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OMEGA AND SADHANA POLYNOMIALS OF AN IFANITE FAMILY OF FULLERENES

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The Sadhana polynomial is defined as $\mathrm{Sd}(G,x)=\sum_c m(G,c)\cdot x^{|E|-c}$, where m(G, c) is the number of strips of length c. This new polynomial has been defined to evaluate the Sadhana index of a molecular graph. The relation between this new polynomial and omega polynomial is investigated. In particular, a method of computing Sadhana polynomial and then Sadhana index for for an infinite family of fullerene has been described.

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Keywords: Omega Polynomial, Sadhana Polynomial, Fullerene.

1. Introduction

Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms. Fullerenes C_n can be drawn for $n = 20$ and for all even $n \geq 24$. 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. In 1988, Hosoya[3] introduced what he termed the Wiener (and latter called Hosoya) polynomial of a graph as $H(G,x)=\sum_{1<k<l} m(G,k)\cdot x^k$, where m($G$,$k$) is the number of pairs of vertices in G that are distance k apart, and l is the maximum value of k or the diameter of G. Sagan, Yeh and Zhang[4] produced a treatment apparently independent of Hosoya's. Perhaps the most interesting property of $H(G,x)$ is the first derivative, evaluated at $x = 1$, which equals the Wiener index: $H'(G,1)=W(G)$.

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

$$e\ co\ e$$

$$e\ co\ f \Leftrightarrow f\ co\ e$$

$$e\ co\ f\ ,\ f\ co\ h \Rightarrow e\ co\ h$$

though the last relation is not always valid.

Set C(e):= {f ∈ E(G) | 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) is the union of disjoint orthogonal cuts. The Omega polynomial Ω(G,x) for counting qoc strips in G was defined by Diudea as $\Omega(G, x) = \Sigma_c m(G, c) \times x^c$, with m(G,c) being the number of strips of length c. The summation runs up to the maximum length of qoc strips in G. If G is bipartite, then a qoc starts and ends out of G and so $\Omega(G, 1) = r/2$, in which r is the number of edges in out of G[6-8]. The Sadhana index Sd(G) for counting qoc strips in G was defined by Khadikar *et. al.*[9,10] as $\mathrm{Sd}(G)=\sum_c m(G,c)(|E(G)|-c)$, where m(G,c) is the number of strips of length c. We now

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define the Sadhana polynomial of a graph G as $Sd(G,x)=\sum_c m(G,c)\cdot x^{|E|-c}$. 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 $x = 1$. Herein, our notation is standard and taken from the standard book of graph theory[11-16]. The aim of this study is to compute the Sadhana polynomial and then Sadhana index of an infinite family of fullerenes.

2. Main results and discussion

The Sadhana polynomial of an infinite family of fullerenes was computed as described above.

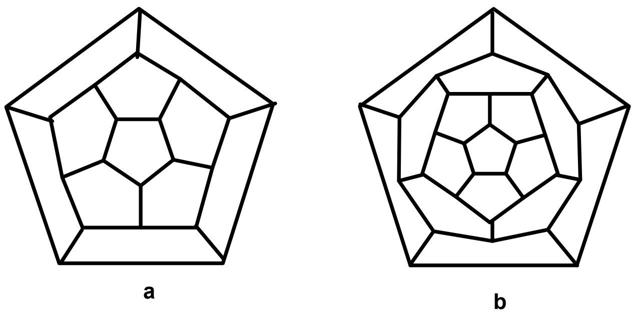


Fig. 1. (a) The Fullerene Graph C_{20}. (b) The Fullerene Graph C_{30}.

Example 1. Suppose C_{20} denotes the fullerene graph on 20 vertices, see Figure 1(a). Then $\Omega(C_{20}, x) = 30x$ and so, $Sd(C_{20},x) = 30x^{29}$.

Example 2. Suppose C_{30} denotes the fullerene graph on 30 vertices, see Figure 1(b). Then $\Omega(G, x) = 20x + 10x^2 + x^5$ and so, $Sd(G, x) = 20x^{44} + 10x^{43} + x^{40}$.

