A Survey on Omega Polynomial of Some Nano Structures

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ABSTRACT

A counting polynomial $C(G, x)$ is a sequence description of a topological property so that the exponents express the extent of its partitions while the coefficients are related to the occurrence of these partitions. Basic definitions and properties of the Omega polynomial $\Omega(G,x)$ and the Sadhana polynomial $Sd(G,x)$ are presented. These polynomials for some infinite classes of fullerenes and nanotubes are also computed. The results of this paper are arranged according to the main Theorems of [9− 43].

Keywords: Omega polynomial, Sadhana polynomial, fullerene, nanotube.

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. Chemical graph theory is an important tool for studying molecular structures. This theory had an important effect on the development of the chemical sciences.

A graph can be described by: a connection table, a sequence of numbers, a derived number (called sometimes a topological index), a matrix, or a polynomial [1].

A finite sequence of some graph-theoretical categories/properties, such as the distance degree sequence or the sequence of the number of *k*-independent edge sets, can be described by so-called counting polynomials:

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$$P(G,x)=\sum_k p(G,k)\cdot x^k \quad (1)$$

where $p(G,k)$ is the frequency of occurrence of the property partitions of G, of length k, and x is simply a parameter to hold k.

Counting polynomials were introduced, in the Mathematical Chemistry literature, by Hosoya with his Z-counting (independent edge sets) and the distance degree polynomials, where initially called ***Wiener*** and later ***Hosoya polynomials*** [2]. Their roots and coefficients are used for the characterization of topological nature of hydrocarbons.

Hosoya proposed the ***sextet polynomial*** [3,4]for counting the resonant rings in a benzenoid molecule. The sextet polynomial is important in connection to the Clar aromatic sextets [5,6] expected to stabilize the aromatic molecules.

The ***independence polynomial*** [7, 8] counts the number of distinct k-element independent vertex sets of G. Other related graph polynomials are the *king*, *color* and *star or clique polynomials* [9].

Vertex contributions to a polynomial $P(G,x)$, based on distance counting, can be written as:

$$P(i,x)=(1/2)\sum_k p(i,k)\cdot x^k \quad (2)$$

Where $p(i,k)$ is the contribution of vertex i to the partition $p(G,k)$ of the global molecular property $P=P(G)$. Note that $p(i,k)$'s are just the entries in ***LM*** or ***SM,*** more exactly 1/2 the value because each vertex contribution is counted twice [10].

Usually, the vertex contribution varies from one atom to another, so that the polynomial for the whole graph is obtained by summing all vertex contributions:

$$P(G,x)=\sum_i P(i,x) \quad (3)$$

In a vertex transitive graph, the vertex contribution is simply multiplied by N:

$$P(G,x)=N\cdot P(i,x) \quad (4)$$

Hence, $P(G)$ is easily obtained as the polynomial value in x=1:

$$P(G)=P(G,x)\,|_{x=1} \quad (5)$$

A ***distance–extended property*** $D\_P(G)$ can be calculated by the *first derivative* of the polynomial in x = 1 [11 – 15]:

$$D\_P(G)=P'(G,x)=\sum_k k\cdot p(G,k)\cdot x^{k-1}\,|_{x=1} \quad (6)$$

In [16], the authors 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: $H'(G,1)=W(G)$. Ashrafi [17]continued the line of the mentioned paper of Sagan *et al*. to introduce the notion of ***PI polynomial*** of a molecular graph G as:

$$PI(G,x)=\sum_{(u,v)=e\in E(G)} x^{N(u,v)} \quad (7)$$

where $N(u,v)=n_{eu}(e|G)+n_{ev}(e|G)$ and $n_{eu}(e|G)$ is the number of edges lying closer to u than v (*i.e*., the ***non–equidistant*** edges) while the number of edges ***equidistant*** to the edge *e* = *uv*$\in$ *E(G)* is given by: $N(e) = |E(G)| - N(u,v)$, where *E*(*G*) denotes the set of all edges of the graph *G*. In [17] the authors have shown that this new polynomial has the same basic properties as the Wiener polynomial. Thus, its first derivative gives the PI index, which can also be calculated by subtracting the total number of equidistant edges in *G* from the square of the edge set cardinality:

$$PI(G) = PI'(G,1) = (|E|)^2 - \sum_e N(e) \quad (8)$$

See also [18 – 20] for more details about PI index. Here, our notations are standard and taken from [21 – 23]. The basic definitions and properties of the Omega polynomial $\Omega(G,x)$ are presented in the second section. In the third section the Omega polynomial of some well–known graphs are computed.

2. MAIN RESULTS AND DISCUSSION

We now recall some algebraic definitions that will be used in the paper. Let *G* be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by *V*(*G*) and *E*(*G*), respectively. Throughout this paper, graph means simple connected graph. The vertex and edge sets of a graph *G* are denoted by *V*(*G*) and *E*(*G*), respectively. If *x, y*$\in$*V*(*G*) then the distance *d*(*x, y*) between *x* and *y* is defined as the length of a minimum path connecting *x* and *y*.

2.1 OMEGA POLYNOMIAL

The ***Omega polynomial*** is a counting polynomial introduced by M. V. Diudea. In recent years, several papers on methods for computing Omega polynomials of molecular graphs have been published [24 – 43].

Let *G* be a connected bipartite graph with the vertex set $V = V(G)$ and edge set $E = E(G)$, without loops. Two edges *e* = *ab* and *f* = *xy* of *G* are called **co-distant** (briefly: *e co f*) if for *k* = 0,1,2,… there exist the relations: *d*(*a,x*) = *d*(*b,y*) = *k* and *d*(*a,y*) = *d*(*b,x*) = *k*+1 or vice versa. For some edges of a connected graph G there are the following relations satisfied:

$$e \; co \; f \quad (9)$$

$$e \; co \; f \Leftrightarrow f \; co \; e \quad (10)$$

$$e \; co \; f \;\&\; f \; co \; g \Rightarrow e \; co \; g \quad (11)$$

though, the relation (11) is not always valid.

Let *C*(*e*):= $\{e' \in E(G)$; *e' co e* $\}$ denote the set of all edges of *G* which are co-distant to the edge *e*. If all the elements of *C*(*e*) satisfy the relations (9–11) 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: $C_1 \cup C_2 \cup ... \cup C_k = E$ and $C_i \cap C_j = \emptyset$ for $i \neq j$, $i, j = 1,2,...,k$.

We now assume that *G* has a plane representation *F*. If *S* is the set of all faces forming the interior regions then every edge appears in at most two members of S.

Suppose T denotes the outside edges of G. Start with an edge e of G. If there is not an edge e_1 different from e with the property that e *co* e_1 and $\{e,e_1\}$ lie in the same face of G then we define $H= \{e_1\}$ and choose another edge f of G. Otherwise, there exists the edge e_1 such that e *co* e_1. Continue this process by e_1 to construct the sequence e *co* e_1 *co* e_2 *co* ... *co* e_r. If $e \in T$ then define $H = \{e, e_1, e_2, ...,e_r\}$. If not, there exists an edge f_1 of G different from e_1 such that f_1 *co* e and $\{e,f_1\}$ lie in the same face of G. By this algorithm a sequence $H= \{f_t, ..., f_1, e, e_1, e_2, ..., e_r\}$ is constructed. H is called a ***quasi–orthogonal cut*** or a ***qoc strip.*** It is an easy fact that a qoc strip is not necessarily transitive. In the case that G is bipartite, then every member of S have an even number of edges and so $f_t, e_r \in T$. Notice that a *qoc* strip starts and ends either out of G (at an edge with endpoints of degree lower than 3, if G is an open lattice,) or in the same starting polygon (if G is a closed lattice). Any *oc* strip is a *qoc* strip but the reverse is not always true.

Suppose $E_1, E_2, ...,E_r$ are *qoc* strips of a connected planar bipartite graph G. We claim that $X = \{E_1, E_2, ...,E_r\}$ is a partition of $E = E(G)$. To do this we assume that $e \in E$ is an arbitrary edge of G. Using a similar argument as those given above one can find a sequence f_t *co* f_{t-1} *co* ... *co* f_1 *co* e *co* e_1 ... *co* e_r. Therefore there exists j, $1 \le j \le r$, such that $\{f_t, ..., f_1, e, e_1, ..., e_r\} \subseteq E_j$. This implies that $e \in E_j$ and so $E = E_1 \cup E_2 \cup ... \cup E_r$. To complete our claim, we must prove $E_i \cap E_j = \emptyset$, for $1 \le i \ne j \le r$. Suppose $E_i = \{e_1,e_2, ..., e_n\}$, $E_j = \{f_1,f_2,...,f_m\}$ and $e \in E_i \cap E_j$. Then there are r, s, $1 \le r \le n$ and $1 \le s \le m$ such that $e = e_r = f_s$. But every edge appears in at most two members of S, so by using an inductive argument $E_i = E_j$. Therefore, X is a partition of E.

The *Omega* $\Omega(G,x)$ polynomial for counting *qoc* strips in G is defined as:

$$\Omega(G,x) = \sum_c m(G,c) \cdot x^c \tag{12}$$

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. On the other hand, one can easily seen that $\Omega'(G,1) = \sum_c m \cdot c = e = |E(G)|$. Two single number descriptors are derived from $\Omega(G,x)$ as:

$$CI(G) = (\Omega')^2 - (\Omega' + \Omega'')\big|_{x=1} \tag{13}$$

$$I_\Omega(G) = (1/\Omega'(G,x)) \cdot \sum_d (\Omega^d(G,x))^{1/d}\big|_{x=1} \tag{14}$$

In case of I_Ω, summation runs over all possible derivatives d in the corresponding polynomial. When one or more edges do not belong to a counted strip, such edges are added as “strips of length 1”.

It is easily seen that, for a single *qoc*, one calculates the polynomial: $\Omega(G,x) = x^c$ and $CI(G) = c^2 - (c + c(c-1)) = 0$. There exist graphs for which *CI* equals *PI*. In fact, the two indices *CI* and *PI* will show identical values if the edge equidistance evaluation in the graph involves only the locally parallel edges. This is occurred for example in partial cubes. In this case, we have:

$$CI(G)=\left(\sum_c m\cdot c\right)^2-\left[\sum_c m\cdot c+\sum_c m\cdot c\cdot(c-1)\right]=e^2-\sum_c m\cdot c^2=PI(G).$$

This counting polynomial is useful in topological description of benzenoid, structures as well as in counting some single number descriptors, *i.e.*, topological indices. The *qoc* strips could give account for the helicity of polyhex nanotubes and nanotori. The Omega 1.1 software program includes the *qoc* strips procedure.

In the end of this section a simple counterexample for equations (9-11) is given in Figure 1. In the graph G_1; {a} and {c} are *oc* strips; {b} and {d} does not have all elements co-distant to each other, so that {b} and {d} are *qoc* strips. In the graph G_2; {a} and {b} and {c} are *oc* strips; {f} and {c} are equidistant but {f} and {c_1 or c_3} do not obey the symmetry relation (8) (and do not belong to one face) thus {f} does not belong to the strip {c}. Therefore, $\Omega(G_1,x)=x^2+2x^4+x^6$ and $\Omega(G_2,x)=5x+2x^2+x^3$.

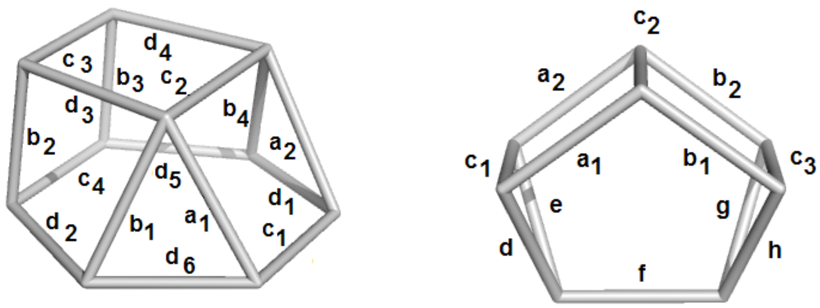


Figure 1. Two Graphs G_1 (left) and G_2 (right).

2.2 EXAMPLES

In this section the Omega polynomial of some well-known graphs are computed. A general formula for computing Omega polynomial of the graph product is presented by which, it is possible to compute the Omega polynomials of nanotubes and nanotori covered by C_4. We begin by some well-known graphs.

Example 1. 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

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

The Cartesian product $G\times H$ of graphs G and H is a graph such that $V(G\times H)=V(G)\times V(H)$, and any two vertices (a,b) and (u,v) are adjacent in $G\times H$ if and only if either a = u and b is adjacent with v, or $b = v$ and a is adjacent with u. The following properties of the Cartesian product of graphs are crucial:

(a) $|V(G \times H)| = |V(G)|\,|V(H)|$ and $|E(G \times H)| = |E(G)|\,|V(H)| + |V(G)|\,|E(H)|$;
(b) $G \times H$ is connected if and only if G and H are connected;
(c) If (a, x) and (b, y) are vertices of $G \times H$ then $d_{G\times H}((a, x), (b, y)) = d_G(a, b) + d_H(x,y)$;
(d) The Cartesian product is associative.

Theorem 2. Let G and H be bipartite connected co-graphs. Then

$$\Omega(G\times H,x)=\sum_{c_1} m(G,c_1).x^{|V(H)|c_1}+\sum_{c_2} m(H,c_2).x^{|V(G)|c_2}.$$

Proof. Suppose that for an edge e = uv of an arbitrary graph L, $N_L(e) = |E| - (n_u(e) + n_v(e))$. Then by definition,

$$N_{G\times H}((a,x),(b,y)) = \begin{cases} |V(G)|\,N(f) & \text{for } a=b \text{ and } xy=f \in E(H) \\ |V(H)|\,N(g) & \text{for } x=y \text{ and } ab=g \in E(G). \end{cases}$$

By above paragraph and definition of the Omega polynomial, we have:

$$\Omega(G\times H,x)=\sum_{c} m(G\times H,c).x^{c}=\sum_{c_1} m(G,c_1).x^{|V(H)|c_1}+\sum_{c_2} m(H,c_2).x^{|V(G)|c_2}$$

which completes the proof.

Corollary 3. Let $G_1, G_2, \cdots, G_n$ be bipartite connected co-graphs. Then we have:

$$\Omega(G_1\times G_2\times\cdots\times G_n,x)=\sum_{i=1}^{n}\sum_{c_i} m(G_i,c_i).x^{\prod_{j=1,\,j\neq i}^{n}|V(G_j)|c_i}.$$

Proof. Use induction on n. By Theorem 2.2, the result is valid for n = 2. Let n ≥ 3 and assume the theorem holds for n - 1. Set $G = G_1 \times \cdots \times G_{n-1}$. Then we have

$$\Omega(G\times G_n,x)=\sum_{c} m(G,c).x^{|V(G_n)|c}+\sum_{c_n} m(G_n,c_n).x^{|V(G)|c_n}$$

$$=\sum_{i=1}^{n-1}\sum_{c_i} m(G_i,c_i).x^{\prod_{j=1,\,j\neq i}^{n}|V(G_j)|c_i}+\sum_{c_n} m(G_n,c_n).x^{|V(G)|c_n}$$

$$=\sum_{i=1}^{n}\sum_{c_i} m(G_i,c_i).x^{\prod_{j=1,\,j\neq i}^{n}|V(G_j)|c_i}.$$

Example 4. In this example the Omega polynomial of nanotubes and nanotori covered by C_4 are calculated. By definitions of Cartesian product of graphs and Omega polynomial, one can easily prove:

$$\Omega(G\times H,x)=\sum_{c_1} m(G,c_1)\times x^{|V(H)|c_1}+\sum_{c_2} m(H,c_2)\times x^{|V(G)|c_2}. \quad (15)$$

Suppose R and S denote a C_4–tube and C_4–torus, respectively. Then by definition $R \cong P_n \times C_m$ and $S \cong C_k \times C_m$. Apply Theorem 2 to deduce that $\Omega(P_n \times P_m, x) = (n-1)x^m + (m-1)x^n$. On the other hand, we have:

$$\Omega(P_n \times C_m, x) = \begin{cases} (n-1)x^m + \frac{m}{2}x^{2n} & 2|m \\ (n-1)x^m + mx^n & 2\nmid m \end{cases},$$

$$\Omega(C_n \times C_m, x) = \begin{cases} nx^m + mx^n & 2\nmid m,\ 2\nmid n \\ nx^m + \frac{m}{2}x^{2n} & 2|m,\ 2\nmid n \\ \frac{n}{2}x^{2m} + mx^n & 2\nmid m,\ 2|n \\ \frac{n}{2}x^{2m} + \frac{m}{2}x^{2n} & 2|m,\ 2|n \end{cases}.$$

Example 5.Consider the molecular graph of a nanocones $G = CNC_4[n]$, Figure 2. This graph has exactly $4(n + 1)^2$ vertices. From Figure 2, one can see that there are $m + 1$ type of edges of G. These are $I_1, I_2,\ldots$ and I_{m+1}. In Table 1, for each type the number of equidistant edges of $G$is computed. By this calculation, we can see that

$$\Omega(G, x) = 2x^{2m+2} + 4(x^{2m+1} + x^{2m} + \ldots + x^{m+2})$$
$$= 2x^{2m+2} + 4(x^{2m+2} - x^{m+2})/(x-1).$$

Table 1. The Number of Parallel Edges.

Edges	Number of Parallel Edges	No
Type I_1 Edges	m+2	4
Type I_2 Edges	m+3	4
Type I_3 Edges	m+4	4
⋮	⋮	4
Type I_{m+1} Edges	2m+2	2

In the end of this section, the Omega polynomials of TWHH[p,q](R) nanotubes and nanotori are computed, Figures 3–5. The molecular graphs of these compounds are denoted by G and H, respectively. From Figures 3-5, one can see that there are two different cases for qoc strips. Suppose e_1 and e_2 are representatives of the different cases. In the molecular graph G, $|C(e_1)| = 2p$ and $|C(e_2)| = 2q+1$. On the other hand, there are q and $2p$ similar edges for each of edges e_1 and e_2, respectively. This implies that $\Omega(G,x) = qx^{2p} + 2px^{2q+1}$. For the graph H, $|C(e_1)| = 2p$ and $|C(e_2)| = 2pq$. On the other hand, there are q and 2 similar edges for the edges e_1, e_2, respectively. Therefore, $\Omega(H,x) = qx^{2p} + 2x^{2pq}$.

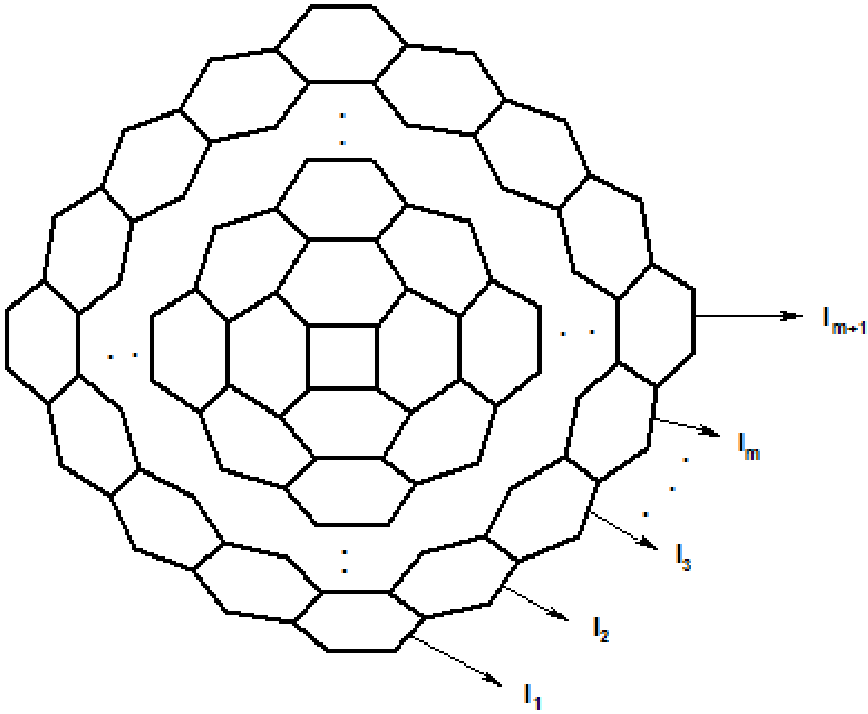


Figure 2. The Molecular graph of carbon nanocones $CNC_4[n]$.

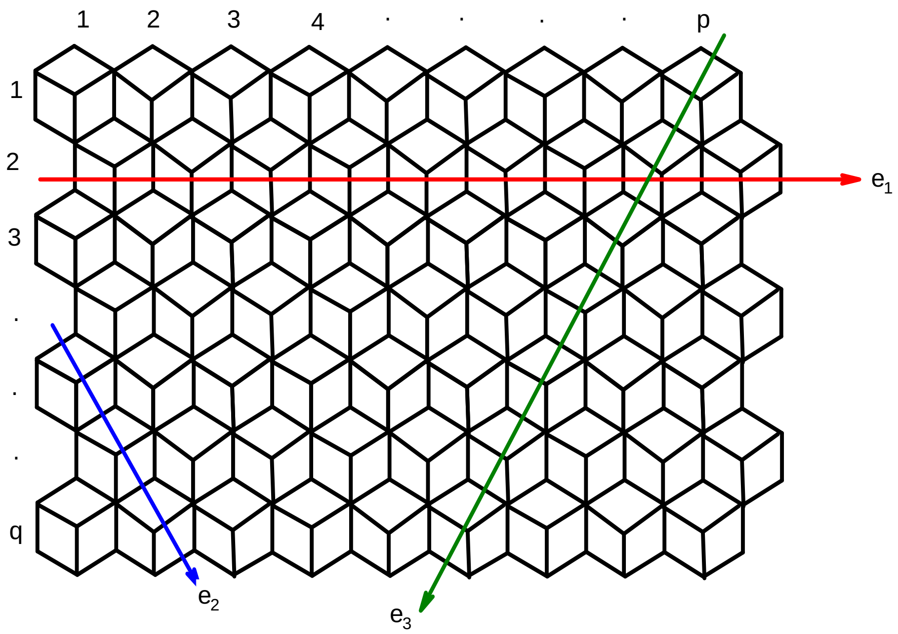


Figure 3. The qoc strips of the 2−dimensional graph of a TWHH[p,q](R) nanotube.

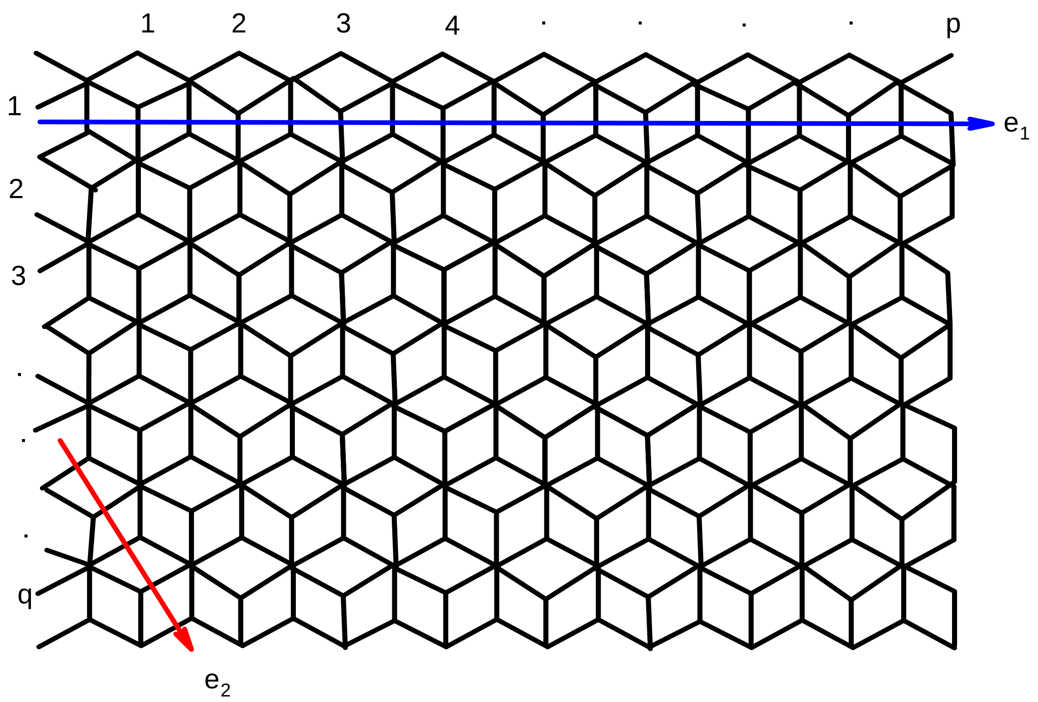


Figure 4. The qoc strips of the nanotube *G*.

