STRUCTURAL PROPERTIES OF FULLERENES

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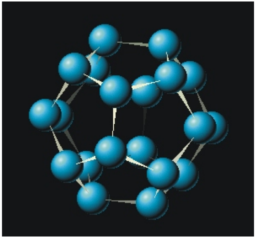
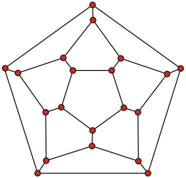
In chemistry: carbon ‘sphere’-shaped molecules

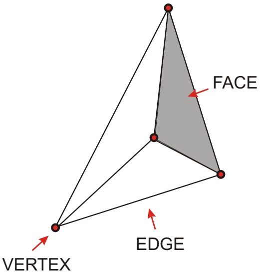




In mathematics: cubic planar graphs, all of whose faces are pentagons and hexagons.

Euler's formula for planar graphs

$$\# \text{ faces} = \# \text{ edges} - \# \text{ vertices} + 2$$



$\Rightarrow$ In a fullerene: 12 pentagons and all other faces hexagonal.

Our motivation for the study of fullerenes - structural properties of fullerenes

The question of finding or proving existence of Hamilton (or long) cycles or paths in graphs has long been an active area of research.

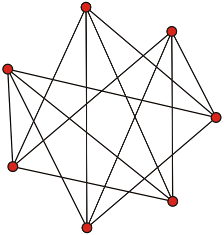
- Hamilton cycle = simple cycle traversing every vertex
- Hamilton path = simple path traversing every vertex

Two particular instances of this general problem are:

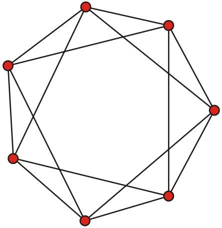
- Hamilton cycles/paths in vertex-transitive graphs (Lovasz,'69)
- Hamilton cycles in fullerenes - a special case of one of Barnette's conjectures.

Does every connected vertex-transitive graph have a Hamilton path?

A graph $X = (V, E)$ *is vertex-transitive if for any pair of vertices u,v there exists an automorphism* α *such that* $\alpha(u) = v$.

