Sadhana polynomial and its index of hexagonal system $B_{a,b}$

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Abstract: Let G be an arbitrary graph. Two edges $e=uv$ and $f=xy$ of G are called *co-distant* (briefly: *e co f*) if they obey the topologically parallel edges relation. The Sadhana polynomial $Sd(G,x)$, for counting *qoc* strips in G was defined by Ashrafi and co-authors as $Sd(G,x) = \sum_c m(G,c) x^{|E(G)|-c}$, where $m(G,c)$, being the number of *qoc* strips of length c. This polynomial is most important in some physico chemical structures of molecules. In this paper, we compute the Sadhana polynomial and its index of an important class of benzenoid system.

Keywords: Molecular Graph, Omega Polynomial, Sadhana Polynomial, Benzenoid, Qoc Strip, Cut Method, Orthogonal Cut

1. Introduction

For a molecular graph G, there exits many topological indices in mathematical 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 a branch of mathematical chemistry which applies graph [1-3].

A topological index of G is a numeric quantity, derived following certain rules in Chemistry, which can be used to characterize the property of molecule and is invariant on the automorphism of the graph.

The Wiener index is the first topological index recognized in chemical graph theory, and it is often referred to as the topological index [3]. *Wiener index* defined as

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

where the distance $d(u,v)$ between two vertices u and v is the number of edges in a shortest path connecting them.

Let G be a simple connected graph in chemical graph theory. The vertex set and edge set of G denoted by $V(G)$ and $E(G)$ respectively and its vertices correspond to the atoms and the edges correspond to the bonds.

Two edges $e=uv$ and $f=xy$ of G are called *codistant* (briefly: *e co f*) if they obey the topologically parallel edges relation [4]. For some edges of a connected graph G there are the following relations satisfied [5-10]

$$e \; co \; e$$

$$e \; co \; f \leftrightarrow f \; co \; e$$

$$e \; co \; f \; \& \; f \; co \; h \rightarrow f \; co \; h$$

though the last relation is not always valid. Set $C(e):=\{f \in E(G)|e \; co \; f\}$. If the relation "co" is transitive on $C(e)$ then C(e) is called an *orthogonal cut "oc"* of the graph G. Thus for a co-graph G, there is the union of disjoint orthogonal cuts for $i \neq j$ and $i, j=1, 2, ..., k$ as $E(G) = \mathcal{C}_1 \cup \mathcal{C}_2 \cup ... \cup \mathcal{C}_{k-1} \cup \mathcal{C}_k$ and $\mathcal{C}_i \cap \mathcal{C}_j = \emptyset$,

The *Omega Polynomial $\Omega(G,x)$* for counting *qoc* strips in G was defined by *Diudea* as

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

where $m(G,c)$, be the number of *qoc* strips of length c (*i.e.*, the number of cut-off edges) in the graph G. The summation runs up to the maximum length of *qoc* strips in G.

In 2008, *Ashrafi* and co-authors [11] introduced the *Sadhana polynomial $Sd(G,x)$*, was defined as

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

The Sadhana index $Sd(G)$, for counting *qoc* strips in G was defined by *Khadikar et.al* [12, 13] as first derivative of

sadhana polynomial (in $x = 1$),

$$Sd(G) = \sum_c m(G,c)(|E(G)|-c)$$

For some chemical applications of these counting polynomial see papers [14-20]. The aim of this study is to compute the Sadhana polynomial and Sadhana index of a benzenoid system and called "hexagonal system $B_{a,b}$". The hexagonal system $B_{a,b}$ is family of molecular graph, which consist several copy of benzene C_6 on circumference. *Shui Ling-Ling* et al. defined a new hexagonal system named jagged-rectangle. An $a\times b$ hexagonal jagged-rectangle whose shape forms a rectangle and the number of hexagonal cells in each chain alternate a and $a-1$. For $a \geq 2$, the vertex set of $B_{a,b}$ defined as [21-23].

$$V(B_{a,b}) = \{(x,y) \mid 0 \leq x \leq 2a, 0 \leq y \leq 2b-1\}$$
$$\cup \{(x,-1) \mid 0 \leq x \leq 2a-1\} \cup \{(x,2b) \mid 1 \leq x \leq 2a-1\}$$

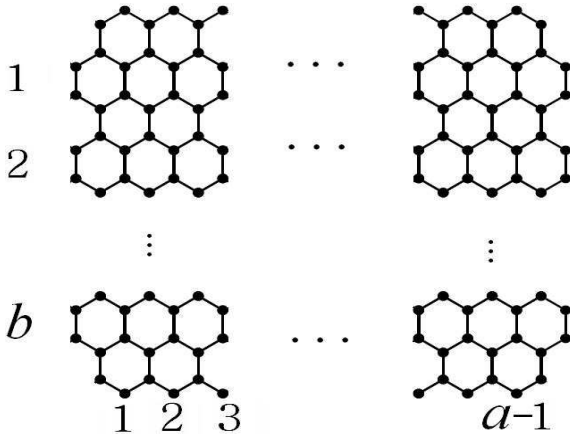Reader can see general representation of this benzenoid system in Figure 1.