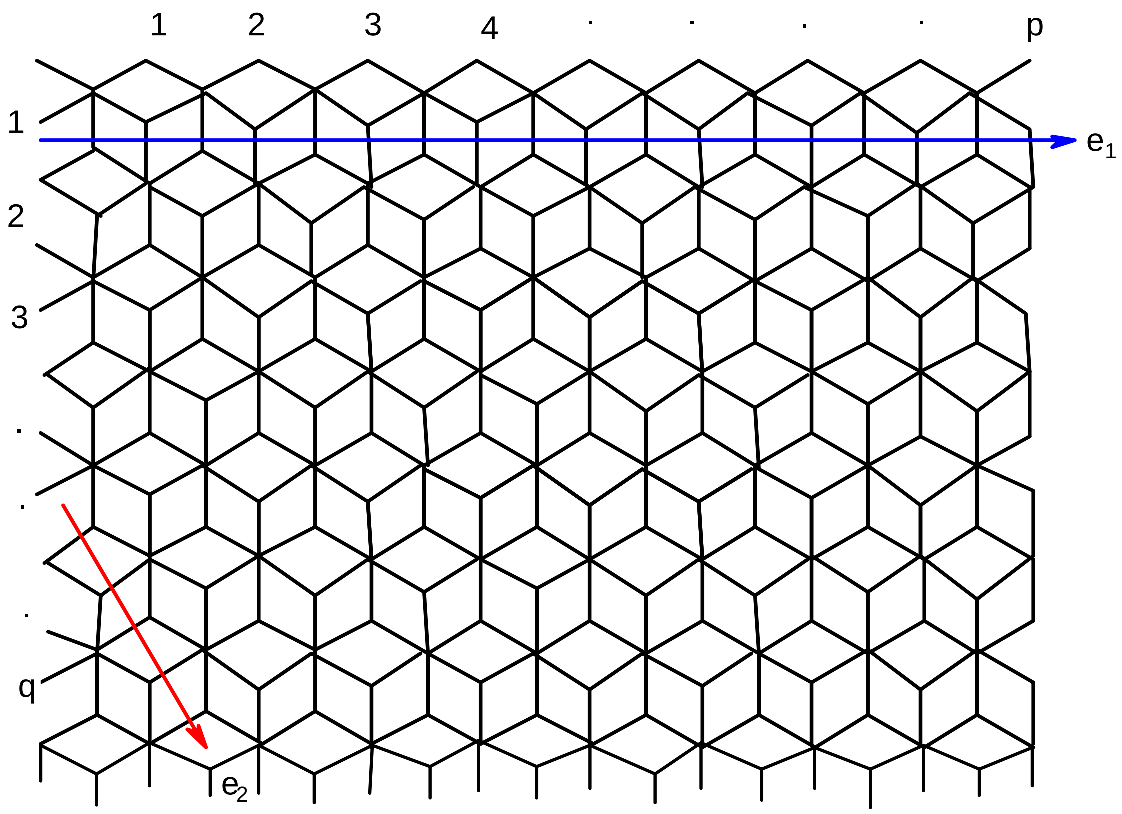
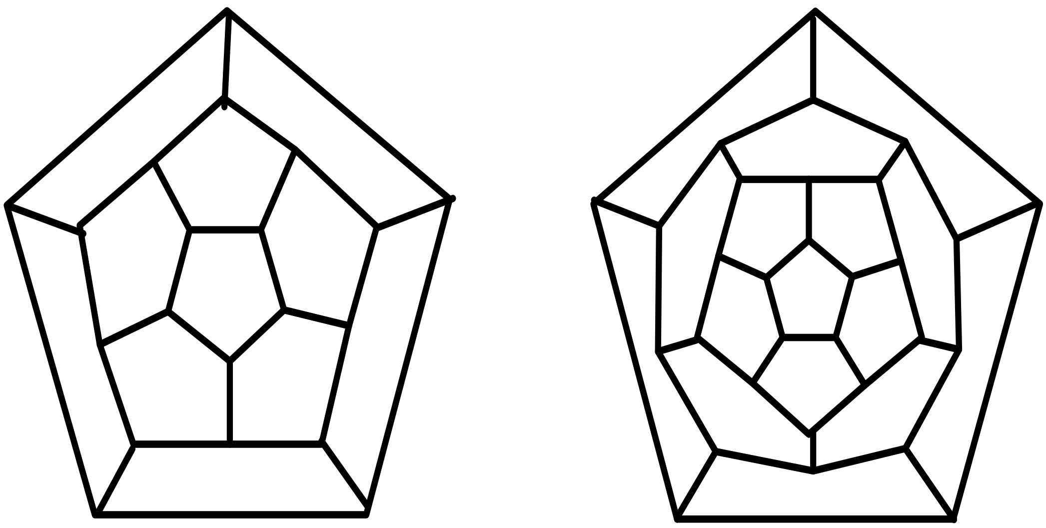


Figure 5. The qoc strips of the nanotorus *H*.

2.3 *OMEGA POLYNOMIAL OF FULLERENES*

The fullerene era was started in 1985 with the discovery of a stable C_{60} cluster and its interpretation as a cage structure with the familiar shape of a soccer ball, by Kroto and his co-authors [44,45]. The well-known fullerene, the C_{60} molecule, is a closed-cage carbon molecule with three-coordinate carbon atoms tiling the spherical or nearly spherical surface with a truncated icosahedral structure formed by 20 hexagonal and 12 pentagonal rings. Let p, h, n and m be the number of pentagons, 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 $n = (5p+6h)/3$, the number of edges is $m = (5p+6h)/2 = 3/2n$ and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $(5p+6h)/3 - (5p+6h)/2 + p + h = 2$, and therefore $p = 12$, $v = 2h + 20$ and $e = 3h + 30$. This implies that such molecules made up entirely of n carbon atoms and having 12 pentagonal and $(n/2 - 10)$ hexagonal faces, where $n \neq 22$ is a natural number equal or greater than 20.

In this section, the Omega polynomials of some infinite classes of fullerenes are investigated. Begin by small fullerenes C_{20} and C_{30} depicted in Figure 6.



a b

Figure 6. (*a*) The fullerene graph C_{20} (*b*) The fullerene graph C_{30}.

Then by our method $\Omega(C_{20}, x) = 30x$ and $\Omega(C_{30}, x) = 20x + 10x^2 + x^5$. We now compute the Omega of an infinite family of fullerene graphs with $40n + 6$ vertices, Figure 7.

Theorem 6. The Omega polynomial of fullerene graph $G = C_{40n+6}$ is computed as follows:

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

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

Proof. From Figure 7, one can see that there are ten distinct cases of ops strips in G. We denote the corresponding edges by e_1, e_2, …,e_{10}. By using calculations given in Table 2 and the Figure 8, the proof is completed.

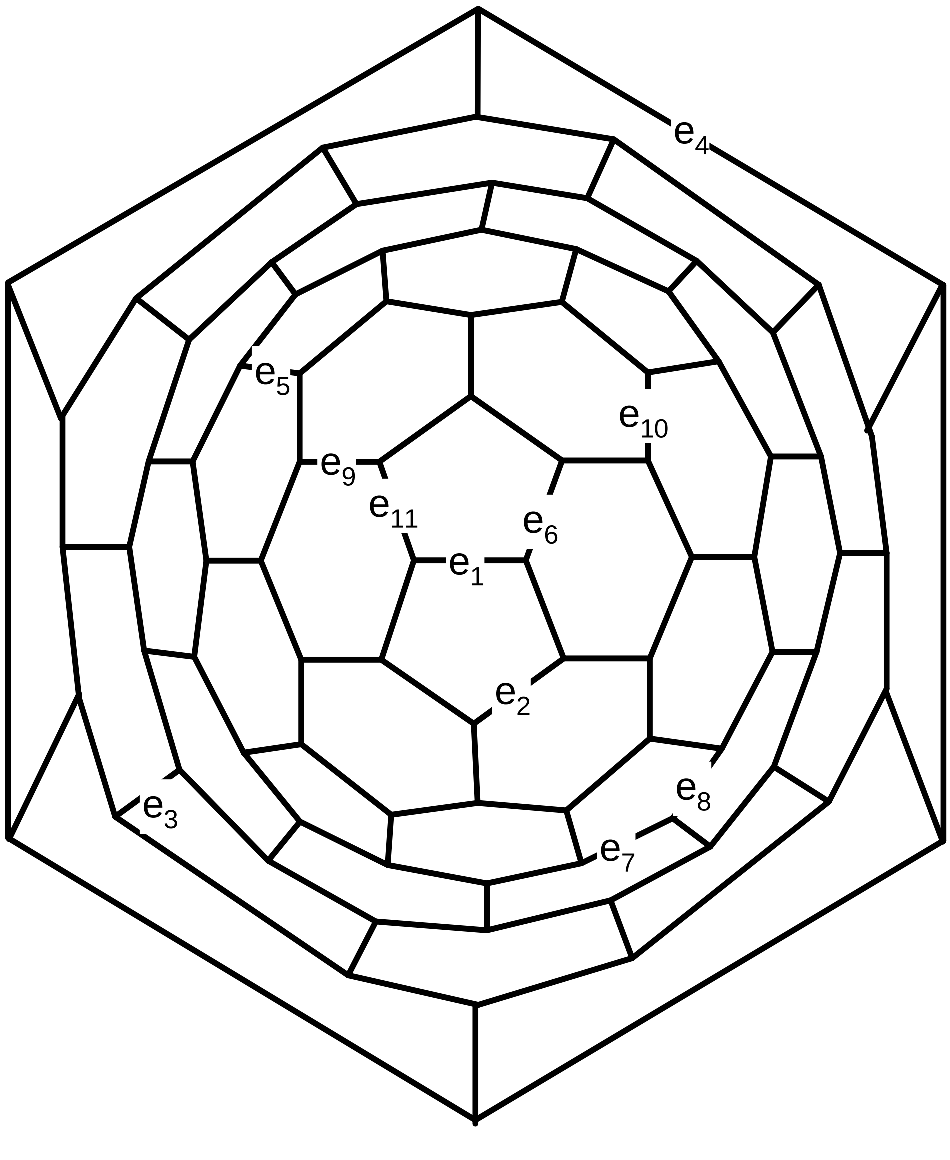
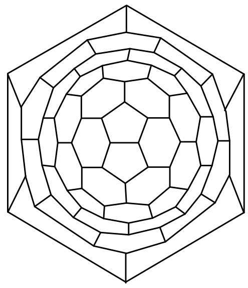


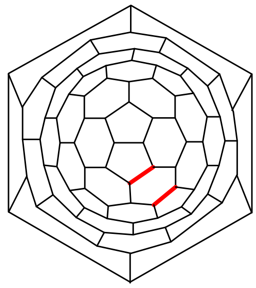
Figure 7. The Graph of fullerene C_{40n+6}, when n = 2.

Table 2. The number of Co–distant edges of e_i, $1 \leq i \leq 10$.

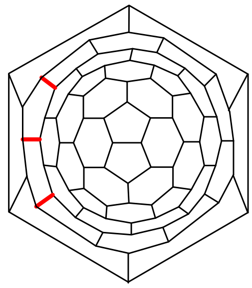
No.	Number of Co-Distant Edges	Type of Edges
1	1	e_1
9	2	e_2
4	3	e_3
2	4	e_4
2n-3	10	e_5
2	$\begin{cases} 2n+1 & 5 \mid n \\ 4n+3 & 5 \mid n-1 \\ 2n & 5 \mid n-4, n-2 \\ 2n+2 & 5 \mid n-3 \end{cases}$	e_6
$\begin{cases} 2 \\ 4 \\ 4 \end{cases}$	$\begin{cases} 4n-1 & 5 \mid n-3 \\ 2n & 5 \mid n, n-2 \\ 2n-2 & 5 \mid n-1, n-4 \end{cases}$	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}



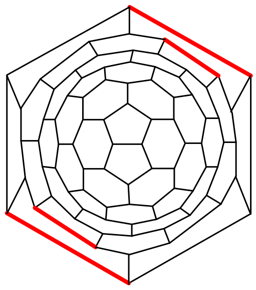
Graph of fullerene C_{40n+6}



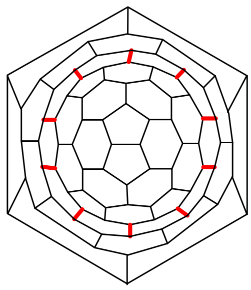
Edges codistant to e_1



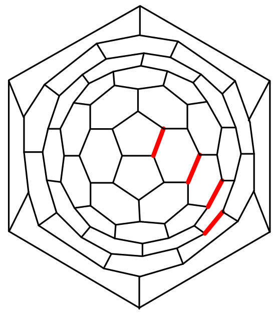
Edges codistant to e_2



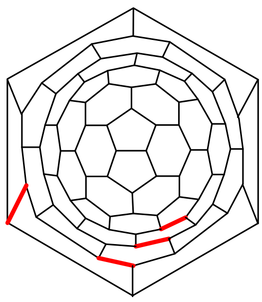
Edges codistant to e_3



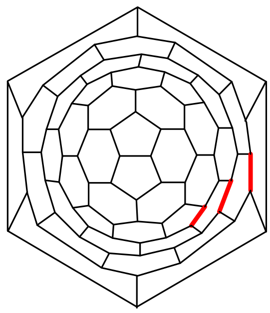
Edges codistant to e_4



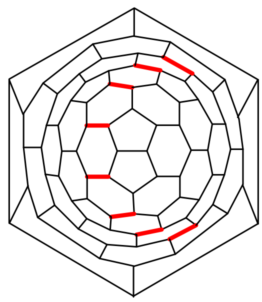
Edges codistant to e_5



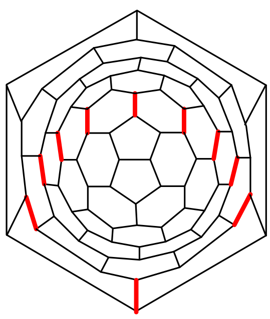
Edges codistant to e_6



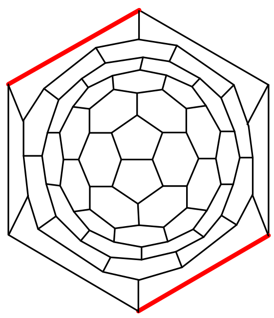
Edges codistant to e_7



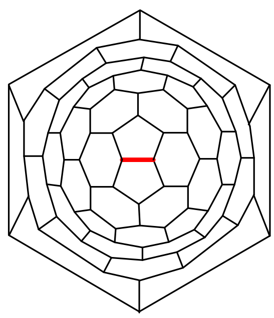
Edges codistant to e_8



Edges codistant to e_9



Edges codistant to e_{10}



Edges codistant to e_{11}

Figure 8. The main cases of C_{40n+6} fullerenes regarding Co−distant edges.

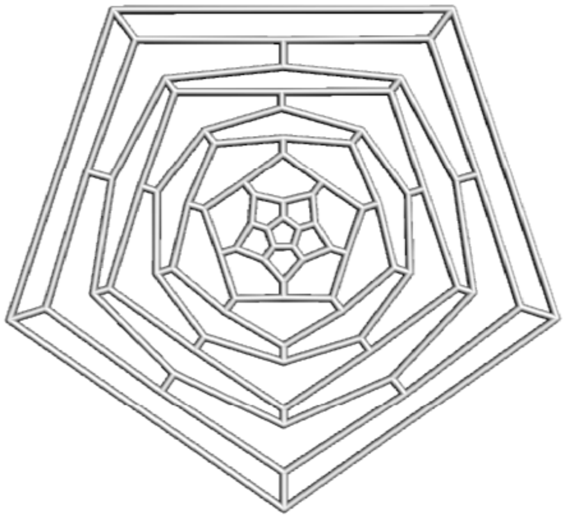


Figure 9. The fullerene graph F_n, $n = 8$.

Next, we consider a class of fullerenes with exactly 10n vertices, Figure 9. From Figure 10, there are six distinct cases of qoc strips as follows:

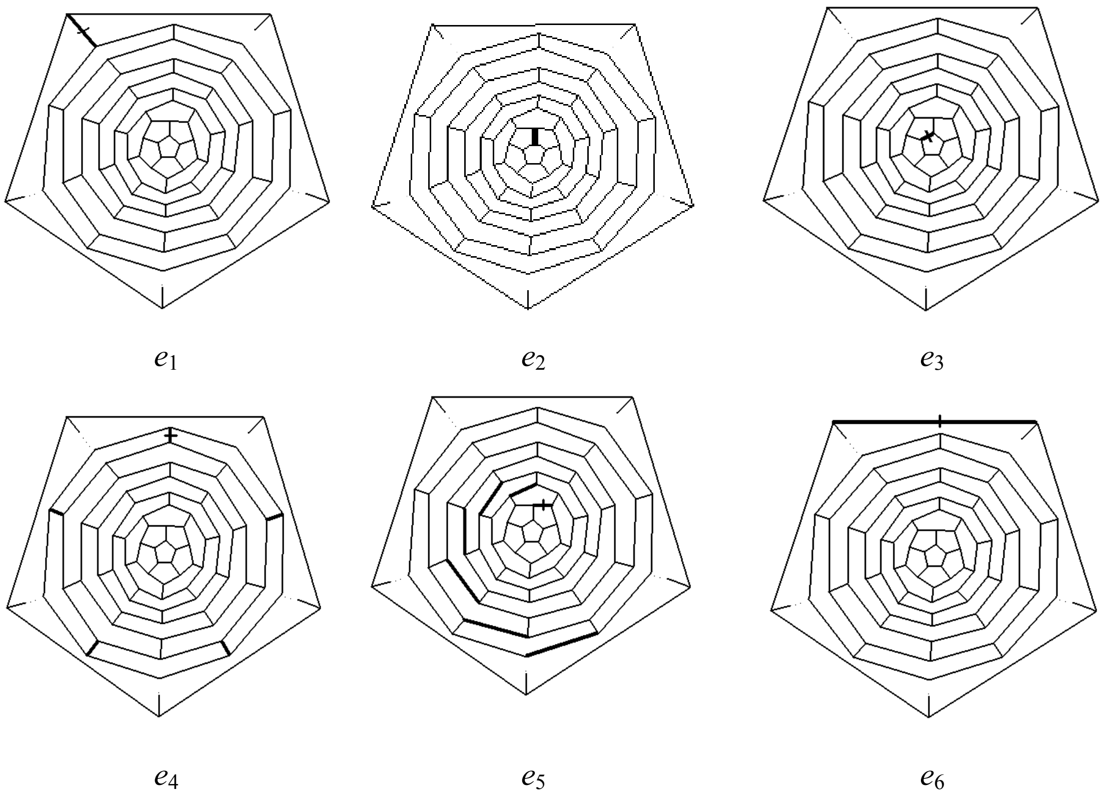


Figure 10. The qoc strips of edgese_1, e_2, …,e_6 in F_n.

We denote the corresponding edges by e_1, e_2, …,e_6. Then |C(e_1)| = |C(e_2)| = |C(e_3)| = |C(e_6)| = 1, |C(e_4)| = 5 and |C(e_5)| = n – 1. On the other hand there are five similar edges for each of edges e_1, e_2, e_3 and e_6, n – 2 edges similar to e_4 and 10 edges similar to e_5. Therefore,

$$\Omega(F_n, x) = 20 \cdot x + (n-2) \cdot x^5 + 10 \cdot x^{(n-1)}.$$

In what follows, a new class of fullerenes with 10n carbon atoms are considered, see Figure 11. In Table 3, we lists the Omega polynomial of $F_n$for $n \leq 9$.

Table 3. The Omega Polynomial of F_n for $n \leq 9$.

Fullerenes	**Ω Polynomials**
C_{20}	$30x$
C_{30}	$20x+x^5+10x^2$
C_{40}	$20x+2x^5+10x^3$
C_{50}	$20x+3x^5+10x^4$
C_{60}	$20x+4x^5+10x^5$
C_{70}	$20x+5x^5+10x^6$
C_{80}	$20x+6x^5+10x^7$
C_{90}	$20x+7x^5+10x^8$

Theorem 7. Consider the fullerene graphs C_{10n}, $n \geq 2$. Then the Omega polynomial of C_{10n} is computed as follows:

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

Proof. To compute the Omega polynomial of C_{10n}, it is enough to calculate C(e) for every e ∊ E(G). In Tables 4 and 5, the number of co-distant edges of this fullerene, are computed. From calculations given in Tables 4, 5 and Figure 11, 12 the equation is obtained which completes the proof.

Table 4. The Number of Co-Distant Edges, when $2|n$.

Type of Edges	**Number of Co-Distant Edges**	**No**
e_1	3	10
e_2	n/2	10
e_3	n – 3	10

Table 5. The Number of Co-Distant Edges, when $2 \nmid n$.

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

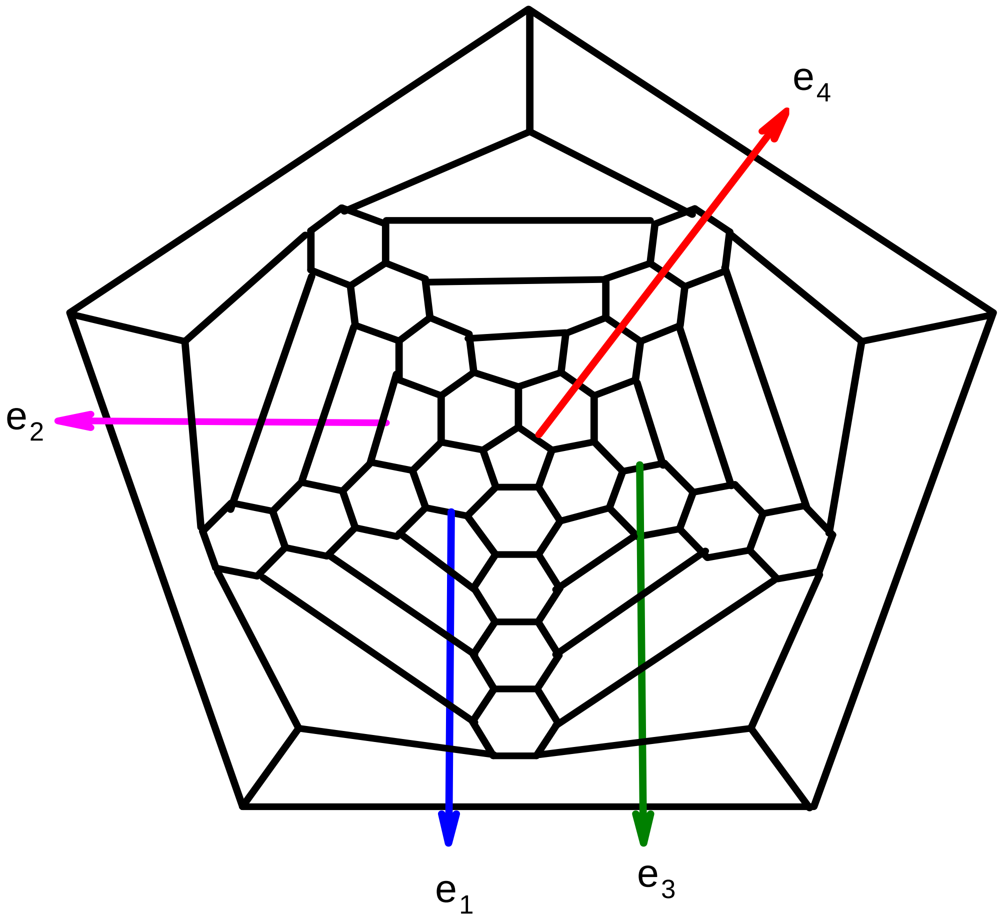


Figure 11. The fullerene graph C_{10n} (n is odd).

