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COUNTING POLYNOMIALS OF A NEW INFINITE CLASS OF FULLERENES

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ABSTRACT. Let m(G,c) be the number of strips of length c. The omega polynomial was defined by M. V. Diudea as $\Omega(G,x)=\sum_c m\cdot x^c$. One can obtain the Sadhana polynomial by replacing x^c with $x^{|E|-c}$ in omega polynomial. Then the Sadhana index will be the first derivative of Sd(G,x) evaluated at x = 1. In this paper, the Omega and Sadhana polynomials of a new infinite class of fullerenes is computed for the first time.

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

INTRODUCTION

The discovery of C_{60} bucky-ball, which is a nanometer-scale hollow spherical structure, in 1985 by Kroto and Smalley, revealed a new allotrope of carbon element other than graphite, diamond and amorphous carbon [1,2]. Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms and having pentagonal and hexagonal faces. In this paper, the [4,6] fullerenes C_{8n^2} with tetragonal and hexagonal faces are considered. Let p, h, n and m be the number of tetragons, hexagons, carbon atoms and bonds between them, in a given fullerene F. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is n = (4p+6h)/3, the number of edges is m = (4p+6h)/2 = 3/2n and the number of faces is f = p + h. By the Euler's formula n − m + f = 2, one can deduce that (4p+6h)/3 – (4p+6h)/2 + p + h = 2, and therefore p = 6. This implies that such molecules, made entirely of n carbon atoms, have 6 tetragonal and (n/2 – 4) hexagonal faces.

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. The distance d(x,y) between x and y is defined as the length of a minimum path between x and y. Two edges e = ab and f = xy of G are called codistant, "e co f", if and only if d(a,x) = d(b,y) = k and d(a,y) = d(b,x) = k+1 or vice versa, for a non-negative integer k. It is easy to see that the relation "co" is reflexive and

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symmetric but it is not necessary to be transitive. 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 a co-graph if and only if the edge set E(G) is 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. Three counting polynomials have been defined on the ground of qoc strips [3-7]:

$$\Omega(G,x) = \sum_c m \cdot x^c \tag{1}$$

$$\Theta(G,x) = \sum_c m \cdot c \cdot x^c \tag{2}$$

$$\Pi(G,x) = \sum_c m \cdot c \cdot x^{e-c} \tag{3}$$

$\Omega(G,x)$ and $\Theta(G,x)$ polynomials count equidistant edges in G while $\Pi(G,x)$, non-equidistant edges. In a counting polynomial, the first derivative (in x=1) defines the type of property which is counted; for the three polynomials they are:

$$\Omega'(G,1) = \sum_c m \cdot c = e = |E(G)| \tag{4}$$

$$\Theta'(G,1) = \sum_c m \cdot c^2 \tag{5}$$

$$\Pi'(G,1) = \sum_c m \cdot c \cdot (e-c) \tag{6}$$

The Sadhana index Sd(G) for counting qoc strips in G was defined by Khadikar et al.[8,9] as $Sd(G) = \sum_c m(G,c)(|E(G)|-c)$. We now define the Sadhana polynomial of a graph G as $Sd(G,x) = \sum_c m x^{|E|-c}$. By definition of Omega polynomial, one can obtain the Sadhana polynomial by replacing x^c with $x^{|E|-c}$ in Omega polynomial. Then the Sadhana index will be the first derivative of Sd(G, x) evaluated at x = 1.

A topological index of a graph G is a numeric quantity related to G. The oldest topological index is the Wiener index, introduced by Harold Wiener. Padmakar Khadikar [10,11] defined the Padmakar–Ivan (PI) index as $PI(G) = \sum_{e=uv \in E(G)} [m_u(e|G) + m_v(e|G)]$, where $m_u(e|G)$ is the number of edges of G lying closer to u than to v and $m_v(e|G)$ is the number of edges of G lying closer to v than to u. Edges equidistant from both ends of the edge uv are not counted.

Ashrafi [12,13] introduced a vertex version of PI index, named the vertex PI index and abbreviated by PI_v. This new index is defined as $PI_v(G) = \sum_{e=uv \in E(G)} [n_u(e|G) + n_v(e|G)]$, where $n_u(e|G)$ is the number of vertices of G lying closer to u and $n_v(e|G)$ is the number of vertices of G lying closer to v. If G is bipartite then $n_u(e|G) + n_v(e|G) = n$ and so, $PI_v(G) = n\,|E(G)|$. Throughout this paper, our notation is standard and taken from the standard book of graph theory [14]. We encourage the reader to consult papers by Ashrafi et al and Ghorbani et al [15-23].

RESULTS AND DISCUSSION

The aim of this paper is to compute the counting polynomials of equidistant (Omega, Sadhana and Theta polynomials) of C_{8n^2} fullerenes with $8n^2$ carbon atoms and $12n^2$ bonds (the graph G, Figure 1, is n=2).

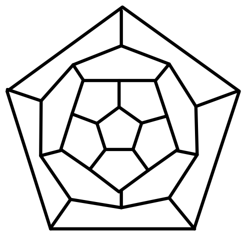

Figure 1. The Fullerene Graph C_{30}.

