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Fullerene graphs with pentagons and heptagons

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ABSTRACT. A fullerene is a three connected cubic planar graph. In this paper, we introduce a new class of fullerenes, with pentagonal and heptagonal rings.

Keywords: molecular graph, fullerene, chemical graph theory.

1. INTRODUCTION

A graph is a collection of points and lines connecting them. Let us to call these points and lines by vertices and edges, respectively. Two vertices x and y are adjacent, if $e = uv$ be an edge of graph. A graph whose all pairs of vertices are connected by a path is called a connected graph. A simple graph is a graph without loop and parallel edges. For example, the graph depicted in Figure 1 has a loop and two parallel edges and so it is not simple.

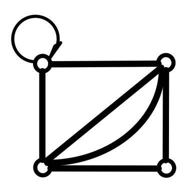

Figure 1. A graph with a loop and two parallel edges.

The vertex and edge-sets of graph G are represented by $V(G)$ and $E(G)$, respectively [1]. A molecular graph (chemical graph) is a labeled simple graph whose vertices and

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edges correspond to the atoms and chemical bonds, respectively. In a molecular graph, it is convenient to omit hydrogen atoms.

A fullerene is a molecule composed of carbon atoms in the form of many shapes such as hollow sphere, ellipsoid, tube, etc. The most important fullerenes are spherical fullerenes or buckyballs. Carbon nanotubes or buckytubes are cylindrical fullerenes. Fullerenes are similar in structure to graphite, but they may also contain triangle, square, pentagonal, hexagonal or sometimes heptagonal rings [2]. The molecular graph of a given fullerene molecule is called a fullerene graph. The aim this paper is to compute the number of triangles, squares, pentagons, hexagons or heptagons in a given fullerene graph.

Theorem 1 (Euler's Formula). Let G be a planar graph and n, m, f are the number of vertices, edges and faces, respectively. Then

$$n - m + f = 2.$$

Here our notation is standard and mainly taken from Refs [3-11].

2. MAIN RESULTS AND DISCUSSIONS

In this section we study four classes of fullerene graphs, (3,6)-fullerenes, (4,6)-fullerenes, (5,6)-fullerenes and (5,7)-fullerenes. Among them (4,6) and (5,6) – fullerenes are very important.

(3,6) fullerenes

In recent years (3,6)–fullerenes have been studied by chemists due to their similarity to ordinary fullerenes. The smallest (3,6)–fullerene is the tetrahedron and its point group symmetry is isomorphic to the symmetric group S_4.

Suppose F is an (3,6)–fullerene and t, h, n and m are the number of triangles, hexagons, carbon atoms and bonds between them. Since each atom lies in exactly 3 faces and each edge lies in two faces, the number of atoms is $n = (3t+6h)/3$, the number of edges is $m = (3t+6h)/2 = 3/2n$ and the number of faces is $f = t + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $(3t + 6h)/3 - (3t+6h)/2 + t + h = 2$, and therefore $t = 4$, $n = 2h + 4$ and $m = 3h + 6$. This implies that such molecules made up entirely of n carbon atoms having 4 triangular faces and $(n/2 - 2)$ hexagonal faces, where n is a natural even number equal or greater than 4, see Figure 2.

(4,6) fullerenes

Let s, h, n and m be the number of squares, hexagons, carbon atoms and bonds between them, in a given (4,6) fullerene F. Since F is cubic, $m = 3n/2$ and by Euler's theorem $n - 3n/2 + f = 2$. This means that $f = 2 + n/2 = s + h$. On the other hand, $n - m +$

$f = (4s + 6h)/3 - (4s + 6h)/2 + s + h = 2$ leads us to conclude that $s = 6$. Hence, $h = n/2 - 4$, while $n \neq 10$ is a natural number equal or greater than 8, see Figure 3.