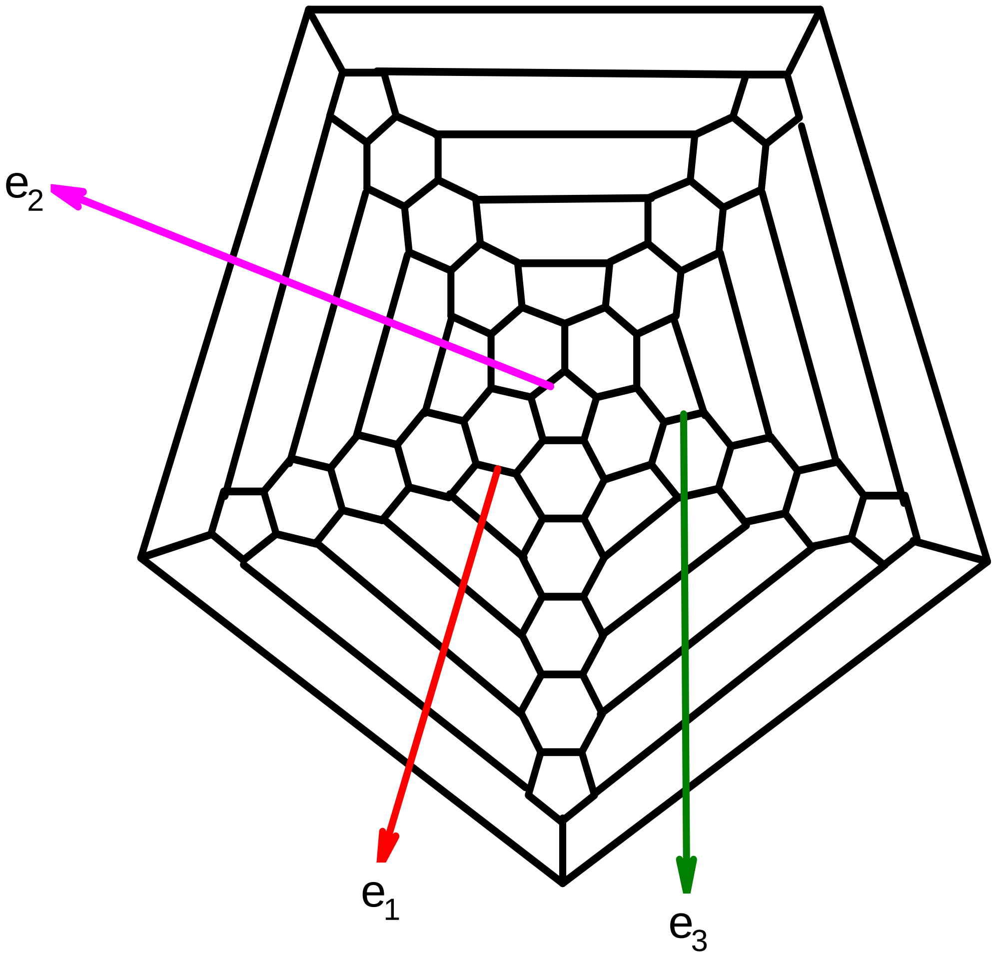


Figure 12. The fullerene graph C_{10n} (n is even).

Theorem 8. Suppose G is the molecular graph of C_{24n} fullerene. Then the Omega polynomial of G is $\Omega(G,x)=3x^{2n}+6x^{n}+12x^{2n-3}+12x^{3}$.

Proof. It is easy to see that there are four different type of edges, f_1, f_2, f_3 and f_4, Figure 13. The number of edges co–distant to f_1, f_2, f_3 and f_4 are $2n$, $2n$-3, 3 and n, respectively. On the other hand, there are 3 edges similar to f_1, 12 edges similar to f_2, 12 edges similar to f_3 and 6 edges similar to f_4, Figure 13. Therefore,

$$\Omega(G,x)=3x^{2n}+6x^{n}+12x^{2n-3}+12x^{3}.$$

Theorem 9. The omega polynomial of fullerene graph C_{12n+4}(Figure 14) is as follows:

$$\Omega(C_{12n+4},x)=18x+4x^{2}+(n-2)x^{6}+8x^{n-1}+4x^{n}.$$

Proof. By Figure 15, there are five distinct cases of qoc strips. We denote the corresponding edges by $e_1, e_2, \ldots, e_5$. By table 1 one can see that $|C(e_1)|=2$, $|C(e_2)| = n-1$, $|C(e_3)|$ = n, $|C(e_4)| = 1$ and $|C(e_5)| = 6$. On the other hand, there are 4, 8, 4, 18 and n-2 similar edges for each of edges e_1, e_2, e_3, e_4 and e_5, respectively. So, we have

$$\Omega(C_{12n+4},x)=18x+4x^2+(n-2)x^6+8x^{n-1}+4x^n.$$

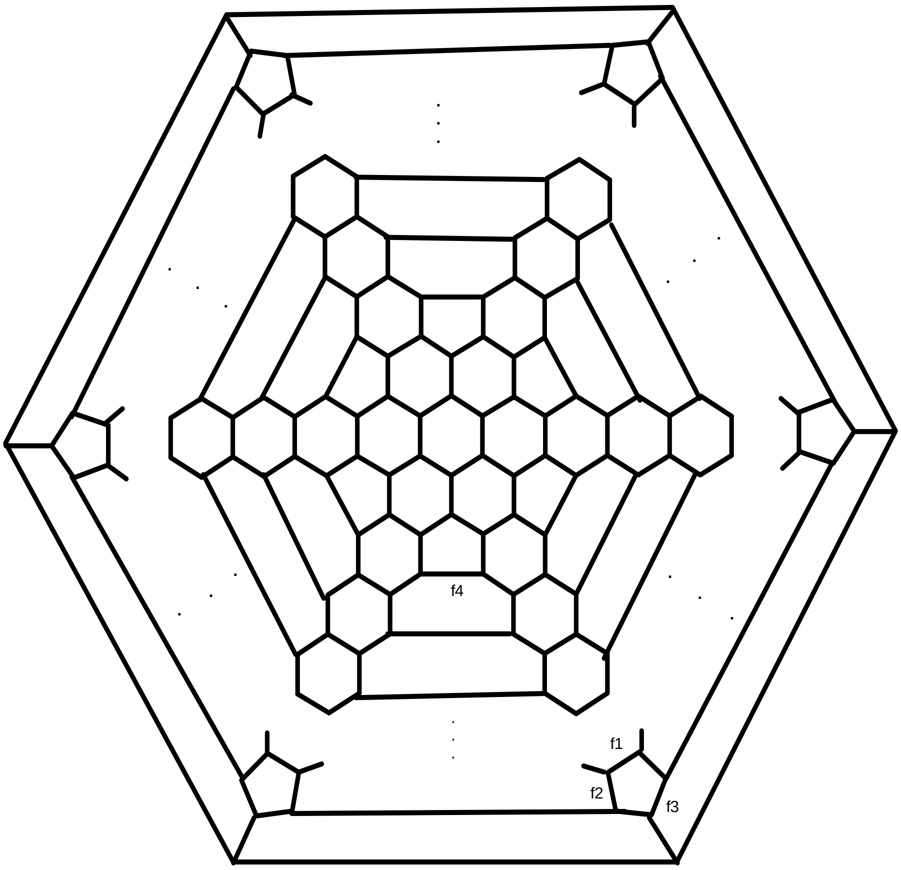


Figure 13. The Schlegel graph of C_{24n} fullerene.

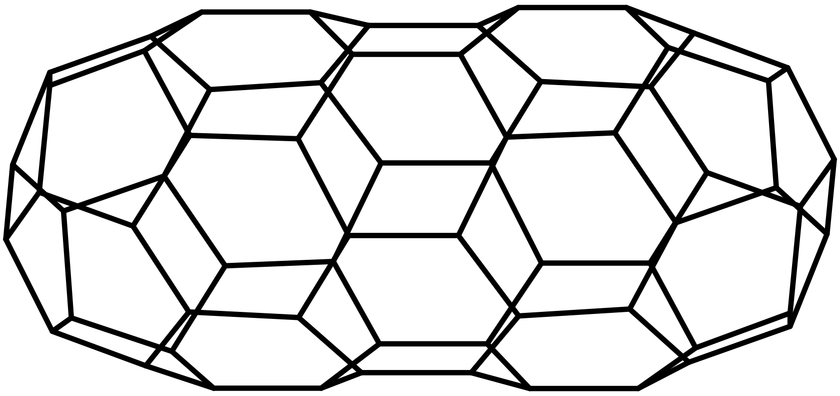


Figure 14. The molecular graph of C_{12n+4} fullerene.

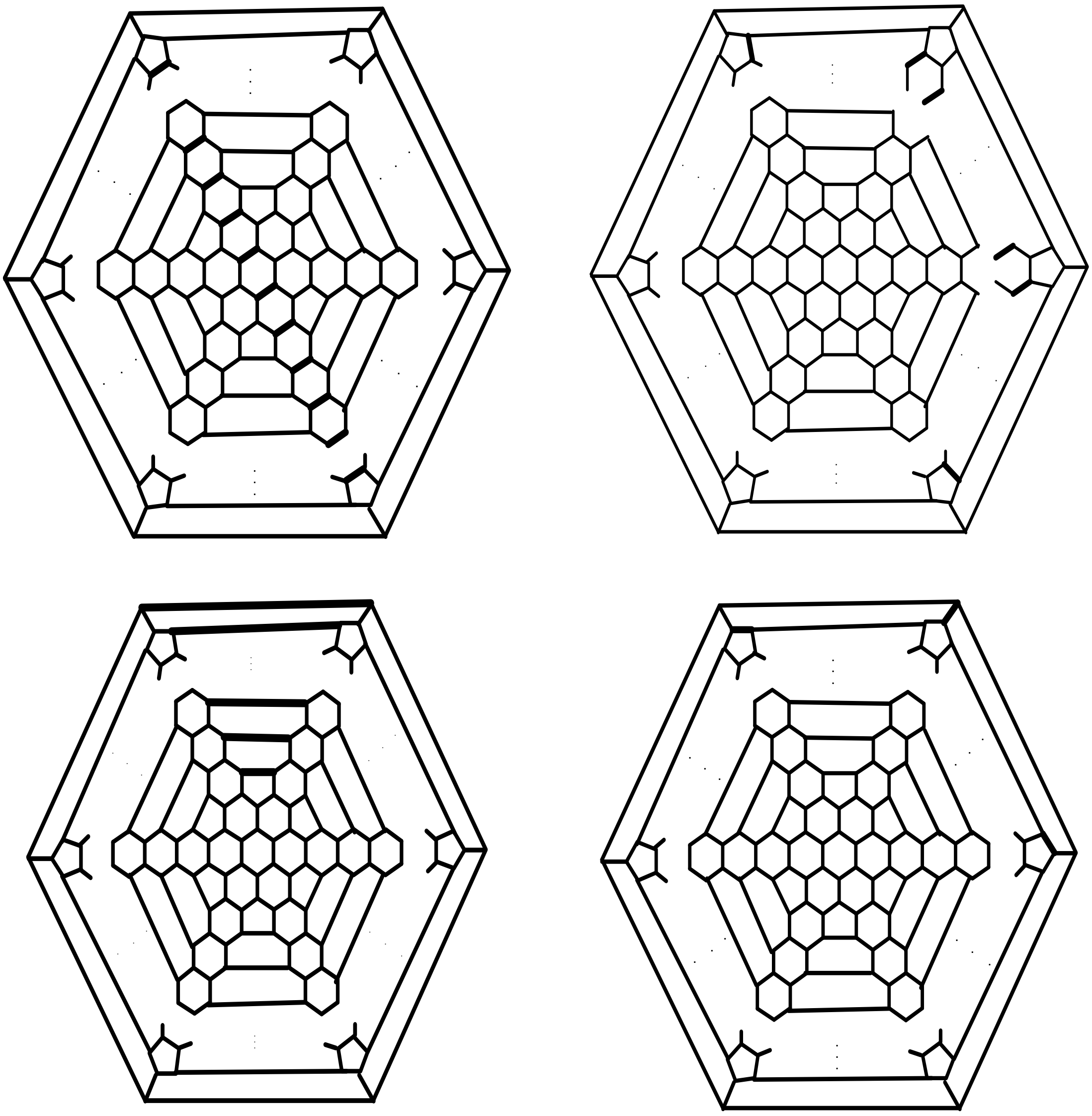


Figure 15. Four different types of edges in C_{24n} Fullerene.

Table 6. The Number of Co–Distant Edges of e_i, $1 \leq i \leq 5$.

No.	Number of Co-Distant Edges	Type of Edges
4	2	e_1
8	$n-1$	e_2
4	n	e_3
18	1	e_4
$n-2$	6	e_5

Theorem 10. The Omega polynomial of the fullerene graph $C_{12(2n+1)}$ is as follows:

$$\Omega(G,x) = 12x^{3} + 12x^{2n-2} + 6x^{n-1} + 3x^{2n+4}, \quad n \geq 2$$

Proof. By Figure 16, there are four distinct cases of qoc strips. We denote the corresponding edges by e_1, e_2, e_3 and e_4. By table 1 one can see that $|C(e_1)|=3$, $|C(e_2)| = 2n - 2$, $|C(e_3)| = 2n + 4$ and $|C(e_4)| = n - 1$. On the other hand, there are 12, 12, 3, and 6 similar edges for each of edges e_1, e_2, e_3, and e_4, respectively. So, we have $\Omega(G,x) = 12x^{3} + 12x^{2n-2} + 6x^{n-1} + 3x^{2n+4}$, $n \geq 2$.

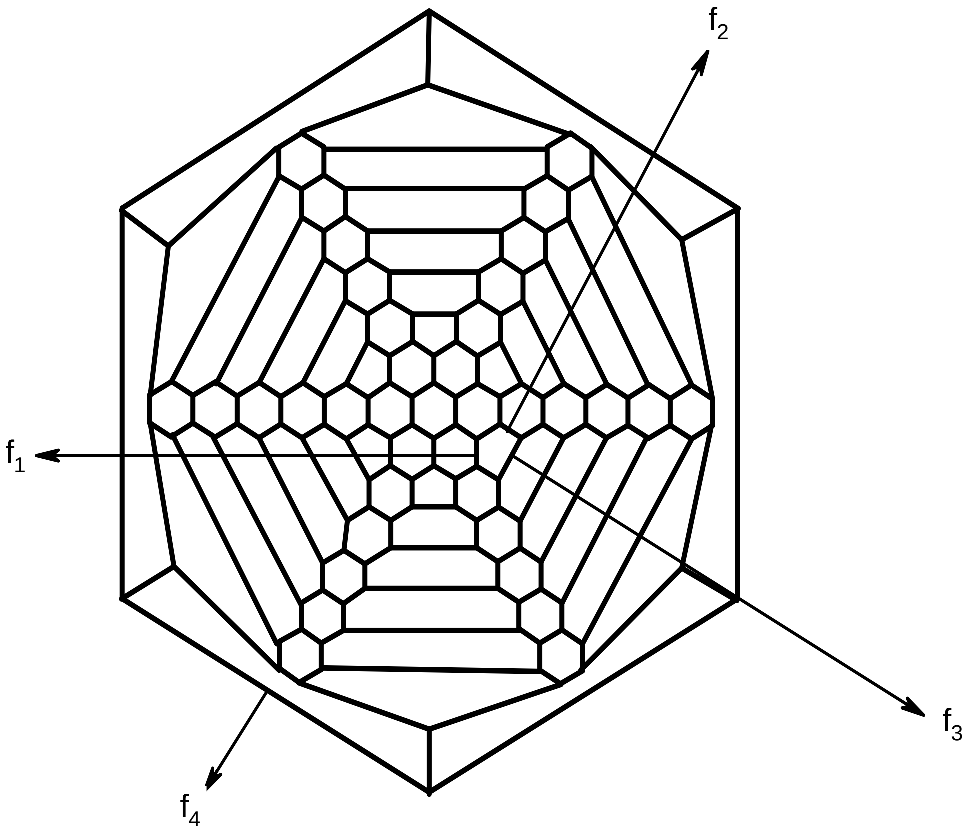


Figure 16. The qoc strips of edges in graph of fullerene $C_{12(2n+1)}$.

Table 7. The number of co-distant edges of e_i, $1 \leq i \leq 4$.

Edge	**The Number of Co Distant Edges**	**No.**
e_1	3	12
e_2	$2n$-2	12
e_3	$2n$+4	3
e_4	n-1	6

Theorem 11. Let F be a fullerene. Then, $\Omega'(G,0)=0$ if and only if F be an IPR fullerene.

Proof. Let $\Omega'(G,0)=0$. This implies the multiplicity of x in definition of Omega polynomial is zero. Since every hexagonal face has 3 strips of length 2, thus none of the pentagons make contact with each other. Conversely, if F be an IPR fullerene, then the length of every strip is greater than 2. Hence, $\Omega'(G,0)=\lambda_1 x+\lambda_2 x^2+\ldots\big|_{x=0}=0$.

Lemma 12. Let G be a graph on n vertices, m edges and α be number of its *qoc* strips. Then

$$\alpha=\frac{Sd(G)}{m}+1. \quad (15)$$

Proof. By using definition of Sadhana index we have:

$$Sd(G)=\sum_s m_s(|E(G)|-s)=\sum_s m_s|E(G)|-\sum_s m_s\cdot s=(\alpha-1)m.$$

Corollary 13. Let F_1 and F_2 be fullerenes of order n. Then

$$Sd(F_1)\le Sd(F_2)\Leftrightarrow \alpha(F_1)\le\alpha(F_2).$$

Proof. Since $Sd(G)=(\alpha-1)m$ the proof is straightforward.

Theorem 14. Suppose F be an IPR fullerene, then

$$Sd(G)\le m(m-2)/2.$$

Proof. For every *qoc* strip C of F, $|C|\ge 2$. Since $2\alpha\le m$, thus $\frac{Sd(G)}{m}+1\le m/2$ and so $Sd(G)\le m(m-2)/2$.

Theorem 15. Let F be afullerene graph. Then $Sd(F)\ge(2+\Omega'(G,0))m$.

Proof. Let r and s be the number of *qoc* strips of length 1 and 2, respectively. Clearly $r=\Omega'(0)$ and since every hexagonal face has at least 3 *qoc* strips of length 2, thus $\alpha\ge 3+\Omega'(G,0)$. By using equation (15) the proof is completed.

Conjecture 16. Among all of fullerenes F on n vertices the IPR fullerene has the minimum value of $Sd(F)$.

Let G be a fullerene graph on n vertices. A leapfrog transform G^l of G is a graph on $3n$ vertices obtained by truncating the dual of G. Hence, $G^l = Tr(G^*)$, where G^* denotes the dual of G. It is easy to check that G^l itself is a fullerene graph. We say that G^l is a leapfrog fullerene obtained from G and write $G^l = Le(G)$. In the other word, for a given fullerene F_n put an extra vertex into the centre of each face of F_n. Then connect these new vertices with all the vertices surrounding the corresponding face. Then the dual polyhedron is again a fullerene having $3n$ vertices 12 pentagonal and $(3n/2)-10$

hexagonal faces. A sequence of stellation–dualization rotates the parent s–gonal faces by π/s. Leapfrog operation is illustrated, for a pentagonal face, in Figure 17.

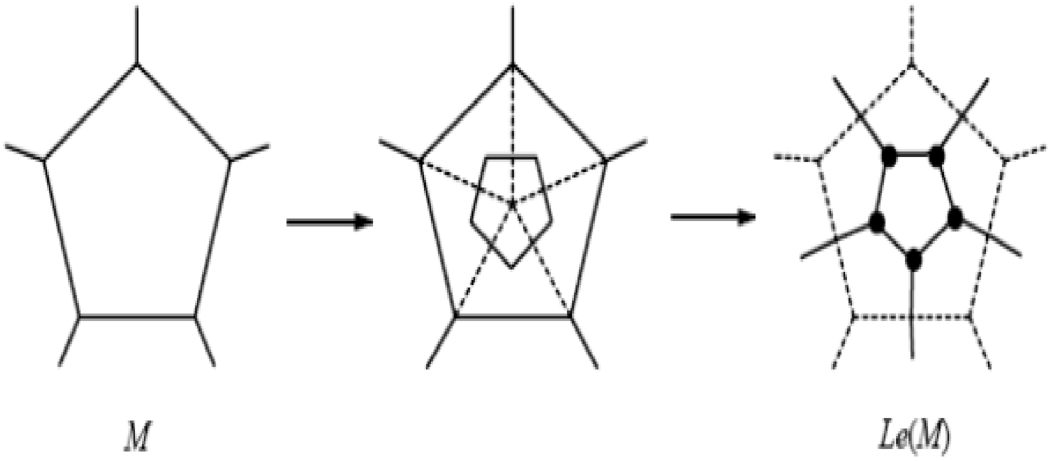
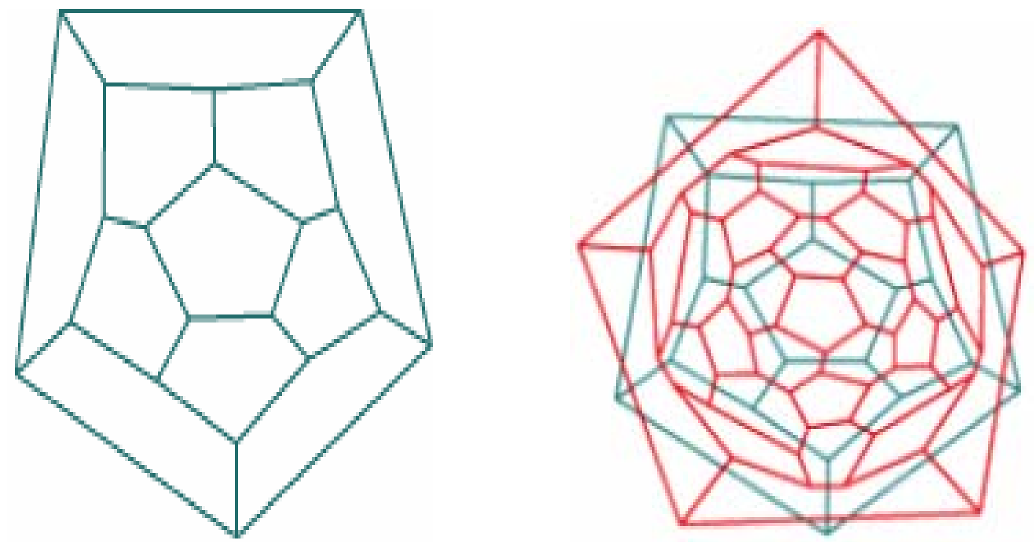


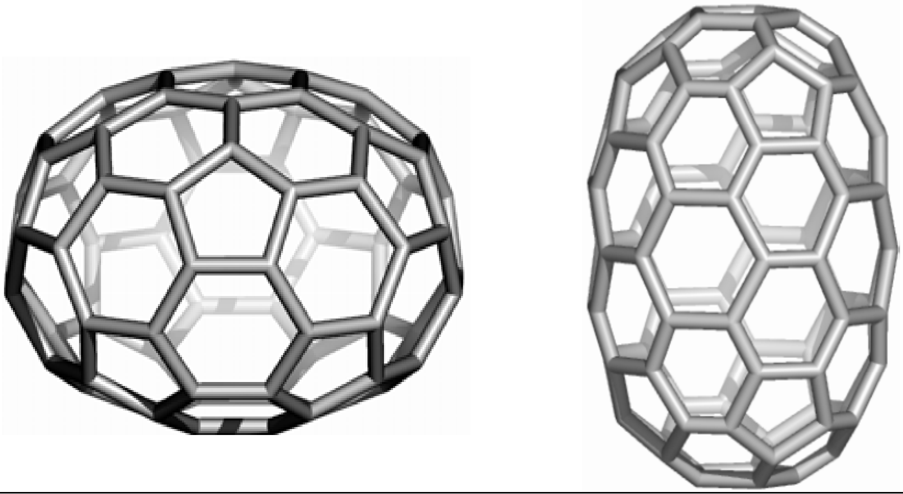
Figure 17. Leapfrog of a pentagonal face.

In Figure 18, one can see that the fullerene graph C_{20} and its Leapfrog, namely C_{60}. Also, in Figure 19 the 3 dimensional leapfrog graph of C_{24} and C_{30} are depicted. We denote the Leapfrog of graph *G* by Le(F).



$Le(C_{20}) = C_{60}$.

