Symmetry of Fulleroids

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Chapter 1

Symmetry of Fulleroids

One of the important features of the structure of molecules is the presence of symmetry elements. Symmetry arguments can e.g. tell us whether the molecule is chiral and so it could be optically active. Structure of the symmetry group of a molecule affects several spectroscopic aspects and vice-versa. Thus, it is clearly important to know the possible symmetries of fullerenes and similar structures.

In this chapter, we study symmetry groups of fulleroids. In the most general manner, a *fulleroid* can be viewed as a cubic (i.e. 3-valent) convex polytope with all faces of size at least five. This definition is a natural generalization of the notion of fullerenes.

Fulleroids can also be represented by planar graphs. In the first section, we recall the basic definitions and properties of convex polyhedra and planar graphs. In the second section, we mention connections between symmetries of convex polyhedra and automorphisms of planar graphs, which allow us not to distinguish between a polyhedron with its symmetry group and a graph with its automorphism group.

In the third section, all groups that can act as symmetry groups of convex polyhedra are listed and described. For each such group, its symmetry elements are listed in a table, and a few more information is then mentioned in the text. We also provide examples and constructions of polyhedra and/or their graphs with particular symmetry groups.

The fourth section gives basic relations between rotational symmetries and faces sizes of fulleroids, which imply some easy to see necessary conditions on face sizes for the existence of fulleroids with particular symmetry groups.

The fifth section brings a brief overview of results concerning symmetries of fullerenes. One can find a list of all possible fullerene symmetry groups and counts of vertices of the smallest representatives of them.

In the next two sections, we study fulleroids with icosahedral symmetry and fulleroids with the symmetry group being a subgroup of an icosahedral group. We provide constructions of fulleroids with icosahedral symmetry group with pentagonal and n-gonal faces only for each $n \geq 7$. We also mention constructions, which assure that there are infinitely many such structures for each $n \geq 7$. It turns out that for subgroups of the icosahedral group $\mathscr{I}_h$, one can find examples of fulleroids with any faces sizes.

In the next section, we study symmetry of fulleroids with multi-pentagonal faces. We use tools from both algebra and geometry to prove nonexistence of fulleroids for the seven groups. Therefore, for the remaining seven groups without local constrains, there are values of integer n such that the corresponding fulleroids with pentagonal and n-gonal faces do not exist.

In the ninth section, we complete the characterization of symmetry of fulleroids by listing the results concerning fulleroids with octahedral, prismatic, or pyramidal symmetry.

In the last section of this chapter, we focus on fulleroids with pentagonal and heptagonal faces and their symmetry. We list all possible symmetry groups and for each of them, we provide examples with minimal number of vertices.

1.1 Convex polyhedra and planar graphs

Fullerene-like molecules are often represented by convex polyhedra, where the atoms are placed in the vertices of a polyhedron, whereas the bonds among atoms are realized along the edges of the polyhedron. Combinatorial structure of convex polyhedra can be represented by planar graphs. A *graph* is a pair $G = (V, E)$ of finite sets such that the elements of E are 2-element subsets of V. The elements of V are the *vertices* of the graph G, the elements of E are its *edges*.

A graph G is *planar*, if it can be represented in the 2-dimensional plane $\mathbb{R}^2$ in such a way that vertices of G are distinct points in $\mathbb{R}^2$, edges of G are arcs between the vertices, such that different edges have different sets of endpoints and the interior of an edge contains no vertex and no point of any other edge. Such representation is called *drawing* or *planar embedding* of G. For every drawing of a graph G, the regions of $\mathbb{R}^2 \setminus G$ are the *faces* of G. One of the faces is always unbounded – the *outer* face; the other faces are its *inner* faces.

Given a convex polyhedron P, the vertices and the edges of P form a graph, called the *graph of* P and denoted by $G(P)$. One can find a planar drawing of $G(P)$ by projecting P into a face f of P. Such drawing of the graph $G(P)$ of a convex polyhedron P is also called the *Schlegel diagram* of P. Any face of P can be chosen to be the outer face in the diagram.

A graph G is *polyhedral* if it is (isomorphic to) a graph of some convex polyhedron. For every convex polyhedron P, the graph $G(P)$ is planar and 3-connected. On the other hand, these conditions are also sufficient for the graph to be polyhedral, by *Steinitz' theorem*.

Theorem 1.1 (Steinitz) *(Cromwell 1997) A graph G is polyhedral if and only if G is planar and 3-connected.*

Convex polyhedra P_1 and P_2 are *equivalent*, if the corresponding graphs $G(P_1)$ and $G(P_2)$ are isomorphic. In this case, we say P_1 and P_2 are *of the same type*.

An arbitrary planar graph can have several different drawings, with the faces of different size. Another important property of 3-connected planar graphs is given by *Whitney's theorem*.

Theorem 1.2 (Whitney) *(Diestel 1997) Any two drawings of a 3-connected graph are equivalent.*

It means that the faces (their boundaries and sizes) of a drawing of G are uniquely determined by the graph itself. Therefore, we can speak about the faces of a 3-connected planar graph without specifying its drawing. Whitney's theorem also says that each 3-connected planar graph corresponds to precisely one type of convex polyhedra. Hence, we can identify a convex polyhedron P with its graph $G(P)$; we represent the fulleroids by 3-connected planar graphs with all faces of size at least five.

To find more information about convex polyhedra, we refer the reader to the books (Cromwell 1997) and (Grünbaum 2003). The recommended introductory book for the graph theory is the book of Chartrand and Lesniak (1972).

1.2 Polyhedral symmetries and graph automorphisms

An *automorphism* of a graph G is an isomorphism of G onto itself. The set of all automorphisms of a graph G together with the composition operation forms the *automorphism group* of G and is denoted by $Aut(G)$. For every graph G the group $Aut(G)$ is nonempty and finite.

Symmetry is a property of a convex polyhedron which causes it to remain invariant under certain classes of transformations (such as rotation, reflection, inversion, or more abstract operations). Strictly speaking, a *symmetry* of a convex polyhedron P is an isometry of the 3-dimensional space $\mathbb{R}^3$, under which the polyhedron P remains invariant. The set of all symmetries of a convex polyhedron P together with composition operation forms the *symmetry group* of P and is denoted by $\Gamma(P)$. For every convex polyhedron P the group $\Gamma(P)$ is nonempty and finite.

If ϕ is a symmetry of a convex polyhedron P, then ϕ restricted to the vertices and edges of P is an automorphism of the graph $G(P)$. Moreover, the group $\Gamma(P)$ is (isomorphic to) a subgroup of the group $Aut(G(P))$. Stronger connection between automorphisms of polyhedral graph and symmetries of corresponding polyhedra is given by the theorem of Mani:

Theorem 1.3 (Mani) *(Mani 1971) Let G be 3-connected planar graph. Then there is a convex polyhedron P whose graph is isomorphic to G and $\Gamma(P)$ is isomorphic to $Aut(G)$.*

This theorem allows us not to distinguish between a polyhedron P with the group $\Gamma(P)$, and its graph G with the group $Aut(G)$. Therefore, to give examples of convex polyhedra with the symmetry group Γ it is sufficient to find polyhedral graphs such that $Aut(G) \cong \Gamma$.

1.3 Point symmetry groups

As mentioned above, the symmetry groups of convex polyhedra are nonempty and finite. But not all finite groups can be symmetry groups of convex polyhedra. The characterization of all the groups that act as a symmetry group of a convex polyhedron is known. The list of all such groups, their structure and properties, can be found in Cromwell (1997). Another source of general information on finite groups is the book of Coxeter and Moser (1972).

Every symmetry of a convex polyhedron P has at least one fixpoint (its centre of gravity), and this point is common for all symmetries of P. The group $\Gamma(P)$ is thus called a *point group*.

According to the number of rotational symmetry axes and their relative position all point groups can be divided into icosahedral, octahedral, tetrahedral, dihedral, skewed, pyramidal and others. The list of all groups that can act as symmetry groups of convex polyhedra is in Table 1.1.

