*Kragujevac J. Sci.* 35 (2013) 61-70. UDC 541.27:541.6

# On Omega and Sadhana Polynomials of Leapfrog Fullerenes

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*(Received July 11, 2012)*

**ABSTRACT.** 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. In this paper, the Omega and Sadhana polynomials of a new infinite class of Leapfrog fullerenes are computed for the first time. The topology of this fullerene is described in terms of Omega counting polynomial. The topological description can be used in structure interpretation analysis.

## INTRODUCTION

In mathematics, groups are often used to describe symmetries of objects. This is formalized by the notion of a group action: every element of the group "acts" like a bijective map (or "symmetry") on some set. To clarify this notion, we assume that $G$ is a group and $X$ is a set. $G$ is said to act on $X$ when there is a map $\phi : G \times X \longrightarrow X$ such that all elements $x \in X$, (i) $\phi(e,x) = x$ where $e$ is the identity element of $G$, and, (*ii*) $\phi(g, \phi(h,x)) = \phi(gh,x)$ for all $g,h \in G$. In this case, $G$ is called a transformation group, $X$ is called a $G$-set, and $\phi$ is called the group action. For simplicity we define $gx = \phi(g,x)$. In a group action, a group permutes the elements of $X$. The identity does nothing, while a composition of actions corresponds to the action of the composition. For a given $X$, the set $\{gx \mid g \in G\}$, where the group action moves $x$, is called the group orbit of $x$. The subgroup which fixes is the isotropy group of $x$.

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

A chemical graph is a graph theoretical representation of a molecule whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds.

The fullerene era was started by discovery of a stable cluster of $C_{60}$ in 1985 by Kroto [1-4]. A fullerene graph is a cubic 3-connected plane graph. 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 $m = (5p+6h)/2 = 3n/2$ 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, $n$ = 2$h$ + 20 and $m$ = 3$h$ + 30. This implies that such molecules, made entirely of $n$ carbon atoms, have 12 pentagonal and ($n$/2 − 10) hexagonal faces, while $n \neq 22$ is a natural number equal or greater than 20.

Let $G$ be a fullerene graph on $n$ vertices. A Leapfrog transform $G^l$ of $G$ is a graph on 3$n$ 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 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 3$n$ vertices 12 pentagonal and (3$n$/2)-10 hexagonal faces. A sequence of stellation-dualization rotates the parent $s$-gonal faces by $\pi/s$. Leapfrog operation is illustrated, for a pentagonal face, in Fig. 1.

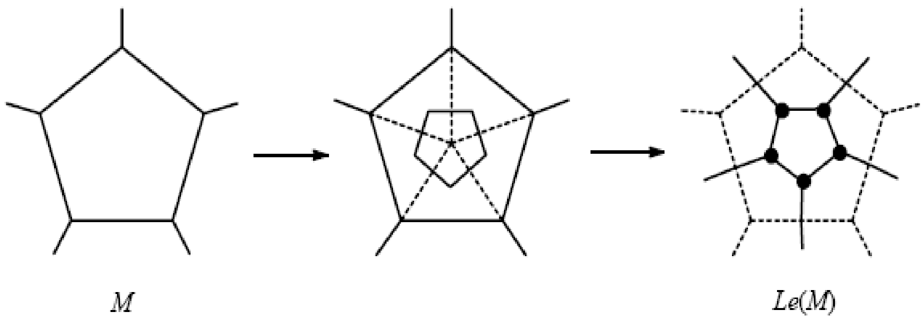



**Fig. 1**. Leapfrog of a pentagonal face.

For a more thorough introduction and treatment of Leapfrog fullerenes we refer the reader to [5, 6]. Through this paper all notations are standard and mainly taken from [7 – 16].

