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More icosahedral fulleroids

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The discovery of the famous fullerene has raised an interest in the study of other candidates for a modeling of carbon molecules. Motivated by a P. Fowler's question Delgado Friedrichs and Deza defined $I(a,b)$-fulleroids as cubic convex polyhedra having only a-gonal and b-gonal faces and the symmetry groups isomorphic with the rotation group of the regular icosahedron. In this note we prove that for every $n \geqslant 8$ there exist infinitely many $I(5,n)$-fulleroids. This answers positively questions posed recently by Delgado Friedrichs and Deza.

KEY WORDS: fullerene, fulleroid, icosahedral group of symmetry, convex polytope, plane graph

AMS subject classification: 05C25, 52B10, 92E10

1. Introduction

Cubic convex polyhedra are good models for carbon molecules. These models have the following structure: atoms of the carbon are the vertices of such polyhedra and edges of these polyhedra realise bonds between pairs of atoms. With every carbon atom four bonds are associated but the polyhedron is cubic (i.e., every its vertex is trivalent). This means that along one edge at each vertex a double bond has to be realized. This is possible because the graph of every cubic convex polyhedron (i.e., the structure defined by vertices and edges of the polyhedron) has a 1-factor (or, equivalently, a perfect matching or a Kekulé structure) as proved by Petersen's theorem [1], or also [2]. In fact, as shown by Klein and Liu [3,4], every cubic convex polyhedron has at least three mutually disjoint 1-factors. Along edges of this 1-factor double bonds can be realized.

The discovery of the famous fullerene C_{60} in 1985 [5] has raised an interest in the study of other candidates for modelling of carbon molecules. Patrick Fowler in 1995, see [6,7], asked whether a fullerene-like structure with 260 vertices consisting of pentagons and heptagons (7-gonal faces) only and exhibiting an icosahedral symmetry could exist. The answer was given by Dress and Brinkmann [7]. The question of Fowler will be generalized later in this note.

First, we introduce some definitions. A *p-vector* (or a *face-vector*, cf. [8,9]) of a cubic, convex polyhedron P is a sequence $\{p_i(P),\ i \geqslant 3\}$, where $p_i(P)$ denotes the number of i-gonal faces of P. The famous Euler's polyhedral formula yields the following relation for terms of the p-vector

$$3p_3(P) + 2p_4(P) + p_5(P) = 12 + \sum_{j \geqslant 7} (j - 6)p_j(P). \tag{1}$$

The problem to characterize which sequences of nonnegative integers $p = \{p_i,\ i \geqslant 3\}$ can be p-vectors of convex polyhedra is a classical problem of Eberhard [21] (cf. [8]). A characterization of such sequences can be found in [9].

Delgado Friedrichs and Deza [6] introduced the following definitions. A *fulleroid* is a cubic convex polyhedron. A Γ-*fulleroid* is a fulleroid which has the group Γ as its symmetry group. In particular, an I-*fulleroid* is a fulleroid which has its symmetry group isomorphic with the rotation group of the regular icosahedron while an I_h-fulleroid is one having its symmetry group isomorphic to the full symmetry group of the regular icosahedron (including inversion, reflections, and improper rotations). A given Γ-fulleroid F is of type (a, b) or a $\Gamma(a, b)$-*fulleroid* if $p_i(F)$ is nonzero only for $i \in \{a, b\}$. Let $a = 5$. The case $b < 5$ is not possible. For $a = b = 5$, the only possible $I_h(5, 5)$-fulleroid is the dodecahedron. The case $(a, b) = (5, 6)$ is the classical fullerene case.

We say that an $\Gamma(a, b)$-fulleroid is *smallest* if it has the smallest possible number of vertices. Note that (1) points that the relation between the numbers p_a and p_b in an $\Gamma(a, b)$-fulleroid is linear. This further implies that v, the number of vertices, is a linear function of any of them. Therefore we can use any one of these three quantities to measure the size of an $\Gamma(a, b)$-fulleroid. However for $I(5, n)$-fulleroids, it will turn out to be most convenient to use p_n.