First seven point groups ($\mathscr{I}_h$, $\mathscr{I}$, $\mathscr{O}_h$, $\mathscr{O}$, $\mathscr{T}_h$, $\mathscr{T}_d$, and $\mathscr{T}$) can be interpreted as the symmetry groups of platonic solids or their subgroups. They contain more than one axis of at least 3-fold rotation.

i) The group $\mathscr{I}_h$ is the full symmetry group of a regular icosahedron (and a regular dodecahedron). It is also the symmetry group of the most famous fullerene, the bucky-ball C_{60}. It is isomorphic to $\mathbb{A}_5 \times \mathbb{Z}_2$, where $\mathbb{A}_5$ is the group of even permutations of 5 elements.

$$\mathscr{I}_h \cong \langle\, x, y, z \mid x^2 = y^2 = z^2 = (xy)^2 = (xz)^3 = (yz)^5 = 1 \,\rangle.$$

ii) The group $\mathscr{I}$ is the group of rotations of a regular icosahedron. It is a subgroup of $\mathscr{I}_h$ of index 2 and it is isomorphic to $\mathbb{A}_5$.

$$\mathscr{I} \cong \langle\, a, b \mid a^2 = b^3 = (ab)^5 = 1 \,\rangle.$$

Group	Order	Rotations	Reflections	Inversion
$\mathscr{I}_h$	120	$6C_5, 10C_3, 15C_2$	15	yes
$\mathscr{I}$	60	$6C_5, 10C_3, 15C_2$	–	–
$\mathscr{O}_h$	48	$3C_4, 4C_3, 6C_2$	9	yes
$\mathscr{O}$	24	$3C_4, 4C_3, 6C_2$	–	–
$\mathscr{T}_d$	24	$4C_3, 3C_2$	6	–
$\mathscr{T}_h$	24	$4C_3, 3C_2$	3	yes
$\mathscr{T}$	12	$4C_3, 3C_2$	–	–
$\mathscr{D}_{nh}$	$4n$	C_n, nC_2	$n+1$	if n even
$\mathscr{D}_{nd}$	$4n$	C_n, nC_2	n	if n odd
$\mathscr{D}_n$	$2n$	C_n, nC_2	–	–
$\mathscr{S}_{2n}$	$2n$	C_n	–	if n odd
$\mathscr{C}_{nh}$	$2n$	C_n	1	if n even
$\mathscr{C}_{nv}$	$2n$	C_n	n	–
$\mathscr{C}_n$	n	C_n	–	–
$\mathscr{C}_s$	2	–	1	–
$\mathscr{C}_i$	2	–	–	yes
$\mathscr{C}_1$	1	–	–	–

Table 1.1: Point symmetry groups. Each row of the table lists one such group, its order, the number and sort of rotational symmetry axes, the number of mirror symmetry planes and presence of point inversion in the group.

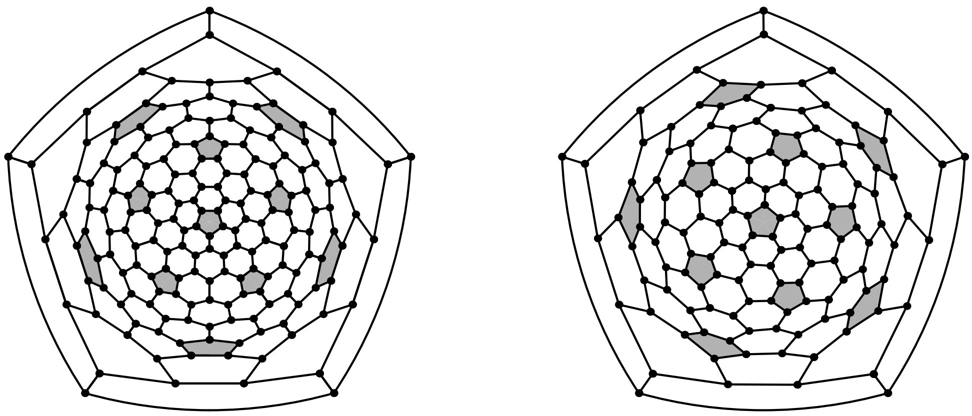

Figure 1.1: Examples of fullerenes with symmetry group $\mathscr{I}_h$ and $\mathscr{I}$, respectively. Pentagonal faces (except for the outer face) are grey.

iii) The group $\mathscr{O}_h$ is the full symmetry group of a regular octahedron (and of a cube). It is isomorphic to $S_4 \times \mathbb{Z}_2$, where S_4 is the group of all permutations of 4 elements.

$$\mathscr{O}_h \cong \langle\ x, y, z \mid x^2 = y^2 = z^2 = (xy)^2 = (xz)^3 = (yz)^4 = 1\ \rangle.$$

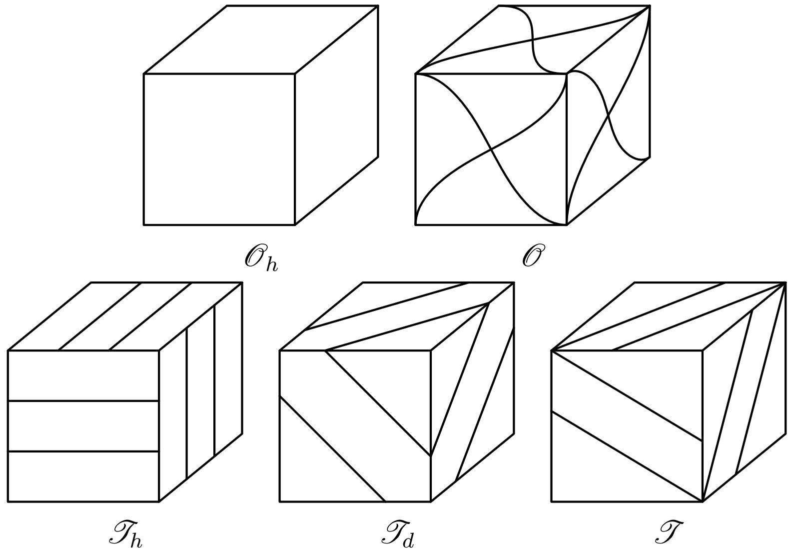

Figure 1.2: The groups $\mathscr{O}_h$, $\mathscr{O}$, $\mathscr{T}_h$, $\mathscr{T}_d$ a $\mathscr{T}$ can be represented as groups of symmetries of a cube respecting certain patterns drawn on it.

iv) The group $\mathscr{O}$ is the group of rotations of a regular octahedron. It is a subgroup of $\mathscr{O}_h$ of index 2 and it is isomorphic to S_4.

$$\mathscr{O} \cong \langle\ a, b \mid a^2 = b^3 = (ab)^4 = 1\ \rangle.$$

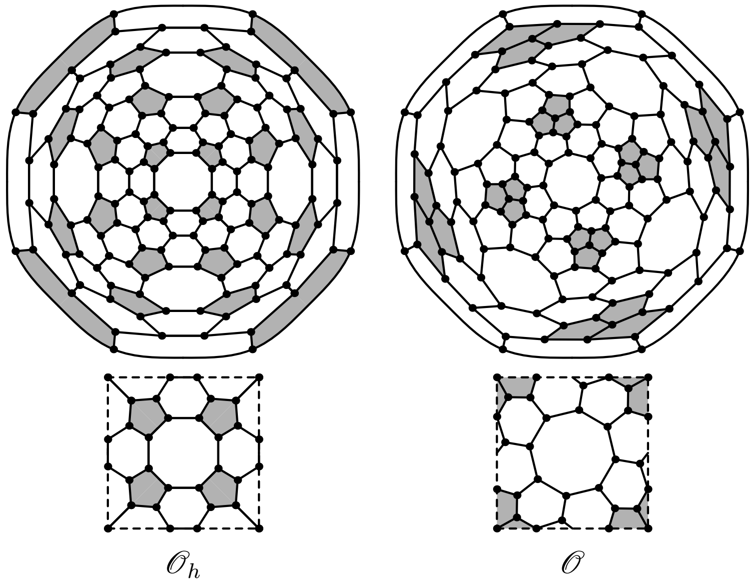

Figure 1.3: Examples of fulleroids with symmetry group $\mathscr{O}_h$ and $\mathscr{O}$, respectively, with the same number of vertices and the same number of faces of size 5, 6, and 8. Pentagonal faces are grey. To obtain the graph of the fulleroid, it suffices to draw the corresponding graph segment onto all faces of a cube.

v) The group $\mathscr{T}_h$ is the full symmetry group of a volleyball ball, or of a pyritohedron. It is a subgroup of both $\mathscr{O}_h$ and $\mathscr{I}_h$ and is a supergroup of $\mathscr{T}$. It is isomorphic to $\mathbb{A}_4 \times \mathbb{Z}_2$, where $\mathbb{A}_4$ is the group of even permutations of 4 elements.

$$\mathscr{T}_h \cong \langle\ a, b \mid a^2 = b^3 = (abab^{-1})^2 = 1\ \rangle.$$

vi) The group $\mathscr{T}_d$ is the full symmetry group of a regular tetrahedron. It is a subgroup of $\mathscr{O}_h$ and it is isomorphic to S_4 (and $\mathscr{O}$ indeed).

$$\mathscr{T}_d \cong\ \langle x, y, z \mid x^2 = y^2 = z^2 = (xy)^2 = (xz)^3 = (yz)^3 = 1\ \rangle.$$

vii) The group $\mathscr{T}$ is the group of rotations of a regular tetrahedron. It is a subgroup of index 2 of both $\mathscr{T}_h$ and $\mathscr{T}_d$ and it is isomorphic to $\mathbb{A}_4$.