Two edges $e = ab$ and $f = xy$ of graph $G$ are called codistant, "$e$ $co$ $f$", if and only if $d(a,x) = d(b,y) = k$ and $d(a,y) = d(b,x) = k+1$ or vice versa, for a non-negative integer $k$. It is easy to check that the relation "$co$" is reflexive and symmetric but it is not necessary to be transitive. Set $C(e) = \{f \in E(G) \mid f \ co \ e\}$. If the relation "$co$" is transitive on $C(e)$ then $C(e)$ is called an orthogonal cut "$oc$" of the graph $G$. The graph $G$ is called co-graph if and only if the edge set $E(G)$ a union of disjoint orthogonal cuts. If any two consecutive edges of an edge-cut sequence are topologically parallel within the same face of the covering, such a sequence is called a quasi-orthogonal cut $qoc$ strip. Let $G$ be an arbitrary connected graph and $s_1, s_2, ..., s_k$ be the oposite edges, $ops$ strips of a plane graph $G$. Then the $ops$ strips form a partition of $E(G)$ and the Ω-polynomial of $G$ is defined as [15]

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

Respect to $qoc$ strips the Omega polynomial is defined as follows:

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

with $m(G, c)$ being the number of strips of length $c$. The summation runs up to the maximum length of $qoc$ strips in $G$. This index can be useful in correlating properties with molecular structures. In other words, Diudea [10] proved that the total energy of some molecular structures has a correlation with Omega polynomial.

Another polynomial also related to the ops in $G$, but counting the non-opposite edges is the *Sadhana Sd* polynomial defined as [17]

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

The Sadhana index $Sd(G)$ for counting *qoc* strips in $G$ was defined by Khadikar et al. [12, 13] as $Sd(G) = \sum_{i=1}^{k} |E(G)| - |S_i|$. By definition of Omega polynomial, one can obtain the Sadhana polynomial by replacing $x^{|S_i|}$ with $x^{|E|-|S_i|}$ in omega polynomial. Then the Sadhana index will be the first derivative of $Sd(x)$ evaluated at $x = 1$.

## MAIN RESULTS AND DISCUSSION

The aim of this section is computing Omega and Sadhana polynomials of Leapfrog fullerenes constructed from $F_{36}$. In other word, by using the Leapfrog principle we can construct an infinite class of fullerenes denoted by $F_{36\times 3^n}$. Finally, we compute Omega and Sadhana polynomials of $F_{36\times 3^n}$. To do it at first we should consider the following examples [17 – 28].

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

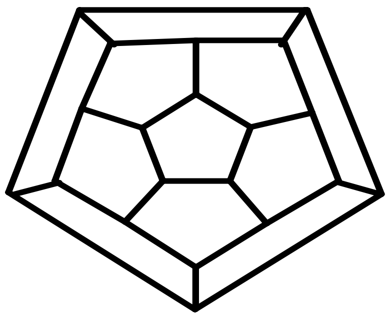
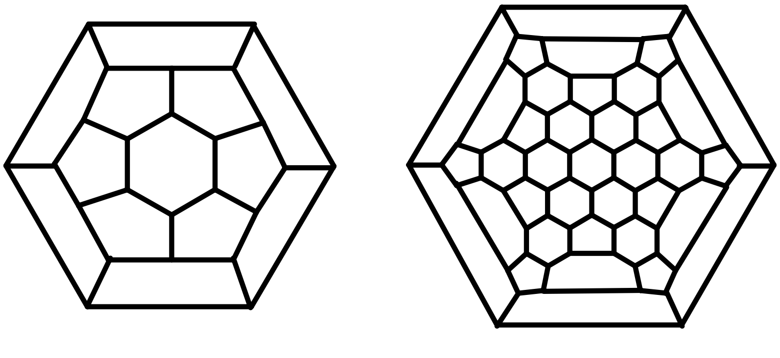


**Fig. 2.** The graph of fullerene $F_{20}$.

**Example 2.** Consider the fullerene graph $F_{24}$ in Fig. 3. 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 Fig. 3 the planer graphs of $F_{24}$ and $Le(F_{24})$ are shown.

