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**Research Article**

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# The Sadhana polynomial and the Sadhana index of polycyclic aromatic hydrocarbons $PAH_K$

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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. The topological index of a graph G is a numeric quantity related to G which is invariant under automorphisms of G. The Omega polynomial Ω(G,x) for counting qoc strips in G is defined as* $\Omega(G,x)=\sum_c m(G,c)x^c$ *with m(G,c) being the number of strips of length c. Also, know that the Sadhana polynomial and the Sadhana Index are equal to* $Sd(G,x)=\sum_c m(G,c)x^{|E(G)|-c}$ *and* $Sd(G)=\sum_c m(G,c)(|E(G)|-c)$*, respectively. The aim of this paper is to compute this counting polynomial and its index of an family of hydrocarbons that we named: Polycyclic Aromatic Hydrocarbons* $PAH_k$ *(* $\forall k\geq 1$*).*

**Keywords:** Molecular Graph, Polycyclic Aromatic Hydrocarbons PAHk, Sadhana Polynomial Omega polynomial, qoc strip, Cut Method.

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## 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. We consider three representations of molecules as graphs “molecular graphs”. In molecular graph, vertices are atom types, edges are bond type.

In chemical graph theory and mathematical chemistry, *Topological Indices* are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure [1-14]. The simplest topological indices do not recognize double bonds and atom types.

One of the oldest graph invariants is the *Wiener index*, *W(G)*, introduced by the chemist *Harold Wiener* [11] in 1947. It is defined as the sum of topological distances *d(u,v)* between any two atoms in the molecular graph (summation runs over all the unordered pairs *u,v* of distinct vertices in *G*.)

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

where the distance $d(u,v)$ between $u$ and $v$ is defined as the length of a minimum path between $u$ and $v$.

Suppose $G$ is an arbitrary simple connected molecular graph with the vertex set $V(G)$ and edge set $E(G)$ and $x,y\in V(G)$. 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 $k$. It is easy to see that the relation "co" is reflexive and symmetric but it is not necessary to be transitive [15, 16].

Set $C(e):=\{f\in E(G) \mid f \text{ co } e\}$. 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.

In 2006 [17], *M.V. Diudea* introduced the Omega polynomial $\Omega(G,x)$ for counting qoc strips in $G$ as

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

Such that $m(G,c)$ being the number of strips of length $c$ and this summation runs up to the maximum length of *qoc* strips in $G$. Also, first derivative of omega polynomial (in $x=1$), equals the number of edges in the graph $G$. For more study, see papers [15-29]:

$$\Omega'\left(\mathrm{G},1\right)=\sum\nolimits_{c}\mathrm{m}\left(\mathrm{G},c\right)\times c=\left|E\left(G\right)\right|.$$

In 2008, *Ashrafi* and co-authors [23] introduced the *Sadhana polynomial Sd(G,x)*, was defined as

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

The Sadhana index $Sd(G)$, for counting *qoc* strips in $G$ was defined by *P.V. Khadikar et.al* [30, 31] as first derivative of the Sadhana polynomial (in $x=1$)

$$Sd(G)=\sum\nolimits_{c} m\left(G,c\right)\left(\left|E\left(G\right)\right|-c\right).$$

In this present study, we compute the Sadhana polynomial and its index of an family of hydrocarbon molecular graph that we named: *Polycyclic Aromatic Hydrocarbons* $PAH_k$ $(\forall k\geq 1)$.

## RESULTS AND DISCUSSION

In this section is to compute the Omega polynomial of a family of hydrocarbon molecules, which called *Polycyclic Aromatic Hydrocarbons* $PAH_k$.

The *Polycyclic Aromatic Hydrocarbons* $PAH_k$ is ubiquitous combustion products. They have been implicated as carcinogens and play a role in graphitization of organic materials [32]. In addition, they are of interest as molecular analogues of graphite [33] as candidates for interstellar species [34] and as building blocks of functional materials for device applications [32-34]. Synthetic routes to Polycyclic Aromatic Hydrocarbons $PAH_k$ are available [35] and a detailed knowledge of all these features would therefore be necessary for the tuning of molecular properties towards specific applications.

In references [32-66] some properties and more historical details of this family of hydrocarbon molecules are studded. Reader can see that some first members of the *Polycyclic Aromatic Hydrocarbons* $PAH_k$ in Figure 1.

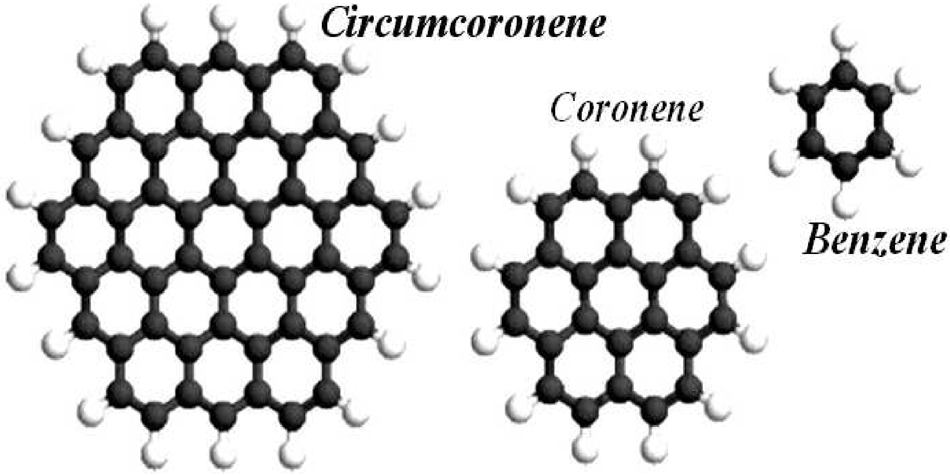


**Figure 1. Some first members (Benzene, Coronene and Circumcoronene) of the Polycyclic Aromatic Hydrocarbons $PAH_k$**

Consider the general representation of this *Polycyclic Aromatic Hydrocarbons* $PAH_k$ ($\forall k\geq 1$) with $6k^2+6k$ vertices/atoms such that $6k^2$ of them are Carbon atoms and also $6k$ of them Hydrogen atoms and the number of edge/chemical bonds in $PAH_k$ is equal to:

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

Now, for computing the Sadhana polynomial and Sadhana index of this Polycyclic Aromatic Hydrocarbons, we should calculate all opposite edge strips *ops.*

By using the Cut Method for the Polycyclic Aromatic Hydrocarbons $PAH_k$, we can see that $PAH_k$ is a co-graph (The *Cut Method* and its general form studied by *S. Klavžar* [67] and others [68-70]).

Thus from Figure 2 and using the Cut method, one can see that there are $k+1$ distinct cases of *qoc strips* for $PAH_k$, such that the size of a *qoc strip* $C_i$ for $i=1.k-1$ is equal to $k+i$ and $\forall e\in C_i$ there are $k+i-1$ co-distant edges with $e$ and the number of repetition of these *qoc strip* $C_i$ is six. Also, for first cut $C_0$, $|C_0|=k$. From Figure 2, for especial *qoc strip* $C_k$ with three repetition, $|C_k|=2k$.

Now by using above mentions, we can compute the Sadhana polynomial and its index of Polycyclic Aromatic Hydrocarbons $PAH_k$ $\forall k\geq 1$ as follow:

The Sadhana polynomial of $PAH_k$ is equal to:

$$Sd(PAH_k,x)=\sum_c m\left(PAH_k,c\right)\mathrm{x}^{|E(PAH_k)|-c}$$

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

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

$$=6x^{9k^2+2k}+6x^{9k^2+2k-1}+\ldots+6x^{9k^2+k+1}+3x^{9k^2+k}$$

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

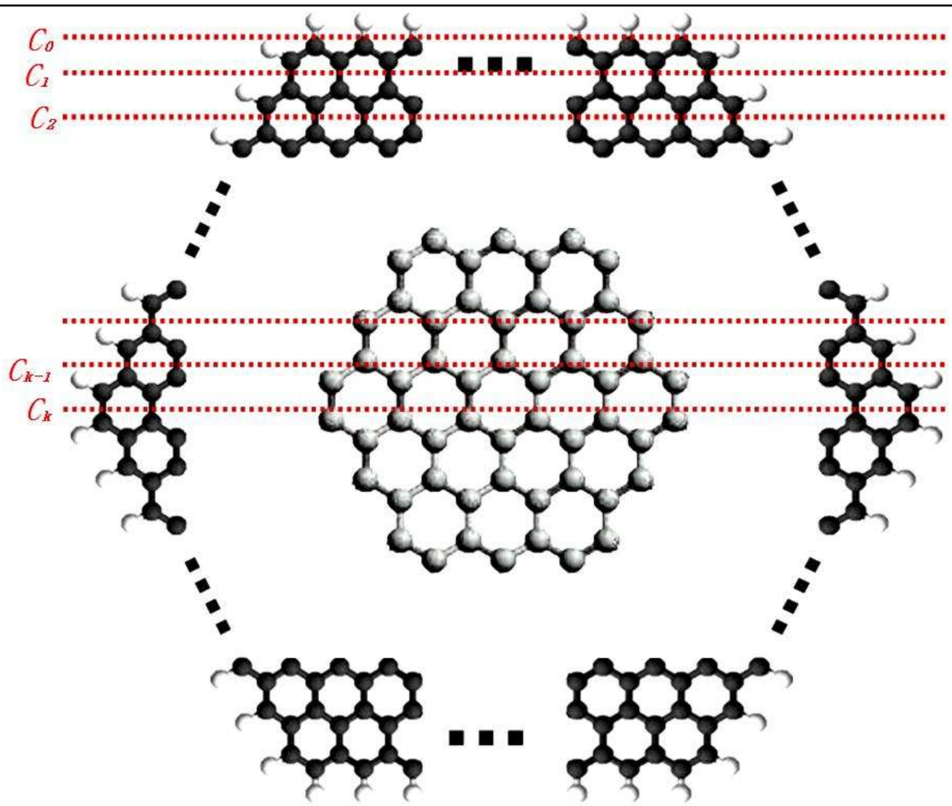


**Figure 2.** ***The presentation of quasi-orthogonal cuts qoc strips of Circumcoronene PAHk.***

The Sadhana index of $PAH_k$ is equal to:

$$Sd(PAH_k)=Sd'(PAH_k,x)\,\Big|_{x=1}=\left[\sum_{i=1}^{k}\left(6x^{9k^2+k+i}\right)+3x^{9k^2+k}\right]_{x=1}$$

$$=\left[\sum_{i=1}^{k}6\left(9k^2+k+i\right)x^{9k^2+k-1+i}+3\left(9k^2+k\right)x^{9k^2+k-1}\right]_{x=1}$$

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

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

$$=6k^2(9k+1)+6[\tfrac{1}{2}k(k+1)]+3k(9k+1)$$

$$=54k^3+36k^2+6k.$$

Thus, the Sadhana polynomial and Sadhana index of this Polycyclic Aromatic Hydrocarbons $PAH_k$ will be

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

$$Sd(PAH_k)=6k(3k+1)^2. \qquad \blacksquare$$

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