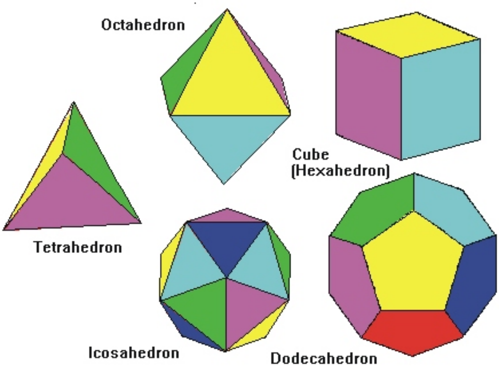


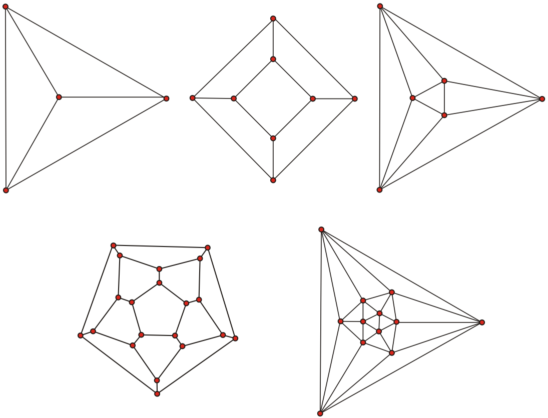
Is not VT



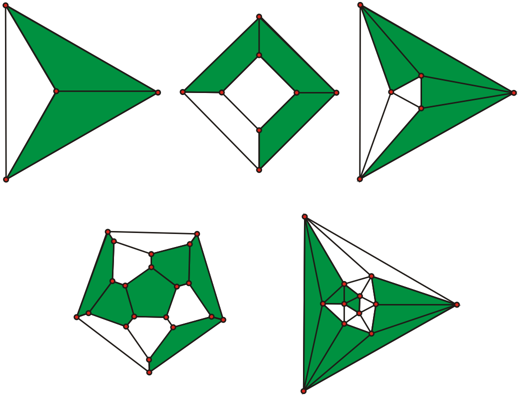
Is VT

Examples


Octahedron
Cube
(Hexahedron)
Tetrahedron
Icosahedron
Dodecahedron



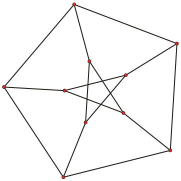
Examples

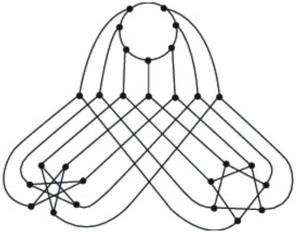


Only four connected VTG ($n > 2$) without Hamilton cycle are known:

- Petersen graph
- truncated Petersen graph
- Coxeter graph
- truncated Coxeter graph

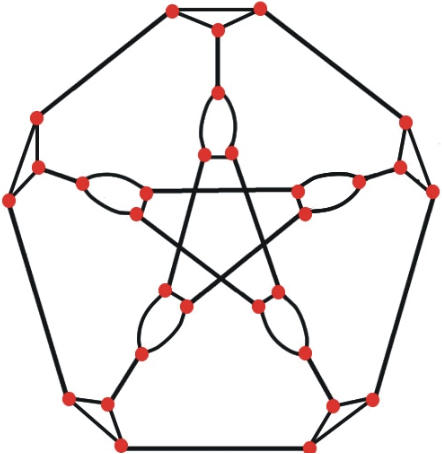
The Petersen graph





The Coxeter graph

The truncation of the Petersen graph



Given a group G and a subset S of $G \setminus \{1\}$ such that $S = S^{-1}$, the Cayley graph $\mathrm{Cay}(G, S)$ has vertex set G and edges of the form

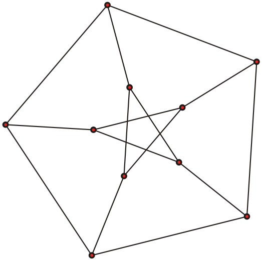
$$\{g, gs\} \text{ for all } g \in G \text{ and } s \in S.$$

- Every Cayley graph is vertex-transitive.
- There exist vertex-transitive graphs that are not Cayley.

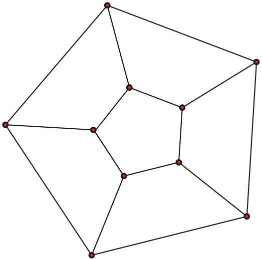
Conjecture

Every connected Cayley graph has a Hamilton cycle.

Example



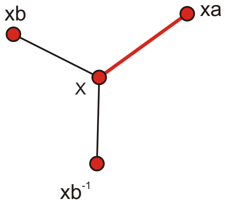
Is not Cayley



Is Cayley

Given a group G and a generating set S of G, the Cayley graph $\mathrm{Cay}(G, S)$ is cubic iff $|S| = 3$ and

- $S = \{a, b, c \mid a^2 = b^2 = c^2 = 1\}$ or
- $S = \{a, b, b^{-1} \mid a^2 = b^s = 1\}$.



Theorem (Glover, Marušič, 2007)

Let $s \geq 3$ be an integer, let G be a group with a presentation $G = \langle a, b \mid a^2 = b^s = (ab)^3 = 1, ect.\rangle$, and let $S = \{a, b, b^{-1}\}$. Then

- if $|G| \equiv 2(mod\ 4)$ the Cayley graph $Cay(G, S)$ has a Hamilton cycle, and
- if $|G| \equiv 0(mod\ 4)$ the Cayley graph $Cay(G, S)$ has a cycle missing out only two adjacent vertices and therefore a Hamilton path.

