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FULLERENES VIA THEIR AUTOMORPHISM GROUPS

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Abstract

A semiregular element of a permutation group is a non-identity element having all cycles of equal length in its cycle decomposition. The existence of semiregular automorphisms in fullerenes is discussed. In particular, the family of fullerene graphs is described via the existence of semiregular automorphisms in their automorphism groups.

1 Introductory remarks

A *fullerene graph* (in short a *fullerene*) is a 3-connected cubic planar graph, all of whose faces are pentagons and hexagons. By Euler formula the number of pentagons is 12. From a chemical point of view, fullerenes correspond to carbon 'sphere'-shaped molecules, the important class of molecules which is a basis of thousands of patents for a broad range of commercial applications [42, 43]. In this respect, graph-theoretic observations on structural properties of fullerenes play an important role [5, 7, 8, 9, 11, 12, 14, 15, 20, 21, 22, 23, 40, 45,

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46]. Some recent developments with regards to certain open problems about the chemistry of fullerenes together with the methods used to answer these problems find their natural environment in a graph-theoretic context. An example of such a problem is a long standing conjecture that an arbitrary fullerene contains a Hamilton cycle, that is, a simple path going through all vertices of the fullerene (see [37]). Not much progress has been made with regards to this conjecture. It has been verified for graphs on at most 176 vertices (see [2]), and to the best of our knowledge, the most general result in this topic is the result on the existence of Hamilton cycles and paths in the so-called Leapfrog fullerenes (see [34]).

In this paper fullerenes are described via their automorphism groups, and the obtained results give possible directions this area of research is likely to take in the near future. Motivated by the problem posed by the second author in 1981 (see [31, Problem 2.4]) who asked if it is true that a vertex-transitive digraph contains a nonidentity automorphism with all orbits of equal length, in short, a *semiregular automorphism*, fullerenes are characterized with regards to the existence of semiregular automorphisms in their automorphism groups (see Theorem 3.8). There exist fullerenes with non-trivial automorphism groups without semiregular automorphisms. In particular, it is shown at the end of Section 3 that there exists an infinite family of fullerenes with the automorphism group isomorphic to $\mathbb{Z}_3$ or S_3 with no semiregular automorphisms.

In the context of vertex-transitive graphs the existence of semiregular automorphisms helps proving the existence of Hamilton paths/cycles for some classes of such graphs, see for example [1, 26, 28, 33, 35, 36]. (The problem of whether every connected vertex-transitive graph contains a Hamilton path is a long standing open problem posed by Lovász in [29].) It seems reasonable to expect that methods similar to those used for finding Hamilton paths/cycles in vertex-transitive graphs could be applied, at least in some cases, to fullerenes as well. An example of this is given in Section 2.

Throughout this paper graphs are simple and finite, undirected and connected. For group-theoretic terms not defined here we refer the reader to [41, 44, 47]. Given a graph X we let $V(X)$, $E(X)$, $A(X)$ and $\mathrm{Aut}X$ be the vertex set, the edge set, the arc set and the automorphism group of X, respectively. For adjacent vertices u and v in X, we write

$u \sim v$ and denote the corresponding edge by uv. If $u \in V(X)$ then $N(u)$ denotes the set of neighbors of u. A sequence $(u_0, u_1, u_2, \dots, u_k)$ of distinct vertices in X is called a *k-arc* if u_i is adjacent to u_{i+1} for every $i \in \{0, 1, \dots, k-1\}$. By an n-cycle we shall always mean a cycle with n vertices.

2 Representation of graphs admitting semiregular automorphisms

Let G be a permutation group on a finite set V. A *semiregular* element of G is a non-identity element having all cycles of equal length in its cycle decomposition. In particular, a (k,n)-*semiregular* element of G is a non-identity element having k orbits of length n and no other orbit. For a graph X and a partition $\mathcal{W}$ of $V(X)$, we let $X_{\mathcal{W}}$ be the associated *quotient graph* of X relative to $\mathcal{W}$, that is, the graph with vertex set $\mathcal{W}$ and edge set induced naturally by the edge set $E(X)$. In the case when $\mathcal{W}$ corresponds to the set of orbits of a semiregular automorphism $\rho \in \mathrm{Aut}X$, the symbol $X_{\mathcal{W}}$ will be replaced by X_ρ.

