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Tetrahedral fulleroids

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Fulleroids are cubic convex polyhedra with faces of size 5 or greater. They are suitable models of carbon molecules. In this paper sufficient and necessary conditions for existence of fulleroids of tetrahedral 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.

KEY WORDS: fullerene graphs, fulleroids, symmetry of polyhedra, tetrahedral symmetry

MSC: 05C10, 05C90, 52B10, 52B15

1. Introduction

Fullerenes have been objects of interest and study in recent decades. A fullerene is a 3-regular (or cubic) 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. The fullerenes can also be represented by graphs. In fact, a fullerene graph is a planar, 3-regular and 3-connected graph, 12 of whose faces are pentagons and any remaining faces are hexagons.

The concept of fullerenes can be generalized in several ways. Patrick Fowler in 1995, see [1,2], 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 [1] introduced the following definition:

Definition 1. A fulleroid is a tiling of the sphere 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 be symmetry group of a convex polyhedron [3]. They can be divided into icosahedral, octahedral, tetrahedral, dihedral, cyclic and others. Symmetry of fullerenes has been studied deeply. Babić, Klein and Sah [4] studied fullerenes with up to 70 vertices and divided them according to the symmetry group. Graver [5] published a catalog of all fullerenes with ten or more symmetries.

The full symmetry group of a regular icosahedron is denoted by I_h; its subgroup of rotational symmetries is I. Delgado Friedrichs and Deza [1] found $I_h(5,n)$-fulleroids for $n=8$, 9, 10, 12, 14 and 15 and asked several questions concerning $I(5,n)$-fulleroids. Most of their questions have been answered by Jendrol' and Trenkler [6], who found infinite series of examples of $I(5,n)$-fulleroids for all $n \geqslant 8$.

Kardoš and Jendrol' [7] found a necessary and sufficient condition for existence of $O_h(5,n)$-fulleroids, where O_h denotes the full symmetry group of regular octahedron.

In this paper, the question of existence of tetrahedral fulleroids will be answered. We will focus on three symmetry groups: the group of all symmetries of regular tetrahedron T_d, the group of rotational symmetries of regular tetrahedron T and the group T_h, which is a subgroup of the group O_h, with four 3-fold rotational symmetry axes, three 2-fold rotational symmetry axes and a point of inversion. Cubes with a pattern in figure 1 are examples of solids with symmetry groups T_h, T_d and T, respectively.

2. Operations used to generate examples

To prove that for some number n and for some group Γ (in fact, T_h, T_d or T) 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 how to create new one from the old one.

If there are four adjacent pentagons in a configuration as in figure 2 left, by adding certain number of edges and vertices inside central two pentagons in a way as in figure 2 right, one can create from four pentagons two new n-gons and $2n-8$ new pentagons ($n \geqslant 6$) [6]. This step can be repeated as many times as

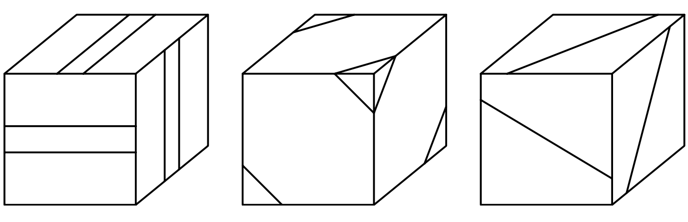

Figure 1. Examples of solids with symmetry group T_h, T_d, and T, respectively.

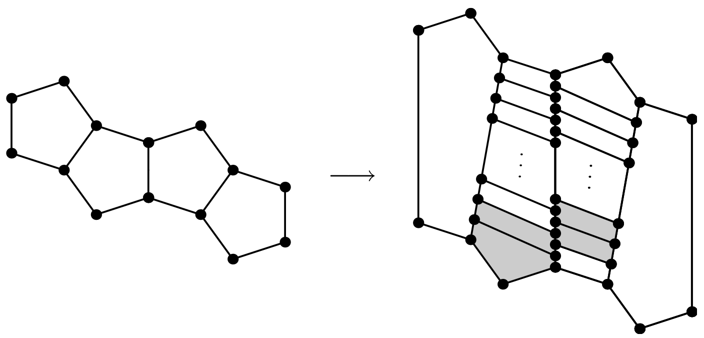

Figure 2. The step to create two new n-gons.

