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On Omega and Sadhana polynomial of a class of nanohorns

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Let G be an arbitrary connected graph and s_1, s_2, ..., s_k be the oposite edges, ops strips of a plane graph G. Then the ops strips form a partition of $E(G)$ and the Ω-polynomial1 of G is defined as $\Omega(x) = \sum_{i=1}^{k} x^{|S_i|}$. In this paper we compute the Omega polynomial of an infinite class of nanohorns.

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1. Introduction

By a graph G means a pair $G = (V, E)$ in which V and E denote to the set of vertices and edges, respectively. For two vertices x and y belong to V, x is adjacent to y if and only if $xy \in E(G)$. G is connected, if for every pair (x, y) of V, there is a path between them. In this paper all of graphs are connected. A chemical graph is a graph theoretical representation of a molecule whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds.

Two edges $e = ab$ and $f = xy$ of graph 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 check that the relation "*co*" is reflexive and symmetric but it is not necessary to be transitive. Set $C(e) = \{f \in E(G) \mid f \ co \ e\}$. 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. Let G be an arbitrary connected graph and s_1, s_2, ..., s_k be the oposite edges, *ops* strips of a plane graph G. Then the *ops* strips form a partition of $E(G)$ and the Ω-polynomial [1-3] of G is defined as

$$\Omega(x) = \sum_{i=1}^{k} x^{|S_i|} .$$

Another polynomial also related to the ops in G, but counting the non-opposite edges is the *Sadhana Sd* polynomial defined as[4]

$$Sd(x) = \sum_{i=1}^{k} x^{|E|-|S_i|} .$$

The Sadhana index $Sd(G)$ for counting *qoc* strips in G was defined by Khadikar et al[5-8] as $Sd(G) = \sum_{i=1}^{k} |E(G)| - |S_i|$. By definition of Omega polynomial, one can obtain the Sadhana polynomial by replacing $x^{|S_i|}$ with $x^{|E|-|S_i|}$ in omega polynomial. Then the Sadhana index will be the first derivative of $Sd(x)$ evaluated at $x = 1$.

Carbon exists in several forms in nature. One is the so-called nanotube which was discovered for the first time in 1991. Unlike carbon nanotubes, carbon nanohorns can be made simply without the use of a catalyst [9,10]. The tips of these short nanotubes are capped with pentagonal faces; see Fig. 1. Let p, h, n and m be the number of pentagons, hexagons, carbon atoms and bonds between them, in a given nanohorn H. Then one can see that $n = r^2 + 22r + 41$, $m = \frac{3r^2 + 65r + 112}{2}$ (r = 0,1,…) and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $p = 5$ and $h = \frac{r2 + 21r + 24}{2}$, r = 1, 2, ….

In This paper by using definition of Omega polynomial we compute it for infinite class of nanohorn H depicted in Fig. 1. Throghout this paper our notation is standard and mainly taken from standard book of graph theory such as [11, 12]. For a more thorough introduction and treatment of Omega polynomial we refer the reader to [13 -19].

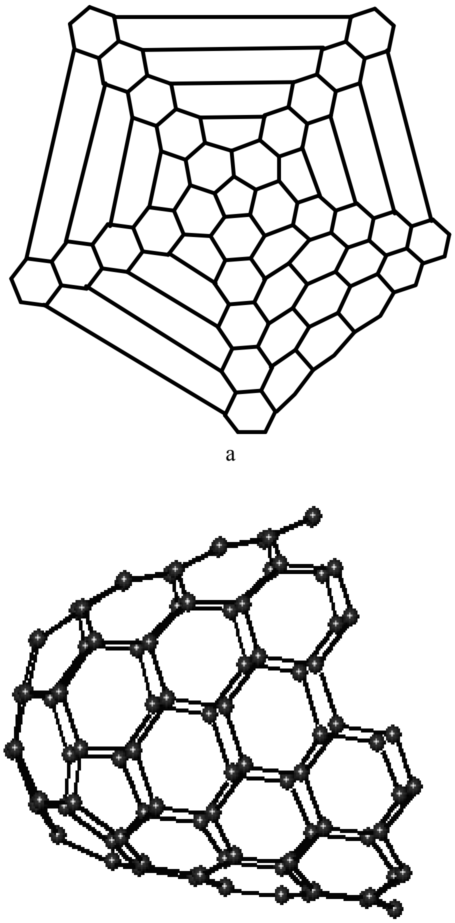

Fig. 1. 2-D and 3- D graph of nanohorn H.

2. Main result and discussion

The aim of this section is computing Omega and Sadhana polynomials of nanohorn H depicted in Fig. 1. To do this at first we should consider the following examples.

Example 1. Let F_{20} be a fullerene with 20 vertices depicted in Fig. 2. It is easy to see that $|E(F_{20})| = 30$. By computing the *qoc* strips of F_{20} one can see that the Omega and Sadhana polynomials are $\Omega(x) = 30x$ and $Sd(x) = 30x^{29}$, respectively.