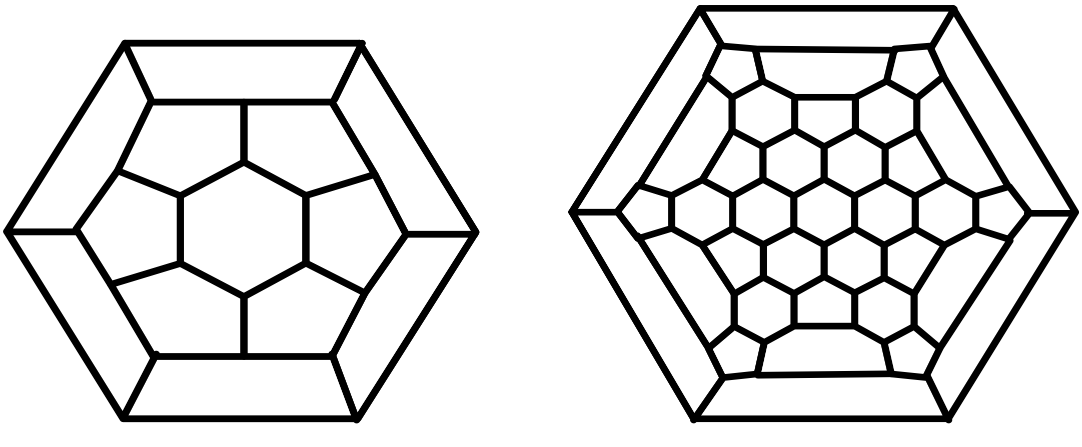
Figure 18. Fullerene graph C_{20} and its Leapfrog.



$L(C_{20}) = C_{60}$.

Figure 19. $Le(C_{24})$ and $Le(C_{30})$.

Example 17. Consider the fullerene graph F_{24} in Figure 20. This fullerene graph has 36 edges. Similar to example 1 one can see that $\Omega(x) = 24x + 6x^2$ and so $Sd(x) = 24x^{35} + 6x^{34}$. In Figure 20 one can see the planer graphs F_{24} and $Le(F_{24})$.

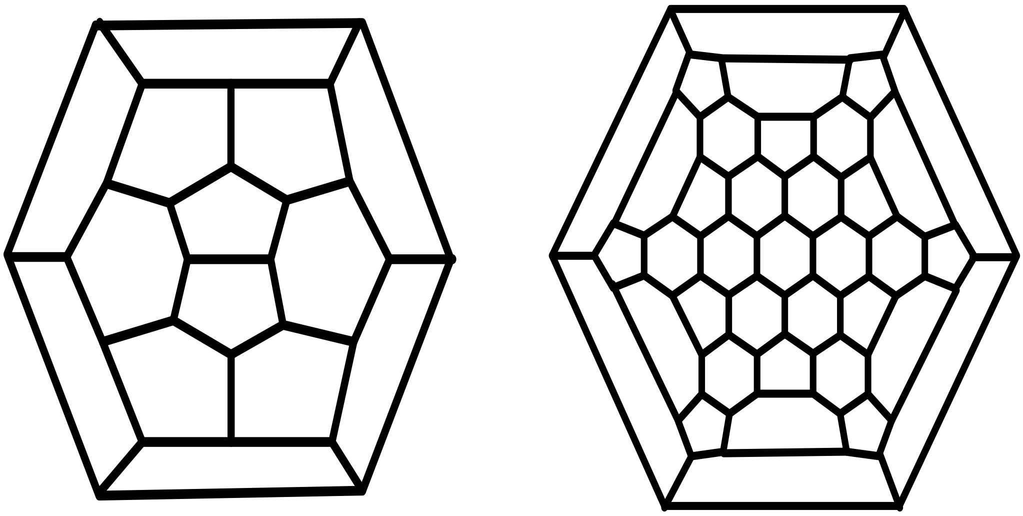


F_{24} $Le(F_{24})$

Figure 20. The Leapfrog of graph F_{24}.

Example 18. Consider the fullerene graph F_{26} depicted in Figure 21. This fullerene graph has 39 edges. Similar to examples 1 and 2 one can see that $\Omega(F_{26}, x) = 21x + 9x^2$ and so, $Sd(F_{24}, x) = 21x^{38} + 9x^{37}$. By computing these polynomials for the Leapfrog fullerene we have:

$$\Omega(G, x) = 24x^3 + 6x^6 + x^9.$$



F_{26} $Le(F_{26})$

Figure 21. The Leapfrog of graph F_{26}.

An automorphism of the graph $G = (V, E)$ is a bijection σ on V which preserves the edge set e, i. *E*., if $e = uv$ is an edge, then $\sigma(e) = \sigma(u)\sigma(v)$ is an edge of E. Here the image of vertex u is denoted by $\sigma(u)$. The set of all automorphisms of G under the composition of mappings forms a group which is denoted by $Aut(G)$. $Aut(G)$ acts transitively on V if for any vertices u and v in V there is $\alpha \in Aut(G)$ such that $\alpha(u) = v$. Similarly $G = (V, E)$ is called edge-transitive graph if for any two edges $e_1 = uv$ and $e_2 = xy$ in E there is an element $\beta \in Aut(G)$ such that $\beta(e_1) = e_2$ where $\beta(e_1) = \beta(u)\beta(v)$. Furthermore, if F be a fullerene graph then, $Aut(F) = Aut(Le(F))$.

As a result of Lemma 32 we compute the Omega polynomial of a hyper – cube. The vertex set of the hypercube H_n consist of all n–tuples $b_1b_2\ldots b_n$with $b_i \in \{0,1\}$. Two vertices are adjacent if the corresponding tuples differ in precisely one place. So the hyper – cube H_n has 2^n vertices and $n.2^{n-1}$ edges. On other word, $H_n \cong \underbrace{K_2 \times K_2 \times \cdots \times K_2}_{n}$.

It is well – known fact that H_n is vertex and edge transitive. We use of this result and we have the following Theorem:

Theorem 19. $\Omega(H_n) = nx^{2^{n-1}}$.

Proof. Let $e = uv$ be an arbitrary edge of H_n. By computing the qoc strips one can see that $c = |C(e)| = 2^{n-1}$. Furthermore, since $|E(H_n)| = n.2^{n-1}$ the proof is completed.

Now, let $G = (V, E)$ be a graph. If $Aut(G)$ acts edge-transitively on V, then we have the following Lemma:

Lemma 20. Let $e \in E(G)$ be an arbitrary edge and $c = |C(e)|$. Then the Omega polynomial of graph G is as follows:

$$\Omega(G,x) = \frac{|E(G)|}{c} x^c .$$

Proof. Because *Aut*(*G*) acts edge-transitively on *E*, so we can divide *E* to some qoc strips of equal size. One can see that each qoc strip is of length *c*.

Example 21. Consider the fullerene graph C_{20} shown in Figure 22. It is easy to see C_{20} is edge - transitive, |*E*| = 30 and *c*=1. So by using Lemma 19 we have $\Omega(G,x) = 30x$.

Fullerenes C_{20} and C_{60} are the only edge - transitive fullerenes. So it is important how to compute the Omega polynomial for graphs in which *Aut*(*G*) is not edge - transitive. One can apply the following Theorem for this case:

Theorem 22. Suppose *Aut*(*G*) acts on *E* and $E_1, E_2, \ldots, E_n$ be its orbits. Then the Omega polynomial of *G* is as $\Omega(G,x) = \sum_{i=1}^{n} \frac{|E_i|}{c_i} x^{c_i}$, where $e \in E_i$ and $c_i = |C(e_i)|$.

Proof. We know *Aut*(*G*)acts edge-transitively on its orbits. By using Lemma 4 the proof is straightforward.

Theorem 22 implies when the acting *Aut*(*G*) is not edge – transitive then, $m(G,c)$'s in equation 1, determine exactly the qoc strips of orbits of *Aut*(*G*). In the other word for an arbitrary edge *e* belong to *E*(*G*), when we say *m*(*G,c*) = *k*, it means there exist an orbit such that Δ with *c* = |*C*(*e*)| and *m*(*G,c*) = | Δ | = *k*. Thus for a given graph of high order it is sufficient to compute all of orbits of *Aut*(*G*) acting on *E*.

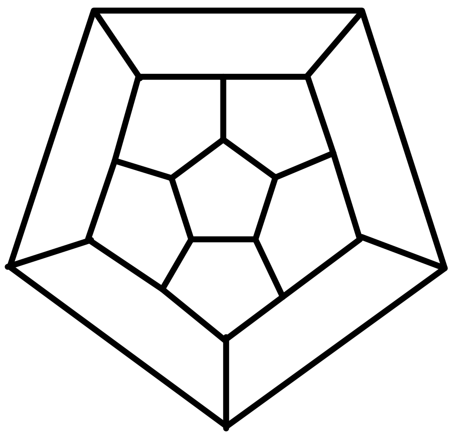


Figure 22. The graph of fullerene C_{20}.

By continuing our methods described in this paper one can consult the graph of fullerene $F_{26\times 3^n}$. Hence, we have the following Theorem:

Theorem 23. Consider the fullerene graph $F_{36\times 3^n}$ ($n \geq 2$) depicted in Figure 23. Then the Omega polynomial is as follows:

$$\Omega(G,x)=\begin{cases}18x^{3^{(\frac{n}{2})}}+15x^{3^{(\frac{n}{2})}\times 2}+(2\times 3^{(\frac{n}{2})}-1)x^{3^{(\frac{n}{2}+1)}\times 2}+6(3^{(\frac{n}{2})}-1)x^{3^{(\frac{n}{2})}\times 7} & 2\mid n\\ 18x^{3^{(\frac{n+1}{2})}}+12x^{3^{(\frac{n+1}{2})}\times 2}+3(2\times 3^{(\frac{n-1}{2})}-1)x^{3^{(\frac{n+1}{2})}\times 4}+2(3^{(\frac{n-1}{2})}-1)x^{3^{(\frac{n+3}{2})}\times 5} & 2\nmid n\end{cases}.$$

Proof. At first by we can prove $Aut(F_{36})\cong D_{12}$. In other word generators of $Aut(F_{36})$ are as follows, Figure 24:

a := (1,2)(3,6)(4,5)(7,13)(8,12)(9,11)(14,18)(15,17)(20,26)(21,25)(22,24)(19,27)(28,30)(31,36)(32,35)(33,34);
b := (1,2,3,4,5,6)(7,9,11,13,15,17)(8,10,12,14,16,18)(21,23,25,27,29,19)(22,24,26,28,30,20)(31,32,33,34,35,36);

It is necessary to consider two cases. At first suppose n be even. $Aut(F_{36})$ act on edges of F_{36} and it has exactly four orbits. Since for a fullerene graph F, $Aut(F)$ = $Aut(Le(F))$, by using Theorem 7, there are four types of edges for *qoc* strips. We denote them by e_1, e_2, e_3 and e_4. It is not difficult to see that $|C(e_1)| = 3^{n/2}$, $|C(e_2)| = 2\times 3^{n/2}$, $|C(e_3)| = 2\times 3^{(n+2)/2}$ and $|C(e_4)| = 7\times 3^{n/2}$. On the other hand there are 18, 15, $2\times 3^{\frac{n}{2}}-1$ and $6(3^{\frac{n}{2}}-1)$ edges of type e_1, e_2, e_3 and e_4, respectively. Now let n be odd. By the same way we can see there are four types of edges for *qoc* strips namely e_1, e_2, e_3 and e_4, $|C(e_1)| = 3^{(n+1)/2}$, $|C(e_2)| = 2\times 3^{(n+1)/2}$, $|C(e_3)| = 3^{(n+2)/2}\times 4$ and $|C(e_4)| = 5\times 3^{(n+3)/2}$. Also, there are 18, 12, $3(2\times 3^{\frac{n-1}{2}}-1)$ and $2(3^{\frac{n-1}{2}}-1)$ edges of type e_1, e_2, e_3 and e_4, respectively.

Corollary 24. For the fullerene graph $F_{36\times 3^n}$ $(n\geq 2)$ the Sadhana polynomial is as follows:

$$Sd(G,x)=\begin{cases}18x^{|E|-3^{(\frac{n}{2})}}+15x^{|E|-3^{(\frac{n}{2})}\times 2}+(2\times 3^{(\frac{n}{2})}-1)x^{|E|-3^{(\frac{n}{2}+1)}\times 2}\\ +6(3^{(\frac{n}{2})}-1)x^{|E|-3^{(\frac{n}{2})}\times 7} & 2\mid n\\ 18x^{|E|-3^{(\frac{n+1}{2})}}+12x^{|E|-3^{(\frac{n+1}{2})}\times 2}+3(2\times 3^{(\frac{n-1}{2})}-1)x^{|E|-3^{(\frac{n+1}{2})}\times 4}\\ +2(3^{(\frac{n-1}{2})}-1)x^{|E|-3^{(\frac{n+3}{2})}\times 5} & 2\nmid n\end{cases}$$

in which $|E|=2\times 3^{n+3}$.

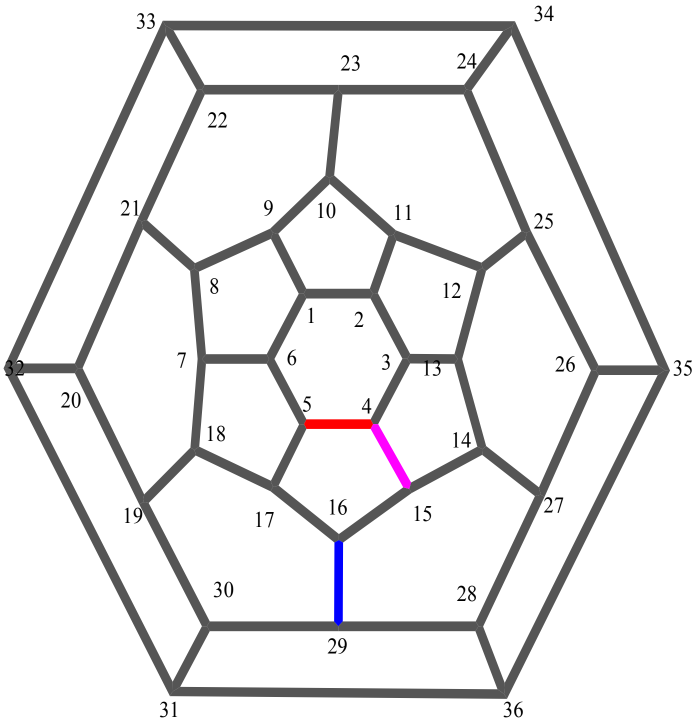


Figure 23. The graph of fullerene F_{36}.

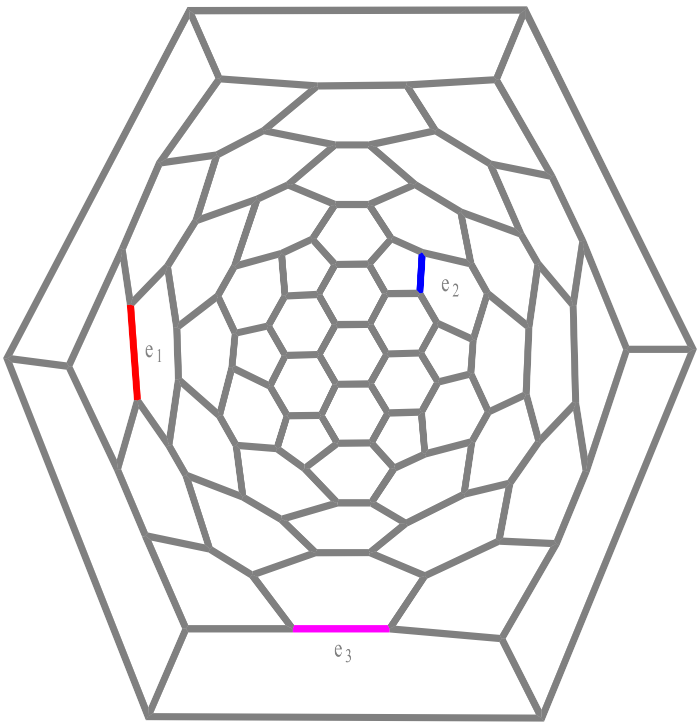


Figure 24(*i*). The graph of $F_{36\times 3^n}$ for $n = 1$.

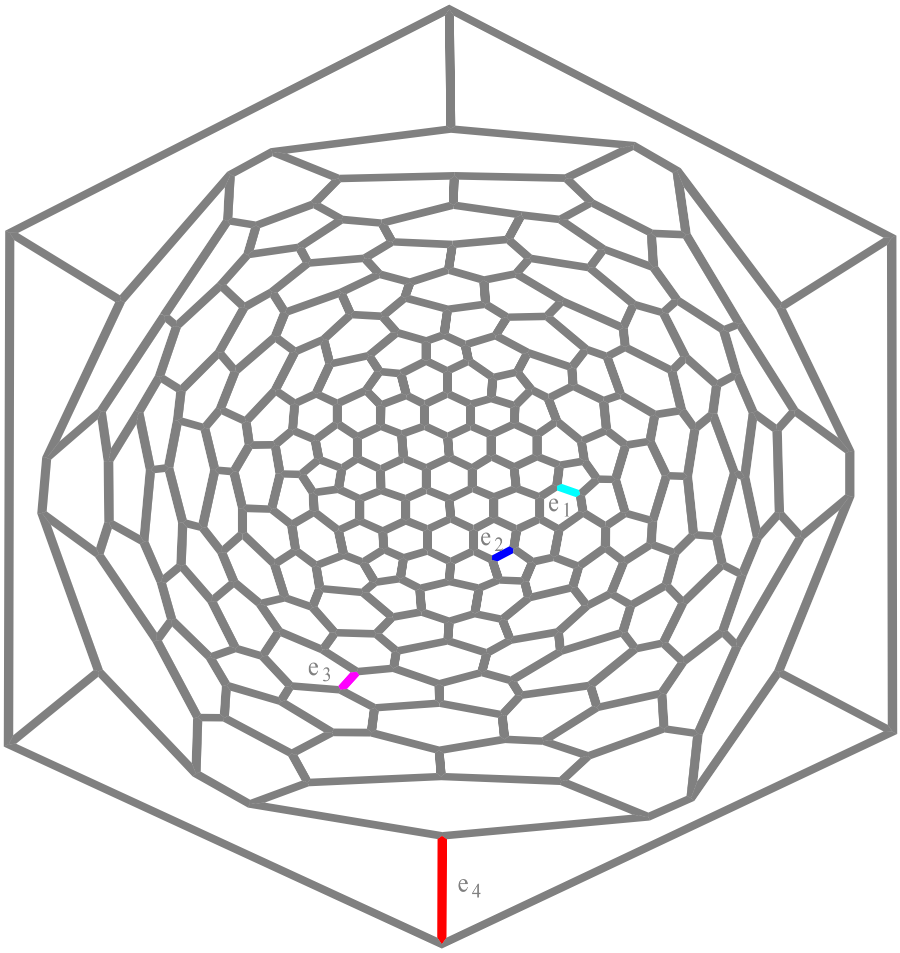


Figure 24(*ii*). The graph of $F_{36\times3^n}$ for $n = 2$.

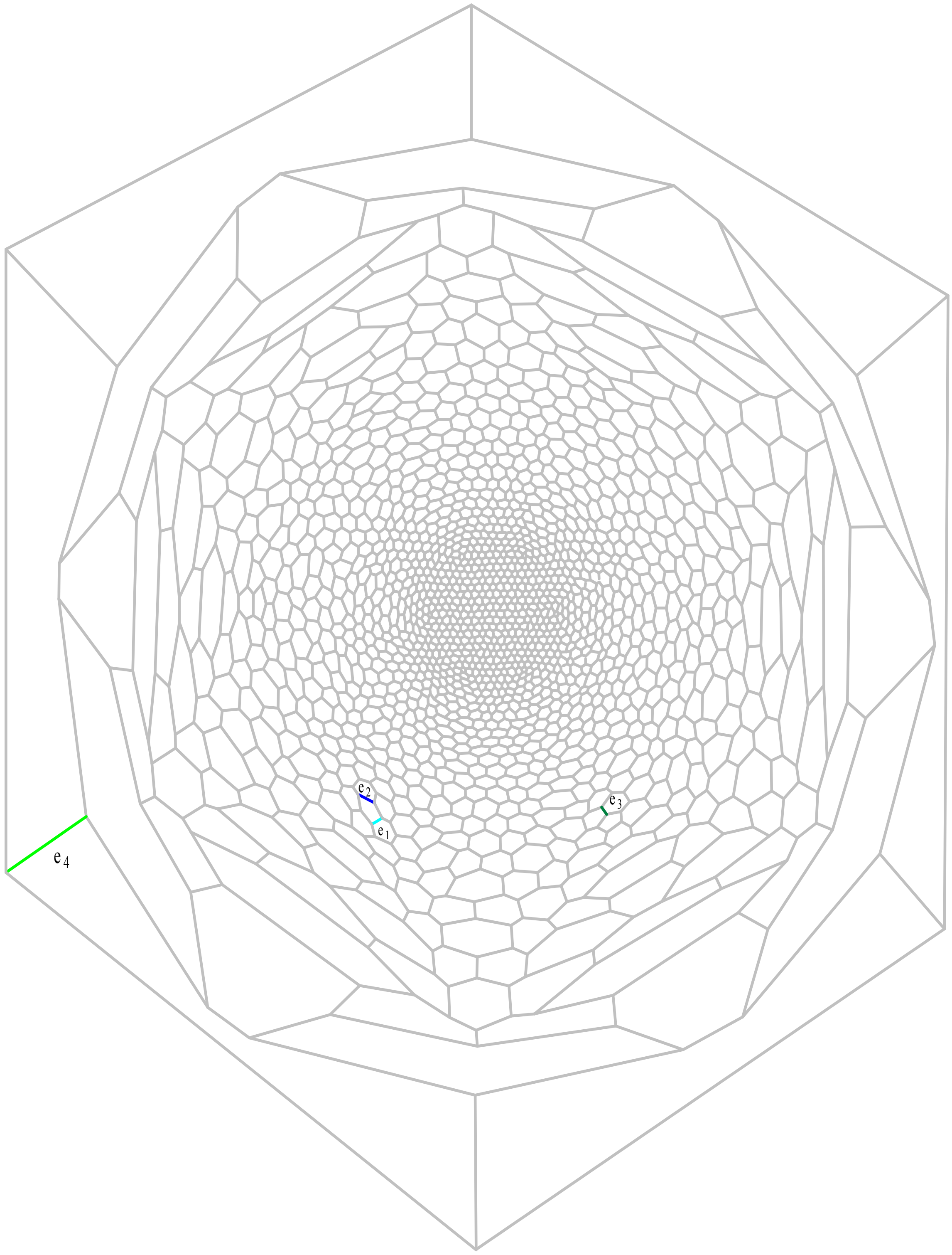


Figure 24(*iii*). The graph of $F_{36\times 3^n}$ for $n = 3$.

In this section by using definition of Omega and Sadhana polynomials, we compute these counting polynomials for a special class of fullerenes, namely $F_{4\times 3^n}$. In other word,

$F_{4\times 3^n}$ is an infinite family of fullerenes with 4×3^n carbon atoms and $2\times 3^{n+1}$ bonds (the graph *G*, Figure 25 is *n*=1) constructed by Leapfrog principle. At first we should to compute some computational examples.

Example 25. Suppose F_{12} denotes the fullerene graph on 12 vertices (Figure 25). The co – distant edges are shown by the same colors. Then $\Omega(x) = 6x^3$ and $Sd(x) = 6x^9$.

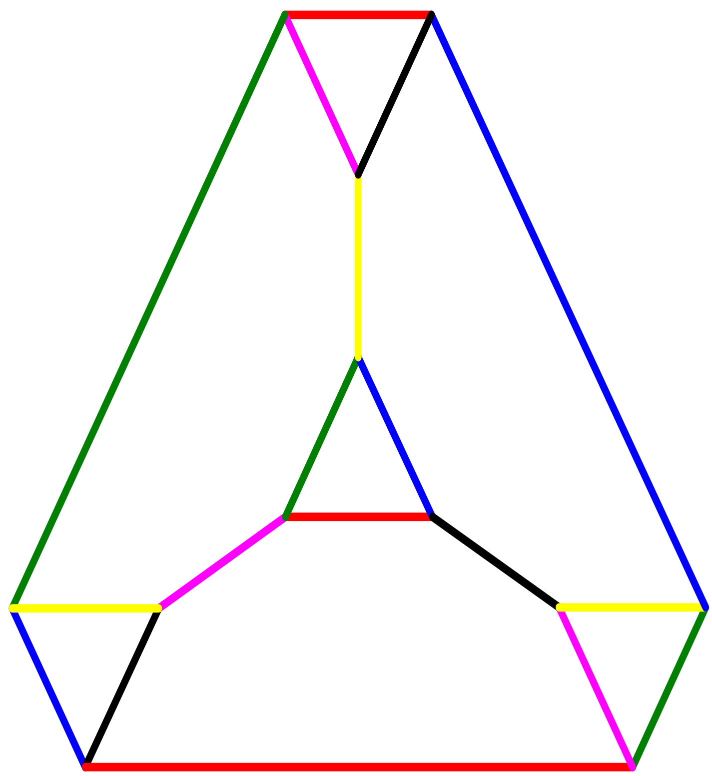


Figure 25. The fullerene graph F_{12}.