Theorem (Glover, KK, Marušič, 2009)

If $s \equiv 0(mod\ 4)$ or s is odd then the Cayley graph $Cay(G, S)$ has a Hamilton cycle.

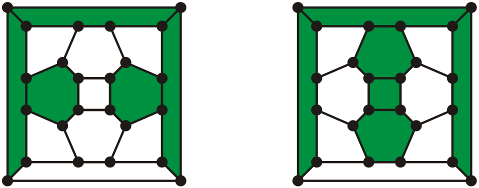
Each Cayley graph we study has a canonical Cayley map given by an embedding of the Cayley graph $X = Cay(G, \{a, b, b^{-1}\})$ of the $(2, s, 3)$-presentation of a group $G = \langle a, b | a^2 = 1, b^s = 1, (ab)^3 = 1, etc. \rangle$ in the closed orientable surface of genus

$$1 + (s - 6)\frac{|G|}{12s}$$

with faces $\frac{|G|}{s}$ disjoint s-gons and $\frac{|G|}{3}$ hexagons.

How is this done?

By finding a tree of faces in this canonical Cayley map whose boundary encompasses all vertices of the graph.



A tree of faces

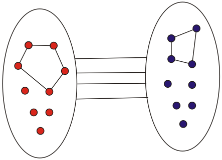
The Buckminsterfullerene is one of only two vertex-transitive fullerenes (the other is the Dodecahedron) and it is in fact a Cayley graph of A_5.

Essential ingredient in this Hamiltonian tree of faces method is the concept of cyclic edge-connectivity and to use a similar method in the context of fullerenes cyclic edge-connectivity of fullerenes need to be studied.

Cyclic edge connectivity of fullerenes

Cycle-separating subset

A subset $F \subseteq E(X)$ of edges of X is said to be cycle-separating (or cyclic-edge cutset) if $X - F$ is disconnected and at least two of its components contain cycles. A cycle-separating subset F of size k is trivial if at least one of the resulting components induces a single k-cycle.



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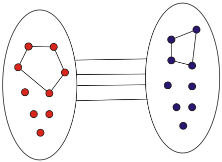
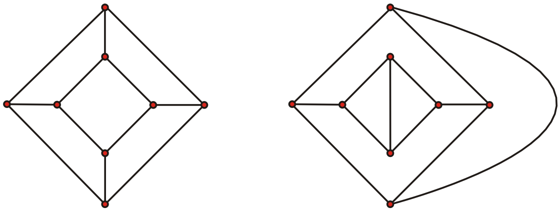


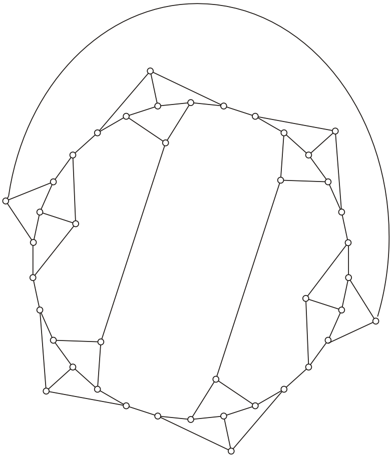
Cyclically k-edge-connected graphs

A graph X is cyclically k-edge-connected, if no set of fewer than k edges is cycle-separating in X.



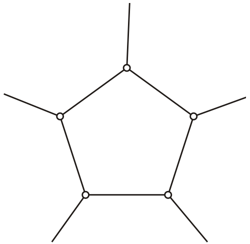
yes no

Is it $c.4.c$?



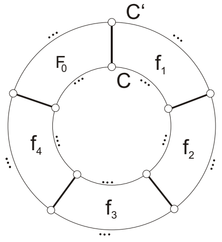
No.

- clearly the cyclic edge-connectivity ≤ 5,
  (since by deleting 5 edges connecting a 5-gonal face, two components each containing a cycle are obtained)

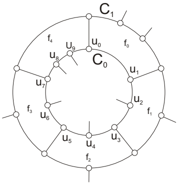


- It was proven that it is in fact precisely 5 (Došlić, 2003).
- The girth of a fullerene is 5.