Let X be a connected graph admitting a (k,n)-semiregular automorphism

$$\rho = (u_0^0 u_0^1 \cdots u_0^{n-1})(u_1^0 u_1^1 \cdots u_1^{n-1}) \cdots (u_{k-1}^0 u_{k-1}^1 \cdots u_{k-1}^{n-1}), \tag{1}$$

and let $\mathcal{W} = \{W_i \mid i \in \mathbb{Z}_k\}$ be the set of orbits $W_i = \{u_i^s \mid s \in \mathbb{Z}_n\}$ of ρ. Using Frucht's notation [19] X may be represented in the following way. Each orbit of ρ is represented by a circle. Inside a circle corresponding to the orbit W_i the symbol n/T, where $T = T^{-1} \subseteq \mathbb{Z}_n \setminus \{0\}$, indicates that for each $s \in \mathbb{Z}_n$, the vertex u_i^s is adjacent to all the vertices u_i^{s+t} where $t \in T$. When $|T| \leq 2$ we use a simplified notation n/t, $n/(n/2)$ and n, respectively, when $T = \{t, -t\}$, $T = \{n/2\}$ and $T = \emptyset$. Finally, an arrow pointing from the circle representing the orbit W_i to the circle representing the orbit W_j, $j \neq i$, labeled by $y \in \mathbb{Z}_n$ means that for each $s \in \mathbb{Z}_n$, the vertex $u_i^s \in W_i$ is adjacent to the vertex u_j^{s+y}. When the label is 0, the arrow on the line may be omitted. Two examples illustrating this notation are given in Figure 1 and Figure 2.

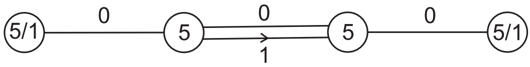

Figure 1: The dodecahedron given in Frucht's notation relative to a $(4,5)$-semiregular automorphism.

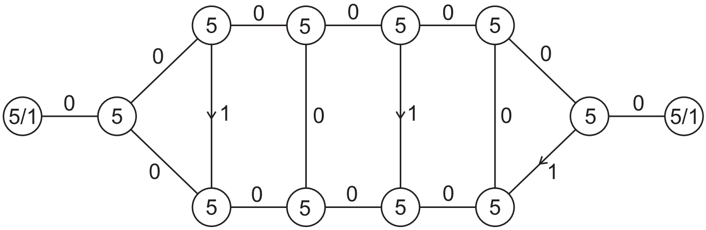

Figure 2: The C_{60} fullerene given in Frucht's notation relative to a $(12,5)$-semiregular automorphism.

As mentioned in Section 1 a frequently used approach to constructing Hamilton cycles in graphs is based on a quotienting/reduction with respect to a suitable semiregular automorphism, preferably one of prime order. Provided the quotient graph contains a Hamilton cycle it is sometimes possible to lift this cycle to construct a Hamilton cycle in the original graph, consistently spiraling through the corresponding orbits. This idea was first introduced in [32] to show existence of Hamilton cycles in particular Cayley graphs. The same idea can be used to show, for example, the existence of a Hamilton cycle in one of the fullerenes of order 32. This fullerene has a $(16,2)$-semiregular automorphism ρ and it can be nicely represented in Frucht's notation as shown in Figure 3. The quotient graph X_ρ with respect to the $(16,2)$-semiregular automorphism ρ has 16 vertices, corresponding to 16 orbits of ρ. Since 1 generates $\mathbb{Z}_2$ the outer cycle of X_ρ lifts to a Hamilton cycle in the fullerene.

3 Automorphism groups of fullerenes

A *map* $\mathcal{M} = \mathcal{M}(X)$ is an embedding of a finite connected graph X into a surface so that it divides the surface into simply-connected regions, called the *faces* of $\mathcal{M}$. To each

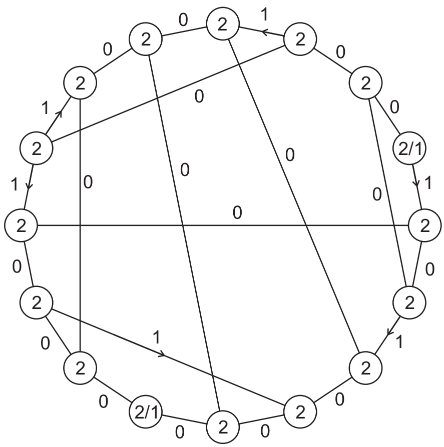

Figure 3: A fullerene of order 32 given in Frucht's notation relative to a $(16, 2)$-semiregular automorphism.