Figure. 1. *A general representation of the hexagonal system $B_{a,b}$ ($a,b \geq 1$).*

2. Main Results

In this section Sadhana polynomial and its index of hexagonal system $B_{a,b}$ are determined. For this computation, suppose that $G=B_{a,b}$ has $4ab+4a+2b-2$ vertices and $6ab+5a+b-4$ edges. In the following theorem we compute the Sadhana polynomial of G (Figure1).

Theorem 1: The Sadhana polynomial of hexagonal system $B_{a,b}$ is equal to

- $\forall \; a \geq b+2$, $Sd(B_{a,b},x) = (b+1)x^{|E(B_{a,b})|-a} + bx^{|E(B_{a,b})|-a-1}$

  $$+4\sum_{i=1}^{b} x^{|E(B_{a,b})|-2i-1} + 2(a-b-1)x^{|E(B_{a,b})|-2b-2}$$

- $\forall \; a \leq b+1$, $Sd(B_{a,b},x) = (b+1)x^{|E(B_{a,b})|-a} + bx^{|E(B_{a,b})|-a-1}$

$$+4\sum_{i=1}^{a-1} x^{|E(B_{a,b})|-2i-1} + 2(b-a+1)x^{|E(B_{a,b})|-2a}$$

Then the Sadhana index of $B_{a,b}$ is

- $\forall \; a \geq b+2$,
  $Sd(B_{a,b}) = 12a^2b+24ab^2+10a^2+14ab-2b^2-16a-14b+6$
- $\forall \; a \leq b+1$,
  $Sd(B_{a,b}) = 12a^2b+24ab^2+10a^2+10ab+4b^2-18a-18b+8$

Proof. Let $G=B_{a,b}$ be the hexagonal system. By using the *Cut Method,* and by using following tables and figures the proof is easy. *Cut Method* and its general form studied by *S. Klavzar* [24] and used in paper series [8, 19, 20, 23-28]. Now by using this method, it is easy to see that hexagonal system is a co-graph. All distinct *qoc strips* of G are shown in Figure 2 and numerated in Table 1 and Table 2.

Table 1. *The number of co-distant edges, when $a \geq b+2$.*

quasi-orthogonal cuts	Number of co-distant edges	No
$C_{2i+1} \;\; \forall \; i=0,...,b$	1	a
$C_{2i} \;\; \forall \; i=1,...,b$	1	$a+1$
$C_i \;\; \forall \; i=1,...,b$	4	$2i+1$
C_{b+1}	$2(a-b-1)$	$2b+2$

Table 2. *The number of co-distant edges, when $a \leq b+1$.*

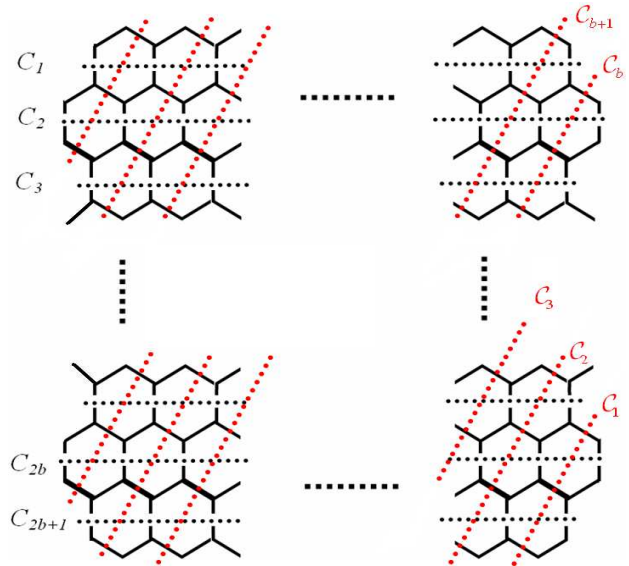| quasi-orthogonal cuts	Number of co-distant edges	No
$C_{2i+1} \;\; \forall \; i=0,...,b$	1	a
$C_{2i} \;\; \forall \; i=1,...,b$	1	$a+1$
$C_i \;\; \forall \; i=1,...,a-1$	4	$2i+1$
C_a	$2(b-a+1)$	$2a$

Figure. 2. *The presentation of quasi-orthogonal cuts (qoc strips) of $B_{a,b}$.*