Let F be a fullerene admitting a nontrivial cycle-separating subset of size 5. Then F contains a ring R of five faces.



$\Rightarrow$ All faces in R are hexagonal.



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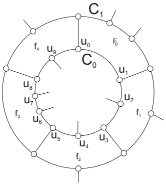

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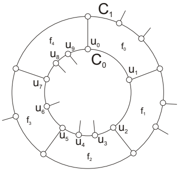

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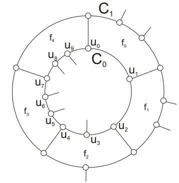

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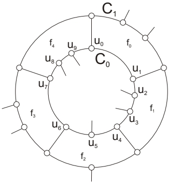

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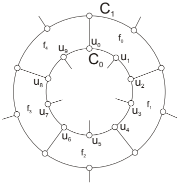

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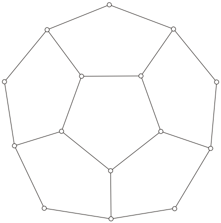
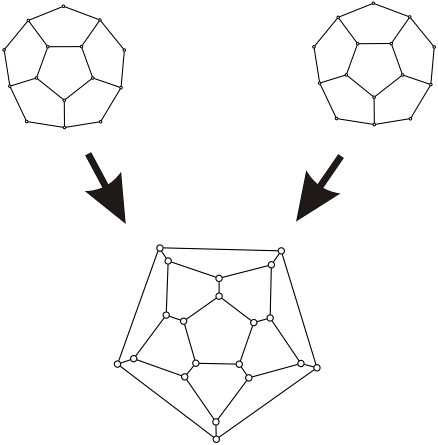


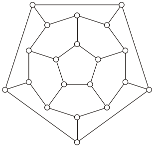
A planar graph on 15 vertices with 7 faces of which one is a 10-gon and six are pentagons.

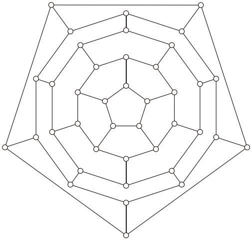
2 pentacaps = the dodecahedron



Theorem (Marušič, KK, 2008 & Kardoš, Škrekovski, 2008)

Let F be a fullerene admitting a nontrivial cyclic-5-cutset. Then F contains a pentacap, more precisely, it contains two disjoint antipodal pentacaps.





Recently Shiu, Li and Chan (Australasian J. Combin., 2010) characterized the spectrum of fullerenes admitting a nontrivial cyclic-5-cutset.

A cyclic cutset F of a fullerene graph X is non-degenerate, if both components of $X - F$ contain precisely six pentagons. Otherwise, F is degenerate.

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- Trivial cyclic cutsets are degenerate.
- Non-trivial cyclic-5-edge cutsets are non-degenerate.

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In 2008 Kardoš and Škrekovski characterized fullerenes admitting a nontrivial cyclic-6-cutset.

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In 2008 Kardoš and Škrekovski characterized fullerenes admitting a nontrivial cyclic-6-cutset.

- Not all the non-trivial cyclic-6-cutsets of fullerenes are non-degenerate.

Kardoš, Krnc, Lužar, Škrekovski, 2010

If there exists a non-degenerate cyclic-7-cutset in a fullerene then the graph is a nanotube unless it is one of the two exceptions given in their paper.

A fullerene is a nanotube, if it can be divided into a cylindrical part containing only hexagons, and two caps, each containing six pentagons and maybe some hexagons. Moreover, at least one of the pentagons should have an edge incident to the outer face of a cap.

Hamilton cycles in fullerenes

Barnette's conjecture

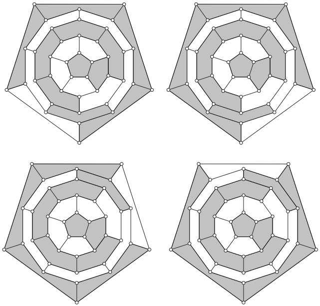
Every 3-connected planar graph with largest face size 6 contains a Hamilton cycle.

