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Fulleroids with dihedral symmetry

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ABSTRACT

Fulleroids are cubic convex polyhedra with faces of size 5 or greater. They are suitable as models of hypothetical all-carbon molecules. In this paper, sufficient and necessary conditions for existence of fulleroids of dihedral symmetry types and with pentagonal and n-gonal faces only depending on number n are presented. Either infinite series of examples are found to prove existence, or nonexistence is proved using symmetry invariants.

1. Introduction

Fullerenes have been objects of interest and study in the past two decades. A *fullerene* is a 3-valent carbon molecule, where atoms are arranged in pentagons and hexagons. It can be seen as a convex polyhedron, where vertices represent atoms and edges represent bonds between atoms. Fullerenes can also be represented by graphs. In fact, a *fullerene graph* is a planar, cubic (i.e. 3-regular) and 3-connected graph, twelve of whose faces are pentagons and the remaining ones hexagons.

The concept of fullerenes can be generalized in several ways. Fowler [5] asked whether a fullerene-like structure consisting of pentagons and heptagons only and exhibiting an icosahedral symmetry, exists. The answer was given by Dress and Brinkmann [2]. Motivated by these examples, Delgado Friedrichs and Deza [4] introduced the following definition:

Definition 1. A *fulleroid* is a convex polyhedron such that all its vertices have degree 3 while all its faces have degree 5 or larger. A *Γ-fulleroid* is a fulleroid on which the group Γ acts as a group of symmetries. A given Γ-fulleroid is of type (a, b) or a $\Gamma(a, b)$-fulleroid if all its faces are either a-gonal or b-gonal.

The set of all $\Gamma(a, b)$-fulleroids will be denoted simply by $\Gamma(a, b)$.

There is a list of groups, that can act as a symmetry group of a convex polyhedron [3]. According to the system of rotational symmetry axes, they can be divided into icosahedral, octahedral, tetrahedral, dihedral, cyclic and others.

Symmetry of fullerenes has been studied deeply. The possible symmetry groups Γ for fullerenes were shown to be limited to a total of 28 point groups [6]. Babić, Klein and Sah [1] divided all fullerenes with up to 70 vertices according to the symmetry group. Fowler and Manolopoulos [5] found symmetry groups of all fullerenes with up to 100 vertices. For each symmetry group Γ they found the smallest Γ-fullerene and the smallest Γ-fullerene obeying IPR (isolated pentagon rule). They described how to create a new fullerene with the same symmetry group having more hexagonal faces and obeying IPR once a fullerene is given. Graver [7] published a catalog of all fullerenes with ten or more symmetries.

Symmetry of fulleroids has also been an object of research in recent years. Among all possible symmetry types, icosahedral symmetry groups were studied first. Let the full symmetry group of a regular icosahedron be denoted by $\mathcal{I}_h$; its subgroup of rotational symmetries by $\mathcal{I}$. Delgado Friedrichs and Deza [4] found $\mathcal{I}_h(5, n)$-fulleroids for $n = 8, 9, 10, 12, 14$ and 15 and asked several questions concerning $\mathcal{I}(5, n)$-fulleroids. Most of their questions were answered by Jendrol' and Trenkler [9], who found infinite series of examples of $\mathcal{I}(5, n)$-fulleroids for all $n \geq 8$.

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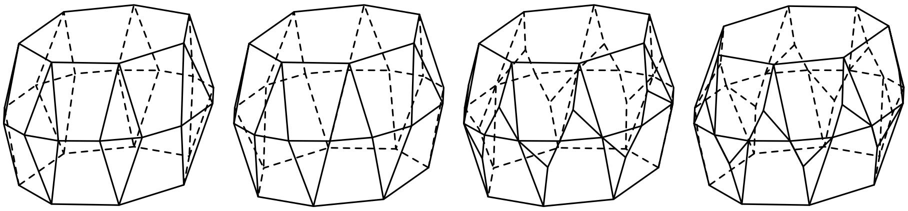

Fig. 1. Examples of polyhedra with $\mathscr{D}_{7h}$, $\mathscr{D}_{7d}$, $\mathscr{D}_7$, and $\mathscr{S}_{14}$ symmetry, respectively.

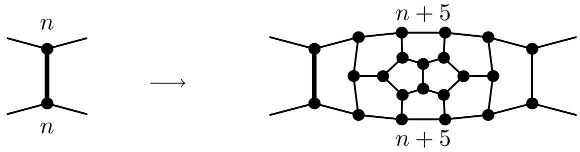

Fig. 2. The step to increase the size of two n-gons by 5.