This implies that

$$Sd(B_{a,b},x) = \sum_c m\left(B_{a,b},c\right)x^{\left|E(B_{a,b})\right|-c}$$

$$= \sum_{i=0}^{b} m\left(B_{a,b},C_{2i+1}\right)x^{\left|E(B_{a,b})\right|-|C_{2i+1}|} + \sum_{i=1}^{b} m\left(B_{a,b},C_{2i}\right)x^{\left|E(B_{a,b})\right|-|C_{2i}|}$$

$$+ \sum_{i=1}^{b} m\left(B_{a,b},C_i\right)x^{\left|E(B_{a,b})\right|-|C_i|} + m\left(B_{a,b},C_b\right)x^{\left|E(B_{a,b})\right|-|C_b|}$$

$$= (b+1)x^{\left|E(B_{a,b})\right|-a} + bx^{\left|E(B_{a,b})\right|-a-1}$$

$$+ 4\sum_{i=1}^{b} x^{\left|E(B_{a,b})\right|-2i-1} + 2(a-b-1)x^{\left|E(B_{a,b})\right|-2b-2}$$

where $|E(B_{a,b})| = 6ab+5a+b-4\ (=e)$.

$$Sd\left(B_{a,b}\right) = Sd'\left(B_{a,b},x\right)\big|_{x=1}$$

$$= \frac{\partial\left((b+1)x^{\left|E(B_{a,b})\right|-a} + bx^{\left|E(B_{a,b})\right|-a-1} + 4\sum_{i=1}^{b} x^{\left|E(B_{a,b})\right|-2i-1} + 2(a-b-1)x^{\left|E(B_{a,b})\right|-2b-2}\right)}{\partial x}\bigg|_{x=1}$$

$$= (e-a)(b+1) + b(e-a-1) + 4\sum_{i=1}^{b}(e-2i-1) + 2(a-b-1)(e-2b-2)$$

$$= \left(e(2b+1)-2ab-a-b\right) + \left(4eb-4b-8\left(\frac{b(b+1)}{2}\right)\right) + \left(2e(a-b-1)+4b-2b^2-2ab-2a+2\right)$$

$$= 12a^2b+24ab^2+10a^2+14ab-2b^2-16a-14b+6$$

And also for $a \leq b+1$

$$Sd\left(B_{a,b}\right) = \frac{\partial\left((b+1)x^{\left|E(B_{a,b})\right|-a} + bx^{\left|E(B_{a,b})\right|-a-1} + 4\sum_{i=1}^{a-1} x^{\left|E(B_{a,b})\right|-2i-1} + 2(b-a+1)x^{\left|E(B_{a,b})\right|-2a}\right)}{\partial x}\bigg|_{x=1}$$

$$= (e-a)(b+1) + b(e-a-1) + 4\sum_{i=1}^{a-1}(e-2i-1) + 2(b-a+1)(e-2a)$$

$$= \left(e(2b+1)-2ab-a-b\right) + \left(4e(a-1)-4a+4-8\left(\frac{a(a-1)}{2}\right)\right) + \left(2e(b-a+1)+4a^2-4ab-4a\right)$$

$$= 12a^2b+24ab^2+10a^2+10ab+4b^2-18a-18b+8$$

Theorem 2: $\forall a \in \mathbb{N}$, the Sadhana polynomial of hexagonal system $B_{a,a}$ is equal to

$$Sd(B_{a,a},x) = ax^{6a^2+5a-5} + (a+1)x^{6a^2+5a-4}$$

$$+ 4\sum_{i=1}^{a-1} x^{6a^2+6a-2i-5} + 2x^{6a^2+4a-4}$$

where $|E(B_{a,b})| = 6a^2+6a-4$.

Also, the Sadhana index of $B_{a,a}$ is equal to

$$Sd(B_{a,a}) = 36a^3+24a^2-36a+8$$

And also, from Table 2, $\forall\ a \leq b+1$:

$$Sd(B_{a,b},x) = \sum_{i=0}^{b} m\left(B_{a,b},C_{2i+1}\right)x^{\left|E(B_{a,b})\right|-|C_{2i+1}|}$$

$$+ \sum_{i=1}^{b} m\left(B_{a,b},C_{2i}\right)x^{\left|E(B_{a,b})\right|-|C_{2i}|} + \sum_{i=1}^{a} m\left(B_{a,b},C_i\right)x^{\left|E(B_{a,b})\right|-|C_i|}$$

$$= (b+1)x^{\left|E(B_{a,b})\right|-a} + bx^{\left|E(B_{a,b})\right|-a-1}$$

$$+ 4\sum_{i=1}^{a-1} x^{\left|E(B_{a,b})\right|-2i-1} + 2(b-a+1)x^{\left|E(B_{a,b})\right|-2a}$$

Also, the Sadhana index of the hexagonal system is equal to

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