face f we associate a closed walk of X with edges surrounding f, to which we shall also refer as a face of $\mathcal{M}$. An *automorphism* of $\mathcal{M}$ is an automorphism of X which preserves its faces. A graph is planar if it underlies a map on the 2-sphere. Finite planar graphs form one of a few families of graphs for which the automorphism groups have been satisfactorily determined, see [3]. In general, the automorphism group of an underlying map $\mathcal{M}(X)$ of a graph X is a subgroup of the full automorphism group $\mathrm{Aut}(X)$ of X, that is, not every automorphism of X can be realized as an automorphism of the map $\mathcal{M}$. However, in 1971 Mani [3, 30] proved that every 3-connected planar graph X can be embedded on the 2-sphere as a convex polytope P in such a way that the automorphism group of X coincides with the automorphism group of the convex polytope P formed by the embedding, that is, the combinatorial automorphisms of X are in fact the same as the topological automorphisms of P. Special cases of this result have been proved in [4, 24].

Proposition 3.1 [30] *For each polyhedral graph X, there exists a 3-dimensional convex polytope P such that every automorphism of X is induced by a symmetry of P.*

Of course, the topological automorphisms of P form a subgroup of the group of all automorphisms of the 2-sphere. Let the subgroup formed by rotations of P be called the *rotation group* of P. Then the above proposition implies that there are precisely two infinite families and three sporadic examples of finite rotation groups of the 2-sphere: the cyclic groups $\mathbb{Z}_n$, the dihedral groups D_{2n}, where $n \in \mathbb{N}$, the alternating group A_4, the symmetric group S_4 and the alternating group A_5. In addition, either the rotation group of P is its full automorphism group or the full automorphism group of P is a product of its rotation group and a reflection. Since fullerenes are planar graphs, these facts imply the following proposition.

Proposition 3.2 *Let $Rot(F)$ be the rotation group of a fullerene F. Then $Rot(F) \cong A_4, S_4, A_5, \mathbb{Z}_n$ or D_{2n}, where $n \in \mathbb{N}$, and either $\mathrm{Aut}(F) = Rot(F)$ or $\mathrm{Aut}(F) = Rot(F) \cup Rot(F)\tau \cong Rot(F) \cdot \mathbb{Z}_2$ where τ is a reflection.*

A stronger result was obtained in 1993 by Fowler, Manolopoulos, Redmond and Ryan [18]. In particular, they gave a list of exactly 28 groups that can occur as the automorphism groups of fullerenes (see also [10]).

In this section a detailed characterization of fullerenes is given based on (non)existence of semiregular automorphisms in their automorphism groups (see Theorem 3.8). We start with a simple observation about the length of cycles in fullerenes which is a direct consequence of the fact that fullerenes are cyclically 5-edge connected. (This means that the maximum number k such that a fullerene cannot be separated into two components, each containing a cycle, by deletion of fewer than k edges, is 5, see [13, Theorem 2] and also [39].)

Lemma 3.3 *Let F be a fullerene. Then every 5-cycle and every 6-cycle in F is a boundary cycle of a face in a planar embedding of F. Moreover, the length of the shortest non-boundary cycle is more than or equal to 8.*

PROOF. This is a direct consequence of the fact that fullerenes are cyclically 5-edge connected and the fact that two adjacent 5-cycles give us an 8-cycle. ■

The next lemma tells us that no nonidentity automorphism in a fullerene fixes a 2-arc.

Lemma 3.4 *Let F be a fullerene, let* $\mathrm{Aut}(F)$ *be its automorphism group and let* $u, v, w \in V(F)$ *be such that* (u, v, w) *is a 2-arc in* F. *Then the stabilizer* $\mathrm{Aut}(F)_{(u,v,w)}$ *of the 2-arc* (u, v, w) *is trivial.*

PROOF. Let $u_0, u_1, u_2 \in V(F)$ be vertices of F such that (u_0, u_1, u_2) is a 2-arc in F. Let $(u_0, u_1, u_2, \ldots, u_l)$, where $l \in \{4, 5\}$, be the boundary cycle of a face f of length $l + 1$ containing the 2-arc (u_0, u_1, u_2) in a planar embedding of F. Let u'_i be the vertex adjacent to u_i, $i \in \{0, 1, \ldots l\}$, not lying on the face f. Suppose that there exists a non-trivial automorphism $\alpha \in \mathrm{Aut}(F)$ that fixes the 2-arc (u_0, u_1, u_2). Then, with no loss of generality, we may assume that $u_l^\alpha = u'_0$ which means that the 3-arc (u'_0, u_0, u_1, u_2) lies on an $(l+1)$-cycle. Since $l \in \{4, 5\}$, Lemma 3.3 implies that this $(l + 1)$-cycle is a boundary cycle of a face in the planar embedding of F. But then the 2-arc (u_0, u_1, u_2) is contained on two different faces of F, a contradiction. ■