$$\mathscr{T} \cong\ \langle a, b \mid a^2 = b^3 = (ab)^3 = 1\ \rangle.$$

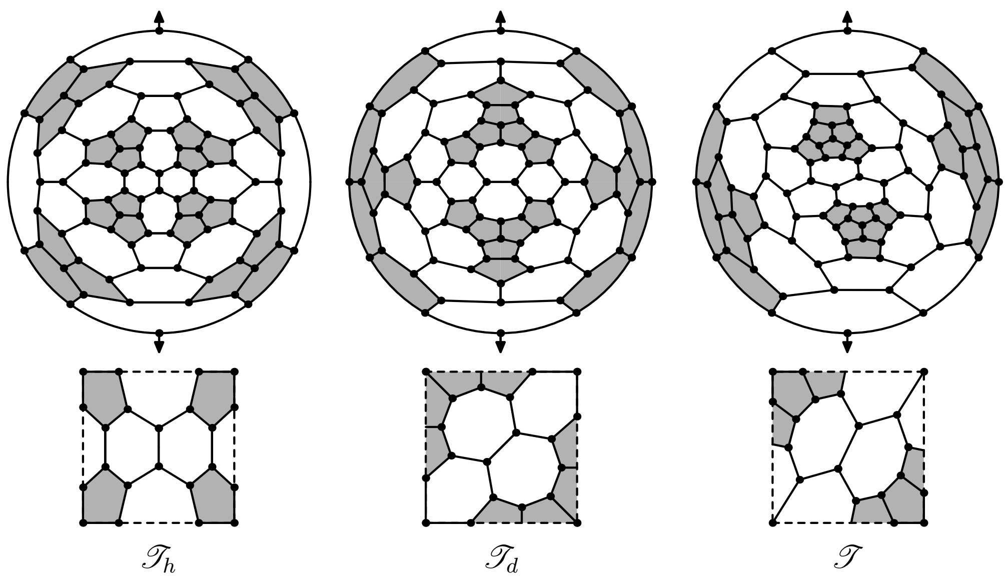

Figure 1.4: Examples of fulleroids with symmetry group $\mathscr{T}_h$, $\mathscr{T}_d$, and $\mathscr{T}$, respectively, with the same number of vertices and the same number of faces of size 5, 6, and 7. Pentagonal faces are grey. To obtain the graph of the fulleroid, it suffices to draw the corresponding graph segment onto all faces of a cube.

Next seven infinite series of groups ($\mathscr{D}_{nh}$, $\mathscr{D}_{nd}$, $\mathscr{D}_n$, $\mathscr{S}_{2n}$, $\mathscr{C}_{nh}$, $\mathscr{C}_{nv}$, and $\mathscr{C}_n$) can be interpreted as symmetry groups of regular prisms or antiprisms or their subgroups.

i) $\mathscr{D}_{mh}$ – full symmetry group of a regular m-sided prism. For m even it is isomorphic to

$D_m \times \mathbb{Z}_2$, for m odd it is isomorphic to D_{2m}. (Here D_k denotes the dihedral group of $2k$ elements.)

ii) $\mathscr{D}_{md}$ – full symmetry group of a regular m-sided antiprism. It is isomorphic to D_{2m}.

iii) $\mathscr{D}_m$ – group of rotations of a regular m-sided prism. It is isomorphic to D_m and is a subroup of index 2 of both $\mathscr{D}_{mh}$ and $\mathscr{D}_{md}$.

iv) $\mathscr{S}_{2m}$ – cyclic group generated by improper rotation (glide) for $\frac{360°}{2m}$ about vertical axis. It is isomorphic to $\mathbb{Z}_{2m}$ and is a subgroup of index 2 of $\mathscr{D}_{md}$.

v) $\mathscr{C}_{mh}$ – group generated by a rotation for $\frac{360°}{m}$ about vertical axis and a reflexion about

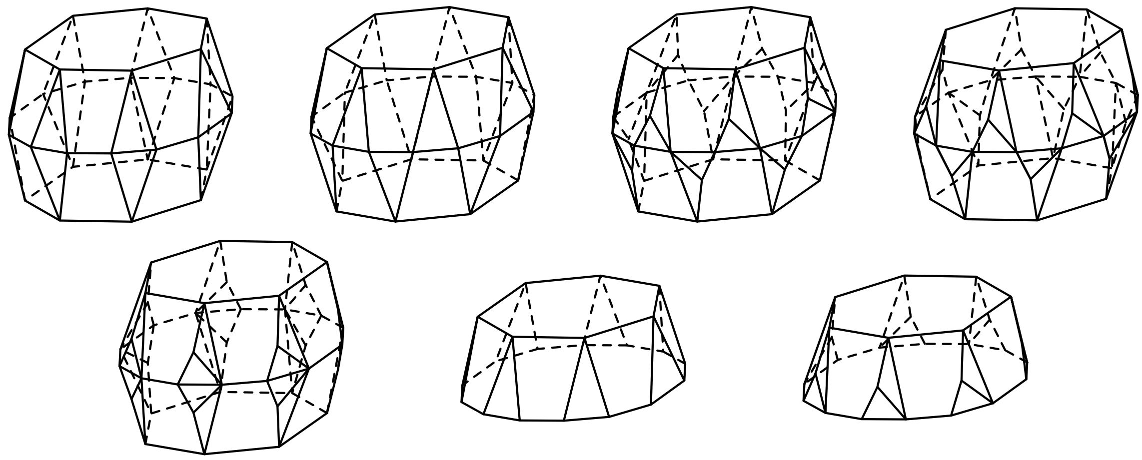

Figure 1.5: Examples of polyhedra with symmetry groups $\mathscr{D}_{7h}$, $\mathscr{D}_{7d}$, $\mathscr{D}_7$, $\mathscr{S}_{14}$, $\mathscr{C}_{7h}$, $\mathscr{C}_{7v}$, and $\mathscr{C}_7$, respectively.

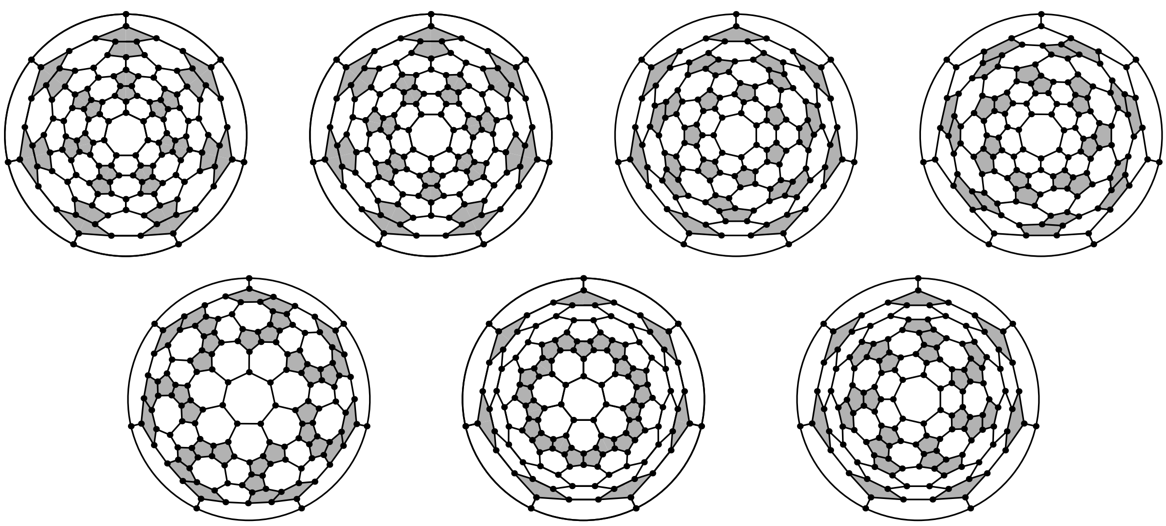

Figure 1.6: Examples of fulleroids with symmetry groups $\mathscr{D}_{7h}$, $\mathscr{D}_{7d}$, $\mathscr{D}_7$, $\mathscr{S}_{14}$, $\mathscr{C}_{7h}$, $\mathscr{C}_{7v}$, and $\mathscr{C}_7$, respectively.

a vertical plane. It is isomorphic to $\mathbb{Z}_m \times \mathbb{Z}_2$ and is a subgroup of index 2 of $\mathscr{D}_{mh}$.

vi) $\mathscr{C}_{mv}$ – full group of symmetries of a regular m-sided pyramid. It is isomorphic to D_n and is a subgroup of index 2 of both $\mathscr{D}_{mh}$ and $\mathscr{D}_{md}$.

vii) $\mathscr{C}_m$ – group of rotations of a regular m-sided pyramid. It is isomorphic to $\mathbb{Z}_m$ and is a subgroup of all groups listed above.

The remaining three groups are the groups of low symmetry.

i) The group C_s contains a mirror reflection and an identity.

ii) The group C_i contains a point inversion and an identity.

iii) The group C_1 contains only an identity.

