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ON OMEGA POLYNOMIALS OF C_{40n+6} FULLERENES

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ABSTRACT. The Omega polynomial is defined as $\Omega(G,x)=\sum_s m\cdot x^s$ where m(G,s) is the number of ops strips of length s. Also, the Sadhana polynomial is defined as $Sd(G,x)=\sum_s m(G,s)\cdot x^{|E|-s}$. This last polynomial has been defined to evaluate the Sadhana index of a molecular graph. In this paper, the Omega and Sadhana polynomials of an infinite family of fullerenes is computed for the first time.

Keywords: Fullerene, Omega and Sadhana Polynomials, Sadhana Index.

INTRODUCTION

Fullerenes are polyhedral molecules, consisting solely of carbon atoms. Fullerenes C_n can be drawn for n = 20 and for all even n ≥ 24. They have n carbon atoms, 3n/2 bonds, 12 pentagonal and n/2-10 hexagonal faces. The most important member of the family of fullerenes is C_{60} [1, 2].

Let G = (V, E) be a connected bipartite graph with the vertex set V = V(G) and the edge set E = E(G), without loops and multiple edges. Two edges e = (u,v) and f = (x,y) of a graph G are called equidistant if the two ends of one edge show the same distance to the other edge. However, the distance between edges can be defined in several modes, as presented below. The distance from a vertex z to an edge e = (u,v) is taken as the minimum distance between the given point and the two endpoints of that edge [3]:

$$d(z,e)=\min\{d(z,u),d(z,v)\} \qquad (1)$$

Then, the edge $e=(u,v)$ is equidistant to $f=(x,y)$ if:

$$d(x,e)=d(y,e) \qquad (2)$$

Or the edges e = (u, v) and f = (x, y) are equidistant if:

$$d(x,e)=d(y,e) \text{ and } d(u,f)=d(v,f) \qquad (3)$$

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A second definition for equidistant edges joins the conditions for (topologically) parallel and perpendicular edges [4]:

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y), \text{ for } \parallel \text{ edges} \quad (4)$$

$$d(u,x) = d(u,y) = d(v,x) = d(v,y), \text{ for } \perp \text{ edges} \quad (5)$$

Omega Polynomial

Two edges e = (u, v) and f = (x, y) 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, 6]:

$$e \text{ co } e \quad (6)$$

$$e \text{ co } f \Leftrightarrow f \text{ co } e \quad (7)$$

$$e \text{ co } f \ \& \ f \text{ co } h \Rightarrow e \text{ co } h \quad (8)$$

though the relation (8) is not always valid.

Let $C(e) := \{f \in E(G); f \text{ co } e\}$ denote the set of edges in G, codistant to the edge $e \in E(G)$. If relation co is an equivalence relation (i.e., all the elements of C(e) satisfy the relations (6) to (8), then G is called a co-graph. Consequently, C(e) is called an orthogonal cut oc of G and E(G) is the union of disjoint orthogonal cuts: $E(G) = C_1 \cup C_2 \cup ... \cup C_k$ and $Ci \cap Cj = \emptyset$ for $i \neq j$, and $i, j = 1, 2,..,k$. Observe co is a Θ relation, (Djoković-Winkler [7,8], relations (6) to (8)), and G is a co-graph if and only if it is a partial cube [9], as Klavžar correctly stated in a recent paper [10].

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 an opposite edge strip ops, which is a quasi-orthogonal cut qoc strip. This means the transitivity relation (8) of the co relation is not necessarily obeyed. Any oc strip is an ops but the reverse is not always true.