Dress and Brinkmann [7] have found two fulleroids with 260 vertices, one is the smallest $I(5, 7)$-fulleroid and the second is the smallest $I_h(5, 7)$-fulleroid, and proved that neither other $I(5, 7)$-fulleroid nor other $I_h(5, 7)$-fulleroid on 260 vertices exists. Delgado Friedrichs and Deza [6] have found the smallest $I_h(5, n)$-fulleroids for $n = 8, 9, 10, 12, 14, 15$, and asked the following questions regarding $I(5, n)$-fulleroids:

- Is there at least one $I(5, n)$-fulleroid for each $n > 6$?
- Is there at least one $I(5, n)$-fulleroid for infinitely many $n > 6$?
- Is there an infinite series of $I(5, n)$-fulleroids for each–infinitely many $n > 6$?
- For which n is there at least one $I(5, n)$-fulleroid realizing the smallest possible p-vector?
- For which n is this smallest $I(5, n)$-fulleroid unique?

The aim of this note is to answer positively the first three questions for $n \geqslant 8$ and bring a partial answer to the fourth. Namely, the main result of this note is the following.

Theorem 1. Let $n \geqslant 8$ and $m \geqslant 1$ be integers. There is an $I(5, n)$-fulleroid $F(m)$ with $p_n(F(m)) = 60m$.

Applying elementary group theory one can easily observe the following.

Theorem 2 [6,10,11]. In an I-fulleroid there is at most one orbit of faces with rotational s-fold symmetries, $s = 2, 3, 5$, respectively. These orbits, if existent, contain exactly 30, 20 and 12 faces, respectively. All the other orbits have exactly 60 faces each. The face sizes of the first three orbits are of the size $2t$, $3t$ and $5t$, respectively, t being a positive integer. Faces of the other orbits can have any size.

Applying these two results we immediately have a partial answer to the fourth question.

Theorem 3. If n is an odd integer, $n \not\equiv 0 \pmod 3$, and $n \not\equiv 0 \pmod 5$ then $F(1)$ is the smallest $I(5, n)$-fulleroid.

2. Preliminaries

The following theorem of P. Mani [12] (see also [13]) plays a very important role in our proofs.

Theorem 4. To every finite 3-connected plane graph H there is a convex polyhedron P such that the graph of P is isomorphic to H and the symmetry group of P is isomorphic to the automorphism group of H.

Clearly, $p_k(H) = p_k(P)$ for every $k \geqslant 3$. Due to Mani's theorem it is enough to construct cubic 3-connected plane graphs which have pentagonal and n-gonal faces and the automorphism groups isomorphic to the group I of rotational symmetries of the icosahedron.

We begin by defining certain configurations and transformations that is, graphs which can occur as induced subgraphs in graphs of $I(5, n)$-fulleroids.

1. For all $t \geqslant 1$ we shall use the graph denoted by $\mathcal{D}_t$ in [14] and defined as follows: Let $\mathcal{D}_1$ be as shown in figure 1 and for $t \geqslant 2$ let $\mathcal{D}_t$ be the graph obtained from $\mathcal{D}_{t-1}$ and $\mathcal{D}_1$ by identifying the edge X_2Y_2 of $\mathcal{D}_{t-1}$ with the edge X_1Y_1 of $\mathcal{D}_1$ and then deleting these labels. The boundary of the exterior face of $\mathcal{D}_t$ has $5t$ edges between successive 2-vertices X_1, X_2 and Y_1, Y_2. The interior

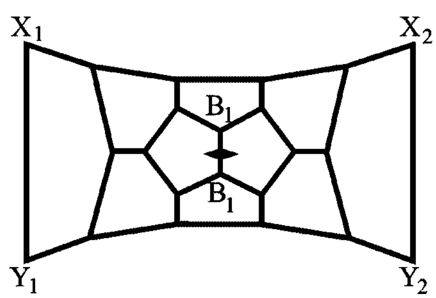

Figure 1. Configuration $\mathcal{D}_1$.

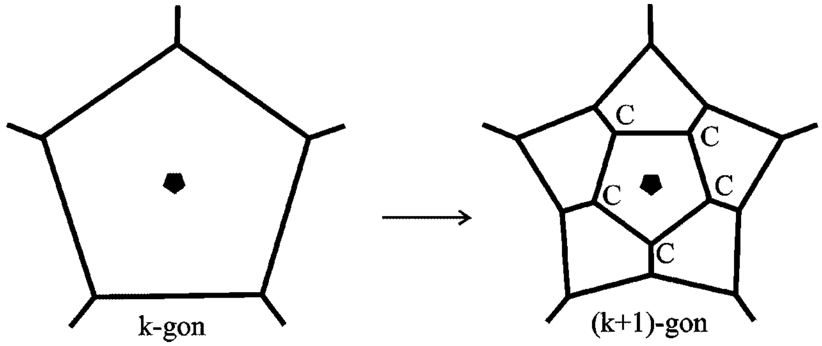

Figure 2.