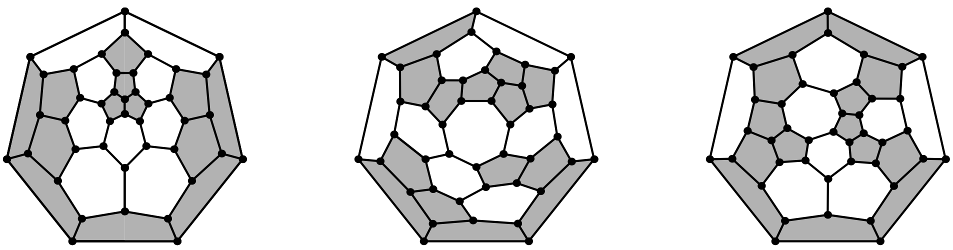

Figure 1.7: Examples of fulleroids with symmetry groups $\mathscr{C}_s$, $\mathscr{C}_i$, and $\mathscr{C}_1$, respectively.

1.4 Local restrictions

In general, the presence of rotational symmetry axes in the symmetry group implies a local rotational symmetry of the sites where the axes intersects the polyhedron:

Lemma 1.1 *Let P be a fulleroid. If an axis of an m-fold rotation intersects a face of size n, then m divides n. If an axis of an m-fold rotation intersects a vertex of P, then $m = 3$. If an axis of an m-fold rotation intersects an edge of P, then $m = 2$.*

These connections, together with the fact that every fulleroid has at least 12 faces of degree 5, give us necessary conditions for the face sizes of fulleroids with given symmetry group. If the symmetry group of a fulleroid P contains an m-fold rotational axis, where $m \neq 2, 3, 5$, then P must have faces of size n, where m divides n.

1.5 Symmetry of fullerenes

In the special case of fullerenes, there are only pentagonal and hexagonal faces. Therefore, by Lemma 1.1 the fullerene symmetry group can contain axes of m-fold rotation only for $m = 2, 3, 5$ and 6. This makes the list of possible symmetry groups be finite; it consist of 36 groups:

$$\begin{array}{l} \mathscr{I}_h, \mathscr{I}, \mathscr{T}_h, \mathscr{T}_d, \mathscr{T}, \\ \mathscr{D}_{6h}, \mathscr{D}_{6d}, \mathscr{D}_6, \mathscr{S}_{12}, \mathscr{C}_{6h}, \mathscr{C}_{6v}, \mathscr{C}_6, \\ \mathscr{D}_{5h}, \mathscr{D}_{5d}, \mathscr{D}_5, \mathscr{S}_{10}, \mathscr{C}_{5h}, \mathscr{C}_{5v}, \mathscr{C}_5, \\ \mathscr{D}_{3h}, \mathscr{D}_{3d}, \mathscr{D}_3, \mathscr{S}_6, \mathscr{C}_{3h}, \mathscr{C}_{3v}, \mathscr{C}_3, \\ \mathscr{D}_{2h}, \mathscr{D}_{2d}, \mathscr{D}_2, \mathscr{S}_4, \mathscr{C}_{2h}, \mathscr{C}_{2v}, \mathscr{C}_2, \\ \mathscr{C}_s, \mathscr{C}_i, \mathscr{C}_1. \end{array}$$

Using more detailed consideration it was proved that whenever a 5-fold or 6-fold rotational axis is present, the structure of the fullerene implies a perpendicular 2-fold rotational axis (Fowler et al. 1993). This means that the groups $\mathscr{S}_{12}, \mathscr{C}_{6h}, \mathscr{C}_{6v}$, and $\mathscr{C}_6$ only occur as subgroups of dihedral groups $\mathscr{D}_{6h}, \mathscr{D}_{6d}$, and $\mathscr{D}_6$; as the groups $\mathscr{S}_{10}, \mathscr{C}_{5h}, \mathscr{C}_{5v}$, and $\mathscr{C}_5$ only occur as subgroups of isosahedral or dihedral groups $\mathscr{I}_h, \mathscr{I}, \mathscr{D}_{5h}, \mathscr{D}_{5d}$, and $\mathscr{D}_5$. The final list of 28 fullerene symmetry groups is therefore:

$$\begin{array}{l} \mathscr{I}_h, \mathscr{I}, \mathscr{T}_h, \mathscr{T}_d, \mathscr{T}, \\ \mathscr{D}_{6h}, \mathscr{D}_{6d}, \mathscr{D}_6, \\ \mathscr{D}_{5h}, \mathscr{D}_{5d}, \mathscr{D}_5, \\ \mathscr{D}_{3h}, \mathscr{D}_{3d}, \mathscr{D}_3, \mathscr{S}_6, \mathscr{C}_{3h}, \mathscr{C}_{3v}, \mathscr{C}_3, \\ \mathscr{D}_{2h}, \mathscr{D}_{2d}, \mathscr{D}_2, \mathscr{S}_4, \mathscr{C}_{2h}, \mathscr{C}_{2v}, \mathscr{C}_2, \\ \mathscr{C}_s, \mathscr{C}_i, \mathscr{C}_1. \end{array}$$

As we will see in the next sections, this is the only case where realizability of a symmetry group is not transferred onto its subgroups.

For each of the 28 fullerene symmetry groups, the smallest examples are known (Fowler and Manolopoulos 1995). The number of vertices of them is listed in Table 1.2.

$\mathscr{I}_h$	$\mathscr{I}$	$\mathscr{T}_h$	$\mathscr{T}_d$	$\mathscr{T}$	$\mathscr{D}_{6h}$	$\mathscr{D}_{6d}$	$\mathscr{D}_6$	$\mathscr{D}_{5h}$	$\mathscr{D}_{5d}$	$\mathscr{D}_5$	$\mathscr{D}_{3h}$	$\mathscr{D}_{3d}$	$\mathscr{D}_3$
60	140	92	28	44	36	24	72	30	40	60	26	32	32
$\mathscr{S}_6$	$\mathscr{C}_{3h}$	$\mathscr{C}_{3v}$	$\mathscr{C}_3$	$\mathscr{D}_{2h}$	$\mathscr{D}_{2d}$	$\mathscr{D}_2$	$\mathscr{S}_4$	$\mathscr{C}_{2h}$	$\mathscr{C}_{2v}$	$\mathscr{C}_2$	$\mathscr{C}_s$	$\mathscr{C}_i$	$\mathscr{C}_1$
68	62	34	40	40	36	28	44	48	30	32	34	56	36

Table 1.2: The counts of vertices of the smallest representatives of 28 fullerene symmetry groups.

1.6 Icosahedral fulleroids

It was Fowler who first asked whether there is fullerene-like structure consisting of pentagons and heptagons only and exhibiting icosahedral symmetry. The answer came immediately, when Brinkmann and Dress (1996) found two such structures with a minimal possible number of vertices and proved that there are only two of them. They also defined $\Gamma(a,b)$-fulleroid to be a fulleroid with only a-gonal and b-gonal faces, on which the group Γ acts as a group of symmetries. Delgado Friedrichs and Deza (2000) found more icosahedral fulleroids with pentagonal and n-gonal faces for $n = 8, 9, 10, 12, 14$, and 15. Jendrol' and Trenkler (2001) constructed $\mathscr{I}(5,n)$-fulleroids for all $n \geq 8$.

The properties and structure of two-faces maps (including fulleroids) are studied in the book of Deza and Dutour Sikirić (2008).

The results (Brinkmann and Dress 1996; Delgado Friedrichs and Deza 2000; Jendrol' and Trenkler 2001) are all concerned with the group $\mathscr{I}$. But the largest fullerene symmetry group is $\mathscr{I}_h$, hence we focus now on $\mathscr{I}_h(5,n)$-fulleroids.

Theorem 1.4 *For any $n \geq 6$ there are infinitely many $\mathscr{I}_h(5,n)$-fulleroids.*

Proof. For $n = 6$ we get the case of $\mathscr{I}_h$-fullerenes, which are completely characterized in the catalogue of Graver (2005). They can be divided into two infinite series.

To depict an $\mathscr{I}_h(5,n)$-fulleroid, it is not necessary to draw whole its graph. If we cut the regular dodecahedron D along all its mirror planes, it falls into 120 congruent triangular pieces, called *flags*. The flags have the shape of a right triangle ABC with $|BC| < |AB| < |AC|$, where A (B, resp. C) represents the point where the 5-fold (2-fold, resp. 3-fold) rotational axis intersects the polyhedron – the face centre, the egde midpoint, and the vertex of D.

If a graph is drawn onto one flag and it is copied onto all other flags, altogether we get a graph with the automorphism group isomorphic to $\mathscr{I}_h$. If this graph is cubic, planar, and 3-connected, with all faces of size at least 5, we get an example of a graph of an $\mathscr{I}_h$-fulleroid.

For $n = 7$, examples of $\mathscr{I}_h(5,7)$-fulleroids are obtained, if the graphs from Figure 1.8 are used this way.

To prove there are infinitely many $\mathscr{I}_h(5,7)$-fulleroids, one can search for a configuration of four pentagons (see Figure 1.9, left) and change them into two heptagons and six pentagons (in every flag). Since there is such a configuration again, the operation can be carried out arbitrarily many times.