Let m(G,s) be the number of ops of length s (i.e., the number of cut-off edges) in the graph G; for the sake of simplicity, m(G,s) will hereafter be written as m. The counting polynomials, defined on the ground of ops strips, [3, 5, 11-14] are as follows:

$$\Omega(G,x) = \sum_s m \cdot x^s \quad (9)$$

$$Sd(G,x) = \sum_s m x^{(|E(G)|-s)} \quad (10)$$

In a counting polynomial, the first derivative (in x=1) defines the type of property which is counted:

$$\Omega'(G,1) = \sum_s m \cdot s = e = |E(G)| \quad (11)$$

$$Sd'(G,1) = \sum_s m(|E(G)| - s) = Sd(G) \quad (12)$$

The Sadhana index Sd(G) of a graph G was defined by Khadikar *et al*. [12, 13] while the Sadhana polynomial by Ashrafi *et al*. [14]. From the definition of Omega polynomial, one can obtain the Sadhana polynomial by replacing x^s with $x^{|E(G)|-s}$ in Omega polynomial. Then the Sadhana index will be the first derivative of Sd(G,x) evaluated in x=1 [14]. Our notations are standard as taken from the textbooks and articles on Graph Theory [15-24].

Example 1. Suppose K_n denotes the complete graph on n vertices (see Figure 1). Then we have:

$$\Omega(K_n, x) = \binom{n}{2} x = (1/2)n(n-1)x \; ; \quad Sd(K_n, x) = (1/2)n(n-1)x^{(1/2)(n^2-n-2)}$$

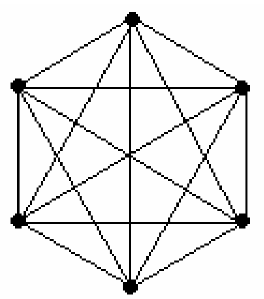

Figure1. Complete graph K_6.

Example 2. Let C_n denotes the cycle of length n. Then we have:

$$\Omega(C_n, x) = \begin{cases} \frac{n}{2}x^2 & 2 \mid n \\ nx & 2 \nmid n \end{cases} \; ; \quad Sd(C_n, x) = \begin{cases} \frac{n}{2}x^{n-2} & 2 \mid n \\ nx^{n-1} & 2 \nmid n \end{cases}.$$

Example 3. Let T_n be a tree on n vertices. We know that $|E(T_n)| = n-1$. Thus, $\Omega(T_n, x) = (n-1)x$; $Sd(T_n, x) = (n-1)x^{n-2}$.

RESULTS AND DISCUSSION

The aim of this section is to compute the counting polynomials of equidistant edges (Omega and Sadhana polynomials) of an infinite family C_{40n+6} of fullerenes with 40n+6 carbon atoms and 60n+9 bonds (the graph in Figure 2 is n = 2).

Theorem. The omega polynomial of fullerene graph C_{40n+6} is as follows:

$$\Omega(G,x)=\begin{cases} a(x)+4x^{2n}+4x^{2n+1}+4x^{4n-1}+2x^{4n} & 5\,|\,n \\ a(x)+2x^{4n+3}+8x^{2n-2}+2x^{4n+4}+2x^{4n+1} & 5\,|\,n-1 \\ a(x)+8x^{2n}+4x^{2n-1}+2x^{4n}+2x^{4n+2} & 5\,|\,n-2 \\ a(x)+4x^{2n-2}+4x^{2n+2}+4x^{4n-1}+2x^{4n+2} & 5\,|\,n-3 \\ a(x)+4x^{2n-2}+4x^{2n-1}+4x^{2n}+2x^{4n+3}+x^{8n+6} & 5\,|\,n-4 \end{cases}$$

in which $a(x)=x+9x^2+4x^3+2x^4+(2n-3)x^{10}$.

Proof. By Figure 2, there are ten distinct cases of ops strips. We denote the corresponding edges by e_1, e_2, …, e_{10}. By using Table 1 and Figure 3 the proof is completed.