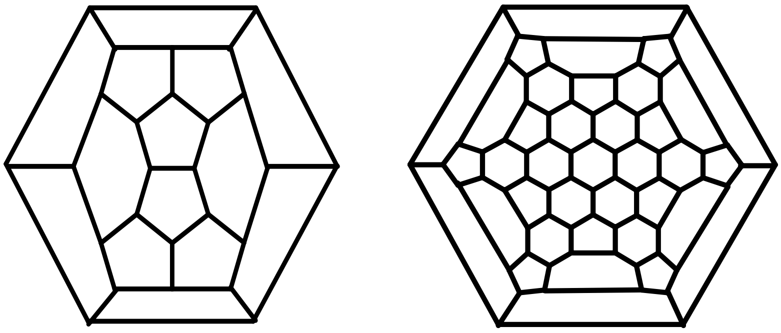


$F_{24}$ $Le(F_{24})$

**Fig. 3.** The Leapfrog of graph $F_{24}$.

**Example 3.** Consider the fullerene graph $F_{26}$ depicted in Fig. 4. This fullerene graph has 39 edges. Similar to Examples 1 and 2,it is not difficult to check $\Omega(F_{26}, x) = 21x + 9x^2$ and $Sd(F_{24}, x) = 21x^{38} + 9x^{37}$. By computing these polynomials for related Leapfrog fullerene we have:

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



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

**Fig. 4.** The Leapfrog of graph $F_{26}$.

An automorphism of the graph $G = (V, E)$ is a bijection $\sigma$ 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 $Aut(F) = Aut(Le(F))$. Now let $G = (V, E)$ be a graph. If $Aut(G)$ acts edge-transitively on $E$, then we have the following Lemma:

**Lemma 4.** Let $e \in E(G)$ be an arbitrary edge and $c = |C(e)|$. Then the Omega polynomial of graph $G$ is as follows:

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

**Proof.** Because $Aut(G)$ acts edge-transitively on $E$, so we can divide $E$ to some qoc strips of equal size $c$.

As a result of Lemma 4 we can 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. In other word, $H_n \cong K_2 \times K_2 \times \underbrace{\cdots}_{n} \times K_2$. Darafsheh [29] proved $H_n$ is vertex and edge transitive. We use from this result and so, the following Theorem is deduced:

**Theorem 5.**

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

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

**Example 6.** Consider the fullerene graph $C_{20}$ shown in Fig. 5. This fullerene is edge - transitive, $|E| = 30$ and $c=1$. So by using Lemma 4 we have $\Omega(G,x) = 30x$.

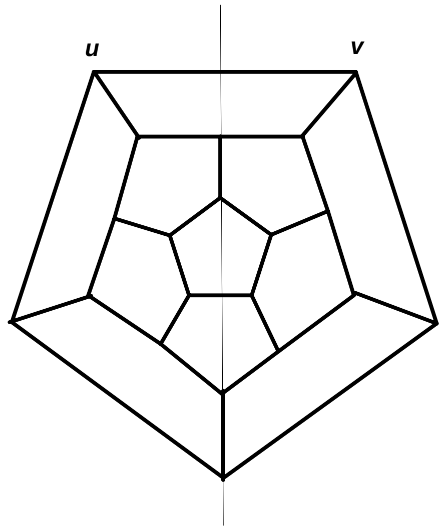



**Fig. 5.** The graph of fullerene $C_{20}$.

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

**Theorem 7.** Suppose *Aut*(*G*) acts on *E* and $E_1$, $E_2$, …,$E_n$ be its orbits. Then the Omega polynomial of *G* is $\Omega(G) = \sum_{i=1}^{n} \frac{|E_i|}{c_i} x^{c_i}$ , 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 7 implies in the case that *Aut*(*G*) is not edge – transitive then, $m(G,c)$ in equation 1, determine exactly the number of elements of any orbit of *Aut*(*G*). In other words for an arbitrary edge *e* belong to *E*(*G*), when we say $m(G,c) = k$, it means that there exist an orbit such as $\Delta$ in which $c = |C(e)|$ and $m(G,c) = |\Delta| = k$. Thus for a given graph of high order to enumeration of $m(G,c)$ it is sufficient to compute all orbits of *Aut*(*G*) acting on *E*.