Weaker conjecture

Every fullerene contains a Hamilton cycle.

Theorem (Marušič, KK, 2008)

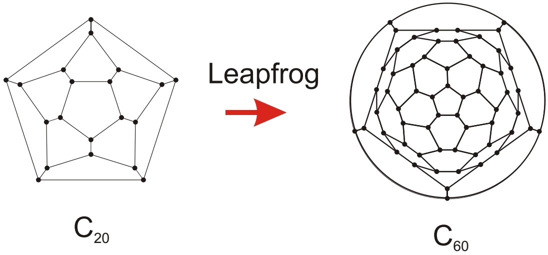
Let X be a fullerene admitting a nontrivial cyclic 5-cutset. Then X has a Hamilton cycle.

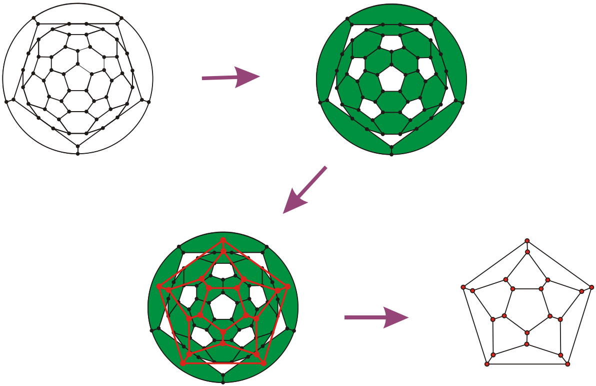


Leapfrog fullerenes

Leapfrog Leap is a composite operation which can be written as

$$\mathrm{Leap}(F) = Tr(Du(F))$$

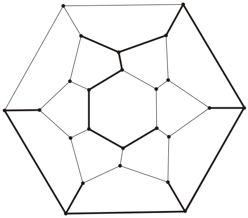


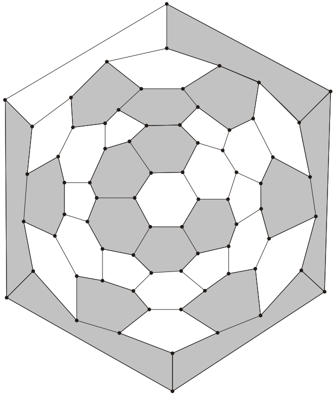


Theorem (Marušič, 2007)

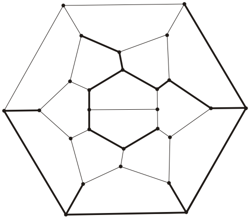
Let X be a fullerene with n vertices. Then the leapfrog-fullerene $Le(X)$ has a Hamilton cycle if $n \equiv 2 \pmod 4$ and contains a long cycle missing out only two adjacent vertices if $n \equiv 0 \pmod 4$.

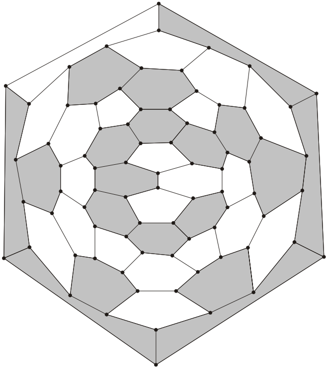
$Leap(C_{24})$





$Leap(C_{26})$



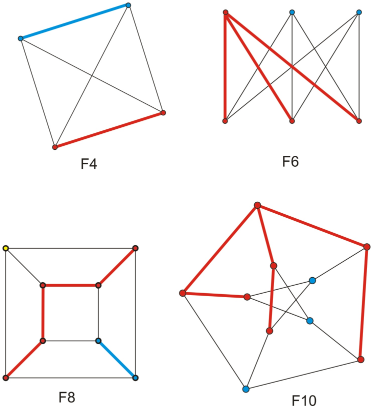


Theorem (Payan, Sakarovitch, 1975)

Let X be a cyclically 4-connected cubic graph of order n, and let S be a maximum cyclically stable subset of $V(X)$. Then $|S| = \lfloor (3n-2)/2 \rfloor$ and more precisely, the following hold.

