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Article

COMPUTING OMEGA AND SADHANA POLYNOMIALS OF HEXAGONAL TRAPEZOID SYSTEM $T_{B,A}$

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ABSTRACT

Let $G(V,E)$ be a connected graph, with the vertex set $V(G)$ and edge set $E(G)$. Omega polynomial $\Omega(G,x)$, was proposed by *M.V. Diudea.* It was defined on the ground of “opposite edge strips” *ops*. The Sadhana polynomial *Sd* can also be calculated by ops counting and was proposed by *Ashrafi* and co-authors. In this paper we compute the Omega and Sadhana polynomial s and their indices of a Hexagonal system $T_{b,a}$..

Keywords: Molecular graph, Omega polynomial, Sadhana Polynomial, qoc strip, Hexagonal trapezoid system.

1. INTRODUCTION

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. In chemical graph theory and in mathematical chemistry, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory.

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A topological index is a numerical value associated with chemical constitution purporting for correlation of chemical structure properties, chemical reactivity or biological activity.

Let *G*(*V*, *E*) be a connected molecular graph without multiple edges and loops, with the vertex set *V*(*G*) and edge set *E*(*G*), and vertices/atoms $x, y\in V(G)$. Two edges $e=uv$ and $f=xy$ of G are called co-distant, "*e* co *f*", if and only if they obey the following relation: [1, 2]

$$d(v,x)=d(v,y)+1=d(u,x)+1=d(u,y)$$

Relation *co* is reflexive, that is, *e co e* holds for any edge *e* of *G*; it is also symmetric, if *e co f* then *f co e* and in general, relation *co* is not transitive. If "*co*" is also transitive, thus an equivalence relation, then *G* is called a *co-graph* and the set of edges is $C(e):=\{f\in E(G)|e\ co\ f\}$), called an *orthogonal cut* (denoted by *oc*) of *G*. In other words, *E*(*G*) being the union of disjoint orthogonal cuts:

$$E(G)=C_1\cup C_2\cup C_3\cup\ldots\cup C_{k-1}\cup C_k$$

and $C_i\cap C_j=\acute{\emptyset}$ for $i\neq j$ and $i, j=1, 2, \ldots, k$.

Klavžar [3] has shown that relation *co* is a theta *Djoković*-*Winkler* relation [4, 5].

Let $m(G,c)$ be the number of qoc strips of length *c*(i.e., the number of cut-off edges) in the graph *G.*

The *Omega Polynomial* $\Omega(G,x)$ [6-9] for counting *qoc* strips in *G* was defined by *Diudea* as

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

The summation runs up to the maximum length of *qoc* strips in *G*. The first derivative (in *x*=1) equals the number of edges in the graph

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

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

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

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

$\Omega(G,x)$ and $\Theta(G,x)$ polynomials count *"equidistant edges"* in *G* while $Sd(G,x)$ and $\Pi(G,x)$, *"non-equidistant edges"*. The first derivative (computed at $x=1$) of these counting polynomials provide interesting topological indices:

The Sadhana index *Sd*(*G*) was defined by *Khadikar et al*. [10,11] as

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

where $m(G,c)$ is the number of strips of length *c*. The Sadhana polynomial *Sd*(*G*,*x*) was defined by *Ashrafi* and co-authors in 2008, [12].

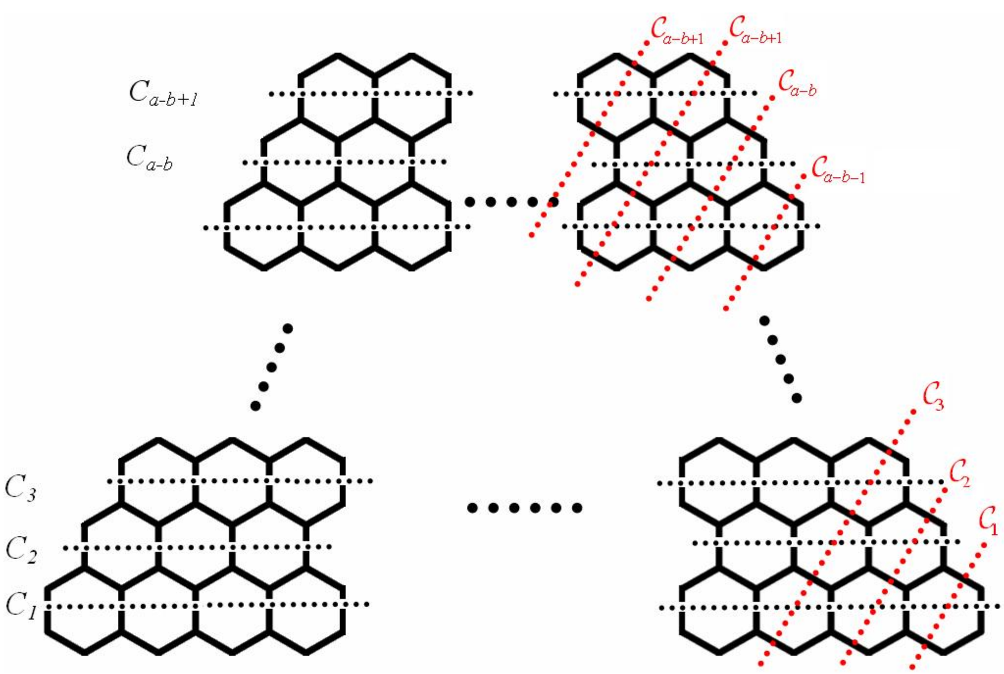
Clearly, the Sadhana polynomial can be derived from the definition of Omega polynomial by replacing the exponent c by $|E(G)|$-c.