Example 3. Consider table 3. In this table we compute the omega polynomial for some fullerene graphs[17].

Theorem 1. Suppose K_n denotes the complete graph on n vertices. Then $\Omega(K_n, x) = \frac{n(n-1)}{2}x$ and so $Sd(K_n, x) = \frac{n(n-1)}{2}x^{\frac{n(n-3)}{2}}$.

Proof. For every $e \in E(K_n)$, $C(e) = 1$ and by using definition of Omega polynomial the proof is obvious.

Theorem 2. Suppose T is a tree on n vertices. Then $\Omega(T, x) = (n-1)x$ and so, $Sd(T, x) = (n-1)x^{n-2}$.

Theorem 3. Consider the fullerene graphs C_{10n}, $n \geq 10$ (Figures 2,3). Then the Omega and Sadhana polynomials of C_{10n} are computed as follows:

$$\Omega(C_{10n},x)=\begin{cases}10x^3+10x^{\frac{n}{2}}+10x^{n-3} & 2\mid n\\ 10x^3+5x^{\frac{n-3}{2}}+5x^{\frac{n+3}{2}}+10x^{n-3} & 2\nmid n\end{cases}$$

$$Sd(C_{10n},x)=\begin{cases}10x^{15n-3}+10x^{\frac{29n}{2}}+10x^{14n+3} & 2\mid n\\ 10x^{15n-3}+5x^{\frac{29n+3}{2}}+5x^{\frac{29n-3}{2}}+10x^{14n+3} & 2\nmid n\end{cases}$$

Proof. To compute the omega polynomial of C_{10n}, it is enough to calculate C(e) for every e in E(G). By using Table 1 and Table 2 the proof is complete.

Table 1. The number of co-distant edges, when n is even.

Type of Edges	Number of co-distant edges	No
e_1	3	10
e_2	$\frac{n}{2}$	10
e_3	n-3	10

Table 2. The number of co-distant edges, when n is odd.

Type of Edges	Number of co-distant edges	No
e_1	3	10
e_2	$\frac{n-3}{2}$	5
e_3	$\frac{n+3}{2}$	5
e_4	n-3	10

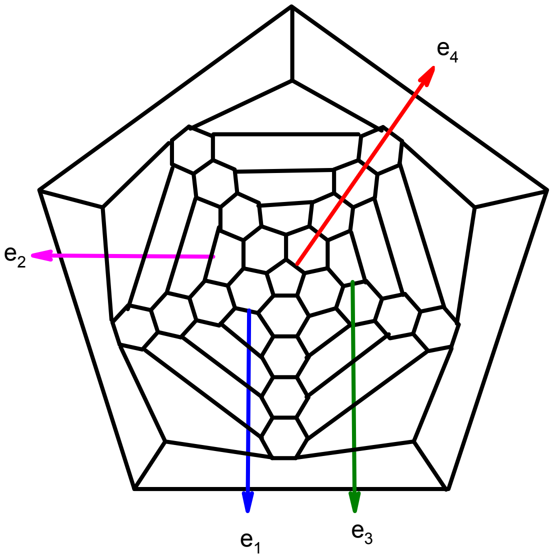


Fig. 2. The Fullerene Graph C_{10n} (n is odd).