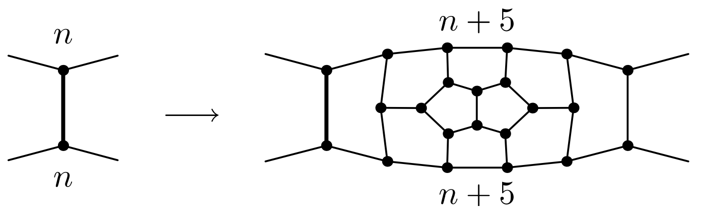

Figure 3. The step to increase size of two n-gons.

required, because the configuration of four pentagons can be found among the new pentagons again (shaded pentagons in figure 2 right).

If the desirable configuration of pentagons can not be found, other operations are used to generate infinite series of fulleroids.

There is one more useful operation. It is used when the size n should be increased. If two n-gons are connected by an edge (see figure 3), by inserting 10 pentagons they are changed to $(n+5)$-gons. Again this step can be carried out arbitrarily many times, so the size of these two faces can be increased by any multiple of 5.

3. $T_h(5, n)$-fulleroids

In figure 4 one fullerene with symmetry group T_h is shown. It is easy to see that underlying graph can be drawn as a regular pattern onto a cube; one face of such a cube is in figure 5, left. Because the symmetry is required, it is sufficient to know only one quarter of the square face of the cube (e.g., the one in figure 5 right) and whole fullerene is then determined. We will use this to draw all other $T_h(5, n)$-fulleroids. Only a quarter of a square face of a cube will be shown, the remaining structure will be given by symmetry. The dashed lines represent edges of the cube; the dotted lines represent the symmetry axes of a square faces of the cube.

$T_h(5, 6)$-fulleroids are in fact fullerenes with symmetry group T_h. Graver [5] in his paper characterised all fullerenes with 10 or more symmetries, including

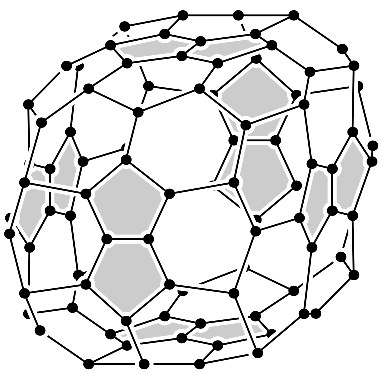

Figure 4. Example of a fullerene with T_h symmetry.

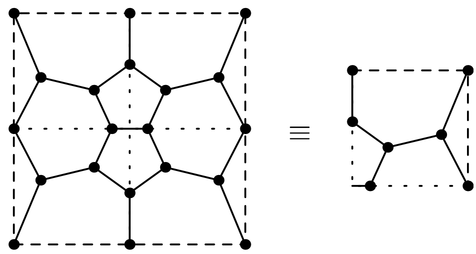

Figure 5. Representing T_h-fulleroids by a quarter of a square face of cube.

the symmetry group T_h. The T_h-fullerenes are split into three infinite families. The example in figure 4 is the second smallest one of them.

Theorem 1. For every $n > 6$ the set of all $T_h(5, n)$-fulleroids has infinitely many elements.

In figure 6 two examples of $T_h(5, 7)$- and two examples of $T_h(5, 8)$-fulleroids are given. In each of these pairs the left one has the smallest number of faces among all fulleroids of that type. The right one can be used to generate infinite family of examples, if operation from figure 2 is applied to dashed pentagons repeatedly.

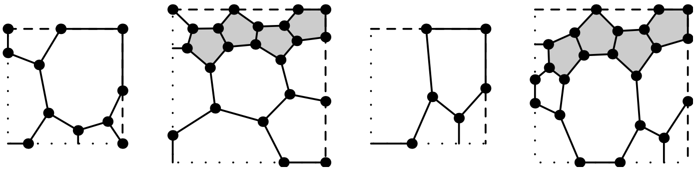

Figure 6. $T_h(5, 7)$- and $T_h(5, 8)$-fulleroids.

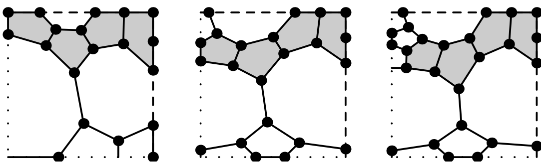

Figure 7. $T_h(5, n)$-fulleroids for $n = 9$, 10, and 11.