Examples of $\mathscr{I}_h(5,n)$-fulleroids for $n = 8, 9 \ldots 17$ are obtained, if the graphs from Figure 1.10 and Figure 1.11 are drawn into all the flags of a regular dodecahedron.

Figure 1.8: The segments of the graph of the smallest $\mathscr{I}_h(5,7)$-fulleroid and another $\mathscr{I}_h(5,7)$-fulleroid.

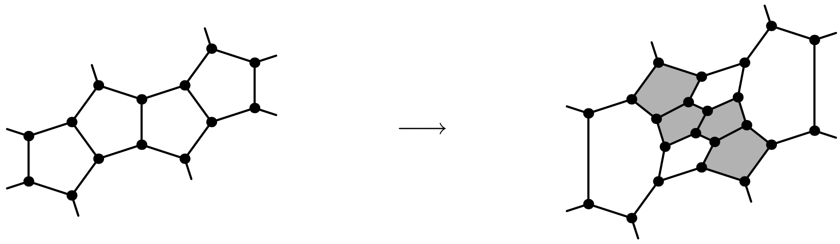

Figure 1.9: The step to create two new heptagons.

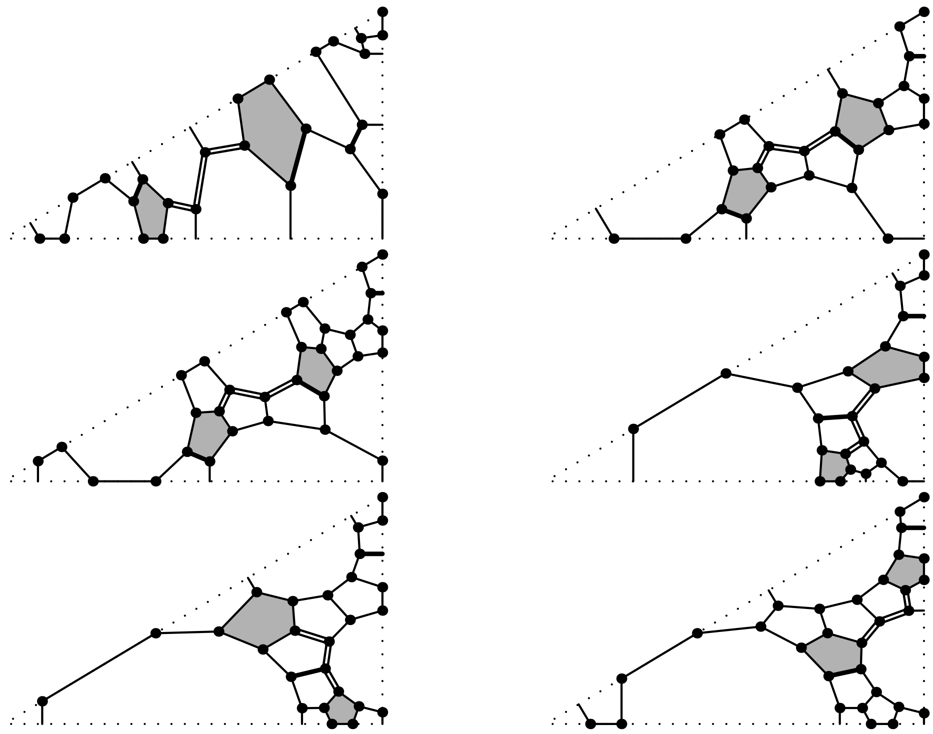

Figure 1.10: The segments of the graphs of $\mathscr{I}_h(5,n)$-fulleroids for $n = 8+10k$, $9+10k$, $10+10k$, $11+10k$, $12+10k$, and $13+10k$.

To prove that for some number n the set of all $\mathscr{I}_h(5,n)$-fulleroids is infinite it is sufficient to find an infinite series of corresponding graphs. We start with an example of fulleroid with pentagonal and m-gonal faces, where $m \in \{8, 9, \ldots 17\}$ such that 10 divides $n - m$, e.g. some of those in Figures 1.10 and 1.11. We first change all the m-gonal faces to n-gons and then

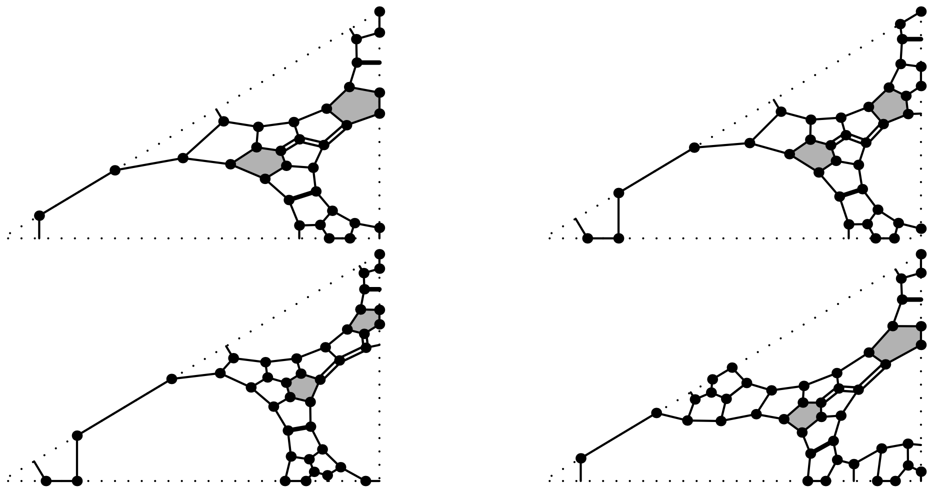

Figure 1.11: The segments of the graphs of $\mathscr{I}_h(5,n)$-fulleroids for $n = 14+10k$, $15+10k$, $16+10k$, and $17+10k$.

increase the number of them.

If the size m of some faces should be increased, two operations can be used. If two m-gons are connected by an edge, by inserting 10 pentagons they are changed to $(m+5)$-gons (see Figure 1.12 for illustration). This step can be carried out arbitrarily many times, so the size of those two faces can be increased by any multiple of 5. In the Figures 1.10 and 1.11, the application of this operation is indicated by thickening the edges.

Figure 1.12: The step to increase the size of two m-gons by 5.

If two m-gons are separated by two faces in the position like in Figure 1.13, left, the size of those faces can be increased arbitrarily (see Figure 1.13, right).

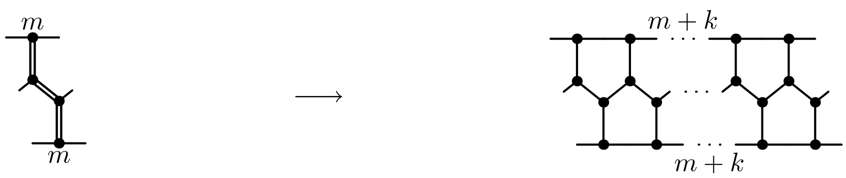

Figure 1.13: The step to increase the size of two m-gons arbitrarily.

As a special case of the second operation we get the following: If original two 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 apropriate position can be found among the new pentagons again. The two pentagons, that can be used this way to create infinitely many examples, are in Figures 1.10 and 1.11 shaded grey and the edges connecting them are doubled. □

It is worth to note that given integers $5 < n_1 < n_2 < \cdots < n_k$, we can make an $\mathscr{I}_h$-fulleroid with faces of sizes 5, n_1, $n_2, \ldots, n_k$ if we start with graph segments from Figures 1.8, 1.10, and 1.11 and use the operations from Figures 1.9, 1.12, and 1.13.

1.7 Subgroups of $\mathscr{I}_h$

In the previous section we proved that there are infinitely many $\mathscr{I}_h(5, n)$-fulleroids for any $n \geq 7$. It is natural to ask for which groups Γ there are infinitely many $\Gamma(5, n)$-fulleroids for any $n \geq 7$.