Example 26. Consider the fullerene graph F_{36} with 36 vertices, Figure 26. Then one can see that $\Omega(x) = 6x^6 + 6x^3$ and $Sd(x) = 6x^{30} + 6x^{33}$.

Example 27. The Omega and Sadhana polynomials of fullerene graph F_{108}, Figure 27, are as follows:

$$\Omega(x) = 6x^9 + 6x^{18} \text{ and } Sd(x) = 6x^{90} + 6x^{99}.$$

Theorem 28. Consider the fullerene graph $F_{4\times 3^n}$, see Figure 28. Then

$$\Omega(x) = 6x^9 + (3^{n-1} - 3)x^{18}.$$

Proof. By Figure 28, there are two distinct cases of qoc strips. We denote the corresponding edges by e_1 and e_2. By using table 1 and Figure 28 the proof is completed.

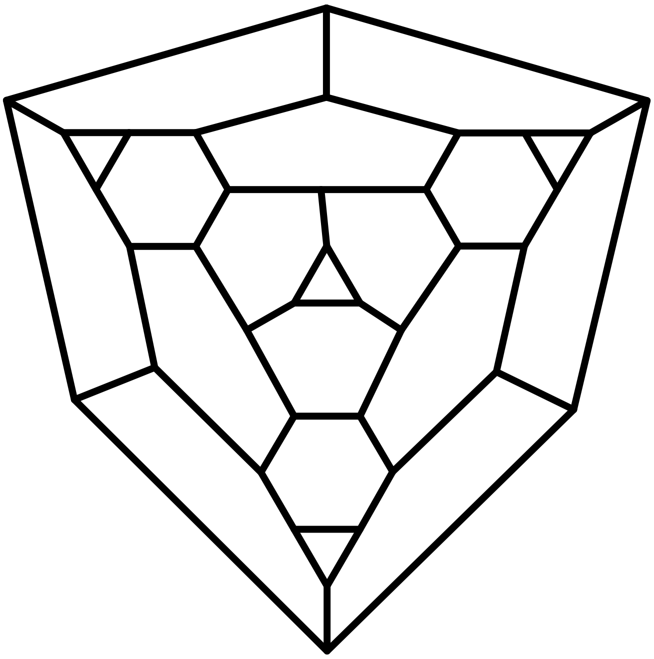


Figure 26. The fullerene graph F_{36}.

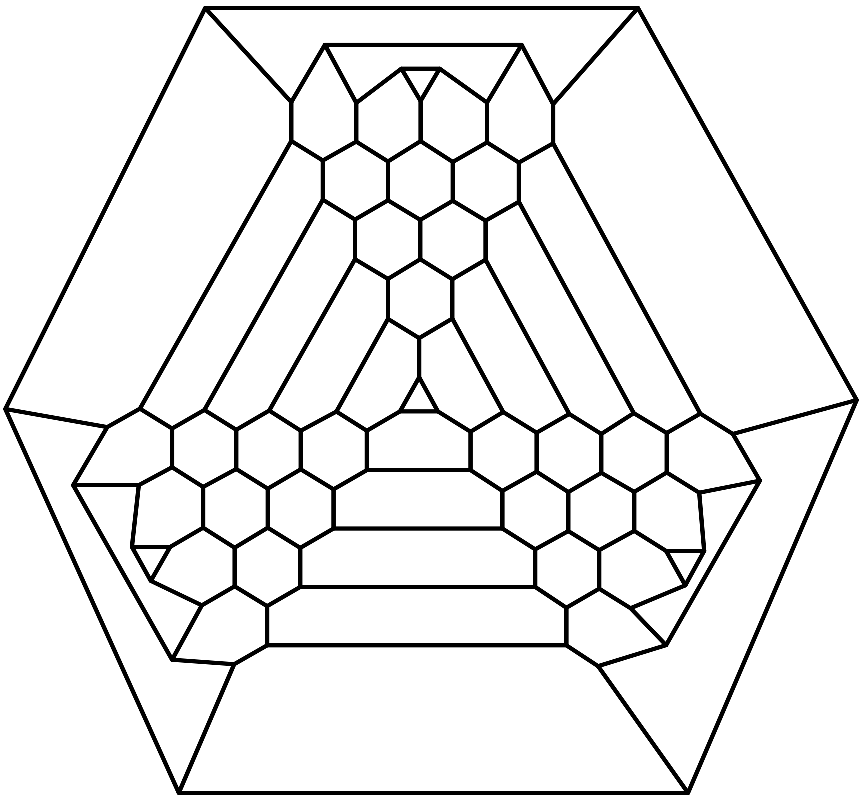


Figure 27.The fullerene graph F_{108}.

Table 8. The number of co-distant edges of e_i, i = 1, 2.

No.	Number of co-distant edges	Type of Edges
$3^{n-1}-3$	18	e_1
6	9	e_2

Corollary 29. $Sd(x) = 6x^{2\times 3^{n+1}-9} + (3^{n-1}-3)x^{2\times 3^{n+1}-18}$.

Corollary 30. $Sd(G) = 4\times 3^{n+2} + 2\times 3^{2n}$.

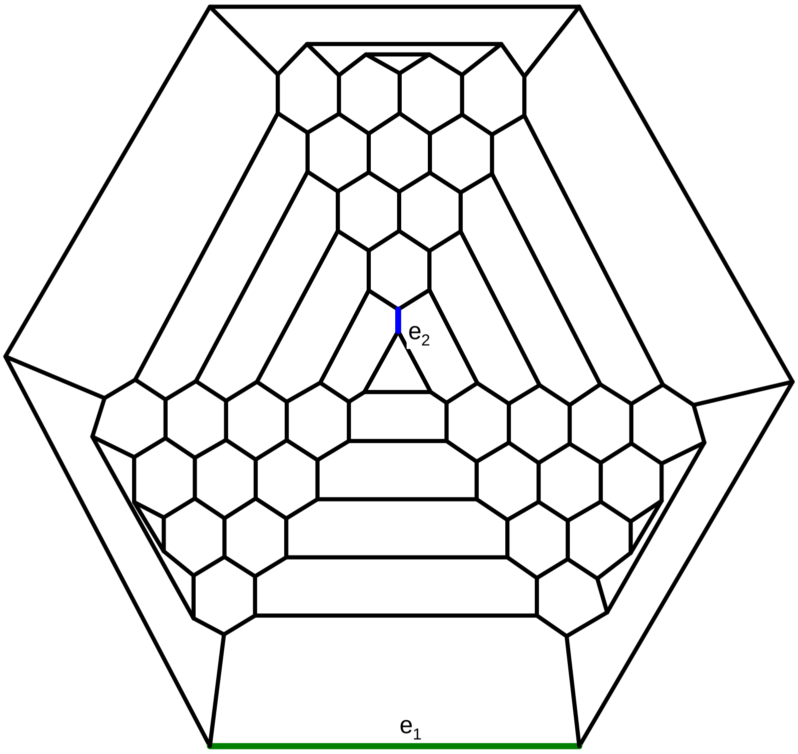
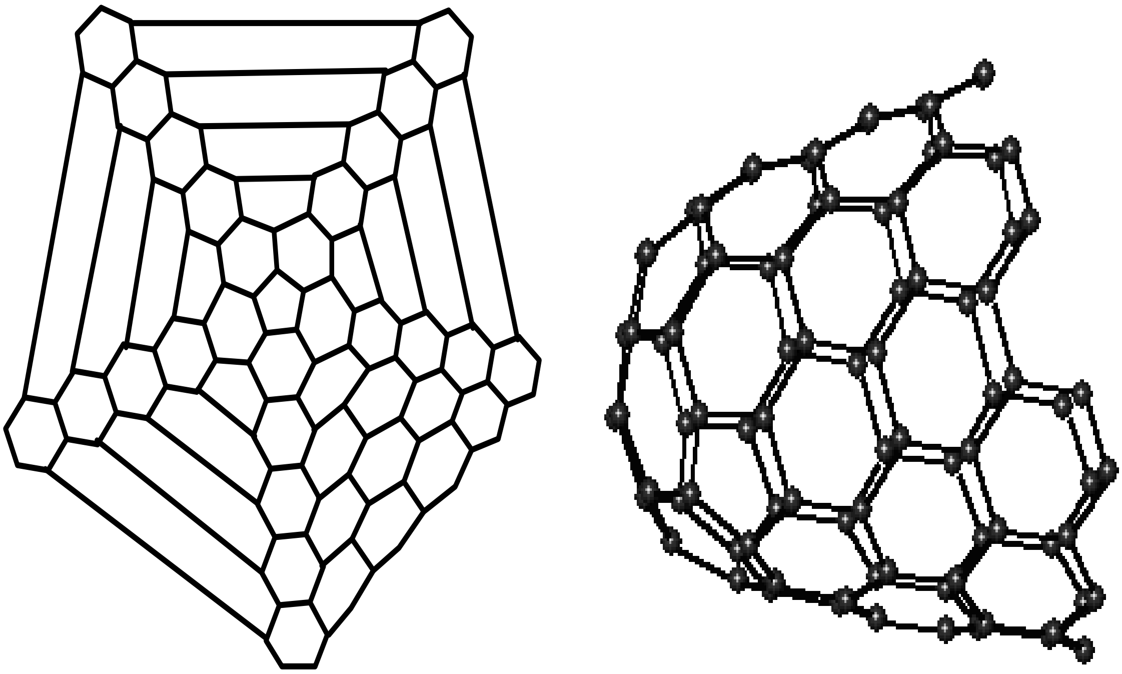


Figure 28. The molecular graph of the fullerene $F_{4\times 3^n}$ for $n = 3$.

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. The tips of these short nanotubes are capped with pentagonal faces; see Figure29. 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, ….



(a) (b)

Figure 29. *2D and 3D graph of nanohorn H.*

In This paper by using definition of Omega polynomial we compute it for infinite class of nanohorn H depicted in Figure29.

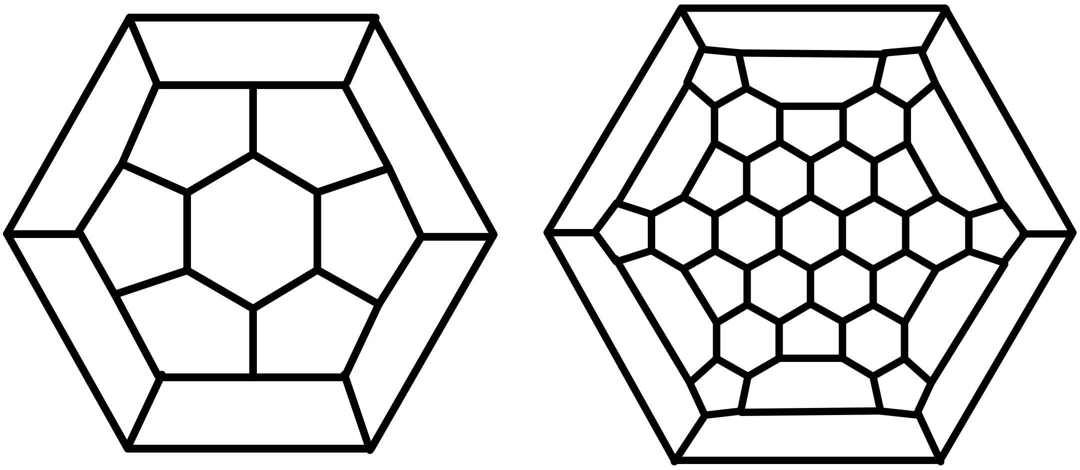
Example 31. Consider the fullerene graph F_{24} in Figure 30. This fullerene graph has 36 edges. Similar to example 1 one can see that $\Omega(x) = 24x + 6x^2$ and so $Sd(x) = 24x^{35} + 6x^{34}$. In Figure 30 one can see the planer graphs F_{24} and $Le(F_{24})$.

Example 32. Consider the fullerene graph F_{26} depicted in Figure 31. This fullerene graph has 39 edges. Similar to Examples 30 and 31 one can see that $\Omega(F_{26}, x) = 21x + 9x^2$ and so, $Sd(F_{24}, x) = 21x^{38} + 9x^{37}$. By computing these polynomials for the Leapfrog fullerene we have:

$$\Omega(x) = 24x^3 + 6x^6 + x^9.$$

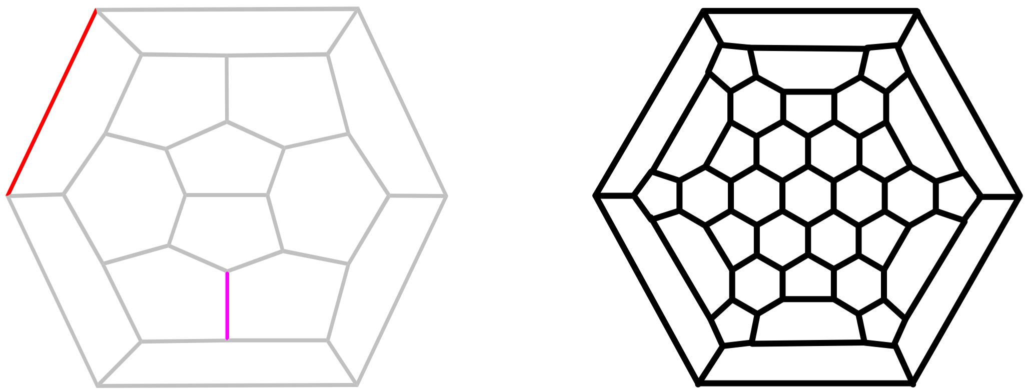
2.4 POLYOMINO CHAINS OF 8–CYCLES

A k–polyomino system is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular $4k$-cycle of length one. In other words, it is an edge-connected union of cells.



F_{24} $Le(F_{24})$

Figure 30. The leapfrog of graph F_{24}.



F_{26} $Le(F_{26})$

Figure 31. The Leapfrog of graph F_{26}.

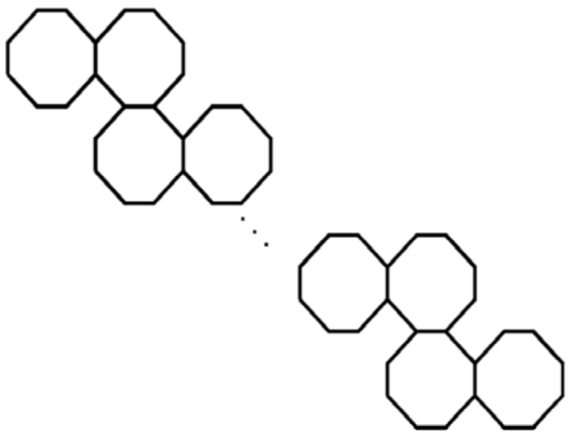


Figure 32. The zig–zag chain of 8-cycles.

Example 33. Consider the graph G shown in Figure 32. One can see this graph has exactly 2 strips C_1 and C_2. On the other hand $|C_1| = 3$ and $|C_2| = 2$. Hence,

$$\Omega(x) = 3x^3 + 10x^2 \text{ and } Sd(x) = 3x^{26} + 10x^{27}.$$

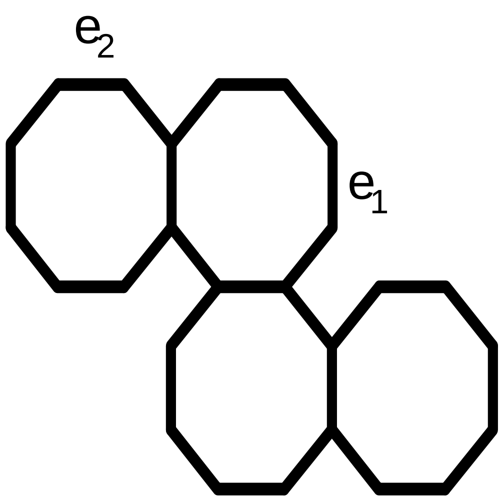


Figure 33. The zig-zag chain of 8-cycles, $n = 1$.

Example 34. For the graph H depicted in Figures33, 34 there exist two distinct strips C_1 and C_2. Similarly, $|C_1| = 3$ and $|C_2| = 2$. Hence,

$$\Omega(x) = 7x^3 + 18x^2 \text{ and } Sd(x) = 7x^{28n-2} + 18x^{28n-1}.$$

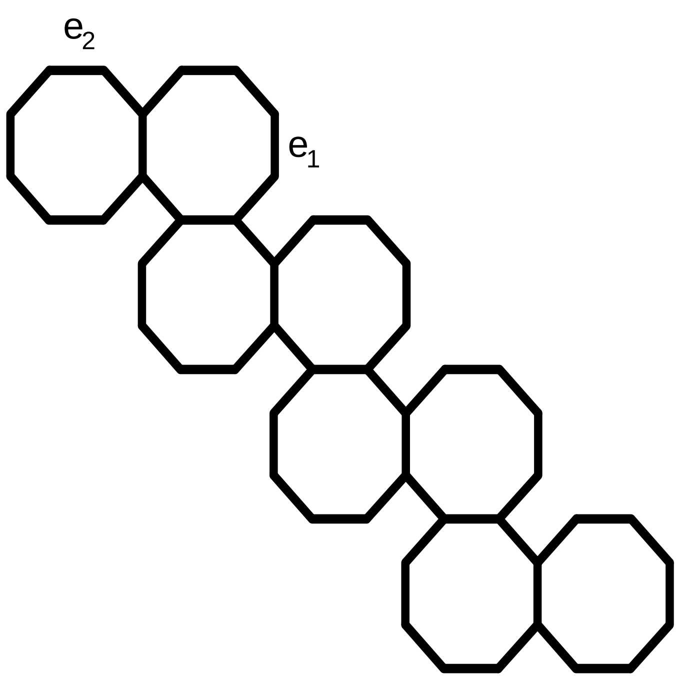


Figure 34. The zig-zag chain of 8-cycles, n =2.

In generally, this graph has two distinct strips of lengths 2 and 3, respectively. In other words we have the following Theorem:

Theorem 35. Consider the graph of 2-polyomino system depicted in Figure 35. Then:

$$\Omega(x) = (4n-1)x^3 + (8n+2)x^2 \text{ and } Sd(x) = (4n-1)x^{28n-2} + (8n+2)x^{28n-1}.$$

Consider now, another version of 2-polyomino system H_n. when $n = 1$, Figure 35, there exist three strips of length 2, 3 and 4, respectively. In other words,

$$\Omega(x) = x^4 + 2x^3 + 13x^2 \text{ and } Sd(x) = x^{32} + 2x^{33} + 13x^{34}.$$

Similarly for n = 2 (Figure 36), there exist three strips of length 2, 3 and 4, respectively. This implies $\Omega(x) = 2x^4 + 5x^3 + 24x^2$ and $Sd(x) = 2x^{67} + 5x^{68} + 24x^{69}$.

By continuing this method it is easy to check that this graph has only three strips of length 2, 3 and 4, respectively. Thus by computing number of strips of equal size and substitute in the Omega polynomial the following Theorem can be deduced:

Theorem 36. Let H_n be the graph of 2-polyomino system shown in Figure 36. Then:

$$\Omega(x) = nx^4 + (3n-1)x^3 + (11n+2)x^2 \textit{ and}$$

$$Sd(x) = nx^{35n-3} + (3n-1)x^{35n-2} + (11n+2)x^{35n-1}.$$

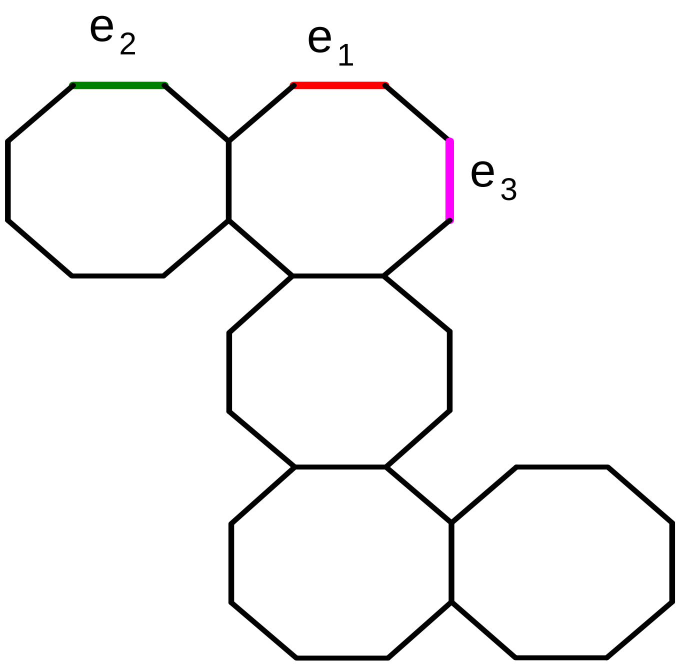


Figure 35. The graph of 2-polyomino system H_n, $n = 1$.

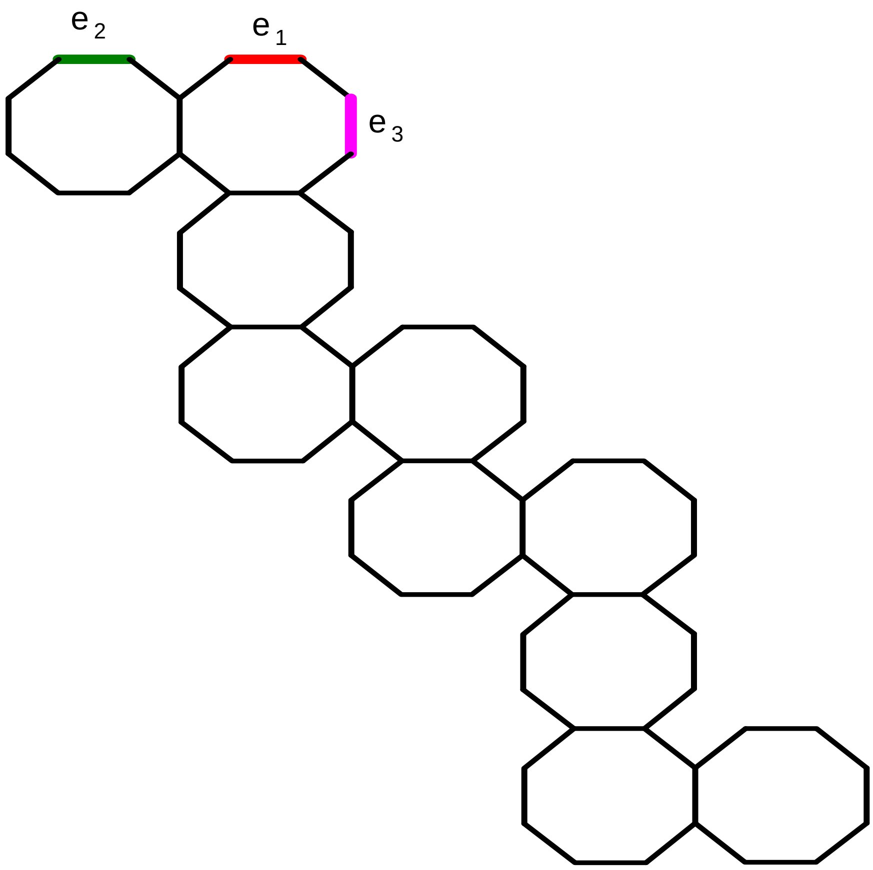


Figure 36. The graph of 2-polyomino system H_n, $n = 2$.

2.5 TRIANGULAR BENZENOID

In this section we compute counting polynomials mentioned in the text of triangular benzenoid graphs (see Figure 37). At first consider the graph of triangular benzenoid $G[n]$ for $n = 1$. The Omega and Sadhana polynomials are $\Omega(x) = 3x^2$ and $\Omega(x) = 3x^4$, respectively. By continuing this method, there exist n strips of length 2, 3, …,n + 1, respectively. In other words, if $C_1, C_2, \ldots, C_n$ be all strips of $G[n]$, then there are 3 strips equivalent with $|C_i|$, $i = 1, 2, \ldots$Hence we proved the following Theorem:

Theorem 37.

$\Omega(G[n],x) = 3(x^2 + x^3 + \cdots + x^{n+1})$ and $Sd(G[n],x) = 3(x^{|E|-2} + x^{|E|-3} + \cdots + x^{|E|-n-1})$, where $|E| = 28n + 1$.