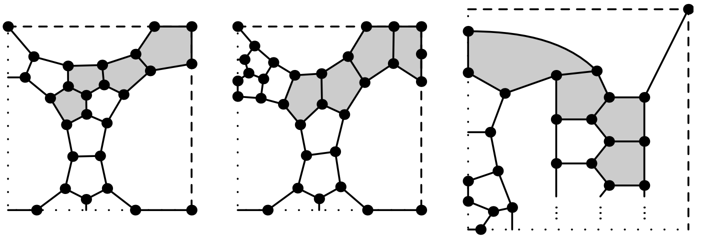

Figure 8. $T_h(5, n)$-fulleroids for $n = 12$ and 13 and for $n \geqslant 14$.

Examples of $T_h(5, n)$-fulleroids for n from 9 to 13 are in figure 7 and figure 8. Analogously infinitely many more of them can be generated by applying operation from figure 2. For $n \geqslant 14$ one example of $T_h(5, n)$-fulleroid can be seen in figure 8, right.

4. $T_d(5, n)$-fulleroids

In figure 9 one fullerene with symmetry group T_d is shown. Again, the underlying graph can be drawn onto a cube, one face of this cube is in figure 10, left. Because the symmetry is now diagonal, it is sufficient to draw one

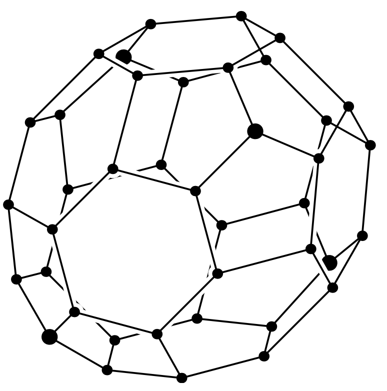

Figure 9. Example of a fullerene with T_d symmetry.

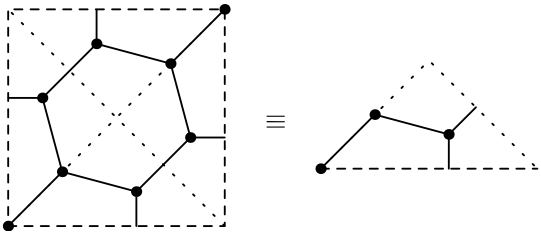

Figure 10. Representing T_d-fulleroids by a triangle-shaped quarter of a square face of cube.

quarter-triangle to determine the structure of whole fullerene, see figure 10, right. So again to describe some T_d-fulleroid only this triangle will be drawn.

$T_d(5,6)$-fulleroids are in fact fullerenes with symmetry group T_d. In Graver's catalog [5] there are all T_d-fullerenes divided into three infinite families. One in figure 9 is the second smallest of them.

The situation about $T_d(5,n)$-fulleroids for $n > 6$ is considerably different from the case of group T_h. Here, the existence depends on the number n:

Theorem 2. Let $n > 6$ be an integer. If $n \equiv 5 \pmod{10}$, then the set $T_d(5,n)$ is empty. If $n \not\equiv 5 \pmod{10}$, then the set of all $T_d(5,n)$-fulleroids has infinitely many elements.

Firstly, we focus on existence in the case of $n \not\equiv 5 \pmod{10}$.

The figure 11 shows two nonisomorphic $T_d(5,7)$-fulleroids with minimum number of faces. In the figure 12 a step to generate infinitely many more examples is given.

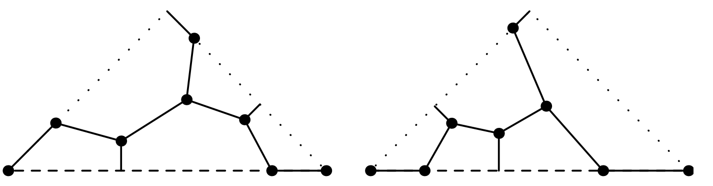

Figure 11. The two smallest $T_d(5,7)$-fulleroids.

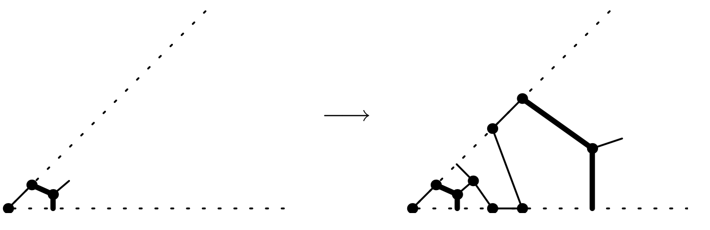

Figure 12. Generating more $T_d(5,7)$-fulleroids.