It is clear that such groups can only contain m-fold rotational axis for $m = 2, 3$, and 5. Therefore, the list of candidates is finite and it is possible to check them one by one. In particular, we get the following 29 groups:

$$\begin{aligned}
&\mathscr{I}_h, \mathscr{I}, \mathscr{T}_h, \mathscr{T}_d, \mathscr{T}, \\
&\mathscr{D}_{5h}, \mathscr{D}_{5d}, \mathscr{D}_5, \mathscr{S}_{10}, \mathscr{C}_{5h}, \mathscr{C}_{5v}, \mathscr{C}_5, \\
&\mathscr{D}_{3h}, \mathscr{D}_{3d}, \mathscr{D}_3, \mathscr{S}_6, \mathscr{C}_{3h}, \mathscr{C}_{3v}, \mathscr{C}_3, \\
&\mathscr{D}_{2h}, \mathscr{D}_{2d}, \mathscr{D}_2, \mathscr{S}_4, \mathscr{C}_{2h}, \mathscr{C}_{2v}, \mathscr{C}_2, \\
&\mathscr{C}_s, \mathscr{C}_i, \mathscr{C}_1.
\end{aligned}$$

Proposition 1.5 *Let Γ be a symmetry group that is a subgroup of the group $\mathscr{I}_h$. Then there are infinitely many $\Gamma(5, n)$-fulleroids for any $n \geq 7$.*

Proof. Since Γ is a subgroup of $\mathscr{I}_h$, it has an action on the set of flags of regular dodecahedron D. Under this action, all 120 flags of D split into $120/|\Gamma|$ orbits, each containing $|\Gamma|$ flags. (Here $|\Gamma|$ denotes the order, i.e. the number of elements of the group Γ.) If we start with an $\mathscr{I}_h$-fulleroid and change the graph in the flags forming one orbit under Γ in such a way that no new symmetries arise, we obtain a Γ-fulleroid. We can use the examples of $\mathscr{I}_h(5, n)$-fulleroids described in the proof of Theorem 1.4 to obtain infinite series of $\Gamma(5, n)$-fulleroids for all $n \geq 7$ and all subgroups Γ of $\mathscr{I}_h$. □

This answers the question of existence of $\Gamma(5, n)$-fulleroids for arbitrary $n \geq 7$ for 22 subgroups of $\mathscr{I}_h$:

$$\begin{aligned}&\mathscr{I}_h, \mathscr{I}, \mathscr{T}_h, \mathscr{T},\\ &\mathscr{D}_{5d}, \mathscr{D}_5, \mathscr{S}_{10}, \mathscr{C}_{5v}, \mathscr{C}_5,\\ &\mathscr{D}_{3d}, \mathscr{D}_3, \mathscr{S}_6, \mathscr{C}_{3v}, \mathscr{C}_3,\\ &\mathscr{D}_{2h}, \mathscr{D}_2, \mathscr{C}_{2h}, \mathscr{C}_{2v}, \mathscr{C}_2,\\ &\mathscr{C}_s, \mathscr{C}_i, \mathscr{C}_1.\end{aligned}$$

As we will conclude later, the condition of being subgroup of $\mathscr{I}_h$ is not only sufficient for the existence of $\Gamma(5, n)$-fulleroid for arbitrary $n \geq 7$, but it is also a necessary condition.

Different constructions of tetrahedral fulleroids can be also found in Kardoš 2007b.

For the remaining 7 groups, $\mathscr{T}_d, \mathscr{D}_{5h}, \mathscr{C}_{5h}, \mathscr{D}_{3h}, \mathscr{C}_{3h}, \mathscr{D}_{2d}$, and $\mathscr{S}_4$, there are values of integer n such that corresponding fulleroids do not exist. All those cases of nonexistence fall within fulleroids with multi-pentagonal faces.

1.8 Fulleroids with multi-pentagonal faces

A face is *multi-pentagonal*, if its size is a multiple of 5. Fulleroids with multi-pentagonal faces play a special role among others, because they can be mapped onto (a graph of) a regular dodecahedron:

Lemma 1.2 *(Jendrol' and Kardoš 2007) Let P be a cubic convex polyhedron such that all faces are multi-pentagons, i.e. the size of each face is a multiple of five. Then there exists an orientation-preserving homomorphism $\Psi: P \to D$, where D denotes a regular dodecahedron.*

By orientation-preserving homomorphism $\Psi: P \to D$ we mean a map from the set $V(P)$ of vertices of the polyhedron P into the set $V(D)$, respecting the adjacency structure, which also preserves the order of the vertices incident with any vertex (up to a cyclic permutation) once an orientation has been assigned to both P and D before.

Lemma 1.3 *(Kardoš 2007a) Let P be a cubic convex polyhedron such that all its faces are multi-pentagons and let $\Psi: P \to D$ be an orientation-preserving homomorphism, where D denotes a regular dodecahedron. If $\varphi \in \Gamma(P)$ is a symmetry of P, then $\Psi \circ \varphi : P \to D$ is also an orientation-preserving homomorphism, moreover, the symmetry φ of P uniquely determines a symmetry $\overline{\Psi}(\varphi)$ of D once Ψ is fixed.*

Theorem 1.6 *(Kardoš 2007a) Let P be a cubic convex polyhedron such that all its faces are multi-pentagons. Then there exists a homomorphism $\overline{\Psi} : \Gamma(P) \to \mathscr{I}_h$, where $\Gamma(P)$ is the symmetry group of P and $\mathscr{I}_h$ denotes the symmetry group of a regular dodecahedron D.*

This theorem is a special case of a result of Malnič et al. (2002) concerning map homomorphisms into regular maps:

Theorem 1.7 *(Malnič, Nedela, and Škoviera 2002) If* $\Psi : N \to M$ *is a map homomorphism with* M *regular, then* $Aut(N)$ *projects.*

The homomorphism $\overline{\Psi} : \Gamma(P) \to \mathscr{I}_h$ is a strong tool for proving nonexistence of fulleroids with multi-pentagonal faces and with symmetry groups which are not subgroups of $\mathscr{I}_h$.

Proposition 1.8 *Let* P *be a cubic convex polyhedron such that the sizes of all its faces are* odd *multiples of five. Then the symmetry group* $\Gamma(P)$ *does not contain the group* $\mathscr{S}_4$ *as a subgroup.*

Proof. Let P be a convex polyhedron satisfying the premise of the claim and let φ be the rotation-reflection that generates $\mathscr{S}_4$ in $\Gamma(P)$. Since all the face sizes are odd, the rotation axis of φ intersects P in the midpoints of two edges, let one of these two edges be denoted by e. Let $e = uv$. Then $\varphi^2(u) = v$ and $\varphi^2(v) = u$. It means φ^2 maps two adjacent vertices u and v onto each other.

Let $\Psi : P \to D$ be the homomorphism given by Lemma 1.2 and $\overline{\Psi} : \Gamma(P) \to \mathscr{I}_h$ be the corresponding homomorphism given by Theorem 1.6. The rotation-reflection φ is an element of order 4 in $\Gamma(P)$. There are no elements of order 4 in $\mathscr{I}_h$, so $\overline{\Psi}(\varphi)$ can be only of order 2 or 1, what implies $\overline{\Psi}(\varphi^2) = \overline{\Psi}(\varphi)^2 = id$. The vertices u and v are adjacent, hence so are the vertices $\Psi(u)$ and $\Psi(v)$. On the other hand,

$$\Psi(v) = \Psi(\varphi^2(u)) = \overline{\Psi}(\varphi^2)(\Psi(u)) = id(\Psi(u)) = \Psi(u),$$

what is a contradiction. □

Corollary 1.9 *There is no fulleroid* P *such that the sizes of all its faces are odd multiples of five with the symmetry group* $\mathscr{S}_4$, $\mathscr{D}_{2d}$, *or* $\mathscr{T}_d$.

Proof. It immediately follows from Proposition 1.8, since $\mathscr{S}_4$ is a subgroup of both $\mathscr{D}_{2d}$ and $\mathscr{T}_d$. □

Proposition 1.10 *Let* P *be a cubic convex polyhedron such that all its faces are multi-pentagons and none of the face sizes is divisible by three. Then the symmetry group* $\Gamma(P)$ *does not contain the group* $\mathscr{C}_{3h}$ *as a subgroup.*

Proof. Let P be a convex polyhedron satisfying the premise of the claim and let ρ and θ be the rotation and the reflection that generate $\mathscr{C}_{3h}$ in $\Gamma(P)$. Since no face of P has the size divisible by three, the rotation axis of ρ intersects P in two vertices, let one of those vertices be denoted by v. Let the neighbours of v be denoted by v_1, v_2, v_3 in such a way that $\rho(v_1) = v_2$, $\rho(v_2) = v_3$, and $\rho(v_3) = v_1$.

Let $\Psi : P \to D$ be the homomorphism given by Lemma 1.2 and $\overline{\Psi} : \Gamma(P) \to \mathscr{I}_h$ be the corresponding homomorphism given by Theorem 1.6. The rotation ρ is an element of order 3 in $\Gamma(P)$.

If $\overline{\Psi}(\rho) = id$, then $\Psi(v_2) = \Psi(\rho(v_1)) = \overline{\Psi}(\rho)(\Psi(v_1)) = \Psi(v_1)$. But $\Psi : P \to D$ maps distinct neighbours of v onto distinct ones, a contradiction. Hence $\mathrm{ord}(\overline{\Psi}(\rho)) = 3$, what implies $\overline{\Psi}(\rho)$ is a rotation by $\pm 120°$.

We know that θ is orientation-reversing symmetry of P and $\mathrm{ord}(\theta) = 2$, so $\overline{\Psi}(\theta)$ must be an orientation-reversing element of $\mathscr{I}_h$ such that $\mathrm{ord}(\overline{\Psi}(\theta)) \leq 2$. The reflection θ has at least one fixpoint on the surface of P (midpoints of edges intersected by the mirror plane), thus also $\overline{\Psi}(\theta)$ must have at least one fixpoint on the surface of D, indeed it can not be a point inversion. So $\overline{\Psi}(\theta)$ it is a reflection.