Jendrol' and Kardoš [8] found a necessary and sufficient condition for the existence of $\mathscr{O}_h(5, n)$-fulleroids, where $\mathscr{O}_h$ denotes the full symmetry group of a regular octahedron. Kardoš [10] characterized $\Gamma(5, n)$-fulleroids, where Γ is the group of all symmetries of a regular tetrahedron $\mathscr{T}_d$, or the group of rotational symmetries of a regular tetrahedron $\mathscr{T}$, or the group $\mathscr{T}_h$, which is a subgroup of the group $\mathscr{O}_h$ with four 3-fold rotational symmetry axes, three 2-fold rotational symmetry axes, and a point of inversion.

In this paper we solve the question of the existence of fulleroids with a symmetry group of dihedral type. In particular, we investigate fulleroids with the symmetry group $\mathscr{D}_m$, $\mathscr{D}_{md}$, and $\mathscr{D}_{mh}$, where $m \geq 2$.

The symmetry groups $\mathscr{D}_m$, $\mathscr{D}_{md}$ and $\mathscr{D}_{mh}$ have one specific property among all possible symmetry groups of convex polyhedra: all rotational symmetry axes with the exception of one axis lie in one plane (called main, horizontal plane) and the only other axis (called main, vertical axis) is perpendicular to this plane.

The group $\mathscr{D}_m$ is the group of all rotational symmetries of a regular m-sided prism. It is isomorphic to the triangle group $T(2, m) = \langle x, y : x^2 = y^m = (xy)^2 = 1\rangle$. The group $\mathscr{D}_{md}$ is the full symmetry group of a regular m-sided antiprism. It is isomorphic to the triangle group $T(2, 2m)$, where the generator of order $2m$ is the rotation-reflection. The group $\mathscr{D}_{mh}$ is the full symmetry group of a regular m-sided prism. It is isomorphic to the full triangle group $\langle x, y, z : x^2 = y^2 = x^2 = 1, (xy)^m = (xz)^2 = (yz)^2 = 1\rangle$.

The group $\mathscr{D}_m$ is a subgroup of index 2 of both $\mathscr{D}_{md}$ and $\mathscr{D}_{mh}$. There is another subgroup of index 2 in the group $\mathscr{D}_{md}$. It is denoted by $\mathscr{S}_{2m}$ and it is generated by the rotation-reflection. The relations among these four symmetry types can be easily observed in Fig. 1, where examples of polyhedra with the symmetry groups $\mathscr{D}_{7h}$, $\mathscr{D}_{7d}$, $\mathscr{D}_7$, and $\mathscr{S}_{14}$ are depicted.

The well-known Steinitz Theorem states that a connected graph G is the graph of a convex polyhedron if and only if it is planar and 3-connected. Thus, in some cases it is useful to study 3-connected planar graphs instead of convex polyhedra and not to distinguish between a convex polyhedron and the corresponding graph. Furthermore, by the theorem of Mani [11] (see also [12]), for each such graph G there is a convex polyhedron P such that the graph of P is isomorphic to G and the symmetry group of P is isomorphic to the automorphism group of G. Therefore, to give an example of a $\Gamma(5, n)$-fulleroid (Γ is either $\mathscr{D}_m$, $\mathscr{D}_{md}$, or $\mathscr{D}_{mh}$), it is sufficient to find a 3-connected cubic planar graph with pentagonal and n-gonal faces whose automorphism group is isomorphic to Γ. Usually, we draw the graph on the surface of regular prism or bipyramid.

2. Operations used to generate examples

To prove that for some number n and for some group Γ ($\mathscr{D}_m$, $\mathscr{D}_{md}$, or $\mathscr{D}_{mh}$) the set of all $\Gamma(5, n)$-fulleroids is infinite, it is sufficient to find an infinite series of corresponding graphs. This can be done by finding one example and a method of creating a new example from the old one.

If the size n of some faces should be increased, two operations are used. If two n-gons are connected by an edge, by inserting 10 pentagons they are changed to $(n + 5)$-gons (see Fig. 2). This step can be carried out arbitrarily many times, so the size of these two faces can be increased by any multiple of 5. When this operation is used later in the paper, it is represented by a rectangle with a number inscribed which denotes the number of edges added to the two adjacent n-gons (see e.g. Fig. 8), or alternatively its application is indicated only by thickening the edges (see e.g. Fig. 11).

If two m-gons (pentagons or n-gons) are separated by two faces in a position as in the left-hand side picture in Fig. 3, the sizes of those faces can be increased equally and arbitrarily (see the right-hand side picture in Fig. 3).

As a special case of the second operation we get the following: If the two original (m-gonal) faces are pentagons, we can change them into two n-gons and $2n - 8$ new pentagons, so the number of n-gonal faces can be increased by two. For $n \geq 8$ this step can be repeated as many times as required, because two pentagons in an appropriate position can be found among the new pentagons again. The new configuration can always be chosen in such a way that possible local symmetry (rotation through 180°) is not destroyed. In the figures used in this paper, the two pentagons that can be used this way to