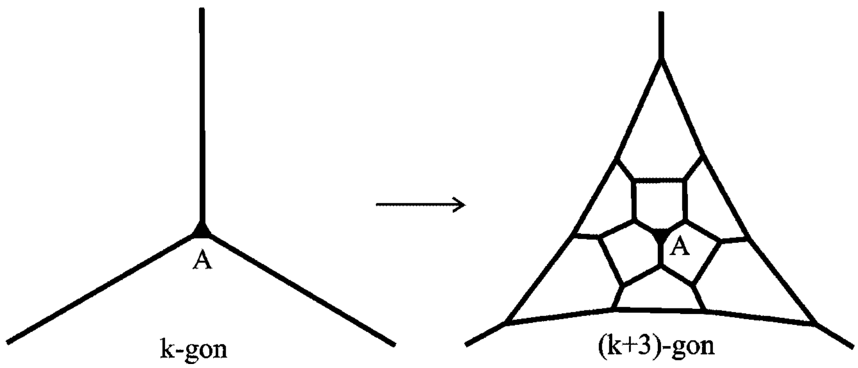

Figure 3.

faces of $\mathcal{D}_t$ are all 5-gons and the number of vertices $v(\mathcal{D}_k)$ of $\mathcal{D}_k$ is $20t$. Let us call the $\mathcal{D}_1$ so added to be the tth compound of $\mathcal{D}_t$. Note that $\mathcal{D}_1$ is centrally symmetric about the center of the edge B_1B_1 (denoted in figure 1 by a small diamond). $\mathcal{D}_{2t+1}$ has 2-fold rotation about to the central point of the B_1B_1 edge of the $(t+1)$st compound of $\mathcal{D}_{2t+1}$ and $\mathcal{D}_{2t}$ has 2-fold rotation according the center of the "former" X_2Y_2 edge of the tth compound.

2. In figure 2 there is a transformation π which enlarges the size of faces neighbour to the pentagonal face by 1. Notice that the graph on this figure admits a 5-fold rotation.

3. Figure 3 shows a transformation ρ which replaces a 3-vertex A with a configuration consisting of nine 5-gons. The graph on this figure admits 3-fold rotation around the vertex A.

4. A *configuration* $\mathcal{K}$, a chain of four pentagons as in figure 4 (do not consider the dashed lines), plays a very important role in our construction.

This configuration is centrally symmetric (posses a 2-fold rotation) about the point C, at the middle point of the edge B_1B_1' (a small diamond in figure 4). We

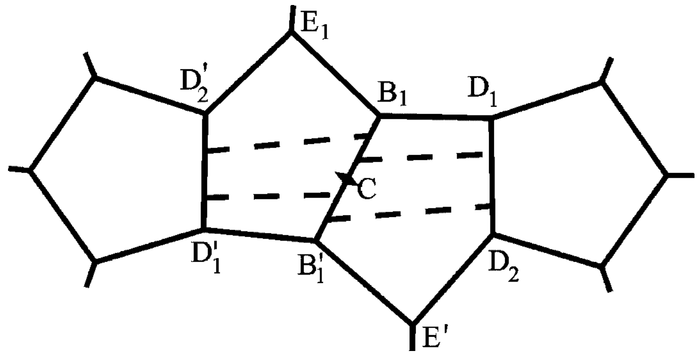

Figure 4.