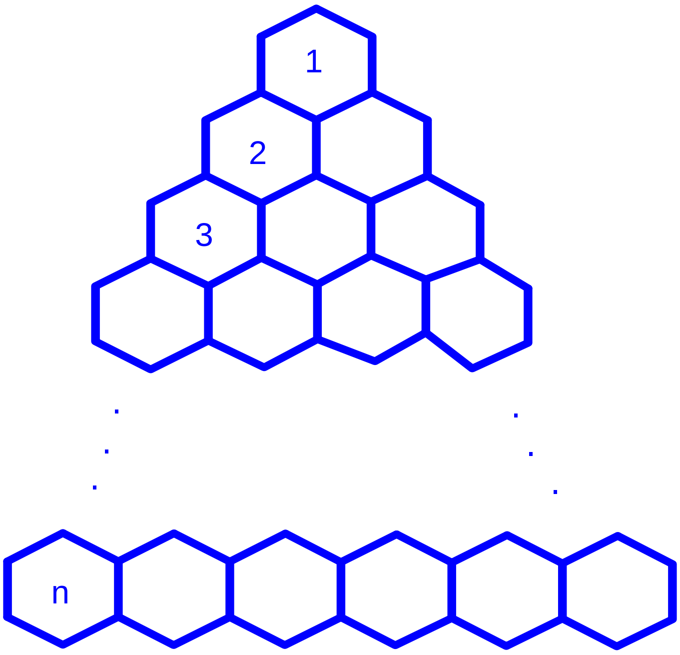


Figure 37. The graph of triangular benzenoid graphs.

3. PI INDEX

Let $\sum$ be the class of finite graphs. A topological index is a function Top from $\sum$ into real numbers with this property that $Top(G) = Top(H)$, if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological index. The Wiener [46] index is the first reported distance based topological index and is defined as half sum of the distances between all the pairs of vertices in a molecular graph. If $x, y \in V(G)$ then the distance $d_G(x, y)$ between x and y is defined as the length of any shortest path in G connecting x and y [47,48].

Khadikar introduced another index called Padmakar-Ivan (PI) index [49]. The PI index of a graph G is defined as:

$$PI = PI(G) = \Sigma\,[m_{eu}(e|G) + m_{ev}(e|G)]$$

where for edge $e = uv$, $m_{eu}(e|G)$ is the number of edges of G lying closer to u than v, $m_{ev}(e|G)$ is the number of edges of G lying closer to v than u and summation goes over all edges of G. Similar to Sadhana polynomial we can define the PI polynomial. Then the PI index will be the first derivative of PI(x) evaluated at x=1.

Let C_e be a strips containing all parallel edges with e. If G be a bipartite graph it is well – known fact that $PI(x) = \sum_S s \times m(G,s) \cdot x^{|E|-s}$. In other words, by using Omega polynomial in bipartite graph we can compute the PI polynomial and then PI index. Hence the following Theorems are resulted from Theorems 1, 2 and 3, respectively:

Theorem 38. Considerthe graph of 2−polyomino system depicted in Figure 35. Then:

$$PI(x) = 3(4n-1)x^{28n-2} + 2(8n+2)x^{28n-1}.$$

Theorem 39. Let H_n be the graph of 2-polyomino system shown in Figure 36. Then:

$$PI(x) = 4nx^{35n-3} + 3(3n-1)x^{35n-2} + 2(11n+2)x^{35n-1}.$$

Theorem 40. For the graph of triangular benzenoid graphs depicted in Figure 37 we have:

$$PI(G[n],x) = 3(2x^{|E|-2} + 3x^{|E|-3} + \cdots + (n+1)x^{|E|-n-1}).$$

where $|E| = 28n + 1$.

4. OMEGA POLYNOMIAL OF INFINITE CLASSES OF NANOSTRUCTURES

Let $G = (V,E)$ be a graph with finite vertex set V and edge set $E \subseteq (V \times V) \setminus \{(v, v) \mid v \in V\}$. An edge $(v,w) \in E$ is directed if $(w, v) \notin E$ and undirected if $(w, v) \in E$. We denote a directed edge (v,w) by $v \to w$ and write $v - w$ if (v,w) is undirected. If $(v,w) \in E$ then v and w are adjacent . If $v \to w$ then v is a parent of w, and if $v - w$ then v is a neighbor of w, see Figure 38.

A path in G is a sequence of distinct vertices $<v_0, \ldots, v_k>$ such that v_{i-1} and $v_i$are adjacent for all $1 \le i \le k$. A path $<v_0, \ldots, v_k>$ is a semi-directed cycle if $(v_i, v_{i+1}) \in E$for all $0 \le i \le k$and at least one of the edges is directed as $v_i \to v_{i+1}$. Here, $v_{k+1} \equiv v_0$. A chain graph is a graph without semi-directed cycles.

Let $G = G(G_1, \ldots, G_k, v_1, \ldots, v_k)$ be a simple connected chain graph in Figure 39. Then $|V(G)| = \sum_{i=1}^{k} |V(G_i)|$ and $|E(G)| = (k-1) + \sum_{i=1}^{k} |E(G_i)|$.

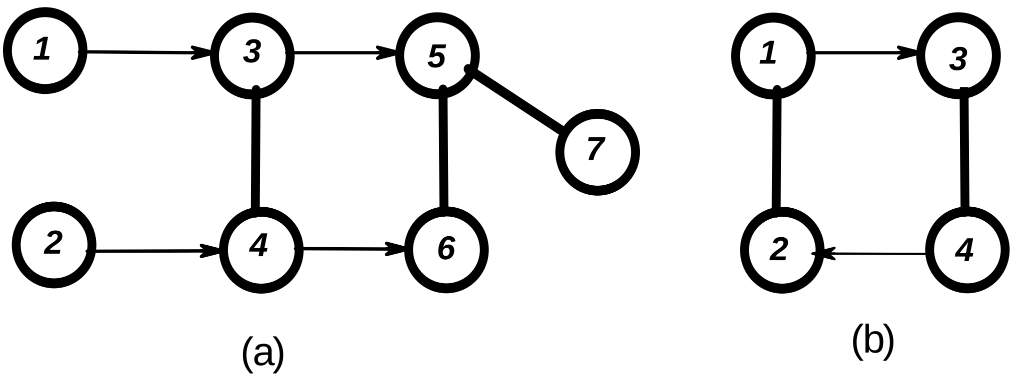


Figure 38. (*a*) Chain graph with chain components {1}, {2}, {3, 4} and {5, 6, 7}; (*b*) a graph that is not a chain graph.

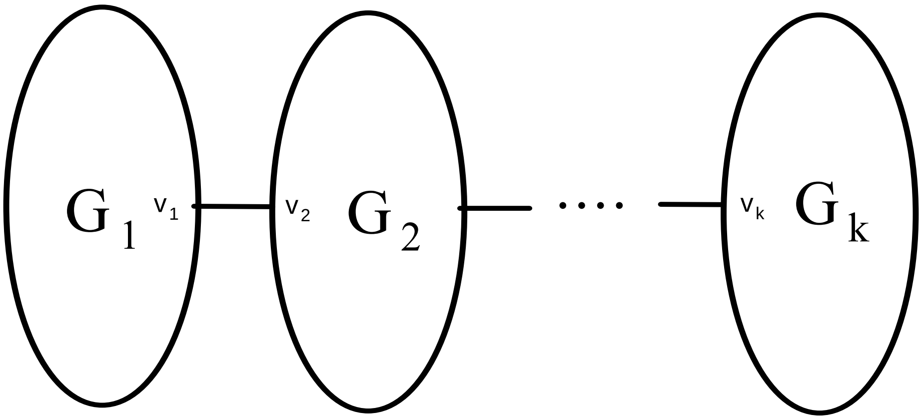


Figure 39. Chain graph $G = G(G_1,...,G_k, v_1,...,v_k)$.

Lemma 41. Let $G = G(G_1,...,G_k, v_1,...,v_k)$ be a simple connected chain graph and $e \in E(G_1)$ and $f \in E(G_2)$. Then the edges e and f don't satisfy in "co" relation. In the other words, $e \not\theta f$.

Proof. Let $e=ab \in G_1$ and $f = xy \in G_2$ be an arbitrary edges. We consider following case:

(**1**) $d(a,v_1) = d(b,v_1) = k_1$ and $d(x,v_2) = d(y,v_2) = k_2$ Then

$d(a,y) = d(a,v_1) + d(v_1,v_2) + d(v_2,y) = k_1 + k_2 + 1$,

$d(a,x) = d(a,v_1) + d(v_1,v_2) + d(v_2,x) = k_1 + k_2 + 1$.

This implies that. $e \not\theta f$.

(**2**) $d(a,v_1) = d(b,v_1) = k_1$ and $d(x,v_2) = k_2, d(y,v_2) = k_2 + 1$. So, $d(a,x) = d(a,v_1) + d(v_1,v_2) + d(v_2,x) = k_1 + k_2 + 1$ and $d(b,x) = d(b,v_1) + d(v_1,v_2) + d(v_2,x) = k_1 + k_2 + 1$. This implies that $e\theta f$ $e \not\theta f$.

(**3**) $d(a,v_1) = k_1, d(b,v_1) = k_1 + 1$ and so, $d(x,a) = d(x,v_2) + d(v_2,v_1) + d(v_1,a) = k_2 + k_1 + 1$ and $d(y,a) = d(y,v_2) + d(v_2,v_1) + d(v_1,a) = k_2 + k_1 + 1$. This implies that. $e \not\theta f$.

Lemma 42. Let $G = G(G_1,...,G_k, v_1,...,v_k)$ be a chain graph and $u \in V(G_i)$ and $v \in V(G_j)$ $(1 \le i, j \le k, i \ne j)$. So, $d(u,v) = d(u,v_i) + d(v_i,v_j) + d(v_j,v) = d(u,v_i) + d(v_j,v) + 1$.

Proof. We know $d(u_i,u_j)=1$ and this complete the proof.

Theorem 43. Let G be a simple connected graph with blocks G_1, G_2 and a cut−edge uv, Figure 40. So, we have, $\Omega(G,x) = x + \Omega(G_1,x) + \Omega(G_2,x)$.

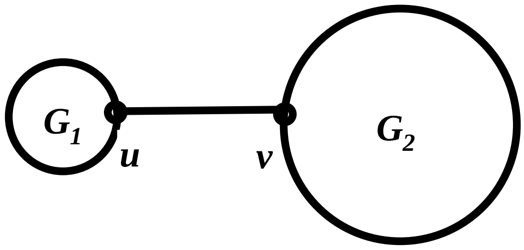


Figure 40. A graph G with a cut–edge uv.

Proof. By using definition of omega polynomial and Lemma 1 one can see that $\Omega(G,x) = x + \sum_{c_1} m(G_1,c_1)x^{c_1} + \sum_{c_2} m(G_2,c_2)x^{c_2} = x + \Omega(G_1,x) + \Omega(G_2,x)$.

Corollary 44. If $G = G(G_1,...,G_k,v_1,...,v_k)$ be a simple connected connected chain graph then we have: $\Omega(G,x) = (k-1)x + \sum_{i=1}^{k}\Omega(G_i,x)$.

Theorem 45. Let $G = G(G_1,G_2,v_1,v_2)$ be simple connected chain graph. Then

$$\theta(G,x) = x + \theta(G_1,x) + \theta(G_2,x),$$

and

$$Sd(G,x) = x^{|E(G)|-1} + \sum_{c_1} m(G_1,c_1)x^{|E(G)|-c_1} + \sum_{c_2} m(G_2,c_2)x^{|E(G)|-c_2}.$$

Corollary 46. Let $G = G(G_1,...,G_k,v_1,...,v_k)$ so:

$Sd(G,x) = (k-1)x^{|E(G)|-1} + \sum_{i=1}^{k}\sum_{c_i} m(G_i,c_i)x^{|E(G)|-c_i}$ and $\theta(G,x) = (k-1)x + \sum_{i=1}^{k}\theta(G_i,x)$.

Corollary 47. Let T be a tree with n vertices and $T = T_n = T(T_{n-1},T_1,v_{n-1},v_1)$. Thus we have $\Omega(T_n,x) = (n-1)x$.

Proof. Let T_{n-1} be a tree with $n-1$ vertices constructed by cutting a vertex of degree 1 of T_n. It is easy to see that $\Omega(T_n,x) - \Omega(T_{n-1},x) = x$, $\Omega(T_{n-1},x) - \Omega(T_{n-2},x) = x$ and $\Omega(T_2,x) - \Omega(T_1,x) = x$. So, $\Omega(T_n,x) = (n-1)x$.

Example 48. Consider graph of dendrimer *D* with n vertices, see Figure 41. Because this graph is a tree with n vertices, we have $\Omega(D,x) = (n-1)x$.

Theorem 49. Consider graph of nanostar dendrimer N with n vertices, see Figure 42. It is easy to see that $|V(G_n)| = 19n$ and $|E(G_n)| = 22n-1$. Now by using a same discussion in corollary 7 We have $G_n = G(G_{n-1}, G_1, v_{n-1}, v_1)$ and then the following relations:

$$\Omega(G_n, x) = x + \Omega(G_{n-1}, x) + \Omega(G_1, x),$$
$$\Omega(G_n, x) - \Omega(G_{n-1}, x) = x + \Omega(G_1, x),$$
$$\Omega(G_{n-1}, x) - \Omega(G_{n-2}, x) = x + \Omega(G_1, x),$$
$$\Omega(G_2, x) - \Omega(G_1, x) = x + \Omega(G_1, x).$$

Now by summation of these relations we have

$\Omega(G_n, x) - \Omega(G_1, x) = (n-1)x + (n-1)\Omega(G_1, x)$. So $\Omega(G_n, x) = (n-1)x + n\Omega(G_1, x)$. But $\Omega(G_1, x) = 3x + 9x^2$. Thus, $\Omega(G_n, x) = (n-1)x + n(3x + 9x^2) = 9nx^2 + (4n-1)x$, $Sd(G_n, x) = (4n-1)x^{22n-2} + 9nx^{22n-3}$ and $\theta(G_n, x) = 18nx^2 + (4n-1)x$.

Example 50.Suppose C_{20} denotes the fullerene graph on 20 vertices, see Figure 43(a). Then $\Omega(C_{20}, x) = 30x$ and so, $Sd(C_{20}, x) = 30x^{29}$.

Example 51. Suppose C_{30} denotes the fullerene graph on 30 vertices, see Figure 43(b). Then $\Omega(G, x) = 20x + 10x^2 + x^5$ and so, $Sd(G, x) = 20x^{44} + 10x^{43} + x^{40}$.

Example 52. Consider Table 3. In this table we compute the omega polynomial for some fullerene graphs.

Theorem 53. 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 trivial.

Theorem 54. Suppose T is a tree on n vertices. Then $\Omega(T, x) = (n-1)x$ and so, $Sd(T, x) = (n-1)x^{n-2}$.

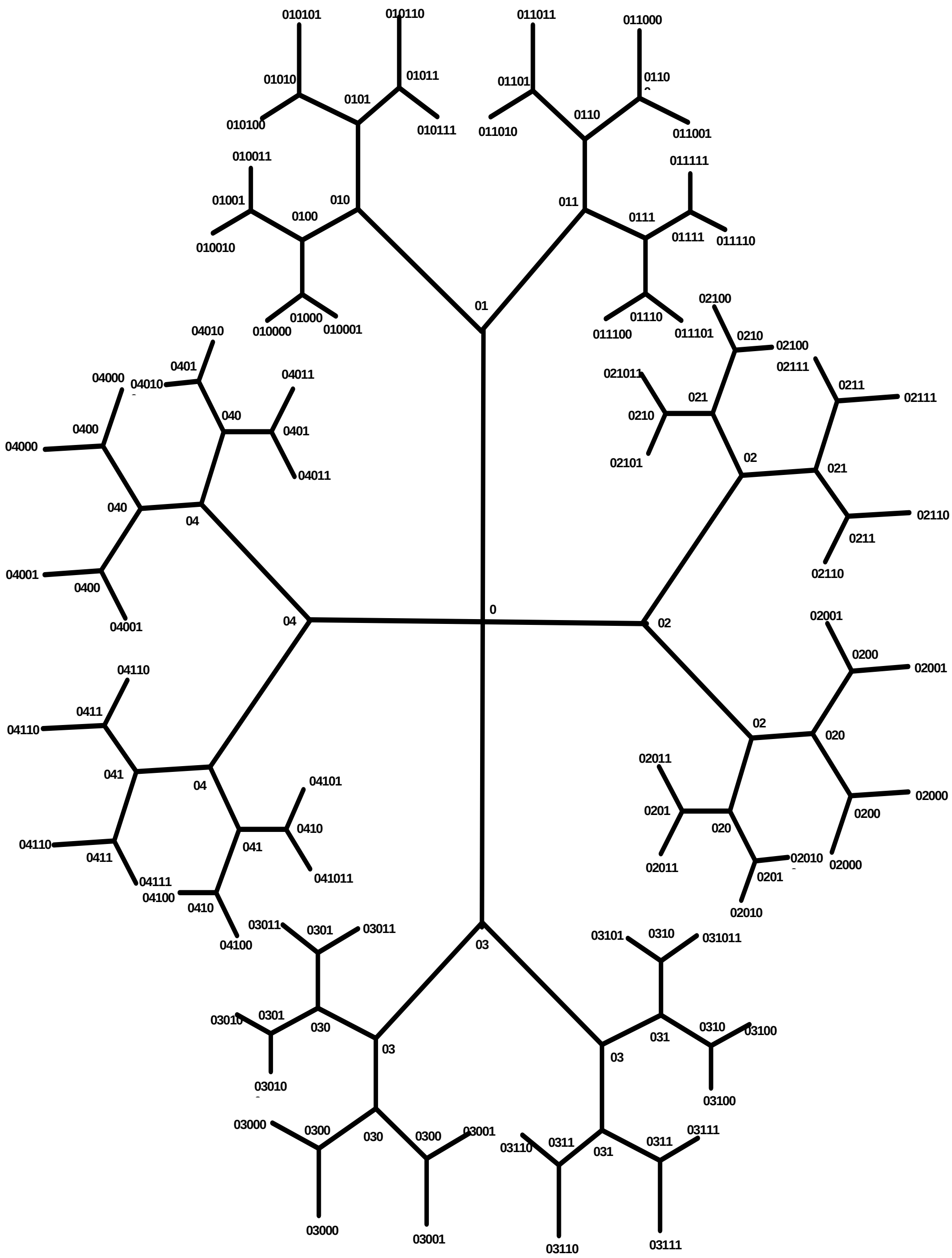


Figure 41. 2*D* graphical representation of a dendrimer *D*.

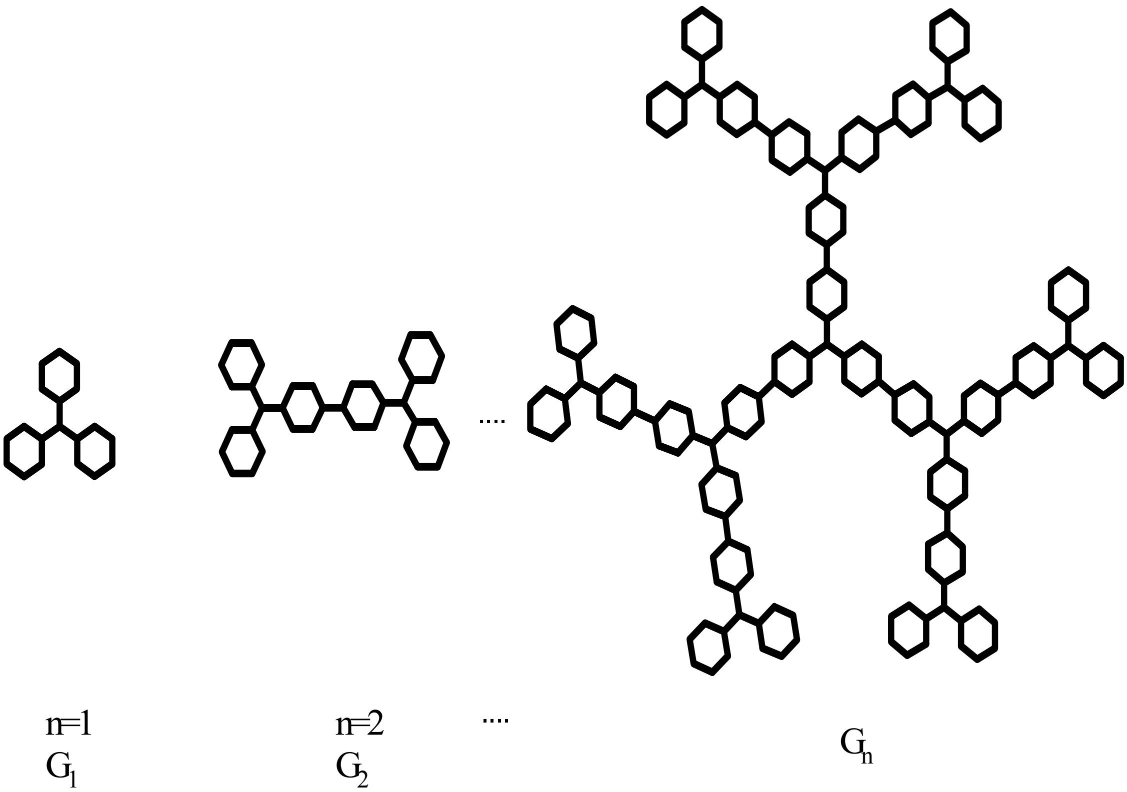


Figure 42. 2*D* graphical representation of a nanostar dendrimer *N*.

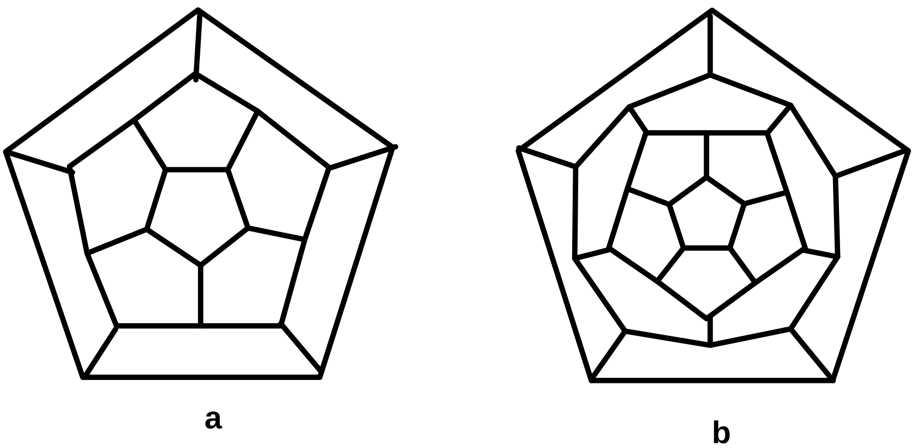


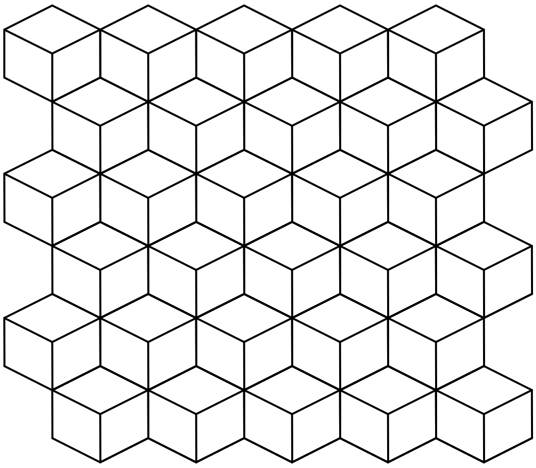
Figure 43. (a) The fullerene graph C_{20} (b) The fullerene graph C_{30}.

5. EXAMPLES FOR CALCULATING OMEGA POLYNOMIAL

1. Case of infinite 2–dimensional graph *K*:
We have the Omega polynomial as $qx^{2p+1} + 2(x^3 + x^5 + ... + x^{2q-1}) + (2p - q + 1)x^{2q+1}$.

