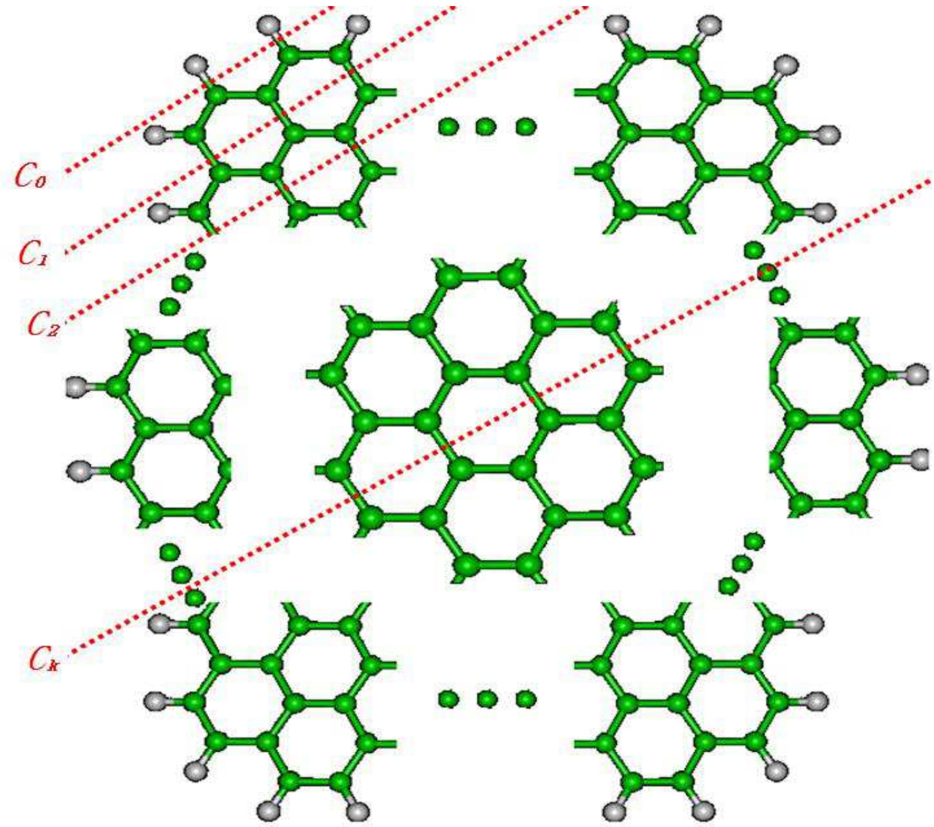

Figure 2. ***All quasi-orthogonal cuts (qoc) strips of* the Polycyclic Aromatic Hydrocarbons PAH_k**

Now, from the definition of Pi index of a graph *G*, we can see the Pi index of *G* is equal to the first derivative of its polynomial (evaluated at $x=1$). So, we can compute the Pi index $\Pi(PAH_k)$ $(\forall k\geq 1)$ of Polycyclic Aromatic Hydrocarbons as follows:

$$\Pi(PAH_k) = \left.\frac{\partial\Pi(PAH_k,x)}{\partial x}\right|_{x=1}$$

$$= \sum_{i=0}^{k} m\left(PAH_k, c_i\right)|C_i|\left(|E(PAH_k)| - |C_i|\right)$$

$$= m\left(PAH_k, c_0\right)|C_0|\left(|E(PAH_k)| - |C_0|\right) + \sum_{i=1}^{k-1} m\left(PAH_k, c_i\right)|C_i|\left(|E(PAH_k)| - |C_i|\right)$$

$$+m\left(PAH_k, c_k\right)|C_k|\left(|E(PAH_k)| - |C_k|\right)$$

$$= 6kx^{|E(PAH_k)|-k} + 6(k+1)x^{|E(PAH_k)|-(k+1)} + \ldots + 6(2k-1)x^{|E(PAH_k)|-(2k-1)} + 3(2k)x^{|E(PAH_k)|-2k}$$

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

$$= 6\left(\sum_{i=1}^{k} i^2 + \sum_{i=1}^{k} k\left(9k+2\right)i + \sum_{i=1}^{k} k^2\left(9k+1\right)\right) + 6k^2(9k+1)$$

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

$$=81k^4+95k^3+15k^2+k.$$

Here the proof of theorem is completed.■

CONCLUSION

In this paper, we were counting a topological polynomial and its topological index of a family of hydrocarbon molecular graphs "Polycyclic Aromatic Hydrocarbon PAH_k". The topological indices and molecular structure descriptors are used for modeling physico-chemical, toxicological, biological and other properties of chemical compounds and nano structure analyzing. The *Pi* polynomial $\Pi(G,x)=\sum_c m(G,c).c.x^{|E(G)|-c}$ and the *Pi* index $\Pi(G)=\sum_c m(G,c).c.(|E(G)|-c)$ are defined recently by Prof. *M.V. Diudea* and many scientists work in this subject.

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