By continuing the methods shown in Examples 1 – 3 one can draw the graph of fullerene $F_{26\times 3^n}$ , see Fig.s 6,7. Hence, by using Theorem 7 we have

**Theorem 8**. Consider the fullerene graph $F_{36\times 3^n}$ $(n \geq 2)$ depicted in Fig. 7. Then the Omega polynomial is as follows:

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

**Proof.** At first by using a *GAP* [30] program(Appendix) we can prove $Aut(F_{36}) \cong D_{12}$. In other words generators of $Aut(F_{36})$ are as follows (see Fig. 6):
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 prove that there are four types of edges for *qoc* strips namely $e_1$, $e_2$, $e_3$ and $e_4$, in which $|C(e_1)| = 3^{(n+1)/2}$, $|C(e_2)| = 2 \times 3^{(n+1)/2}$, $|C(e_3)| = 3^{(n+2)/2} \times 4$ 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. This completes the proof.

**Corollary 9.** For the fullerene graph $F_{36\times 3^n}$ $(n\geq 2)$ the Sadhana polynomial is as follows:

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

where, $|E|=2\times 3^{n+3}$.

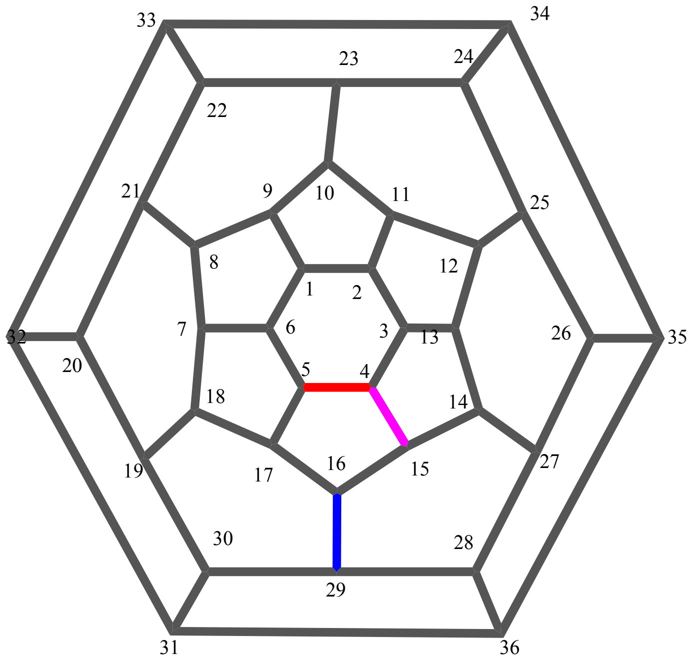



**Fig. 6.** The graph of fullerene $F_{36}$.

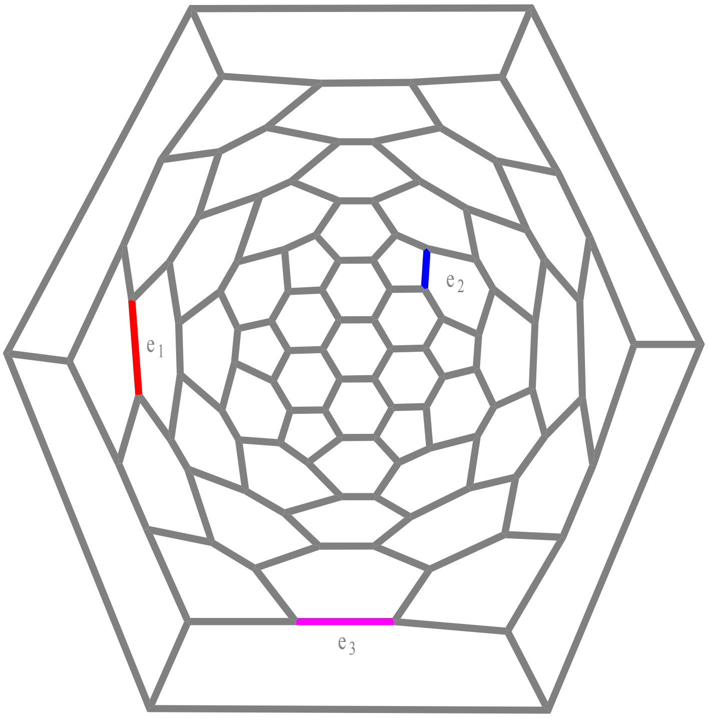



**Fig. 7(i).** The graph of $F_{36\times 3^n}$ for $n$ = 1.

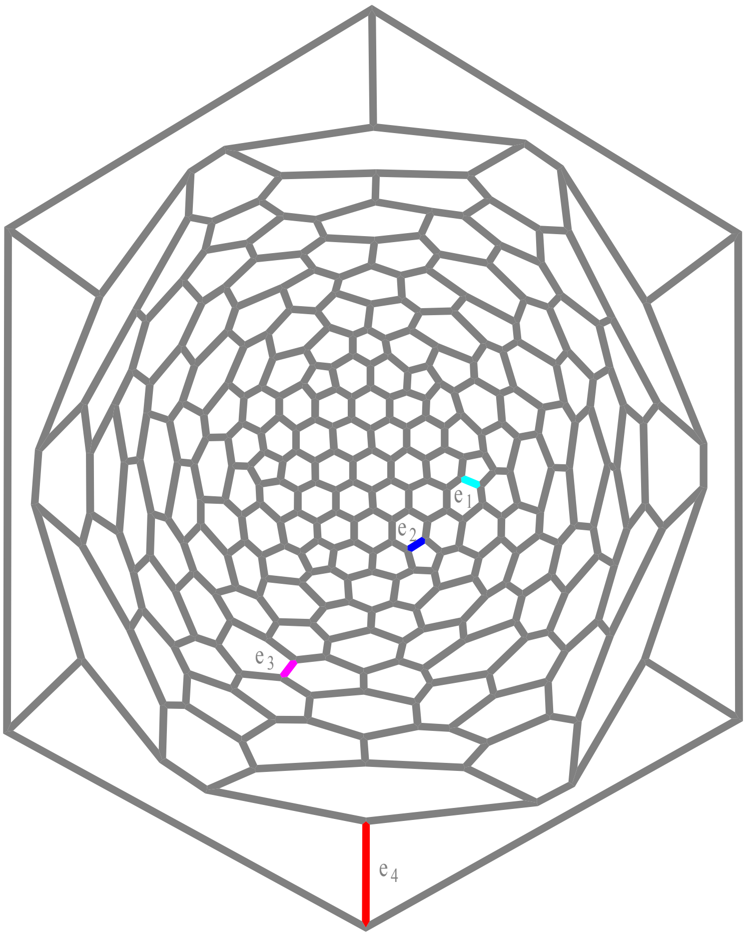