1. 1. Case: $2p > q > p, 2 \mid q$,

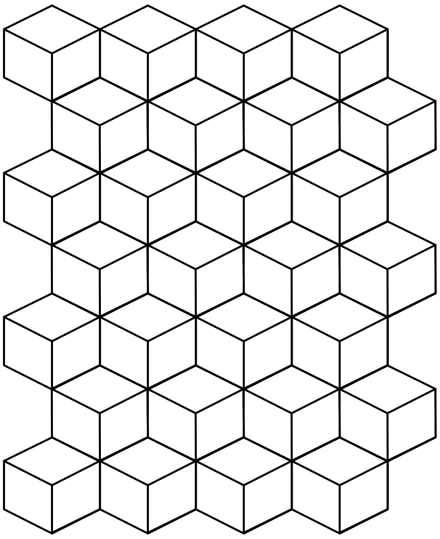
If $q = 6$, $p = 5$ then, the graph is as follows:



and $\Omega(G,x) = 6x^{11} + 2(x^3 + x^5 + x^7 + x^9 + x^{11}) + 5x^{13}$.

1. 2. Case: $2p > q > p, 2 \nmid q$:

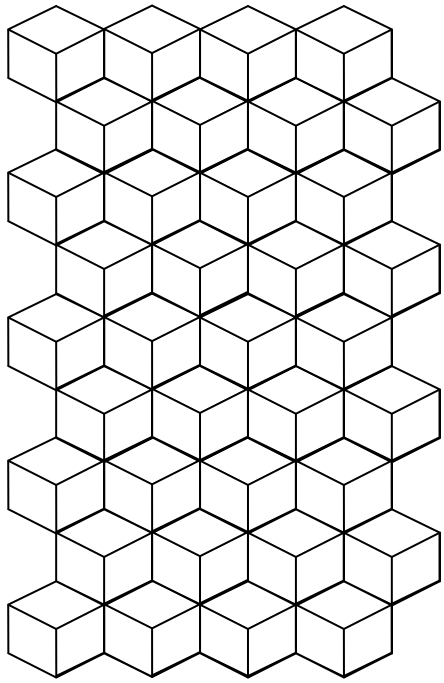
In this case if for instance $p = 4$, $q = 7$ then, the graph is as follows:



and $\Omega(G,x) = 7x^9 + 2(x^3 + x^5 + x^7 + x^9 + x^{13}) + 2x^{15}$. We have also $qx^{2p+1} + 2(x^3 + x^5 + ... + x^{4p-1}) + (q - 2p + 1)x^{4p+1}$.

1.3. Case: $q \geq 2p$

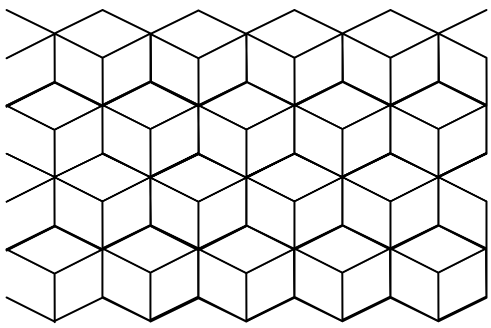
In this case if for instance $p = 4$, $q = 9$ then, the graph is as follows:



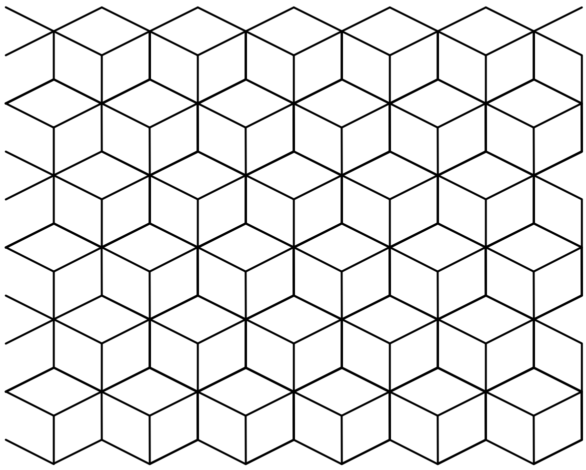
and $\Omega(G,x)=9x^9+2(x^3+x^5+x^7+x^9+x^{11}+x^{13}+x^{15})+2x^{17}$.

2. Case of nanotubes $G[p,q]$.

In this case the Omega polynomial is $\Omega(G,x)=qx^{2p}+2px^{2q+1}$. For example, if p = 5, q = 4 then, the graph is as follows:



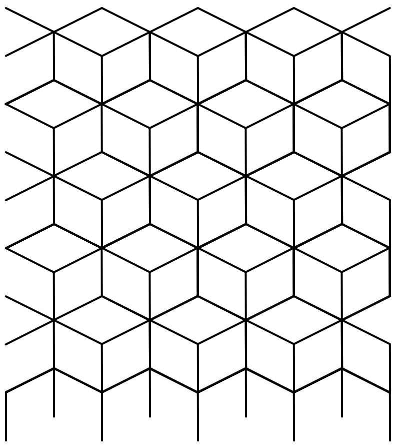
and $\Omega(G,x)=4x^{10}+10x^9$. If p = 6, q = 6 then, the graph is as follows:



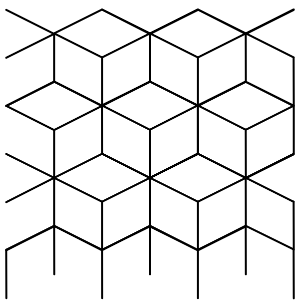
and $\Omega(G,x) = 6x^{12} + 12x^{13}$.

3. Case of nanotori *H* [*p,q*]:

In this case the Omega polynomial is $\Omega(H,x) = qx^{2p} + 2x^{2pq}$. For example if $p = 4$, $q = 5$ then, the graph is as follows:



and $\Omega(H,x) = 5x^{8} + 2x^{40}$. If $p = 3$, $q = 3$, then, the graph is as follows:



and $\Omega(H,x) = 3x^{6} + 2x^{18}$.

6. CALCULATING OMEGA POLYNOMIAL OF TUC_4C_8 NANOTUBES AND NANOTORI

The Sadhana polynomial of a $TUC_4C_8(R)$ nanotube and $TUC_4C_8(S)$ nanotorus were computed as described above. The Sadhana polynomial of the 2-dimensional lattice of $TUC_4C_8(R)$ graph K= KTUC[p,q] (Figure 44) is also computed. We denote a $TUC_4C_8(R)$ nanotube by G = GTUC[p,q] and $TUC_4C_8(S)$ nanotorus by H = HTUC[p,q] (Figures 45 and 46). It is easy to see that $|V(G)| =4p(q+1)$, $|V(H)| =4pq$, $|V(K)| = 4(p+1)(q+1)$, $|E(G)| = 6pq +5p$, $|E(H)| = 6pq$ and $|E(K)| =6pq+5(p+q)+4$. We begin with the molecular graph of K (Figure 44). One can see that there are three separate cases and the number of qoc strips is different. Suppose e_1, e_2 and e_3 are representative edges for these cases. Then our programs described in last section shows that $|C(e_1)| = 2\min\{p,q\}+2$, $|C(e_2)| =p$ and $|C(e_3)| =q$. By definition of Omega polynomial and Table 9 one can see that for $\alpha=\min\{p,q\}$:

$$\Omega(K,x) = qx^{p+1} + px^{q+1} + 2(2x^2 + ... + 2x^{2\alpha} + (|p-q|+1)x^{2\alpha+2}),$$

and so

$$Sd(K,x) = qx^{|E(K)|-p-1} + px^{|E(K)|-q-1} + 2(2x^{|E(K)|-2} + ... + 2x^{|E(K)|-2\alpha} + (|p-q|+1)x^{|E(K)|-2\alpha-2}).$$

We now consider the molecular graph G, Figure 45. Figure 45 shows that there are three different cases and the qoc strips are different. Suppose e_1, e_2 and e_3 are representatives of the different cases. One can see that $|C(e_1)| = 2q+2$, $|C(e_2)| = q+1$ and $|C(e_3)| =p$. On the other hand, there are $2p$, p, q similar edges for each of edges e_1, e_2 and e_3, respectively. This implies that $\Omega(G,x) = qx^p + px^{q+1} + 2px^{2(q+1)}$ and so $Sd(G,x) = qx^{|E(G)|-p} + px^{|E(G)|-q-1} + 2px^{|E(G)|-2(q+1)}$.

Figure 46 shows that there are three separate cases and the number of qoc strips are different. We denote these edges by e_1, e_2 *and* e_3. One can see that $|C(e_1)| = 2pq$, $|C(e_2)|=q$ and $|C(e_3)| = p$ (Figure 46). On the other hand, there are 2, p, q similar edges for each of edges e_1, e_2 and e_3, respectively. Therefore, $\Omega(H,x) = qx^p + px^q + 2x^{2pq}$ and so $Sd(H,x) = qx^{|E(H)|-p} + px^{|E(H)|-q} + 2x^{|E(H)|-2pq}$.

Table 9. The number of co-distant edges of e_i, $1\le i\le 3$.

No.	Number of co-distant edges	Type of edges
$4, \vdots, 4, 2\lvert p-q\rvert+2$	$\begin{cases}2\\4\\\vdots\\2\alpha-2\\2\alpha\end{cases}$, $\alpha=\min\{p,q\}$	e_1
q	$p+1$	e_2
p	$q+1$	e_3

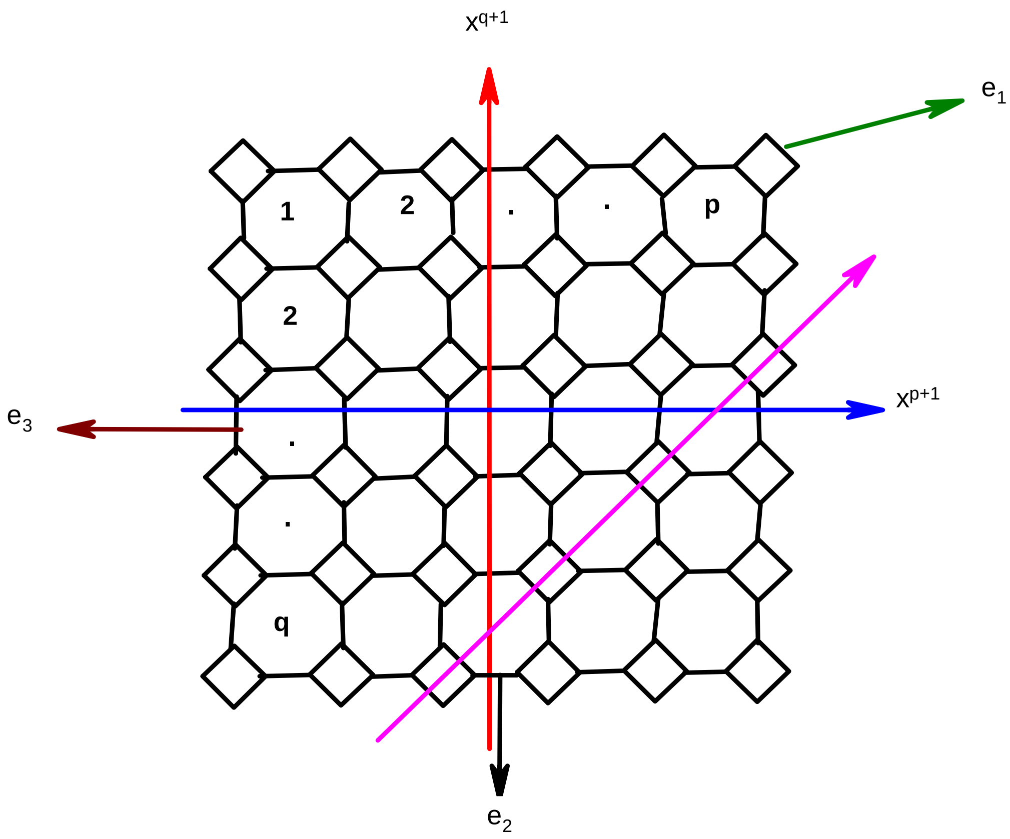


Figure 44. The qoc strips of 2-dimensional graph *K* of the TUC4C8(*R*) nanotube.

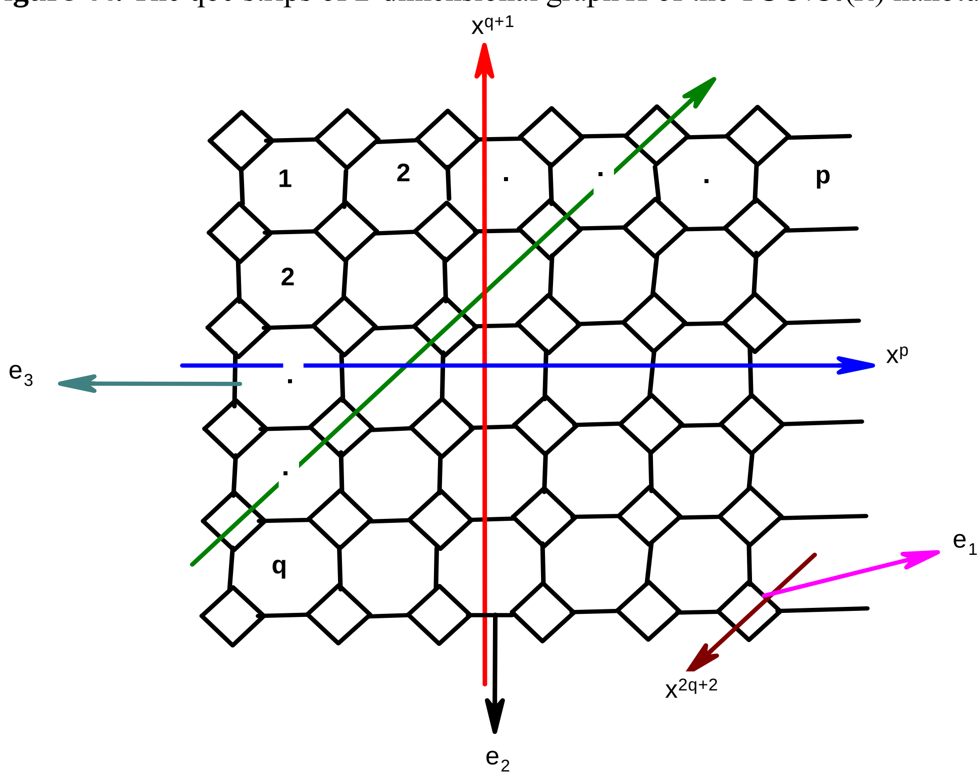


Figure 45. The qoc strips of TUC4C8(*R*) nanotube G = GTUC [*p*,*q*].

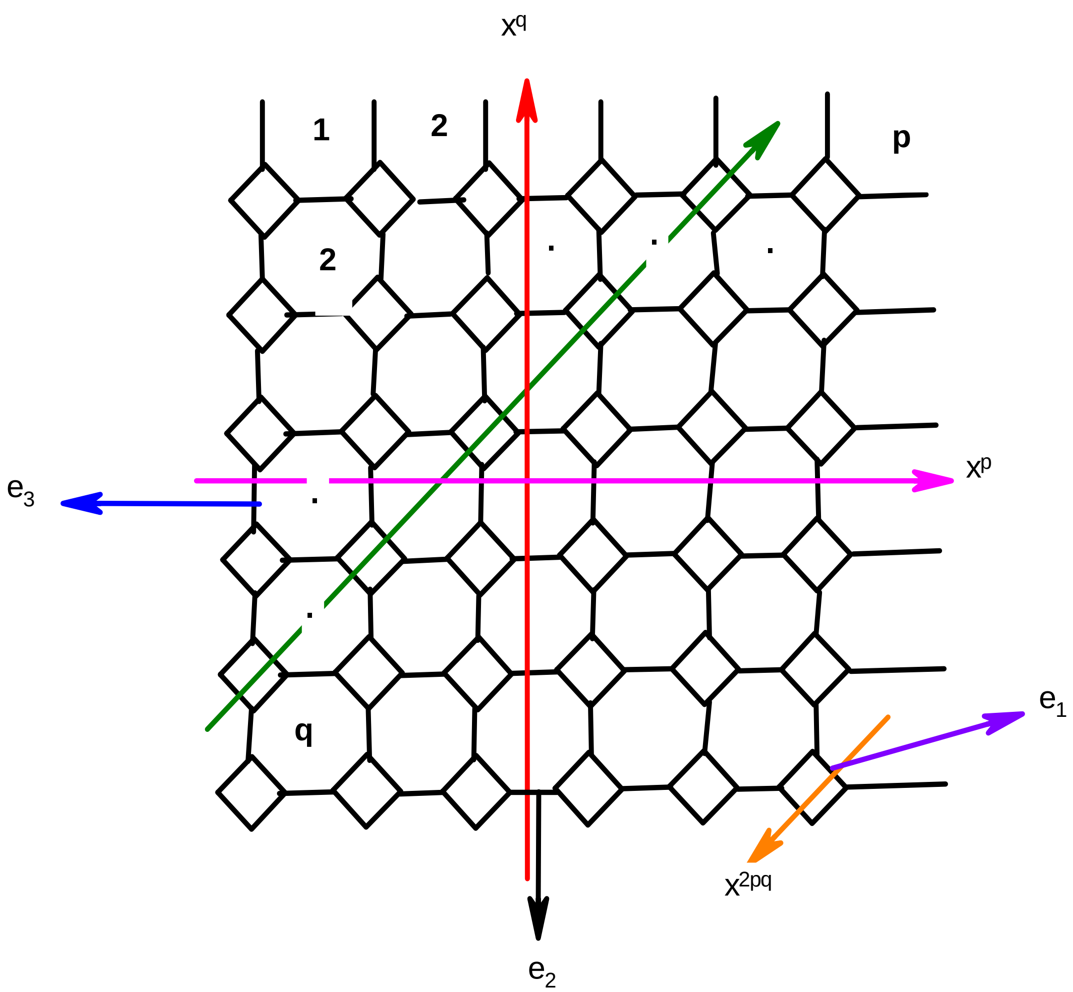


Figure 46. The qoc strips of $TUC_4C_8(S)$ nanotorus $H = HTUC\,[p,q]$.

1. Let P_n be a path of length n, and C_n be a cycle of length n. Then $\Omega(P_n,x) = (n-1)x$ and

$$\Omega(C_n,x) = \begin{cases} \frac{n}{2}x^2 & 2|n \\ nx & 2\nmid n \end{cases}.$$

Consider the ladder graph G with 18 vertices. We know

$$G = P_{10} \times P_2.$$

Here we have a cut of length 9 and 8 cuts of length 2, so $\Omega(G,x) = x^9 + 8x^2$. Also, we know that by using

$\Omega(G \times H, x) = \sum_{c_1} m(G,c_1) \times x^{|V(H)|c_1} + \sum_{c_2} m(H,c_2) \times x^{|V(G)|c_2}$ (1) and so we have $\Omega(P_n \times P_m, x) = (n-1)x^m + (m-1)x^n$, for example $G = P_{10} \times P_2$ and we have $\Omega(G,x) = \Omega(P_9 \times P_2, x) = 8x^2 + x^9$.

2. Now we consider $P_5 \times P_4$. There are 3 cuts of length 5 and 4 cuts of length 4. Thus we have:

$$\Omega(P_5 \times P_4, x) = 3x^5 + 4x^4.$$

3. Now we consider $P_5 \times C_4$. There are 2 cuts of length 10 and 4 cuts of length 4. So, $\Omega(P_5 \times C_4, x) = 2x^{10} + 4x^4$. By using equation (1)

$$\Omega(P_n \times C_m, x) = \begin{cases} (n-1)x^m + \frac{m}{2}x^{2n} & 2|m \\ (n-1)x^m + mx^n & 2\nmid m \end{cases}$$

and so we have $\Omega(P_5 \times C_4, x) = 2x^{10} + 4x^4$.

Now we consider $C_5 \times C_4$. There are 2 cuts of length 10 and 5 cuts of length 4. So, $\Omega(C_5 \times C_4, x) = 2x^{10} + 5x^4$ as another result we have:

$$\Omega(C_n \times C_m, x) = \begin{cases} nx^m + mx^n & 2\nmid m,\ 2\nmid n \\ nx^m + \frac{m}{2}x^{2n} & 2|m,\ 2\nmid n \\ \frac{n}{2}x^{2m} + mx^n & 2\nmid m,\ 2|n \\ \frac{n}{2}x^{2m} + \frac{m}{2}x^{2n} & 2|m,\ 2|n \end{cases},$$

So $\Omega(C_5 \times C_4, x) = 2x^{10} + 5x^4$.

Theorem 55. Let $G_1, G_2, \ldots, G_n$ be bipartite connected co−graphs. Then we have

$$\Omega(G_1 \times G_2 \times \cdots \times G_n, x) = \sum_{i=1}^{n} \sum_{c_i} m(G_i, c_i).x^{\prod_{j=1, j\neq i}^{n} |V(G_j)| c_i}.$$

Theorem 56. The Omega polynomial of fullerene graph $F_{12(2n+1)}$ for $n \geq 2$ is as follows:

$$\Omega(F_{12(2n+1)}, x) = 12x^3 + 12x^{2n-2} + 6x^{n-1} + 3x^{2n+4}.$$

Proof. By Figure 47, there are four distinct cases of qoc strips. We denote the corresponding edges by f_1, f_2, f_3 and f_4. By the Table 10 proof is completed.

The aim of this section is to compute the counting polynomials of equidistant (Omega, Sadhana and Theta polynomials) of an infinite family C_{40n+6} of fullerenes with $40n+6$ carbon atoms and $60n+9$ bonds (the graph G, Figure 48 is $n = 2$).

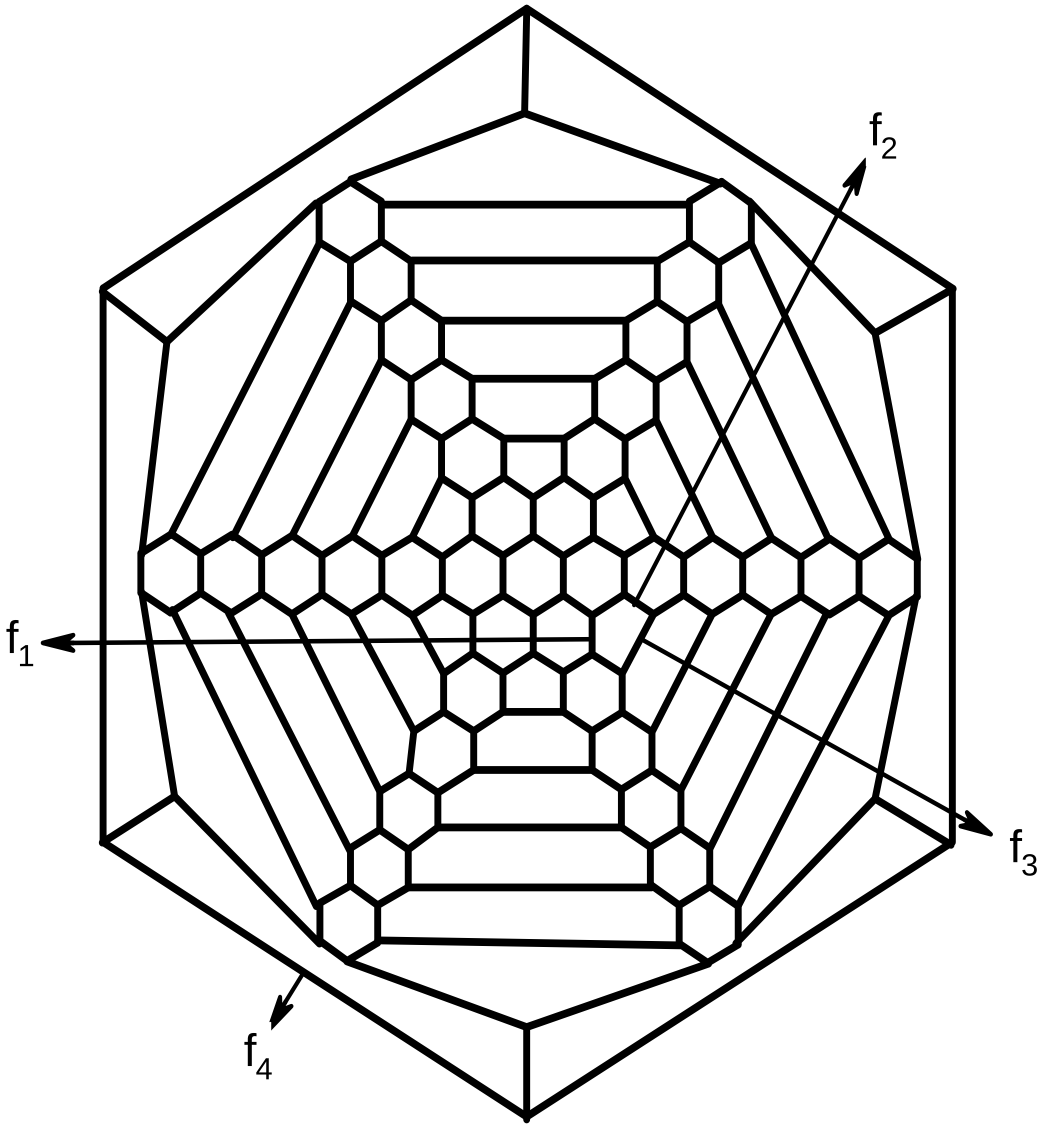


Figure 47. The graph of fullerene $F_{12(2n+1)}$ for $n = 4$.