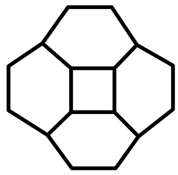

Figure 2. The Carbon Nanocone $CNC_4[1]$ with 16 vertices.

Example 1. Suppose C_{30} denotes the fullerene graph on 30 vertices, see Figure 1. Then $PI_v(C_{30}) = 1090$ and $\Omega(C_{30},x) = x^5 + 10x^2 + 20x$.

Example 2. Consider the carbon nanocones G = $CNC_4[1]$ with 16 vertices, Figure 2. Then $PI_v(G) = 320$ and $\Omega(G,x) = 2x^4 + 4x^3$.

Example 3. Suppose H is the graph of carbon nanocones $CNC_4[2]$ with 36 vertices, see Figure 3. Then $PI_v(H) = 1728$ and $\Omega(H,x) = 2x^6 + 4x^5 + 4x^4$.

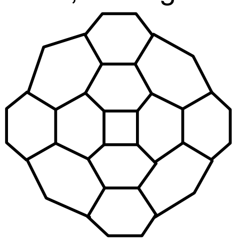

Figure 3. The Carbon Nanocone $CNC_4[2]$ with 36 vertices.

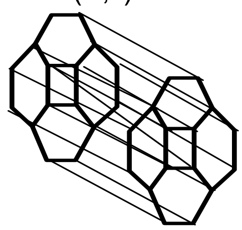

Figure 4. C_{32} obtained from two copies of $CNC_4[1]$.

Example 4. Consider the fullerene C_{32}, Figure 2. One can see that $PI_v(C_{32})=1536$ and $\Omega(C_{32},x) = 3x^8 + 4x^6$.

Lemma. Consider the fullerene graph C_{8n^2}. Then $PI_v(C_{8n^2}) = 96n^4$.

Proof. Because the graph is bipartite, by above discussion we have:
$PI_v(G) = |E(G)||V(G) = 96n^4$.

Consider the fullerene graph C_{8n^2} (Figure 4). Its symmetry group is isomorphic to a non-Abelian group of order 96. The orders of elements of its symmetry group are 1, 2, 3, 4 and 6. The center of its symmetry group is isomorphic with the group C_2. In the Appendix one can see how its symmetry group can be computed by GAP[31] software. We can draw the graph of C_{8n^2} by joining corresponding vertices of two copies of $CNC_4[n-1]$. For example C_{32} is obtained from two copies of $CNC_4[1]$ as follows:

Theorem. $\Omega(C_{8n^2}, x) = 3x^{4n} + 4(n-1)x^{3n}$.

Proof. By Figure 5, there are two distinct cases of qoc strips. We denote the corresponding edges by e_1, e_2, …, e_{10}. By using Table 1 and Figure 5 the proof is completed.

Table 1. The number of co-distant edges of e_i, $1 \le i \le 5$.

No.	Number of co-distant edges	Type of Edges
3	4n	e_1
4(n-1)	3n	e_2

Corollary. $Sd(C_{8n^2}, x) = 3x^{12n^2-4n} + 4(n-1)x^{12n^2-3n}$.

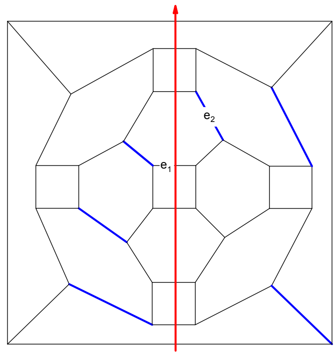

Figure 5. The graph of fullerene C_{8n^2} for n=2.

CONCLUSIONS

Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms. In this paper, by constructing an infinite family of [4,6] fullerenes, we computed Omega and Sadhana polynomials of them for the first time.

Appendix(Symmetry Group of C_{32} Fullerene by GAP Software [31]

a:=(1,2)*(3,4)*(5,6)*(7,8)*(9,10)*(11,12)*(13,14)*(15,16)*(17,18)*(19,20)*(21,22)*(23,24)*(25,26)*(27,28)*(29,30)*(31,32);

b:=(1,3)*(2,4)*(5,7)*(6,8)*(9,11)*(10,12)*(13,15)*(14,16)*(17,19)*(18,20)*(21,23)*(22,24)*(25,27)*(26,28)*(29,31)*(30,32);

c:=(1,4)*(6,7)*(11,24)*(12,22)*(16,30)*(15,32)*(26,27)*(10,21)*(9,23)*(14,29)*(31,13)*(18,19);

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d:=(1,2,3,4)*(7,8,6,5)*(21,12,24,9)*(11,22,10,23)*(15,30,14,31)*(16,32,13,29)*(27,28,26,25)*(19,20,18,17);G:=Group(a,b,c,d);e:=Elements(G);Print("\n");Print(" e= ",Size(e),"\n");
dd:=[ 1, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 226, 227, 228, 229, 230 ];w:=[];ww:=[];tt:=[];

for i in  dd do
ff:=Elements(SmallGroup(96,i));
for j in ff do
AddSet(w,Order(j));
if w=[1,2,3,4,6] then AddSet(ww,i);fi;
od;w:=[];
od;
for i in ww do
if Size(NormalSubgroups(SmallGroup(96,i)))=12 then
Add(tt,i);
fi;
od;
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