Proposition 3.5 *Let F be a fullerene, let* $\mathrm{Aut}(F)$ *be its automorphism group and let* $u \in V(F)$. *Then the stabilizer* $\mathrm{Aut}(F)_u$ *of u is trivial or it is isomorphic to one of the following three groups: the cyclic group* $\mathbb{Z}_2$, *the cyclic group* $\mathbb{Z}_3$ *and the symmetric group* S_3.

PROOF. By Lemma 3.4 the stabilizer of any 2-arc in F is trivial. Consequently, the stabilizer of a vertex $u \in V(F)$ acts faithfully on the neighbors' set $N(u)$. The result is then clear. ■

A finite group G is said to be a $\{p_1, \ldots, p_2\}$-*group* if $\{p_i \mid i \in \{1, 2, \ldots, n\}\}$ is the set of all prime divisors of the order of G. For example, the symmetric group S_3 is a $\{2, 3\}$-group.

Proposition 3.6 *Let F be a fullerene admitting an automorphism* $\alpha \in \mathrm{Aut}(F)$ *of order* 5. *Then α is a semiregular automorphism of F.*

PROOF. By Proposition 3.5 the stabilizer of any vertex in F is a subgroup of a $\{2, 3\}$-group and thus without elements of order 5. Consequently, all orbits of an automorphism

$\alpha \in \mathrm{Aut}(F)$ of order 5 are of length 5. ■

Examples of fullerenes admitting automorphisms of order 5 are, for example, the dodecahedron C_{20}, the soccer-ball-shaped fullerene C_{60}, as well as the infinite family of fullerenes admitting a non-trivial cyclic-5-cutset which were recently classified in [27]. (A set of k edges whose elimination disconnects a graph into two components, each containing a cycle, is called a *cyclic-k-cutset* and moreover, it is called a *trivial cyclic-k-cutset* if at least one of the resulting two components induces a single k-cycle.)

The next lemma can be proved using the list of 28 possible automorphism groups of fullerenes given in [18]. We do, however, for the sake of completeness give an independent proof using elementary concepts from group actions on combinatorial objects.

Lemma 3.7 *Let F be a fullerene. Then its automorphism group* $\mathrm{Aut}(F)$ *is a subgroup of a $\{2,3,5\}$-group. Moreover, the order of* $\mathrm{Aut}(F)$ *divides* $2^3 \cdot 3 \cdot 5$.

PROOF. Let $\mathcal{T}$ be the set of twelve 5-cycles in F and consider the natural action of $A = \mathrm{Aut}(F)$ on $\mathcal{T}$ in a natural way. Let $\mathcal{O}$ be the set of orbits of A on $\mathcal{T}$ and let $O \in \mathcal{O}$. Then cardinality $|O|$ equals l_O for some $l_O \in \{1, 2, \ldots, 12\}$, and thus the quotient group A/K_O is a group of degree l, where K_O is the kernel of the action of A on $O \in \mathcal{O}$. Clearly, by Lemma 3.4, it follows that for any 5-cycle $T \in O$ the restriction $(K_O)^T$ equals K_O, and therefore $K_O = 1$ or $K_O \cong \mathbb{Z}_2$ or $K_O \cong \mathbb{Z}_5$ or $K_O \cong D_{10}$. Moreover, since a 5-cycle cannot be fixed by an automorphism of order 3, Proposition 3.5 implies that the stabilizer $(A/K_O)_T$ of a 5-cycle $T \in \mathcal{T}$ is a subgroup of a $\{2,5\}$-group. In particular, considering the induced action of A/K_O on $\mathcal{T}$ we have that $(A/K_O)_T = 1$ or $(A/K_O)_T \cong \mathbb{Z}_2$ or $(A/K_O)_T \cong \mathbb{Z}_5$ or $(A/K_O)_T \cong D_{10}$. By the well-known orbit-stabilizer property of permutation groups [17] it follows that $|(A/K_O)/(A/K_O)_T| = l_O$, and hence

$$|A| = |K_O| \cdot |(A/K_O)_T| \cdot l_O = 2^{m_O} \cdot 5^{n_O} \cdot l_O \tag{2}$$