In P, the mirror plane corresponding to θ is perpendicular to the rotational axis of ρ. Moreover, $\rho \circ \theta = \theta \circ \rho$ and the subgroup $\mathscr{C}_{3h}$ of $\Gamma(P)$ generated by ρ and θ is commutative. What is the relative position of $\overline{\Psi}(\rho)$ and $\overline{\Psi}(\theta)$? There is no mirror plane of D perpedicular to any of its 3-fold rotational symmetry axis. Moreover, if a 3-fold rotational axis $\overline{\Psi}(\rho)$ is chosen, a mirror plane of D together with $\overline{\Psi}(\rho)$ generate either a non-commutative subgroup of $\mathscr{I}_h$ with 6 elements (the group $\mathscr{C}_{3v}$, if the mirror plane contains the axis), or the whole group $\mathscr{I}_h$ (otherwise), what is a contradiction. □

Corollary 1.11 *There is no fulleroid P such that all its faces are multi-pentagons, none of the face sizes is divisible by three, and the symmetry group of P is $\mathscr{C}_{3h}$ or $\mathscr{D}_{3h}$.*

Proof. It immediately follows from Proposition 1.10, since $\mathscr{C}_{3h}$ is a subgroup of $\mathscr{D}_{3h}$. □

Proposition 1.12 *Let P be a cubic convex polyhedron such that all its faces are multi-pentagons and none of the face sizes is divisible by 25. Then the symmetry group $\Gamma(P)$ does not contain the group $\mathscr{C}_{5h}$ as a subgroup.*

Proof. Let P be a convex polyhedron satisfying the premise of the claim and let ρ and θ be the rotation and the reflection that generate $\mathscr{C}_{5h}$ in $\Gamma(P)$. The rotation axis of ρ intersects P in two faces, let one of those faces be denoted by f. Let v be a vertex incident with f.

Let $\Psi : P \to D$ be the homomorphism given by Lemma 1.2 and $\overline{\Psi} : \Gamma(P) \to \mathscr{I}_h$ be the corresponding homomorphism given by Theorem 1.6. The rotation ρ is an element of order 5 in $\Gamma(P)$. Since no face of P has the size that is a multiple of 25, $\Psi(v)$ and $\Psi(\rho(v)) = \overline{\Psi}(\rho)(\Psi(v))$ are two distinct vertices of the face $\Psi(f)$. Thus, $\overline{\Psi}(\rho)$ is not an identity, so $\overline{\Psi}(\rho)$ is an element of order 5 in $\mathscr{I}_h$, hence $\overline{\Psi}(\rho)$ is a rotation by $\pm 72°$.

Using the same arguments like in the proof of Proposition 1.10 we get that $\overline{\Psi}(\theta)$ it is a reflection.

In P, the mirror plane corresponding to θ is perpendicular to the rotational axis of ρ. Moreover, $\rho \circ \theta = \theta \circ \rho$ and the subgroup $\mathscr{C}_{5h}$ of $\Gamma(P)$ generated by ρ and θ is commutative. What is the relative position of $\overline{\Psi}(\rho)$ and $\overline{\Psi}(\theta)$? There is no mirror plane of D perpedicular to any of its 5-fold rotational symmetry axis. Moreover, if a 5-fold rotational axis $\overline{\Psi}(\rho)$ is chosen, a mirror plane of D together with $\overline{\Psi}(\rho)$ generate either a non-commutative subgroup of $\mathscr{I}_h$ with 10 elements (the group $\mathscr{C}_{5v}$, if the mirror plane contains the axis), or the whole group $\mathscr{I}_h$ (otherwise), what is a contradiction. □

Corollary 1.13 *There is no fulleroid P such that all its faces are multi-pentagons, none of the face sizes is divisible by 25, and the symmetry group of P is $\mathscr{C}_{5h}$ or $\mathscr{D}_{5h}$.*

Proof. It immediately follows from Proposition 1.12, since $\mathscr{C}_{5h}$ is a subgroup of $\mathscr{D}_{5h}$. □

Corollaries 1.9, 1.11, and 1.13 cover all the seven groups, which are not subgroups of $\mathscr{I}_h$, even though they do not force any local restrictions. For all seven of them, there are values of n, for which there are no $\Gamma(5,n)$-fulleroids. On the other hand, for all other values of n not covered by Corollaries 1.9, 1.11, and 1.13, examples of $\Gamma(5,n)$-fulleroids can be found in Kardoš (2007a).

The results mentioned above combined with constructions in sections 1.6 and 1.7 complete the proof of the following characterization:

Theorem 1.14 *Let Γ be a point symmetry group. Then there are infinitely many $\Gamma(5,n)$-fulleroids for any $n \geq 7$ if and only if Γ is a subgroup of the group $\mathscr{I}_h$.*

1.9 Fulleroids with octahedral, prismatic, or pyramidal symmetry

There are groups which contain an m-fold rotational symmetry for $m = 4$ or $m \geq 6$. Local conditions (see Lemma 1.1) do not allow existence of $(5,n)$-fulleroids for arbitrary n — in this case n must be a multiple of m. However this necessary condition is not always also sufficient.

Octahedral symmetry groups $\mathscr{O}_h$ and $\mathscr{O}$ both contain three 4-fold rotational symmetry axes, therefore, the size of some faces must be a multiple of four.

Theorem 1.15 *(Jendrol' and Kardoš 2007) Let $n \geq 6$. There are infinitely many $\mathscr{O}_h(5,n)$-fulleroids and $\mathscr{O}(5,n)$-fulleroids if and only if (i) $n \equiv 0 \pmod{60}$ or (ii) $n \equiv 0 \pmod 4$ and $n \not\equiv 0 \pmod 5$.*

The groups $\mathscr{D}_{mh}, \mathscr{D}_{md}, \mathscr{D}_m, \mathscr{S}_{2m}, \mathscr{C}_{mh}, \mathscr{C}_{mv}$ and $\mathscr{C}_m$ contain m-fold rotational symmetry, therefore, the size of some faces must be a multiple of m.

Theorem 1.16 *(Kardoš 2007a) Let $m = 4$ or $m \geq 6$ and $n \geq 7$ be integers and let Γ be $\mathscr{D}_{md}, \mathscr{D}_m, \mathscr{S}_{2m}, \mathscr{C}_{mv}$ or $\mathscr{C}_m$. Then there are infinitely many $\Gamma(5,n)$-fulleroids if and only if n is a multiple of m.*

Theorem 1.17 *(Kardoš 2007a) Let $m = 4$ or $m \geq 6$ and $n \geq 7$ be integers and let $m \not\equiv 0 \pmod 5$. Let Γ be $\mathscr{D}_{mh}$ or $\mathscr{C}_{mh}$. Then there are infinitely many $\Gamma(5,n)$-fulleroids if and only if n is a multiple of m.*

Theorem 1.18 *(Kardoš 2007a) Let $m \geq 10$ and $n \geq 7$ be integers and let $m \equiv 0 \pmod 5$. Let Γ be $\mathscr{D}_{mh}$ or $\mathscr{C}_{mh}$. Then there are infinitely many $\Gamma(5,n)$-fulleroids if and only if n is a multiple of $5m$.*

Examples and constructions can be found in Kardoš (2007a).

1.10 $(5,7)$-fulleroids

Unlike the case of fullerenes, i.e. $(5,6)$-fulleroids, for $(5,7)$-fulleroids, all point symmetry groups that satisfy local restrictions are realizable.

For the 36 groups Γ, which do not contain m-fold rotation unless $m = 2$, 3, 5, or 7, the numbers of vertices of the smallest examples of $\Gamma(5,7)$-fulleroids are listed in Table 1.3. The examples with dihedral, skewed, pyramidal, and low symmetry are depicted in Figures 1.14–1.17.

$\mathscr{I}_h$	$\mathscr{I}$	$\mathscr{T}_h$	$\mathscr{T}_d$	$\mathscr{T}$	$\mathscr{D}_{7h}$	$\mathscr{D}_{7d}$	$\mathscr{D}_7$	$\mathscr{S}_{14}$	$\mathscr{C}_{7h}$	$\mathscr{C}_{7v}$	$\mathscr{C}_7$
500	260	116	116	68	84	28	140	196	112	112	140
$\mathscr{D}_{5h}$	$\mathscr{D}_{5d}$	$\mathscr{D}_5$	$\mathscr{S}_{10}$	$\mathscr{C}_{5h}$	$\mathscr{C}_{5v}$	$\mathscr{C}_5$	$\mathscr{D}_{3h}$	$\mathscr{D}_{3d}$	$\mathscr{D}_3$	$\mathscr{S}_6$	$\mathscr{C}_{3h}$
60	60	100	140	80	80	100	44	44	44	68	56
$\mathscr{C}_{3v}$	$\mathscr{C}_3$	$\mathscr{D}_{2h}$	$\mathscr{D}_{2d}$	$\mathscr{D}_2$	$\mathscr{S}_4$	$\mathscr{C}_{2h}$	$\mathscr{C}_{2v}$	$\mathscr{C}_2$	$\mathscr{C}_s$	$\mathscr{C}_i$	$\mathscr{C}_1$
68	68	52	36	36	52	44	44	44	44	60	52

Table 1.3: The counts of vertices of the smallest $\Gamma(5,7)$-fulleroid for all 36 possible symmetry groups Γ.