Then the Sadhana index will be the first derivative of $Sd(x)$ evaluated at x=1. The aim of this study is to compute the Omega and Sadhana polynomials of a Hexagonal trapezoid system $T_{b,a}$. Here our notations are standard and mainly taken from [13-16].

2. RESULTS AND DISCUSSION

In this section we compute counting polynomials mentioned in the text of a family of benzenoid graphs (see Figure 1 and references [16-18]) that called Hexagonal trapezoid system Tb,a. A hexagonal trapezoid Tb,a ∀a,b∈ℕ & a≥b is a hexagonal system consisting a−b+1 rows of benzenoid chain in which every row has exactly one hexagon less than the immediate row. An especial case of this family is triangular benzenoid Gn, that is equivalent with a hexagonal trapezoid system T1,n. It is easy to see that the triangular benzenoid Gn ∀n∈ℕ has n2+4n+1 vertices and $\frac{3}{2}n(n+3)$ edges (see Figure 2).

Figure 1: A general representation of the hexagonal trapezoid system $T_{b,a}$ ($\forall a,b \in \mathbb{N}$)



Theorem 1: The Omega polynomial of the Hexagonal Trapezoid System Tb,a ($\forall$a,b$\in\mathbb{N}$) is as follows:

$$\Omega(T_{b,a},x)=\sum_{i=1}^{a-b+1} x^{a+2-i}+\sum_{i=1}^{a-b} 2x^{i+1}+2bx^{a-b+2}$$

Proof. Let $G=T_{b,a}$ be the hexagonal trapezoid system. In general case the number of vertices of hexagonal trapezoid $T_{b,a}$ is equal to $2a+1+\sum_{i=2b+1}^{2a+1} i=a^2-b^2+4a+2$ for all $a,b\in\mathbb{N}$ and the number of edges of $T_{b,a}$ is equal to $2a+\sum_{i=3b+1}^{3a+1} i=\frac{3}{2}(a^2-b^2)+\frac{9}{2}a+\frac{b}{2}+1$.

To compute the Omega polynomial of G, it is enough to calculate $C(e)$ for every e in $E(G)$. Thus, from Table 1 we have

$$\Omega(T_{b,a},x)=\sum_c \mathrm{m}(T_{b,a},c)\mathrm{x}^c$$

$$=\sum_{c_i,i=1}^{a-b+1} \mathrm{m}(T_{b,a},c_i)\mathrm{x}^{c_i}+\sum_{C_i,i=1}^{a-b} \mathrm{m}(T_{b,a},C_i)\mathrm{x}^{C_i}+\mathrm{m}(T_{b,a},C_{a-b+1})\mathrm{x}^{C_{a-b+1}}$$

$$=\sum_{i=1}^{a-b+1} x^{a+2-i}+\sum_{i=1}^{a-b} 2x^{i+1}+2bx^{a-b+2}$$

$$=x^{a-b+2}+x^{a-b+1}+\ldots+x^{a+1}+x^{a}+2x^2+2x^3+\ldots+2x^{a-b+1}+2bx^{a-b+2}$$

Hence we proved Theorem 1. ■

Table 1: The number of co-distant edges for all natural numbers *a,b* such that $a\geq b$

quasi-orthogonal cuts	Number of co-distant edges	No
c_i $\forall i=1,\ldots,a-b+1$	$a-i+2$	1
C_i $\forall i=1,\ldots, a-b$	$i+1$	2
C_{a-b+1}	$a-b+2$	$2b$

Theorem 2: The Sadhana polynomial of the hexagonal trapezoid system $T_{b,a}$ is

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

And the Sadhana index of $T_{b,a}$ is equal to

$$Sd(T_{b,a})=\tfrac{1}{2}(9a^3+27a^2-3b^3-b^2)-6a^2b+6ab+3a$$

Proof. The proof is analogous to the proof of Theorem 1 and by using Table 1, we have