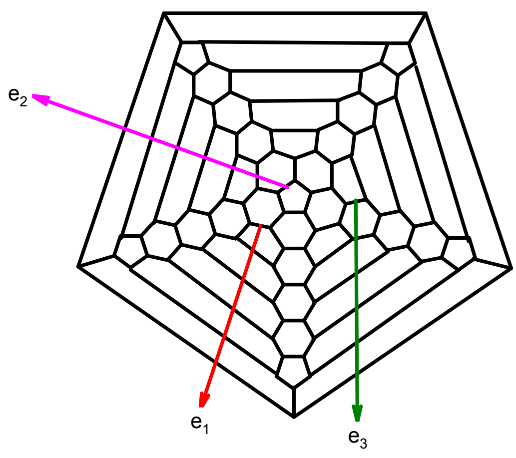
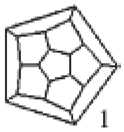
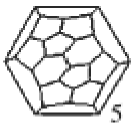
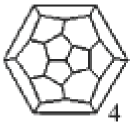
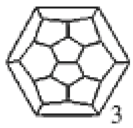
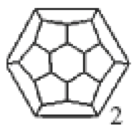
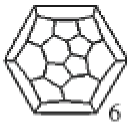
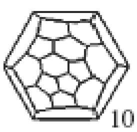
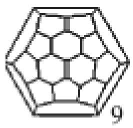
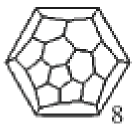
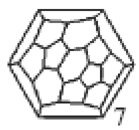
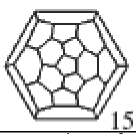
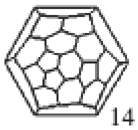
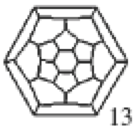
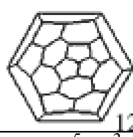
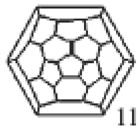
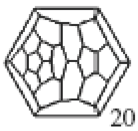
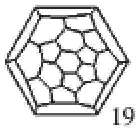
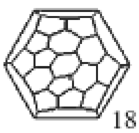
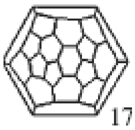
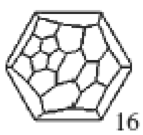
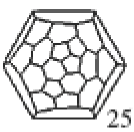
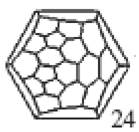
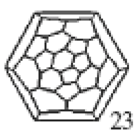
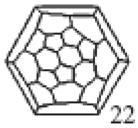
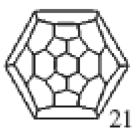


Fig. 3. The Fullerene Graph C_{10n} (n is even).

Table 3. Omega polynomial for some fullerene graphs.