For $n = 11 + 10k$, $13 + 10k$, $14 + 10k$, $16 + 10k$ and $17 + 10k$ one (not necessarily the smallest) example is shown in figure 13. By applying the operation from figure 3 to the double-lined edges k times the size of n-gonal faces can be increased by $10k$; by applying the operation from figure 2 to the shaded faces the number of n-gonal faces can be increased by two repeatedly.

For $n = 8+10k$, $9+10k$ and $12+10k$ the smallest $T_d(5, n)$-fulleroid is shown in figure 14. Again by applying the operation from figure 3 to the double-lined edges k times the size of n-gonal faces can be increased by $10k$. To create new n-gonal faces, the operations from figure 15 can be used.

For n=10+20k the smallest $T_d(5, n)$-fulleroid is in figure 16, left. To increase the size of n-gonal faces by $20k$, again the operation from figure 3 should be applied to the double-lined edges k times. To create new faces, the operation from figure 17 should be performed.

For $n = 20 + 20k$ one example of $T_d(5, n)$-fulleroid is in figure 16, right. To increase the size of n-gonal faces by $20k$, again the operation from figure 3 can be applied to the double-lined edges k times. To create new faces, one can choose two pentagons connected by an edge and apply the operation from figure 3 $(3 + 4k)$ times. It is easy to see that there is always such a pair of pentagons.

The second part of the proof of theorem 2 is to prove that for $n = 15 + 10k$ the set $T_d(5, n)$ is empty. For this purpose following lemma [7] will be used:

Lemma 1. Let $n \equiv 0 \pmod 5$ and P be a convex polyhedron with pentagonal and n-gonal faces only and all vertices of degree 3. Then there exists the homomorphism $\Psi : \; P \to D$, where D denotes the dodecahedron.

By homomorphism $\Psi : \; P \to D$ we mean the mapping of vertices of the polyhedron P onto those of the polyhedron D, respecting the incidence structure. That means if two vertices (edges, faces) of P are adjacent, then also their images are adjacent in D.

Let us assume that there exists a counterexample, that means there is a $T_d(5, n)$-fulleroid for some $n \equiv 5 \pmod{10}$, let us denote it P. By lemma 1 we have homomorphism $\Psi : \; P \to D$. Because T_d is the symmetry group of P, we can draw the graph of P onto a cube and deal with its triangle-shaped quarter, in the same way like when describing the examples above. This triangle will be denoted by ABC, where AB is an edge of a cube while AC and BC are halves of diagonals.

The point C, the midpoint of a face of the cube, is a point of 2-fold rotational symmetry of P. This point cannot be neither a vertex of P, because all vertices are of degree 3, nor a internal point of any face, because faces are of odd degree, so it must be a midpoint of an edge. Then the image $\Psi(C)$ is also a midpoint of some edge of the dodecahedron.

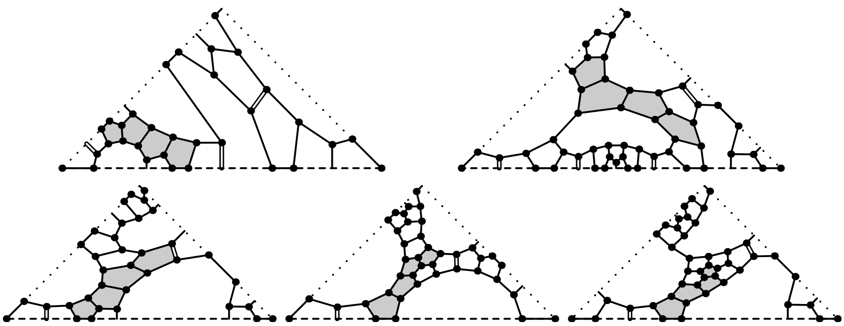

Figure 13. Examples of $T_d(5, n)$-fulleroids for $n = 11, 13, 14, 16$, and 17.

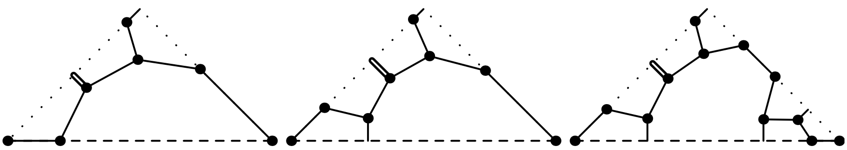

Figure 14. The smallest $T_d(5, n)$-fulleroids for $n = 8, 9$, and 12.