where $m_O \in \{0,1,2\}$ and $n_O \in \{0,1,2\}$. But this holds for every orbit O in $\mathcal{O}$ and so the lengths of two orbits in $\mathcal{O}$, if not coprime (one of length 2, and the other of length 5) and if not equal, may only differ by a factor of 2, 4, 5, or 10. Hence, since $\sum_{O \in \mathcal{O}} l_O = 12$, we have that $l_O \notin \{7, 9, 11\}$. Now checking up the various remaining possibilities it may be seen that A is a subgroup of a $\{2, 3, 5\}$-group, and moreover its order divides $2^4 \cdot 3 \cdot 5^2$. In what follows we show that in fact $|A|$ divides $2^3 \cdot 3 \cdot 5$.

Suppose first that 5 divides $|A|$ and that a Sylow 5-subgroup $\mathrm{Syl}_5(A)$ of A is of order 5^2 and consider its action on the set $\mathcal{T}$ of twelve 5-cycles in F. Now $Syl_5(A)$ being a 5-group, it must have at least two trivial orbits in its action on $\mathcal{T}$. Hence there exist 5-cycles with stabilizers divisible by 25, contradicting the above statements on stabilizers of 5-cycles. It follows that $|\mathrm{Syl}_5(A)| = 5$.

Suppose now that 2 divides $|A|$ and that a Sylow 2-subgroup $\mathrm{Syl}_2(A)$ of A is of order 2^4 and consider its action on the set $\mathcal{T}$ of twelve 5-cycles in F. Using a similar argument as in the preceding paragraph, we infer that there are either three orbits of length 4 or one orbit of length 8 and one of length 4 arising from this action. Now consider the action of $\mathrm{Syl}_2(A)$ on an orbit of length 4 in its action on $\mathcal{T}$. Since, by assumption, $\mathrm{Syl}_2(A)$ is of order 2^4, the orbit-stabilizer property implies that the subgroup of $\mathrm{Syl}_2(A)$ that stabilizes a 5-cycle in this orbit is of order 4, a contradiction. Thus the order of $\mathrm{Syl}_2(A)$ divides 2^3, as claimed. ■

We are now ready to prove the main result of this paper.

Theorem 3.8 *Let F be a fullerene with non-trivial automorphism group. Then either F admits a semiregular automorphism or* $\mathrm{Aut}(F) \cong \mathbb{Z}_2$, $\mathbb{Z}_3$ *or* S_3.

PROOF. In view of Proposition 3.6 and Lemma 3.7 we may assume that $\mathrm{Aut}(F)$ is a subgroup of a $\{2, 3\}$-group with order dividing $2^3 \cdot 3$. Further, assume that the rotational subgroup $\mathrm{Rot}(F)$ of $\mathrm{Aut}(F)$ has even order. Then it has an involuntary rotation, that is, a half-turn rotation. If this rotation was not semiregular, there would be at least one vertex of F lying on the axis of this rotation. But then the set of neighbors of this vertex would not be fixed by this half-turn rotation. We may therefore assume that $\mathrm{Rot}(F)$ is of odd order and hence either trivial or isomorphic to $\mathbb{Z}_3$. Consequently, $\mathrm{Aut}(F)$ is one of $\mathbb{Z}_2$, $\mathbb{Z}_3$ or S_3. ■

There are examples of fullerenes with $\mathbb{Z}_2$, $\mathbb{Z}_3$ and S_3 groups not having semiregular automorphisms (see Figures 4, 5, and 6), and therefore Theorem 3.8 is best possible.

The leapfrog fullerene $\mathrm{Le}(F)$ is obtained from a fullerene F by performing the so-called tripling (leapfrog transformation) [16, 25, 38] which consists in the truncation of the dual $\mathrm{Du}(F)$ of F. That is, $\mathrm{Le}(F) = \mathrm{Trun}(\mathrm{Du}(F))$ and consequently $\mathrm{Aut}(F) = \mathrm{Aut}(\mathrm{Le}(F))$. Observe that a vertex in F corresponds to a hexagonal face in $\mathrm{Le}(F)$ and one can easily see that every non-trivial automorphism of F fixing a vertex 'lifts' to a semiregular automorphism in $\mathrm{Le}(F)$. Therefore the leapfrog transformation enables us to construct an infinite family of fullerenes with a prescribed non-trivial automorphism group and having a semiregular automorphism.