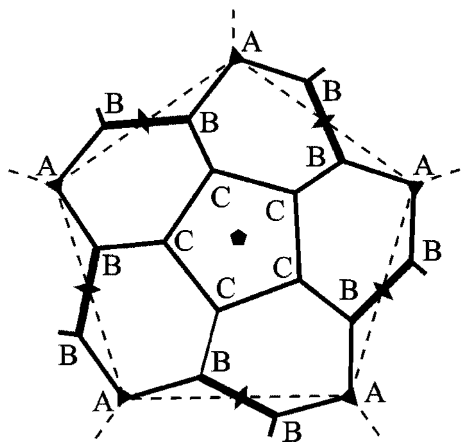

Figure 5.

use this configuration to receive a pair of required m-gons, $m \geqslant 6$. We proceed in the following way: We place $m - 5$ different vertices on the segment B_1C of the edge B_1B_1 (none of them coincides with the point C) and $m - 5$ different vertices on the edge D_1D_2 then we place the images, with respect to the 2-fold rotation about to center C, of placed vertices on the segment $B_1'C$ of the edge B_1B_1' and the edge $D_1'D_2'$.

In the next step we insert $2(m - 5)$ edges joining the vertices added so that the pentagons incident with the edge B_1B_1' are divided into $4(m - 5)$ new pentagons, and the configuration obtained again possesses a 2-fold rotation. (See figure 5 with dashed lines for the case $m = 7$.) Notice that the resulting configuration again contains a configuration $\mathcal{K}$, it is a chain of four pentagons with the edge having the point C as its center. This new configuration $\mathcal{K}$ can be used for receiving the next pair of two m-gons in the same way as described above.

Note. Let us notice that also each configuration $\mathcal{D}_t$ contains a configuration $\mathcal{K}$.

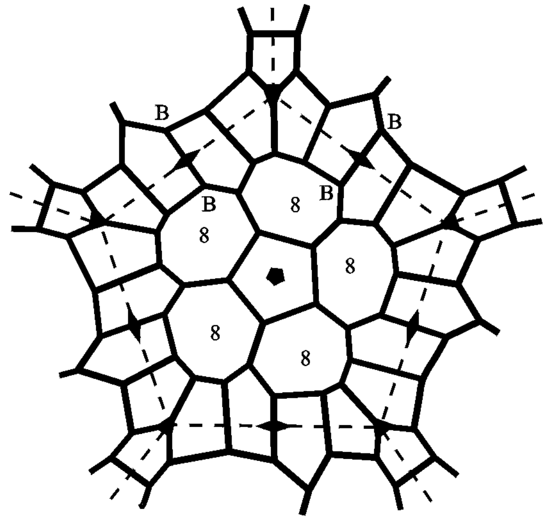

Figure 6.

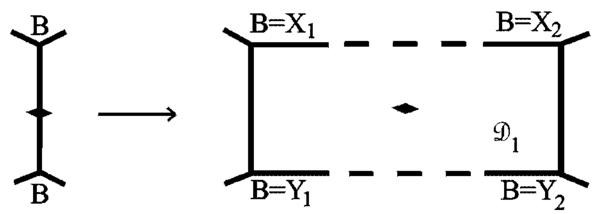

Figure 7.

3. Proof of theorem 1

Our construction begins with two graphs P_0 and Q_0. The graph P_0 is obtained from the icosahedron in the following way. Each of its 5-faces is split into one new 5-face α and six new 6-faces as shown in figure 5. It is easy to see that the automorphism group of the resulting graph P_0 is the rotation group of the icosahedron. The (original) vertices A are poles of 3-fold rotations (denoted in figure 5 by small triangles), the centers of 5-faces are poles of 5-fold rotations (marked in figure 5 by a small pentagon) and the middle points of the BB-edges are poles of 2-fold rotations (marked by small diamonds). In the construction we distinguish five cases. The graph Q_0 is also obtained from the icosahedron by splitting each of its 5-faces with one new 5-face, five octagons and twenty "half faces" as shown in figure 6. The graph Q_0 has 60 octagons, 30 BB-edges which are involved into 30 $\mathcal{K}$-configuration. It is easy to see that (similarly as in the graph P_0) the graph Q_0 has the same rotations as the icosahedron (but has no plane symmetries).

Case 1. If $n = 6 + 5t$, $t \geqslant 0$, then the construction continues by replacing each edge BB of P_0 by the configuration $\mathcal{D}_t$ as in figure 7.

