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The Theta Polynomial Θ(G,x) and the Theta Index Θ(G) of Molecular Graph Polycyclic Aromatic Hydrocarbons PAH_k

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ABSTRACT: The omega polynomial *Ω(G,x),* for counting *qoc* strips in molecular graph *G* was defined by *Diudea* as $\Omega(G,x)=\sum_c m(G,c)x^c$ with *m(G,c),* being the number of *qoc* strips of length *c*. The Theta polynomial *Θ(G,x)* and the Theta index *Θ(G)* of a molecular graph *G* were defined as $\Theta(G,x)=\sum_c m(G,c).c.x^c$ and $\Theta(G)=\sum_c m(G,c).c^2$, respectively.

In this paper, we compute the Theta polynomial *Θ(G,x)* and the Theta index *Θ(G)* of molecular graph *Polycyclic Aromatic Hydrocarbons* PAH_k, for all positive integer number *k*.

Keywords: Molecular graph, Polycyclic Aromatic Hydrocarbons, Omega polynomial, Theta polynomial, Theta index

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1. INTRODUCTION

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 graph can be described by a connection table, a sequence of numbers, a matrix, a polynomial or by a single number (often called a topological index). A counting polynomial can be written as:

$$P(G, x)=\sum_{k} m(G,k)\, X^{k}$$

with the exponents showing the extent of partitions p(G), $\cup p(G)=P(G)$ of a graph property P(G) while the coefficients m(G, k) are related to the number of partitions of extent k.

Let G(V,E) be a connected 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, for a non-negative integer k.

If co is an equivalence relation: [1-3].

$$e\ co\ e$$

$$e\, co\, f \Leftrightarrow f\, co\, e$$

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

Then, C(e):={f∈E(G)| f co e} is the set of edges in G, co-distant to the edge e∈E(G) and G is called a co-graph. Consequently, C(e) is called an orthogonal cut set ocs of G and E(G) is the union of disjoint orthogonal cuts:

$$E(G)=C_1\cup C_2\cup\ldots\cup C_{k-1}\cup C_k \text{ and } C_i\cap C_j=\varnothing,$$

for i≠j and i, j=1, 2, …, k. The relation ops is not necessarily transitive. Observe an ops is an ocs only in partial cubes.

Observe co is a θ relation, (Djokovic-Winkler relation) [4, 5] and G is a co-graph if and only if it is a partial cube, a result due to Klavžar [6]. In a plane bipartite graph, an edge e is in relation θ with any opposite edge f if the faces of the plane graph are isometric (which is the case of the most chemical graphs). Then an orthogonal cut oc with respect to a given edge is the smallest subset of edges closed under this operation and C(e) is precisely a θ-class of G.

The Omega polynomial Ω(G,x) for counting qoc strips in G was defined by M.V. Diudea as [7]

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

where *m*(*G*,*c*) is the number of opposite edge strips of length *c.*

If *ops* is an *ocs*, as in partial cubes, we can write the following counting polynomials [8-23]:

$$Sd(G,x)=\sum_{c} m(G,c)\,x^{|E(G)|-c}$$

$$\Theta(G,x)=\sum_{c} m(G,c).c.x^{c}$$

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

Ω(G,x)and Θ(G,x) count equidistant edges in G while Sd(G, X) and Π(G,x), count non-equidistant edges. The first two polynomials are counted once for a strip while the last two are counted for each edge, so that the coefficients are multiplied with k.

In this present study, we compute the Theta polynomial Θ(G,x) and the Theta index Θ(G) of molecular graph Polycyclic Aromatic Hydrocarbons PAH_k, for all positive integer number k.

2. MAIN RESULTS AND DISCUSSION

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.

Reader can see some first members of this family in Figure 1. In references [24-41] some properties and more historical details of this family of hydrocarbon molecules are studded.

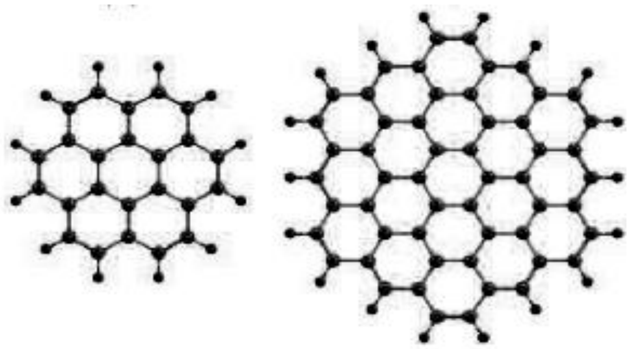

Figure 1. Two first members of the *Polycyclic Aromatic Hydrocarbons* PAH_k.

Theorem 1. The Theta polynomial $\Theta(G,x)$ and the Theta index $\Theta(G)$ $\forall k\geq 1$, are equal to

$$\Theta(PAH_k,x)=\sum_{i=0}^{k-1}6(k+i)x^{k+i}+(6k)x^{2k}$$

$$\Theta(PAH_k)=14k^3-3k^2+k.$$

Proof. Consider be the general representation of *Polycyclic Aromatic Hydrocarbons* PAH_k ($\forall k\geq 1$) with $6k^2+6k$ vertices/atoms and $9k^2+3k$ edge/chemical bonds.

Because, there are $6k^2$ Carbon atoms with degree 3 and $6k$ Hydrogen atoms with degree 1in vertex set $V(PAH_n)$, thus

$$|E(PAH_k)|=\frac{3\times 6k^2+1\times 6k}{2}=9k^2+3k$$

Now, we counting all opposite edge strips *ops* $m(PAH_k,c)$ of the general representation of *Polycyclic Aromatic Hydrocarbons* PAH_k, by using the Cut Method. The *Cut Method* and its general form studied by *S. Klavzar* [42].