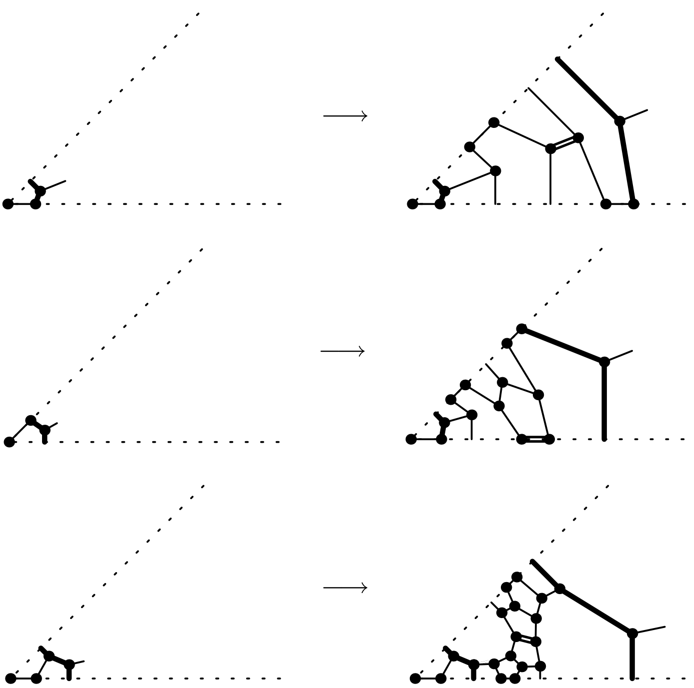

Figure 15. Generating more $T_d(5, n)$-fulleroids for $n = 8, 9$, and 12.

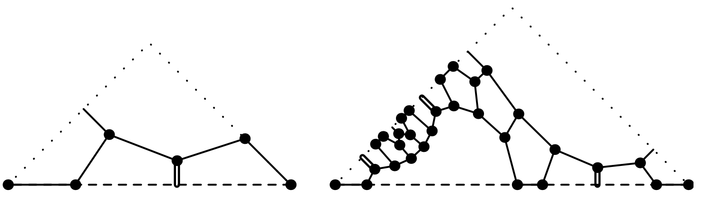

Figure 16. The smallest $T_d(5, 10)$-fuleroid and an example of $T_d(5, 20)$-fulleroid.

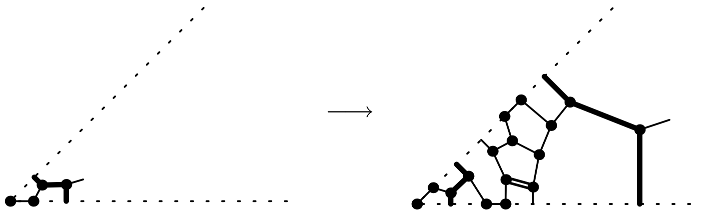

Figure 17. The step to add new n-gonal faces for $n = 10 + 20k$.

As the lines AC and BC are in fact intersections of symmetry planes of P with P itself, when a point x moves from C to A (or from C to B), the image $\Psi(x)$ can move only on certain circular lines on the dodacehedron, two of them visible in figure 18. These lines will be denoted as perimeters of D.

Moreover, the image of line BC is included in the perimeter p_{BC} that is in the same relative position to the perimeter p_{AC} that includes the image of line AC like the perimeters in figure 18.

Since the line AB also represents the symmetry plane, the image of the line AB is also included in one of the perimeters. The relative position of this third perimeter p_{AB} to the first two depends on the local structure of P in the neighbourhood of points A and B.

The points A and B are points where 3-fold rotational symmetry axes intersect P, so the local structure must have 3-fold rotational symmetry. If $n \not\equiv 0 \pmod 3$, then there must be a vertex in both A and B. In that case the

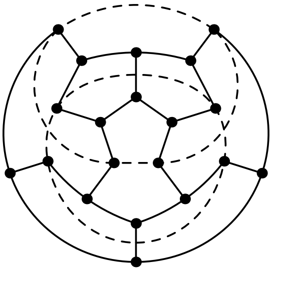

Figure 18. Section circular lines (the perimeters) of the dodecahedron

perimeter p_{AB} must intersect both the perimeters p_{AC} and p_{BC} in vertices. But every perimeter of D that intersects one of those two perimeters in two vertices intersects the other in two midpoints of faces and vice versa, thus there is a contradiction.

In the case $n \equiv 0 \pmod 3$ if we want to avoid the contradiction from previous case there must be an n-gonal face in at least one of the points A and B. Assume there is an n-gonal face in point A. Since n is a multiple of 5, we have $p_{AC} = p_{AB}$. Then p_{AB} and p_{BC} are perpendicular, so there must be a midpoint of an edge in th point B. Then B is not a point of 3-fold rotational symmetry, what is a contradiction again.