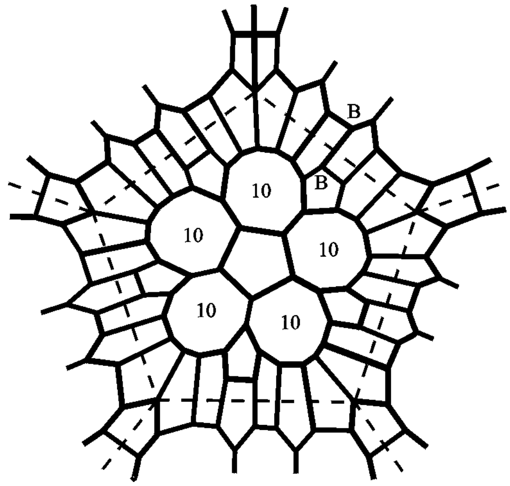

Figure 8.

The result is an $I(5, n)$-fulleroid P_1 with $p_n = 60$ and if $t \geqslant 1$, 30 configurations $\mathcal{K}$. Note that here and in the sequel $\mathcal{D}_0$ means that no replacement of the edge BB is performed.

Case 2. If $n = 7 + 5t$, $t \geqslant 0$, first we construct an $I(5, n-1)$-fulleroid P_1 as in case 1. Then the transformation π is used on each pentagon $[CCCCC]$ of P_1 which has been present already in P_0. The result is a required $I(5, n)$-fulleroid P_2 with 60 n-gonal faces and, if $t \geqslant 1$, 30 configurations $\mathcal{K}$.

Case 3. Let $n = 8 + 5t$, $t \geqslant 0$. Our construction starts with the graph Q_0 in which each edge BB is replaced by the configuration $\mathcal{D}_t$ as in figure 7. The result is an $I(5, n)$-fulleroid Q_1 with $p_n = 60$ and 30 configuration $\mathcal{K}$.

Case 4. If $n = 9 + 5t$, $t \geqslant 0$, we first construct an $I(5, n-1)$-fulleroid Q_1 as in the case 3. Then the construction π is applied to each pentagon of Q_1 which is crossed with an axis of a 5-fold rotation. The resulting graph Q_2 has 60 n-gons and 30 configurations $\mathcal{K}$.

Case 5. If $n = 10 + 5t$, $t \geqslant 1$, we first construct an $I(5, n-3)$-fulleroid P_2 as in the case 2 and then the transformation ρ is applied to each 3-vertex which has been presented in already in P_0. The result is a required $I(5, n)$-fulleroid P_4 with 60 n-gonal faces and 30 configurations $\mathcal{K}$. For $t = 0$ our construction begins with the dodecahedron whose 5-faces are splitted as indicated in figure 8. The result is an $I(5, 10)$-fulleroid Q_3 with $p_{10} = 60$ and 30 configurations $\mathcal{K}$.

Note that our construction has been led in such a way that all 30 configurations $\mathcal{K}$ are in the same orbit of the icosahedral group of the graph P_i, $i = 1, 2, 3$, and of the graph Q_j, $j = 0, 1, 2, 3$. We shall keep this property also in the next constructions of 60 new n-gonal faces which we create in pairs by the construction described in the previous part using these 30 configurations $\mathcal{K}$.

4. Remarks

1. In our proof of theorem 1, case 2 with $t = 0$, we obtain the smallest $I(5,7)$-fulleroid described in [7]. A little modification of our construction (a use a generalization of the configuration $\mathcal{K}$) leads to infinitely many $I(5,7)$-fulleroids. Infinite series of $I_h(5,7)$-fulleroids can be obtained using ideas of Delgado Friedrichs and Deza [6].

2. The problem to investigate p-vectors of Γ-fulleroids has been first formulated by Jucovič [15] in seventieth but in a different language; see also Trenkler [16] where p-vectors of 4-valent polyhedra with prescribed groups of symmetries were investigated. A literature concerning "Eberhard-type theorems" for the chemical relevant subclass of cubic convex polyhedra is rather extensive. The reader is reffered, e.g., to Klein and Liu [3,4] and Liu et al. [17] and the references therein.

3. The question of Fowler's can be generalized in the following way: Let $\Gamma(a,b)$-fulleroids be Γ-fulleroids having only a-gonal and b-gonal faces. For a list of all groups of symmetries that can act on convex polyhedra, see, e.g., Coxeter and Moser [11], or a recent book [18] by Cromwell. For symmetries on fullerenes see the papers by Babić et al. [19], and Fowler et al. [20].

Problem. Characterize $\Gamma(a,b)$-fulleroids for all possible pairs of parameters (a,b) and all possible groups of symmetries Γ.

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