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

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

$$+m(T_{b,a},C_{a-b+1})x^{\left|E(T_{b,a})\right|-C_{a-b+1}}$$

$$=\sum_{i=1}^{a-b+1} x^{|E|+i-a-2}+\sum_{i=1}^{a-b}2x^{|E|-i-1}+2bx^{|E|+b-a-2}$$

where $|E(T_{b,a})|=\frac{3}{2}(a^2-b^2)+\frac{9}{2}a+\frac{b}{2}+1.$

And also the Sadhana index of $T_{b,a}$ is equal to

$$Sd'\left(T_{b,a},x\right)\big|_{x=1}=\left[\sum_{i=1}^{a-b+1}(|E|+i-a-2)x^{|E|+i-a-3}+2\sum_{i=1}^{a-b}(|E|-i-1)x^{|E|-i-2}+2b(|E|+b-a-2)x^{|E|+b-a-3}\right]_{x=1}$$

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

$$=\left(\frac{a^2+b^2+-2ab+3a-3b+2}{2}\right)-2\left(\frac{a^2+b^2+-2ab+a-b}{2}\right)$$

$$+(-a^2+2b^2-ab-5a-2)+|E|(3a-b+1)$$

$$=\left(\frac{3a^2-3b^2+9a+b+2}{2}\right)\left(3a-b+1\right)-\left(\frac{3a^2-3b^2+9a+b+2}{2}\right)$$

$$=\tfrac{1}{2}(9a^3+27a^2-3b^3-b^2)-6a^2b+6ab+3a.\blacksquare$$

Corollary 1. [16] Let G_n be the Triangular Benzenoid.

- The Omega polynomial of G_n is equal to $\Omega(G_n,x)=3x^2+3x^3+\ldots+3x^{n+1}$
- The Sadhana polynomial of G_n is equal $Sd(G_n,x)=3x^{|E|-2}+3x^{|E|-3}+\ldots+3x^{|E|-n-1}$

where $|E|=\frac{3}{2}n(n+3)$ and the Sadhana index $Sd(G_n)=\frac{9n^3}{2}+\frac{15n^2}{2}+9n-2.$

Corollary 2. Let LHn=Tn,n be the Linear Hexagonal Chain with 4n+2 vertices and 5n+1 edges ∀n∈ℕ (see Figure 3). One can see that Ω(Gn,x)=2nx2+xn+1, Sd(LHn,x)=2nx5n-1+x4n and Sd(LHn)=10n2+2n.

Figure 2: Graph of Triangular Benzenoid G_7.

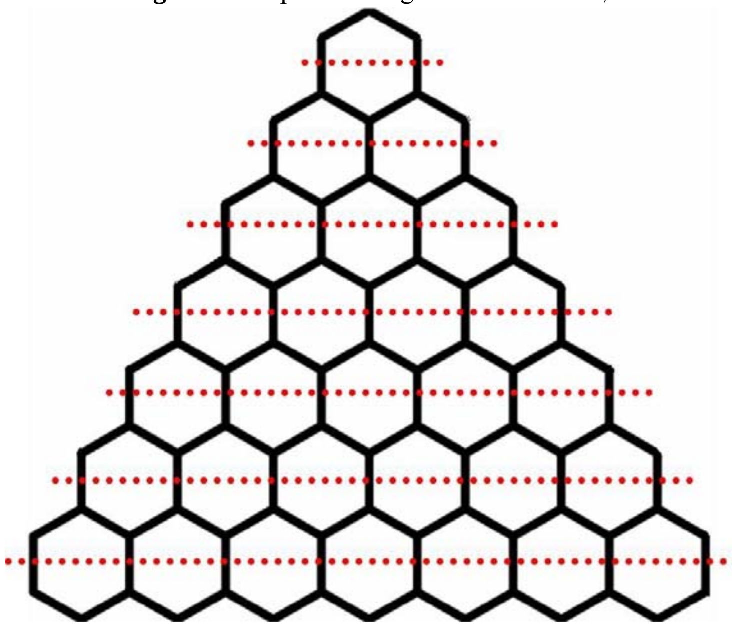
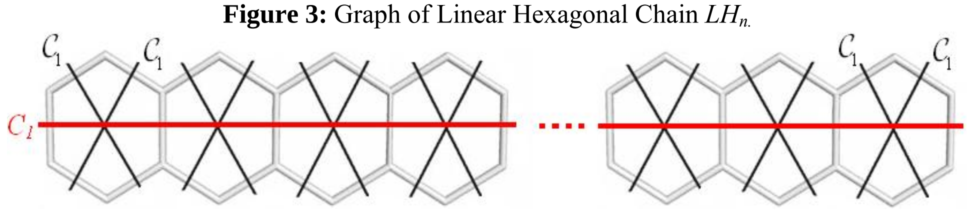


Figure 3: Graph of Linear Hexagonal Chain LH_n.



4. CONCLUSION

In this paper, I was counting a new counting topological polynomial and its index for a family of Hexagonal system "Hexagonal Trapezoid System $T_{b,a}$" and its especial cases "G_n be the Triangular Benzenoid" and "Linear Hexagonal Chain LH_n.". $\Omega(G,x)$ and $Sd(G,x)$ polynomial and their indices are useful for counting the *quasi-orthogonal cut qoc* strip in structure of connected molecular graph, Nanotubes and Nanostructures.

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