C				
C_{20}	***C_{30}***	***C_{28}***	***C_{26}***	***C_{24}***
 1	 5	 4	 3	 2
$\Omega(X)=X^{30}$	$\Omega(X)=x^5+8x^2+24x$	$\Omega(X)=24x+9x^2$	$\Omega(X)=30x+6x^2$	$\Omega(X)=30X+3X^2$
C_{32}	***C_{36}***	***C_{34}***	***C_{32}***	***C_{32}***
 6	 10	 9	 8	 7
$\Omega(X)=11x^2+2x^3+20x$	$\Omega(X)=6x^3+9x^2+18x$	$\Omega(X)=18x+12x^2+3x^3$	$\Omega(X)=4x^3+7x^2+22x$	$\Omega(X)=4x^3+7x^2+22x$
C_{38}	***C_{38}***	***C_{36}***	***C_{36}***	***C_{36}***
 15	 14	 13	 12	 11
$\Omega(X)=2x^4+3x^3+12x^2+16x$	$\Omega(X)=x^6+x^5+x^4+12x^2+18x$	$\Omega(X)=x^6+15x^2+18x$	$\Omega(X)=2x^5+x^3+11x^2+19x$	$\Omega(X)=x^5+x^3+12x^2+22x$
C_{40}	***C_{40}***	***C_{40}***	***C_{40}***	***C_{40}***
 20	 19	 18	 17	 16
$\Omega(X)=2x^5+8x^3+2x^2+22x$	$\Omega(X)=8x^3+11x^2+14x$	$\Omega(X)=x^6+6x^3+x^2+16x$	$\Omega(X)=15x+12x^2+5x^3+x^6$	$\Omega(X)=4x^2+4x^4 4x^3+20x$
C_{44}	***C_{44}***	***C_{44}***	***C_{42}***	***C_{40}***
 25	 24	 23	 22	 21
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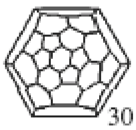
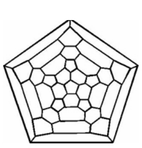
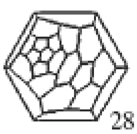
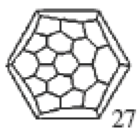
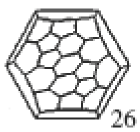
C_{44}	***C_{70}***	***C_{44}***	***C_{44}***	***C_{44}***
 30		 28	 27	 26
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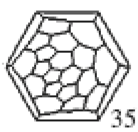
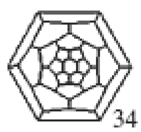
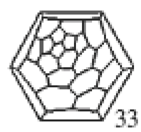
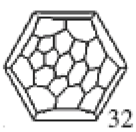
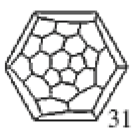
C_{48}	***C_{48}***	***C_{48}***	***C_{48}***	***C_{48}***
 35	 34	 33	 32	 31
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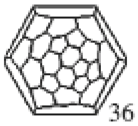
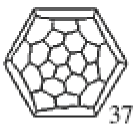
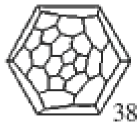
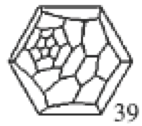
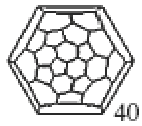
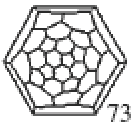
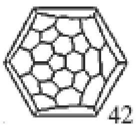
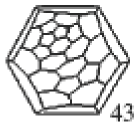
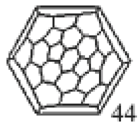
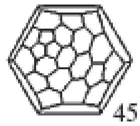
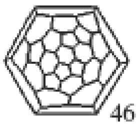
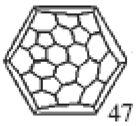
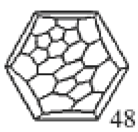
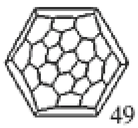
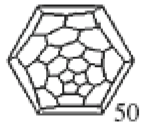
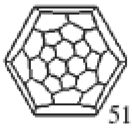
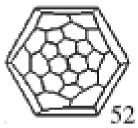
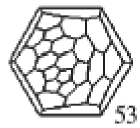
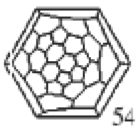
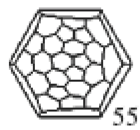
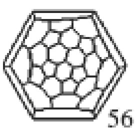
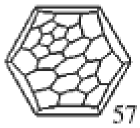
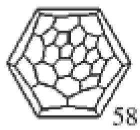