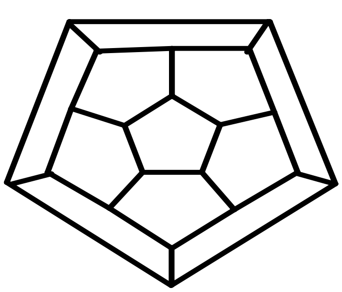

Fig. 2. The graph of fullerene F_{20}.

Example 2. Consider the pattern of TiO_2 lattice depicted in Fig. 3. By calculating Omega and then the Sadhana polynomial we have the following relations"

$\Omega(x) = 3x^3 + 3x^5$; $\Omega'(G,1) = 24 = e(G)$;

$Sd(x) = 3x^{19} + 3x^{21}$; $Sd'(G,1) = 120 = Sd(G)$.

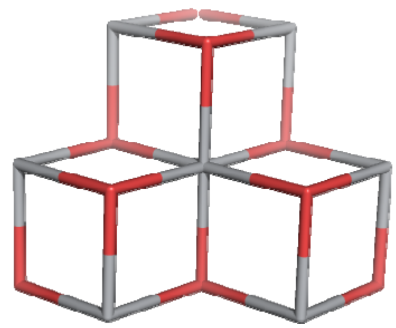

Fig. 3. The pattern of TiO_2 lattice.

Example 3. Suppose T_n, C_n and K_n denote the an arbitrary acyclic graph, cycle and complete graph on n vertices, respectively. Then by simple calculations, one can see that

$$\Omega(K_n, x) = \begin{cases} \frac{n}{2}\left(x^{\frac{n}{2}} + x^{\frac{n}{2}-1}\right) & 2 \mid n \\ nx^{\frac{n-1}{2}} & 2 \nmid n \end{cases},$$

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

Consider now nanohorn H in Fig. 1. It is easy to see that the number of its edges is equal to $|E(G)| = \frac{3p^2 + 65p + 112}{2} (p = 0,1,2,...)$. Then, the Omega and Sadhana polynomials are as follows:

Theorem.

$$\Omega(x) = 4x^{p+1} + 2x^{p+2} + 7x^{p+3} + 5x^{p+4} + 2x^{p+5} + x^{p+7} + x^{p+10} + 3x^3 + x^{p+13} + x^{p+16} + \sum_{i=1}^{p-4} x^{p+16+i}.$$

Proof. There are $p + 7$ separate cases that qoc strips are different. We denote these cases by edges e_1, e_2, e_3, e_4, e_5, e_6 and f_1, ..., f_{p+1}. By this figure and Table 1 the proof is completed.

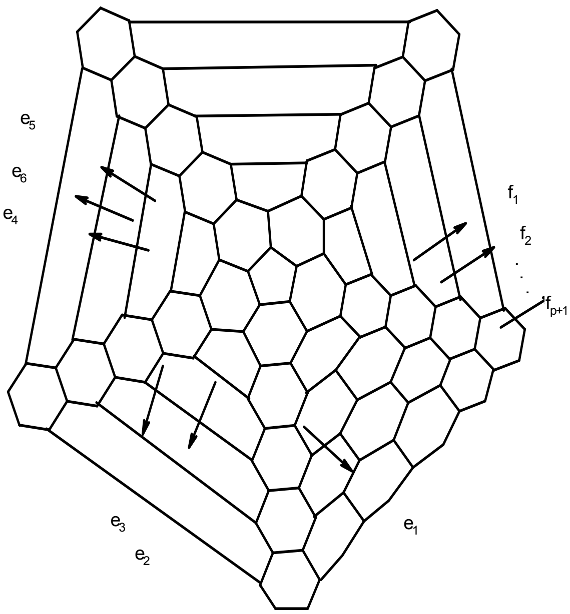

Fig. 4.2 - D graph of nanohorn H.

Corollary. The Sadhana polynomial of nanohorn H is as follows:

$$Sd(x) = 4x^{|E|-p-1} + 2x^{|E|-p-2} + 7x^{|E|-p-3} + 5x^{|E|-p-4} + 2x^{|E|-p-5} + x^{|E|-p-7} + x^{|E|-p-10} + 3x^{|E|-3} + x^{|E|-p-13} + x^{|E|-p-16} + \sum_{i=1}^{p-4} x^{|E|-p-16-i}.$$

Table 1. The Number of Parallel Edges.

Edges	The Number of Parallel Edges	No
e_1	$p+1$	4
e_2	$p+2$	2
e_3	$p+3$	7
e_4	$p+4$	4
e_5	$p+5$	2
e_6	3	3
f_1	$p+4$	1
f_2	$p+7$	1
f_3	$p+10$	1
f_4	$p+13$	1
f_5	$p+16$	1
$\vdots$	$\vdots$	$\vdots$
f_i	$16p+i$	1

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