**Fig. 7(ii).** The graph of $F_{36\times 3^n}$ for $n$ = 2.

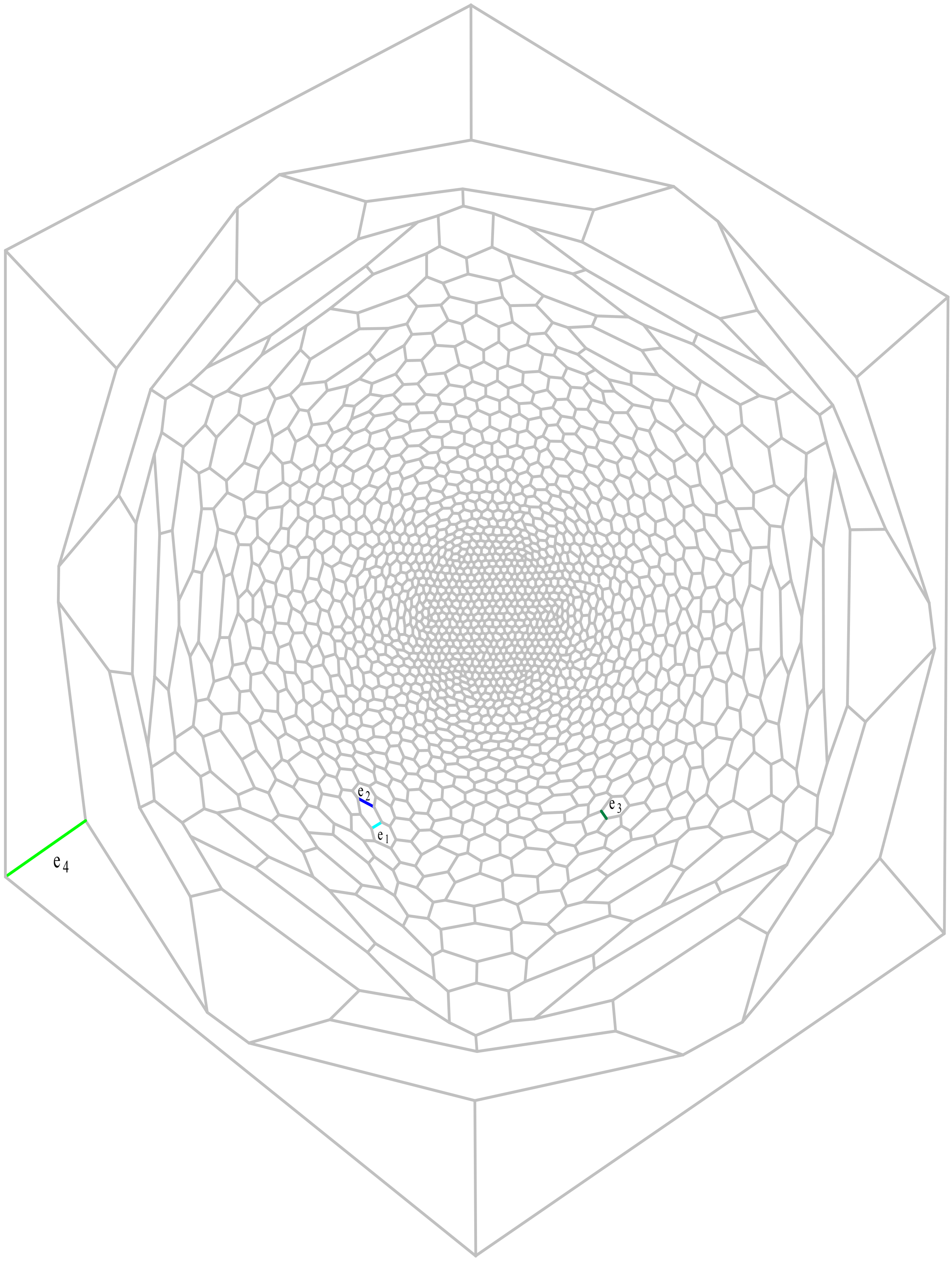



**Fig. 7(iii).** The graph of $F_{36\times 3^n}$ for $n = 3$.

## CONCLUSIONS

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 $\Omega(x)$ and Sadhana polynomial Sd($x$) are presented. These polynomials are also computed for an infinite class of fullerenes.

Omega polynomial introduced by M. V. Diudeacounts the quasi orthogonal cut qoc strips in a graph $G$. 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 fullerenes, 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.

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