On the other hand, there are also infinitely many fullerenes having non-trivial automorphism groups without semiregular automorphisms as is shown by the three examples given in Figures 7,8 and 9. They are the smallest three members of an infinite family of such fullerenes, of order $70 + 24k$, having S_3 as their automorphism group for k even and $\mathbb{Z}_3$ as their automorphism group for k odd. The construction rule is best understood if the point of view is the outer hexagon, that is, the boundary of the infinite region. Its neighboring faces make up a ring of six hexagons, which is in turn followed by a second ring consisting of alternate hexagons and pentagons, six of each. This ring is then followed by k rings each containing twelve hexagons. The last of these rings is followed by a ring consisting of alternate pairs of hexagons and pentagons, three of each, and, to close up the picture, a stack of six hexagons in a triangle shape turned upside down in our figures, in the middle of which is the fixed vertex of the automorphism of order 3. There is an additional reflexive symmetry when k is even, about an axis passing through $10 + k$ vertices, the above central vertex in the $\mathbb{Z}_3$-symmetry being one of them (see Figures 7 and 9). The automorphism group is therefore S_3 in this case. When k is odd this bisective symmetry is broken by the odd number of rings of twelve hexagons between the two rings containing pentagons and thus the group is $\mathbb{Z}_3$ in this case (see Figure 8).

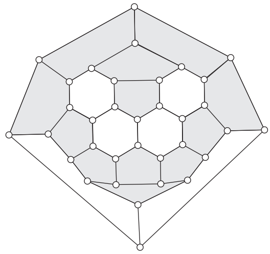

Figure 4: A fullerene of order 34 without a semiregular automorphism with the full automorphism group isomorphic to the cyclic group $\mathbb{Z}_2$.

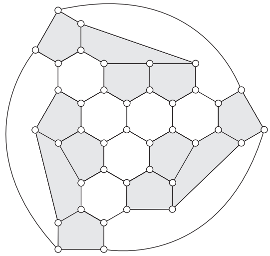

Figure 5: A fullerene of order 40 without a semiregular automorphism with the full automorphism group isomorphic to the cyclic group $\mathbb{Z}_3$.

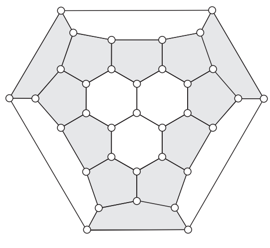

Figure 6: A fullerene of order 34 without a semiregular automorphism with the full automorphism group isomorphic to the symmetric group S_3.

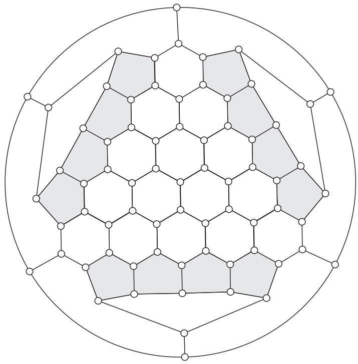

Figure 7: The first fullerene ($k = 0$) in an infinite family of fullerenes without a semiregular automorphism with the full automorphism group isomorphic to the symmetric group S_3.

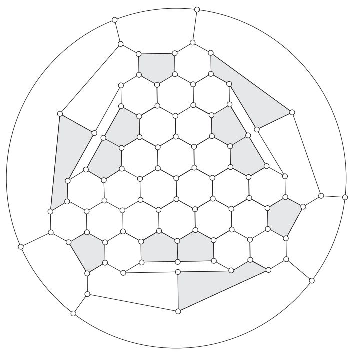

Figure 8: The second fullerene ($k = 1$) in an infinite family of fullerenes without a semiregular automorphism with the full automorphism group isomorphic to the symmetric group $\mathbb{Z}_3$.

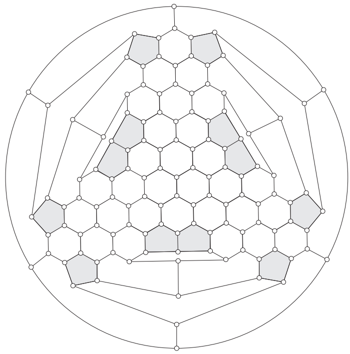

Figure 9: The third fullerene ($k = 2$) in an infinite family of fullerenes without a semiregular automorphism with the full automorphism group isomorphic to the symmetric group S_3.

4 Conclusions

In this paper we have characterized fullerene graphs via their automorphism groups, in particular, via the existence of semiregular automorphisms. We believe that the use of the concept of semiregular automorphisms will prove useful in some open problems regarding fullerenes such as, for example, the hamiltonicity problem.

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