As the assumption of existence of $T_d(5, n)$-fulleroid for $n \equiv 5 \pmod{10}$ leads to a contradiction and infinite series of examples for all other possible $n > 6$ were given, the theorem 2 has been proved.

5. $T(5, n)$-fulleroids

In figure 19 one fullerene with symmetry group T is depicted. Again the underlying graph can be drawn onto a cube, see figure 20, left. Here the only symmetry of a face of such cube is the point of inversion (2-fold rotational symmetry point). To describe some T-fulleroid one face of the cube will be drawn, as in figure 20, right.

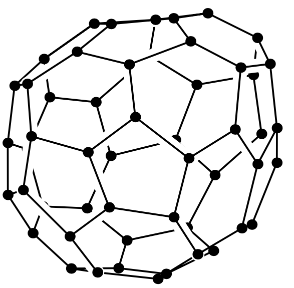

Figure 19. Example of a fullerene with T symmetry.

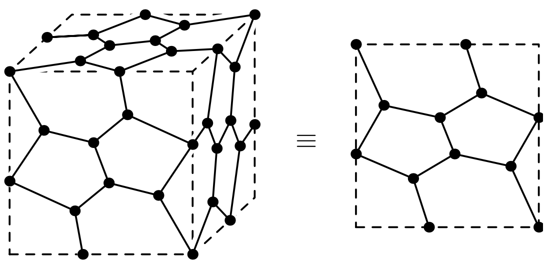

Figure 20. Representing T-fulleroids by the face of the cube.

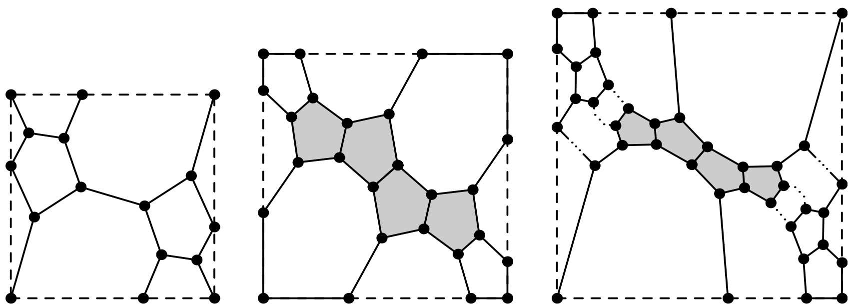

Figure 21. Examples of $T(5, n)$-fulleroids for $n = 7$ and $n \geqslant 8$.

$T(5, 6)$-fulleroids are nothing else but fullerenes with symmetry group T. In Graver's catalog [5] there are all T-fullerenes divided into 15 infinite families. One in figure 19 is the second smallest of them.

The question about existence of $T(5, n)$-fulleroids for bigger numbers n is answered in the following statement:

Theorem 3. For every $n > 6$ the set of all $T(5, n)$-fulleroids has infinitely many elements.

In figure 21 two examples of $T(5, n)$-fulleroids for $n = 7$ and one for $n \geqslant 8$ are depicted. The operation from figure 2 can be carried out repeatedly in such a way that the symmetry will not be broken. This proves the claim.

Acknowledgment

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References

[1] O. Delgado Friedrichs and M. Deza, in: *Discrete Mathematical Chemistry*, eds. P. Hausen, P. Fowler and M. Zheng, DIMACS Series in Discrete Mathematics and Theoretical Computer Science, Vol. 51 (2000) 97–115.

[2] A.W.M. Dress and G. Brinkmann, Match 33 (1996) 87.

[3] P.R. Cromwell, *Polyhedra* (Cambridge University Press, Cambridge, 1997).

[4] D. Babić, D.J. Klein and C.H. Sah, Chem. Phys. Lett. 211 (1993) 235.

[5] J.E. Graver, A Catalog of All Fullerenes with Ten or More Symmetries, Computers and Discovery in Graph Theory With Applications to Chemistry, the Proceedings of the DIMACS Working Group Conference, 2001.

[6] S. Jendrol' and M. Trenkler, J. Math. Chem. 29(4) (2001) 235.

[7] F. Kardoš and S. Jendrol', On Octhedral Fulleroids, Preprint, Institute of Mathematics, Faculty of Science, UPJŠ, Košice, Slovakia (2004).