By using the Cut Method, we see that the Polycyclic Aromatic Hydrocarbons is a co-graph and from Figure 2, one can see that there are $k+1$ distinct case of *qoc strips* for PAH_k such that the size of a *qoc strip* C_i for $\forall i=1,..,k-1$ is equal to $k+i$ ($=|C_i|=c_i$) and for $i=0$, $|C_0|=k$.

In other words,

- For $i=0$; $m(PAH_k,c_0)=6$ and $|C_k|=k$.
- For *all* $i=1,..,k-1$; $m(PAH_k,c_i)=6$ and $|C_i|=k+i$.
- For $i=k$; $m(PAH_k,c_k)=3$ and $|C_k|=2k$.

Thus the Theta polynomial of the Polycyclic Aromatic Hydrocarbons PAH_k ($\forall k\geq 1$) will be

$$\Theta(PAH_k,x)=\sum_c m(PAH_k,c).c.x^c$$

$$=\sum_{i=0}^{k}m(PAH_k,c_i).c_i.x^{c_i}$$

$$=m(PAH_k,c_0)|C_0|x^{|C_0|}+m(PAH_k,c_1)|C_1|x^{|C_1|}+\ldots$$

$$+m(PAH_k,c_{k-1})|C_{k-1}|x^{|C_{k-1}|}+m(PAH_k,c_k)|C_k|x^{|C_k|}$$

$$=6|C_0|x^{|C_0|}+6|C_1|x^{|C_1|}+\ldots+6|C_{k-1}|x^{|C_{k-1}|}+3|C_k|x^{|C_k|}$$

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

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

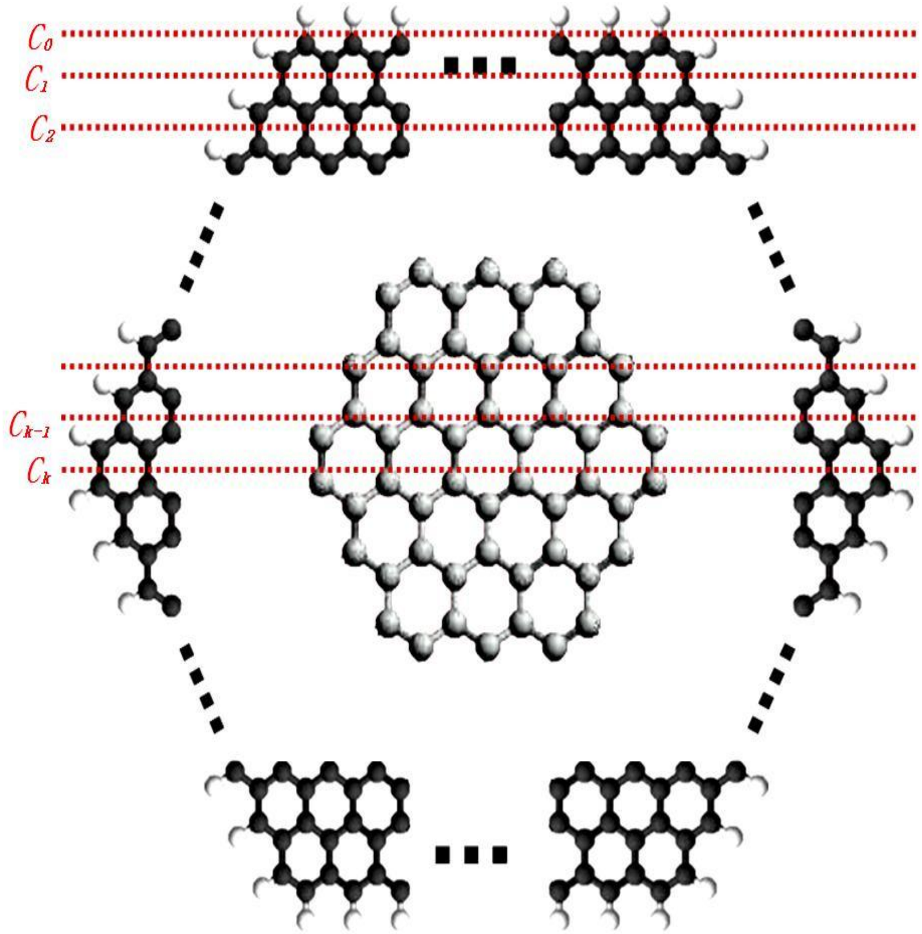

Figure 2. The presentation of quasi-orthogonal cuts qoc strips of Circumcoronene PAH_3.

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

$$=\frac{\partial}{\partial x}\left(6(k)x^k+6(k+1)x^{k+1}+\ldots+6(2k-1)x^{2k-1}+3(2k)x^{2k}\right)_{x=1}$$

$$=\left(6(k)^2x^{k-1}+6(k+1)^2x^k+\ldots+6(2k-1)^2x^{2k-2}+3(2k)^2x^{2k-1}\right)_{x=1}$$

$$=\left(\sum_{i=0}^{k-1}6(k+i)^2\mathrm{x}^{k+i-1}+12k^2x^{2k-1}\right)_{x=1}$$

$$=\sum_{i=1}^{k-1}6(k+i)^2+12k^2$$

$$=6k^2(k-1)+12k\left(\frac{k^2}{2}-\frac{k}{2}\right)+6\left(\frac{k^3}{3}-\frac{k^2}{2}+\frac{k}{6}\right)+12k^2$$

$$=14k^3-3k^2+k$$

Here the proof of theorem is completed.■

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