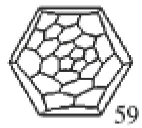
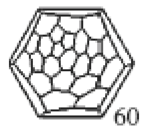
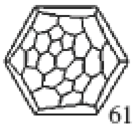
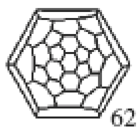
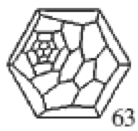
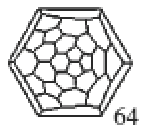
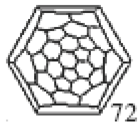
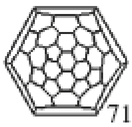
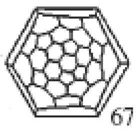
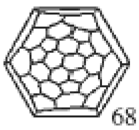
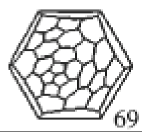
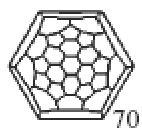
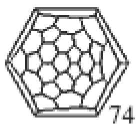
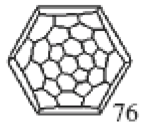
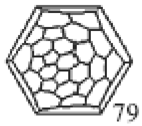
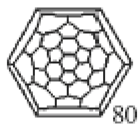
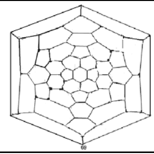
C				
C_{50}	C_{50}	C_{50}	C_{50}	C_{50}
 36	 37	 38	 39	 40
$\Omega(X)=x^8+x^7+x^5+3x^4+x^3+14x^2+12x$	$\Omega(X)=7x^4 4x^3+13x^2+9x$	$\Omega(X)=2x^6+3x^5+x^4+5x^3+7x^2+15x$	$\Omega(X)=x^6+2x^5+2x^4+4x^3+21x$	$\Omega(X)=9x^3+12x^2+4x^4+8x$
C_{60}	C_{52}	C_{52}	C_{52}	C_{52}
 73	 42	 43	 44	 45
$\Omega(X)=x^8+10x^3+14x^2+8x$	$\Omega(X)=2x^8+2x^4+7x^3+11x^2+11x$	$\Omega(X)=2x^6+4x^4+4x^3+4x^2+14x$	$\Omega(X)=x^8+6x^4+2x^3+15x^2+10x$	$\Omega(X)=2x^7+4x^4+2x^5+x^3+11x^2+12x$
C_{52}	C_{52}	C_{52}	C_{52}	C_{52}
 46	 47	 48	 49	 50
$\Omega(X)=x^8+7x^4+2x^3+11x^2+11x$	$\Omega(X)=2x^7+2x^5+3x^4+3x^3+10x^2+13x$	$\Omega(X)=2x^8+2x^4+7x^3+11x^2+11x$	$\Omega(X)=2x^7+4x^4+15x^2+10x$	$\Omega(X)=x^{20}+3x^4+x^3+15x^2+13x$
C_{52}	C_{52}	C_{52}	C_{54}	C_{54}
 51	 52	 53	 54	 55
$\Omega(X)=9x^4+3x^3+12x^2+9x$	$\Omega(X)=3x^6+2x^5+2x^4+2x^3+15x^2+9x$	$\Omega(X)=x^{18}+5x^4+6x^3+4x^2+17x$	$\Omega(X)=4x^6+2x^5+8x^3+7x^2+12x$	$\Omega(X)=5x^5+6x^4+2x^3+9x^2+11x$
C_{20}	C_{20}	C_{20}	C_{20}	C_{20}
 56	 57	 58	 59	 60
$\Omega(X)=3x^7+2x^5+6x^3+13x^2+9x$	$\Omega(X)=2x^6+x^5+5x^4+5x^3+7x^2+13x$	$\Omega(X)=2x^5+11x^4+2x^3+6x^2+12x$	$\Omega(X)=5x^7+x^4+8x^3+2x^2+17x$	$\Omega(X)=2x^6+6x^5+x^4+4x^3+6x^2+14x$
C_{20}	C_{20}	C_{20}	C_{20}	C_{60}
 61	 62	 63	 64	 72
$\Omega(X)=3x^8+5x^3+18x^2+9x$	$\Omega(X)=3x^8+10x^3+8x^2+14x$	$\Omega(X)=7x^5+8x^3+10x^2+8x$	$\Omega(X)=x^7+2x^4+17x^3+8x^2+5x$	$\Omega(X)=x^7+x^6+6x^4+10x^3+8x^2+7x$
C_{60}	C_{60}	C_{60}	C_{60}	C_{60}
 71	 67	 68	 69	 70
$\Omega(X)=x^6+6x^4+10x^3+11x^2+8x$	$\Omega(X)=3x^5+5x^4+11x^3+8x^2+6x$	$\Omega(X)=2x^5+10x^4+6x^3+7x^2+8x$	$\Omega(X)=4x^8+x^6+x^5+9x^3+2x^2+16x$	$\Omega(X)=3x^6+3x^5+12x^3+6x^2+9x$

C_{60}	***C_{60}***	***C_{60}***	***C_{60}***	***C_{80}***
				
$\Omega(X)=x^8+2x^6+2x^5+4x^4+4x^3+12x^2+8x$	$\Omega(X)=3x^9+x^7+x^6+x^3+20x^2+7x$	$\Omega(X)=3x^8+10x^3+14x^2+8x$	$\Omega(X)=25x^3+6x^2+3x$	$\Omega(X)=6x^{10}+30x^2$

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