Corollary. The Sadhana polynomial of the fullerene graph C_{40n+6} is as follows:

$$Sd(G,x)=\begin{cases} b(x)+4x^{|E|-2n}+4x^{|E|-2n-1}+4x^{|E|-4n+1}+2x^{|E|-4n} & 5\,|\,n \\ b(x)+2x^{|E|-4n-3}+8x^{|E|-2n+2}+2x^{|E|-4n-4}+2x^{|E|-4n-1} & 5\,|\,n-1 \\ b(x)+8x^{|E|-2n}+4x^{|E|-2n+1}+2x^{|E|-4n}+2x^{|E|-4n-2} & 5\,|\,n-2 \\ b(x)+4x^{|E|-2n+2}+4x^{|E|-2n-2}+4x^{|E|-4n+1}+2x^{|E|-4n-2} & 5\,|\,n-3 \\ b(x)+4x^{|E|-2n+2}+4x^{|E|-2n+1}+4x^{|E|-2n}+2x^{|E|-4n-3}+x^{|E|-8n-6} & 5\,|\,n-4 \end{cases}$$

in which $b(x)=x^{|E|-1}+9x^{|E|-2}+4x^{|E|-3}+2x^{|E|-4}+(2n-3)x^{|E|-10}$
and $|E|=60n+9$.

Table 1. The number of opposite edges of e_i, $1\le i\le 10$.

No.	Number of opposite edges	Type of Edges
1	1	e_1
9	2	e_2
4	3	e_3
2	4	e_4
2n-3	10	e_5

2	$\begin{cases} 2n+1 & 5 \mid n \\ 4n+3 & 5 \mid n-1 \\ 2n & 5 \mid n-4, n-2 \\ 2n+2 & 5 \mid n-3 \end{cases}$	e_6
$\begin{cases} 2 \\ 4 \\ 4 \end{cases}$	$\begin{cases} 4n-1 & 5 \mid n-3 \\ 2n & 5 \mid n, n-2 \\ 2n-2 & 5 \mid n-1, n-4 \end{cases}$	e_7
$\begin{cases} 4 \\ 4 \\ 2 \end{cases}$	$\begin{cases} 2n-2 & 5 \mid n-1, n-3 \\ 2n-1 & 5 \mid n-2, n-4 \\ 4n-1 & 5 \mid n \end{cases}$	e_8
$\begin{cases} 1 \\ 2 \\ 2 \\ 2 \end{cases}$	$\begin{cases} 8n+6 & 5 \mid n-4 \\ 4n+2 & 5 \mid n-3 \\ 4n+4 & 5 \mid n-1 \\ 4n & 5 \mid n, n-2 \end{cases}$	e_9
2	$\begin{cases} 4n-1 & 5 \mid n, n-3 \\ 4n+1 & 5 \mid n-1 \\ 4n+2 & 5 \mid n-2 \\ 4n+3 & 5 \mid n-4 \end{cases}$	e_{10}
2	$\begin{cases} 2n+1 & 5 \mid n \\ 2n & 5 \mid n-2, n-4 \\ 2n+2 & 5 \mid n-3 \end{cases}$	e_{11}

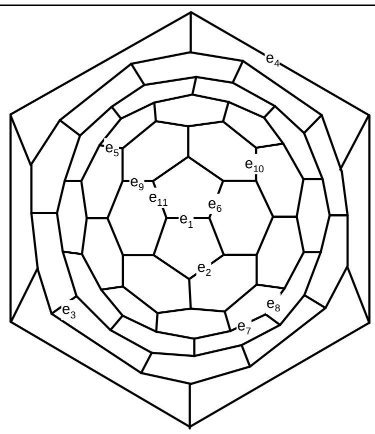

Figure 2. The graph of fullerene C_{40n+6} for n=2.