Table 10. The number of equidistant edges**.**

Edge	#Co distance	Number of edges
f_1	3	12
f_2	$2n$-2	12
f_3	$2n$+4	3
f_4	n-1	6

Theorem 59. 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 49, there are ten distinct cases of qoc strips. We denote the corresponding edges by $e_1, e_2, \ldots, e_{10}$. By using table 1 and Figure 49 the proof is completed.

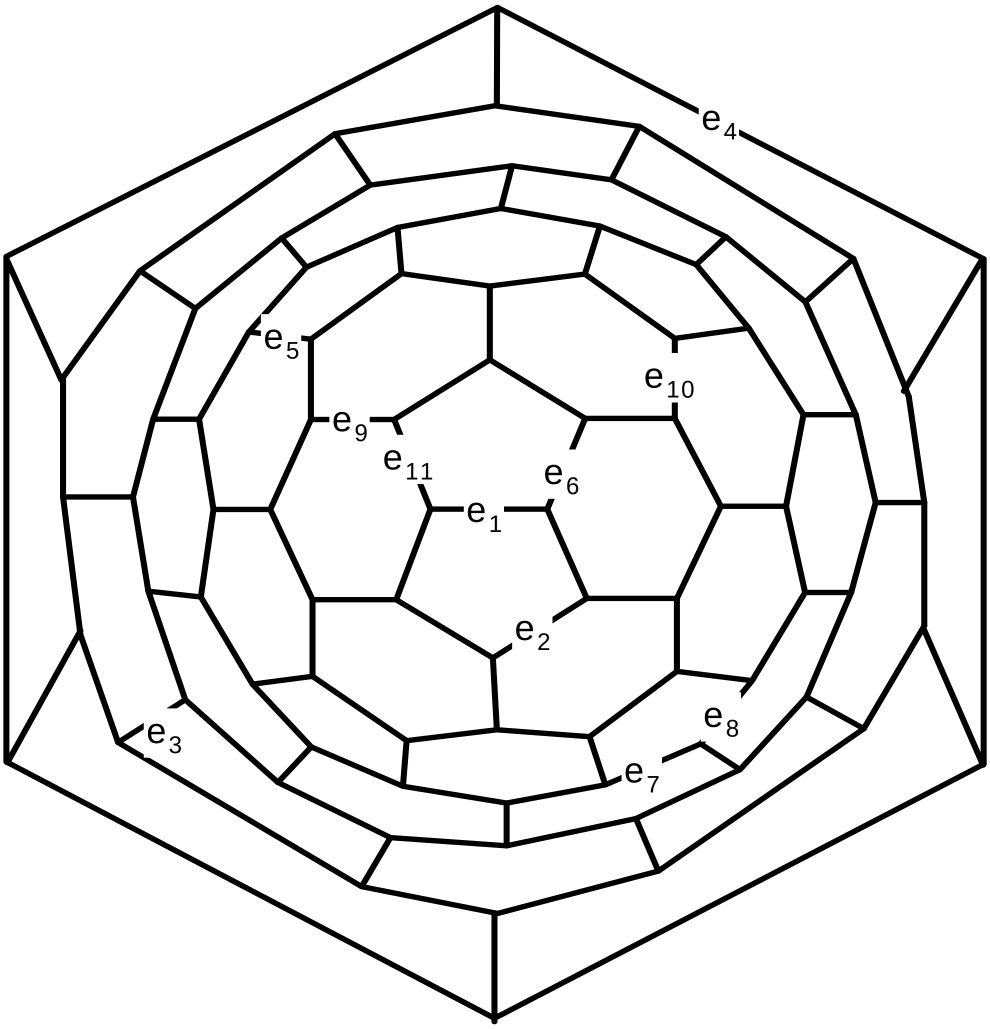


Figure 48. The graph of fullerene C_{40n+6} for $n = 2$.

Table 11. The number of co-distant edges of e_i, $1\leq i \leq 10$.

No.	Number of co-distant 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}

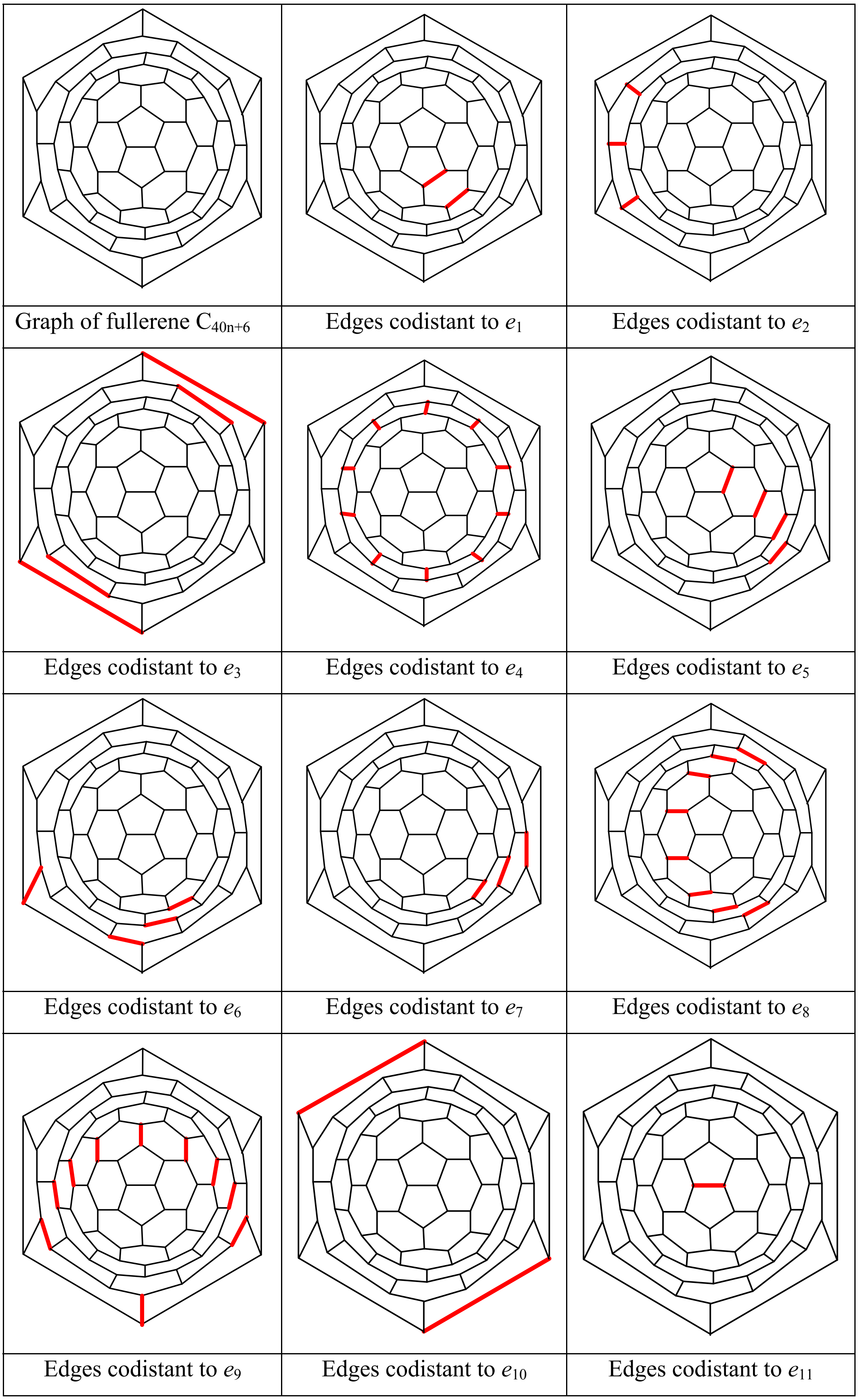


Figure 49. The main cases of fullerenes C_{40n+6} related to computing co-distant edges.

Corollary 60. The Sadhana polynomial of 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 $|E|=60n+9$.

7. DESIGN OF TITANIUM OXIDE LATTICE

A map M is a combinatorial representation of a (closed) surface. Several transformations or operations on maps are known and used for various purposes. We limit here to describe only those operations needed here to build the TiO_2 pattern. *Medial Med* is achieved by putting new vertices in the middle of the original edges. Join two vertices if the edges span an angle (and are consecutive within a rotation path around their common vertex in *M*). Medial is a 4-valent graph and *Med*(*M*) = *Med*(*Du*(*M*)).

Dualization of a map starts by locating a point in the center of each face. Next, two such points are joined if their corresponding faces share a common edge. It is the (Poincaré) *dualDu*(*M*). The vertices of *Du*(*M*) represent faces in *M* and *vice-versa.*

Figure 50 illustrates the sequence of map operations leading to the TiO_2 pattern: *Du*(*Med*(6,6)), the polyhex pattern being represented in Schläfli's symbols. Correspondingly, the TiO_2 pattern will be denoted as: (4(3,6)), squares of a bipartite lattice of 3 and 6 connected atoms, while the medial pattern: ((3,6)4). Clearly, the TiO_2 pattern can be done simply by putting a point in the centre of hexagons of the (6,6) pattern and join it alternately with the points on the center. It is noteworthy that our sequence of operations is general, enabling transformation of the (6,6) pattern embedded on any surface and more over, it provides a rational procedure for related patterns, to be exploited in cage/cluster building.

(a) (b) (c)

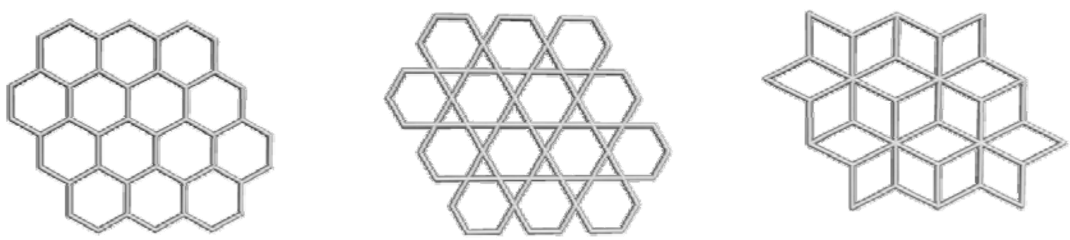


Figure 50. Way to TiO_2 lattice: (a) polyhex (6,6) pattern; (b) Med(6,6); (c) Du(Med(6,6)).

8. OTHER CLASSES OF FULLERENE GRAPHS

The most famous fullerene are (5, 6) fullerenes [50]. Recently some other classes of fullerenes are considered by scientists who work on Mathematical Chemistry area. We denote these classes of fullerenes by$C_{4,6}[n]$ and $C_{3,6}[n]$, respectively. This section is devoted to compute counting polynomial of these classes of fullerenes.

- **(4, 6) Fullerenes:**

By using Euler's formula $n - m + f = 2$, one can deduce that this class of fullerenes have exactly $n/2 - 4$ hexagonal faces and 6 tetragonal faces, where n is number of its vertices. One class of these fullerenes is depicted in Figure 51. This fullerene has $8n^2$ carbon atoms and $12n^2$ bonds. We have the following Theorem for its Omega polynomial:

Theorem 61.

$$\Omega(G,x) = 3x^{4n} + 4(n-1)x^{3n}.$$

Proof. By Figure 51, there are two distinct cases of qoc strips. We denote the corresponding edges by e_1 *and* e_2. By using Table 12 and Figure 51 the proof is completed.

Table 12. 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
$4(n\text{-}1)$	$3n$	e_2

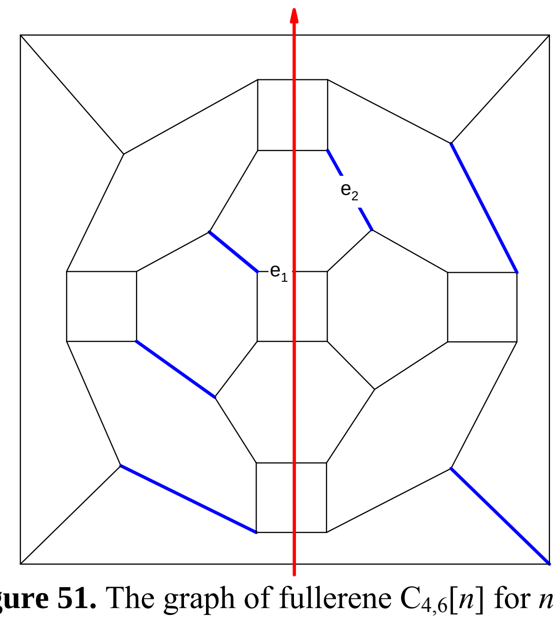


Figure 51. The graph of fullerene $C_{4,6}[n]$ for $n = 3$.

Corollary 62. $Sd(G,x)=3x^{12n^2-4n}+4(n-1)x^{12n^2-3n}$.

Corollary 63. $\Theta(G,x)=12nx^{4n}+12n(n-1)x^{3n}$.

Corollary 64. $PI(G,x)=\Pi(G,x)=12nx^{12n^2-4n}+12n(n-1)x^{12n^2-3n}$.

- **(3, 6) Fullerenes:**

Again Euler's formula for this class of fullerenes results that they have exactly$n/2$ - 2 hexagonal faces and 4 tetragonal faces. In this section we compute Omega and Sadhana polynomials of an infinite class of fullerene graphs, namely C_{8n} fullerenes, see Figures 52, 53. In other words, this family of fullerenes has exactly $8n$ vertices and $12n$ edges.

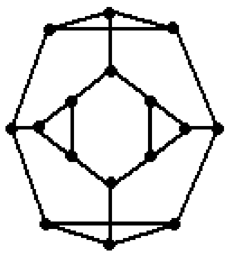


Figure 52. $2D$ graph of fullerene C_{8n} for $n = 2$.

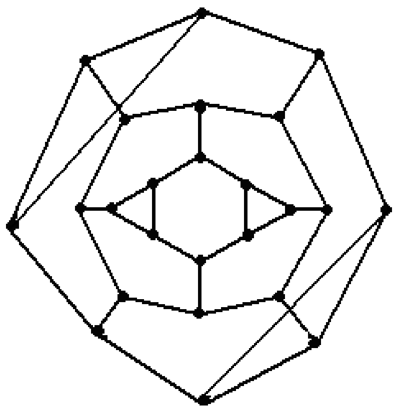


Figure 53. $2D$ graph of fullerene C_{8n} for $n = 3$.

At first suppose $n = 2$ (Figure 52). By computing number of strips and their sizes Omega and Sadhana polynomials are as follows:

$$\Omega(G,x)=2x^2+4x^6+2x^4 \text{ and } Sd(G,x)=2x^{34}+4x^{30}+2x^{32}.$$

When $n = 3$ (Figure 53), one can see that $\Omega(G,x)=2x^2+4x^6+2x^4$ and $Sd(G,x)=2x^{34}+4x^{30}+2x^{32}$. By computing this method we have:

Theorem 65. Consider the fullerene graph C_{8n}(Figure 5). Then:

$$\Omega(F_{8n},x)=\begin{cases}2x^2+(n-1)x^4+4x^{2n} & 2\mid n\\ 2x^2+(n-1)x^4+2x^n+3x^{2n} & 2\nmid n\end{cases},$$

$$Sd(F_{8n},x)=\begin{cases}2x^{12n-2}+(n-1)x^{12n-4}+4x^{10n} & 2\mid n\\ 2x^{12n-2}+(n-1)x^{12n-4}+2x^{11n}+3x^{10n} & 2\nmid n\end{cases}.$$

Proof. To compute qoc strips we should to consider two cases:

Case 1: *n* is even. According to Figure 54(a), there are 3 strips such as $C(e_1)$, $C(e_2)$ and $C(e_3)$ with $|C(e_1)|=2$ ، $|C(e_2)|=4$ and $|C(e_3)|=2n$. On the other hand, there are 2, *n – 1,* 4 stripes of types $C(e_1)$, $C(e_2)$ and $C(e_3)$, respectively. This completes the first claim.

Case 2: *n is odd*. According to Figure 54(b), there are 4 strips such as $C(e_1)$, $C(e_2)$, $C(e_3)$ and $C(e_4)$ with $|C(e_1)|=2$ ، $|C(e_2)|=4$, $|C(e_3)|=n$ and $|C(e_4)|=2n$. On the other hand, there are 2, *n – 1*, 2, 3 stripes of types $C(e_1)$, $C(e_2)$, $C(e_3)$ and $C(e_4)$, respectively. This completes the proof.

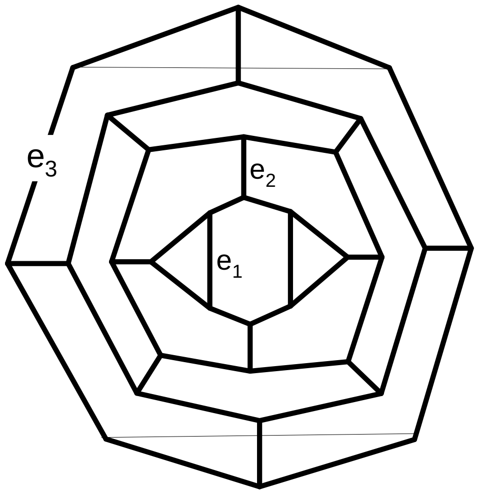


Figure 54(a). 2*D* graph of fullerene C_{8n} when *n* is even.

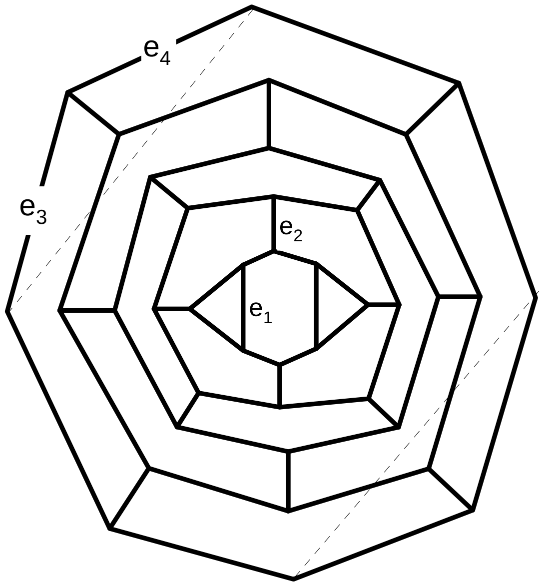


Figure 54(b). $2D$ graph of fullerene C_{8n} when n is odd.

9. NANOSTAR DENDRIMER

The goal of this section is computation of PI, Omega and Sadhana polynomials of nanostar dendrimer G_n, depicted in Figure 55. Let G be a bipartite graph, $e \in E(G)$. It is clear that $C(e) = N(e)$. Hence, by using this note we can compute three counting polynomials.

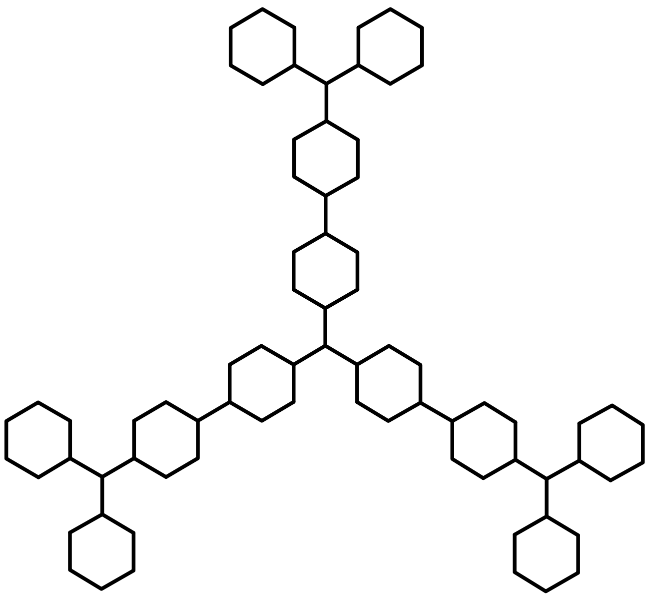


Figure 55. $2D$ graph of nanostar dendrimer G_n for $n = 2$.

At first consider G_1, in Figure 56. Obviously, there are two different strips, *e. g.* F_1 and F_2. On the other hand there are 36 strips of type F_1 and 9 strips of type F_2. Further, $|F_1| = 2$ and $|F_2| = 1$. Thus, we have

$$\Omega(G,x) = 9x^2 + 3x,\ Sd(x) = 9x^{19} + 3x^{20},\ PI(G,x) = 18x^{19} + 3x^{20}.$$

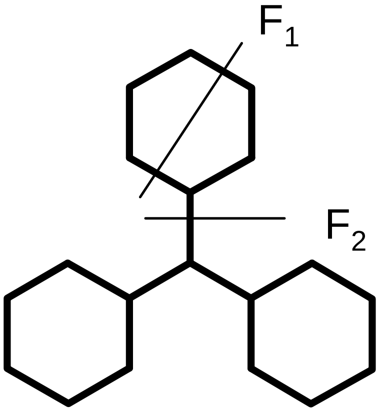


Figure 56. 2*D* graph of nanostar dendrimer G_n for $n = 1$.

Let us consider the graph of G_2 depicted in Figure 55. Similar to the last case, there are two different strips, namely F_1 and F_2, in which $|F_1| = 2$ and $|F_2| = 1$. On the other hand there are 36 strips of type F_1 and 9 strips of type F_2. Further, $|F_1| = 2$ and $|F_2| = 1$. This implies

$$\Omega(G,x) = 36x^2 + 9x,\ Sd(x) = 9x^{85} + 3x^{86},\ PI(G,x) = 72x^{85} + 9x^{86}.$$

In generally, in G_n there are two strips F_1 and F_2, with $|F_1| = 2$ and $|F_2| = 1$. By counting strips equivalent with F_1 and F_2 respectively, it is easy to see that there are $9 + 27 \times 2^{n-2}$ strips of type F_1 and $3 + 12 \times 2^{n-2}$ cut edges. Thus we proved the following Theorem:

Theorem 66. Consider the nanostardendrimerG_n, for $n \geq 2$. Then

$$\Omega(G,x) = (9 + 27 \times 2^{n-2})x^2 + (3 + 12 \times 2^{n-2})x,$$

$$Sd(G,x) = (9 + 27 \times 2^{n-2})x^{|E|-2} + (3 + 12 \times 2^{n-2})x^{|E|-1},$$

$$PI(G,x) = 2(9 + 27 \times 2^{n-2})x^{|E|-2} + (3 + 12 \times 2^{n-2})x^{|E|-1}.$$

where $|E| = |E(G_n)| = 33 \times 2^n - 45$.

10. Conclusion

A counting polynomial C(G,x) is a sequence description of a topological property so that the exponents express the extent of its partitions while the coefficients are related to the occurrence of these partitions. Basic definitions and properties of the Omega polynomial $\Omega(G,x)$ and Sadhana polynomial Sd(G,x) are presented. These polynomials for some infinite classes of fullerenes and nanotubes are also computed.

Omega polynomial introduced by M. V. Diudeacounts the quasi orthogonal cut qoc strips in a graph G=G(V, E). A qoc strip, defined with respect to any edge in G, represents the smallest subset of edges closed under taking opposite edges on faces. The first and second derivatives, in x= 1, of Omega polynomial enables the evaluation of the

Cluj-Ilmenau CI index. Composition rules for Omega polynomial in nanostructures, according to their topology, are derived. In recent years, several papers on methods for computing Omega polynomials of molecular graphs have been published.Good ability of these descriptors in predicting the heat of formation and strain energy in small fullerenes or the resonance energy in planar benzenoids was found. Omega polynomial is useful in describing the topology of tubular nanostructures.

Our calculation was done by a combination of HyperChem [51], TopoCluj [52] and GAP [53]. We first draw the molecule by HyperChem and them load it into TopoCluj. We compute its distance matrix by TopoCluj and then upload this matrix into a GAP program. In this way, we obtain a very fast method for our calculations.

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