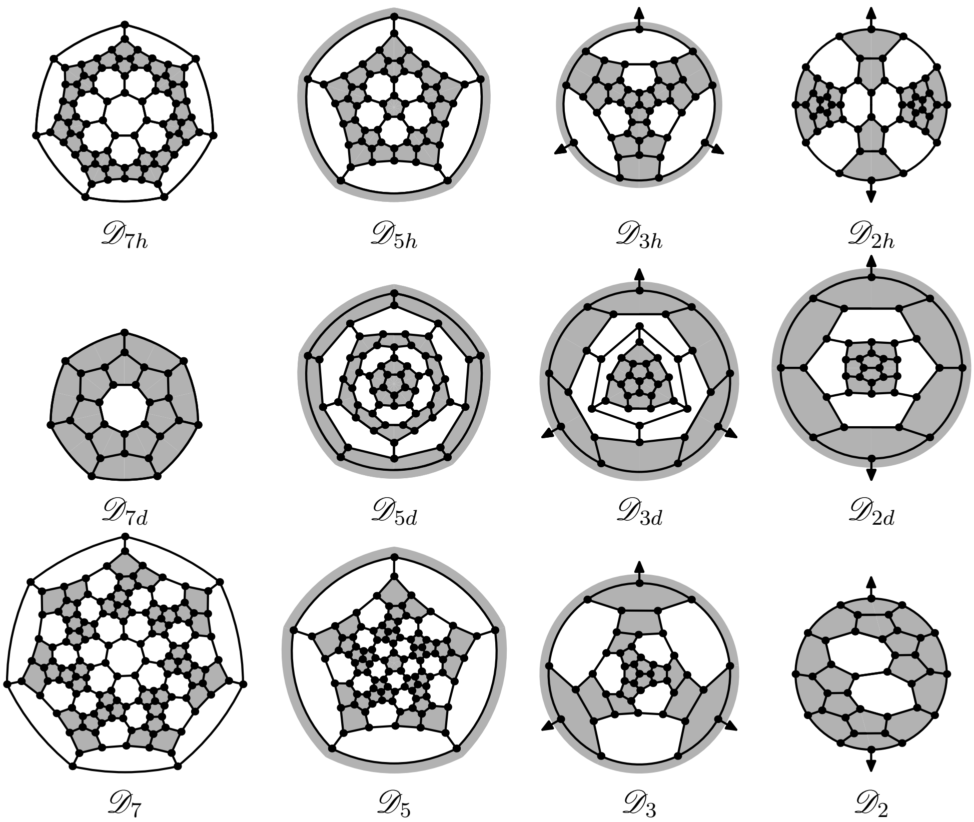

Figure 1.14: The smallest $(5,7)$-fulleroids with dihedral symmetry groups.

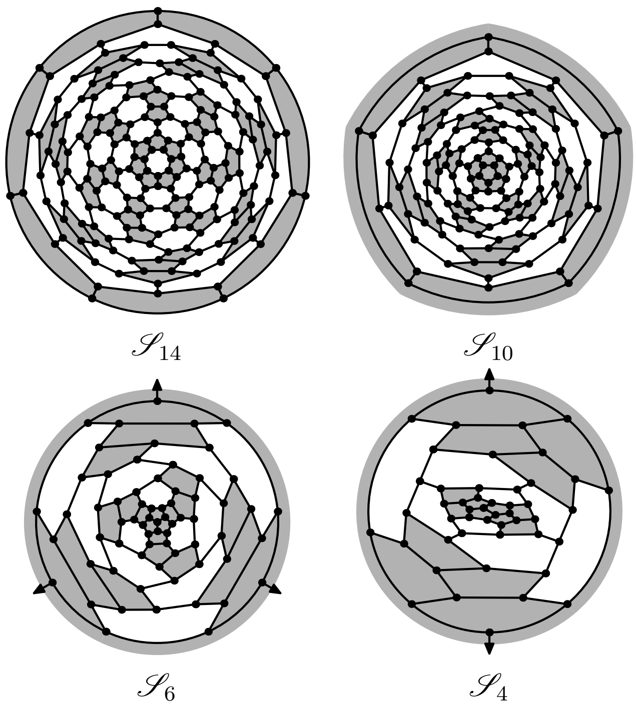

Figure 1.15: The smallest $(5,7)$-fulleroids with skewed symmetry groups.

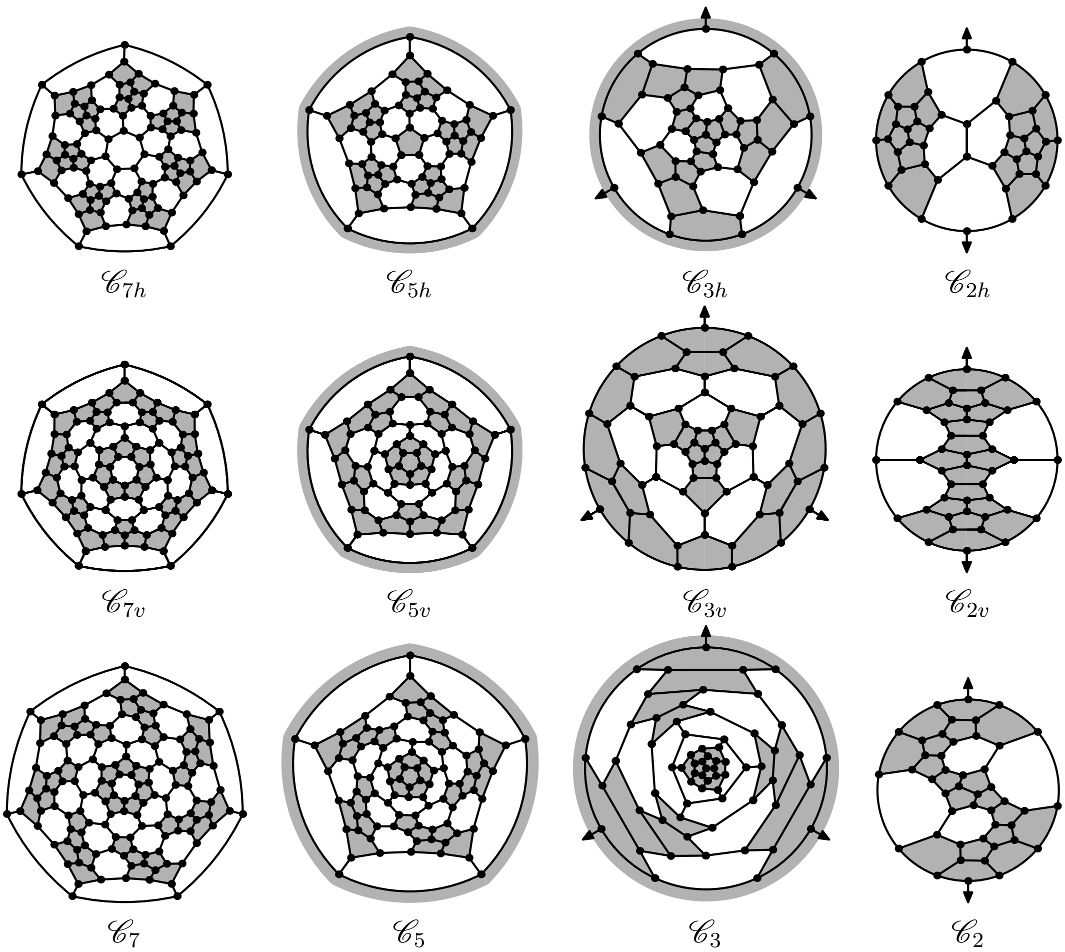

Figure 1.16: The smallest $(5, 7)$-fulleroids with pyramidal symmetry groups.

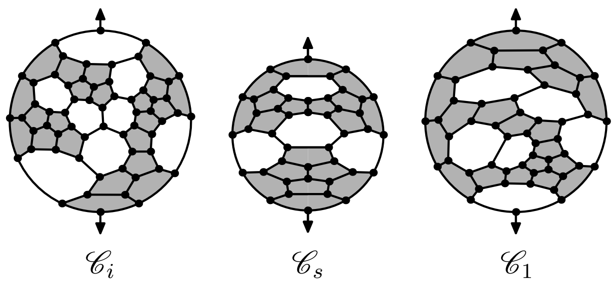

Figure 1.17: The smallest $(5, 7)$-fulleroids with low symmetry.

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