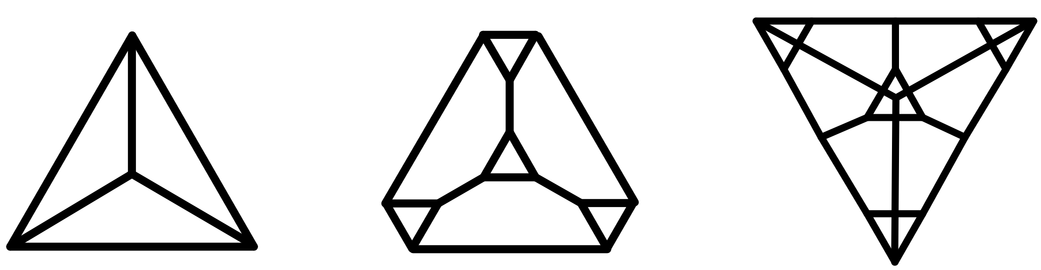
(5,6) fullerenes

These fullerenes are 3–connected cubic planar graphs with only pentagonal and hexagonal faces. The first stable fullerene molecule was discovered by Kroto and his co-authors. [3, 4] Since all faces of ordinary fullerenes are pentagons and hexagons, it is convenient to use the name (5,6)–fullerene as fullerene.

Let p, h, n and m be the number of pentagons, hexagons, carbon atoms and bonds between them, in a given (5,6) 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 $p = 12$. 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, see Figure 4.

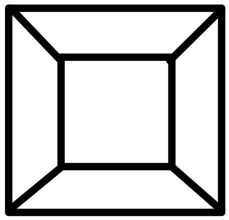
(5,7) fullerenes

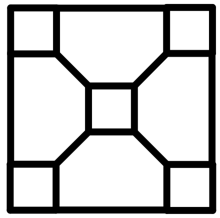
Let p, h, n and m be the number of pentagons, heptagons, carbon atoms and bonds between them, in a given (5,7) fullerene F. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is $n = (5p+7h)/3$, the number of edges is $m = (5p+7h)/2 = 3/2n$ and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $p + h = 2 + n/2$, and therefore $p = n/4 + 7$ and $h = n/4 - 5$. Three members of this class of fullerenes are depicted in Figure, see Figure 5.



A fulleren without hexagons | A fulleren with 4 hexagons. | A fulleren with 6 hexagons.

Figure 2. Some (3,6) fullerene graphs.


A fulleren without hexagons


A fulleren with 4 hexagons.

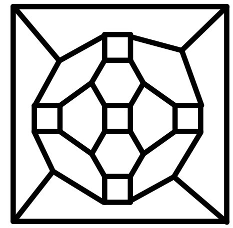
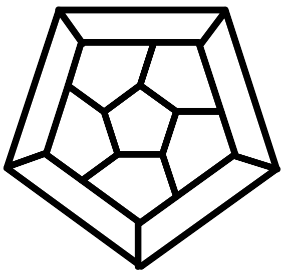
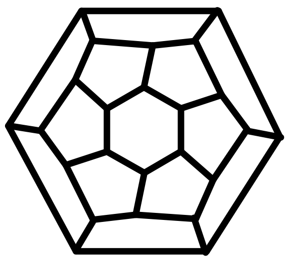

A fulleren with 12 hexagons.

Figure 3. Some (4,6) fullerene graphs.


A fulleren without hexagons


A fulleren with 2 hexagons.

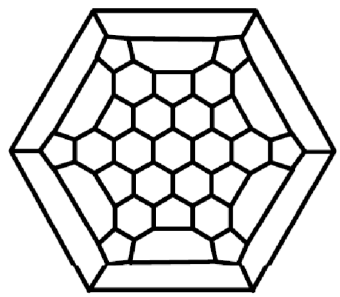
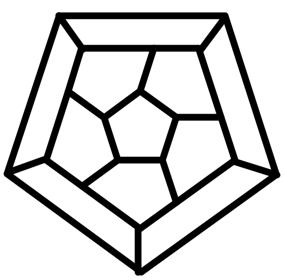
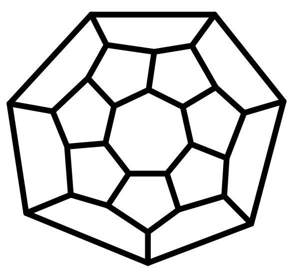

A fulleren with 26 hexagons.

Figure 4. Some (5,6) fullerene graphs.


A fulleren without hexagons


A fulleren with 2 hexagons.

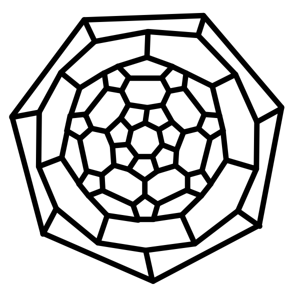

A fulleren with 16 hexagons.

Figure 5. Some (5,7) fullerene graphs.

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