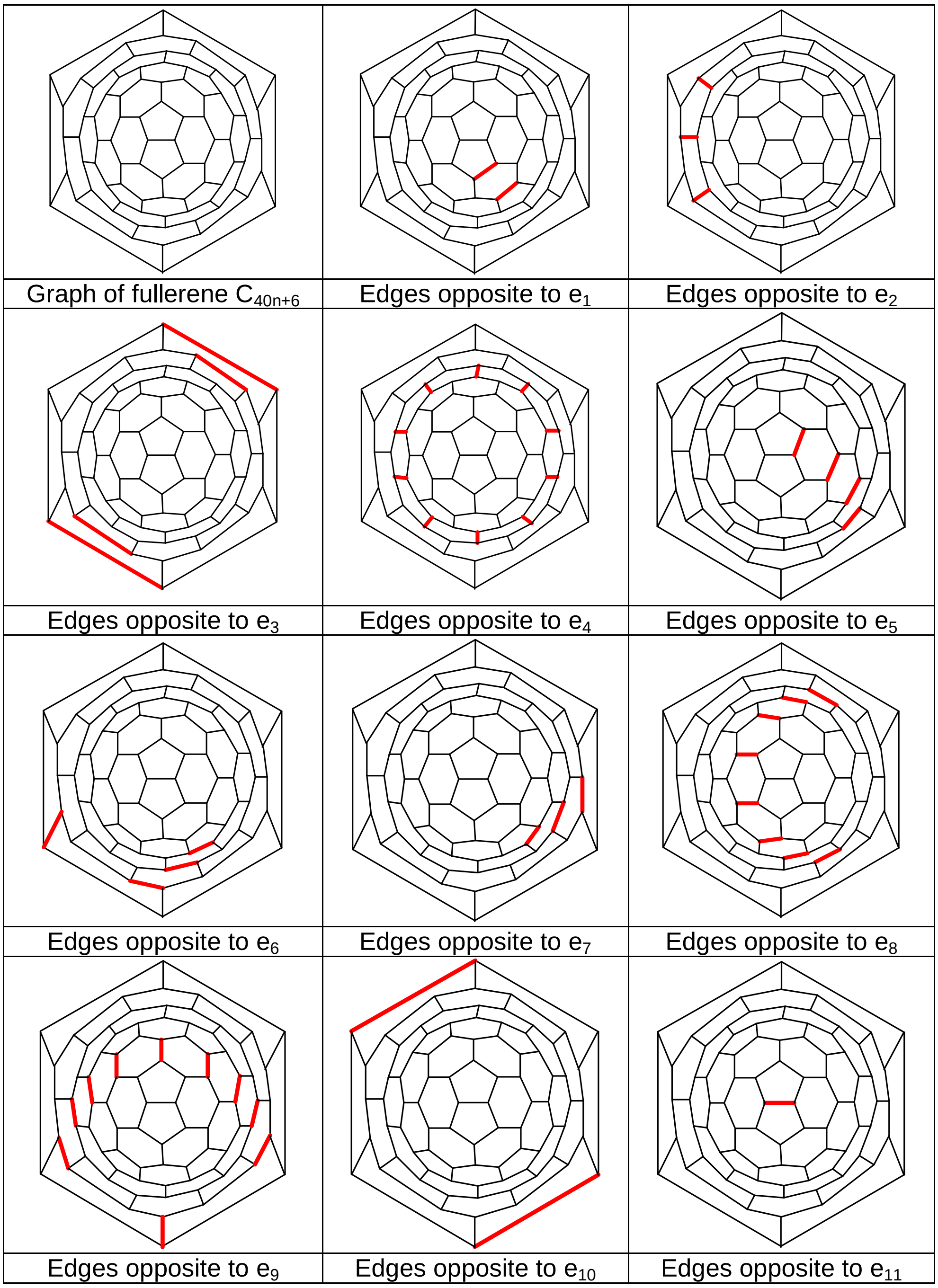

Figure 3. The main cases of opposite edge strips ops in fullerenes C_{40n+6}

CONCLUSIONS

The Omega polynomial was defined by M. V. Diudea in view of counting the opposite edge strips of any length in the graph. He also computed this polynomial for some nanostructures. In this paper, the Omega and the related Sadhana polynomials of an infinite class of fullerenes of formula C_{40n+6} was computed for the first time.

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