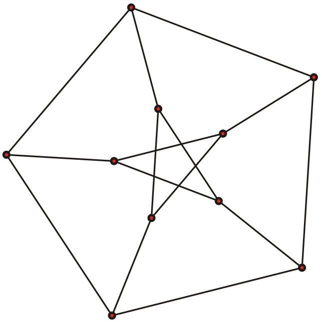
- If $n \equiv 2 \,(mod\, 4)$ then $|S| = (3n-2)/4$, and $X[S]$ is a tree and $V(X) \setminus S$ is an independent set of vertices;
- If $n \equiv 0 \,(mod\, 4)$ then $|S| = (3n-4)/4$, and either $X[S]$ is a tree and $V(X) \setminus S$ induces a graph with a single edge, or $X[S]$ has two components and $V(X) \setminus S$ is an independent set of vertices.

Cyclically stable subsets



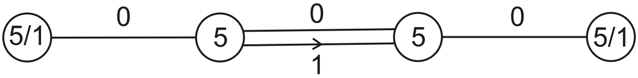
Semiregular automorphisms in fullerenes

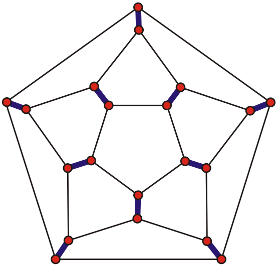
A semiregular element of a permutation group is a non-identity element having all cycles of equal length in its cycle decomposition.



The Petersen graph has a semiregular automorphism with two orbits of size 5.

The dodecahedron given in Frucht's notation relative to a semiregular automorphism with 4 orbits of size 5.





Open problem (Marušič, 1981)

Is it true that a vertex-transitive digraph contains a semiregular automorphism?

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.

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.

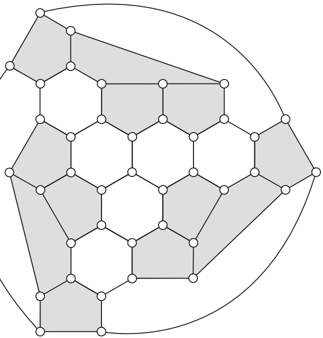
Motivated by this problem we recently characterized fullerenes with regards to the existence of semiregular automorphisms in their automorphism groups.

Theorem (Janežič, Marušič, KK, 2010)

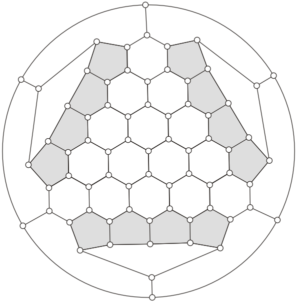
Let F be a fullerene with non-trivial automorphism group. Then either F admits a semiregular automorphism or $\mathrm{Aut}(F) \cong \mathbb{Z}_2$, $\mathbb{Z}_3$ or S_3.

- The automorphism group $\mathrm{Aut}(F)$ of a fullerene F is a subgroup of a $\{2, 3, 5\}$-group (Fowler, Manolopoulos, Redmond and Ryan, 1993).
- Let F be a fullerene admitting an automorphism $\alpha \in \mathrm{Aut}(F)$ of order 5. Then α is a semiregular automorphism of F.
- 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.

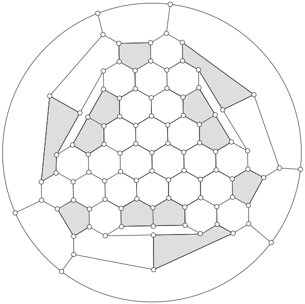
Example of a fullerene having a semiregular automorphism



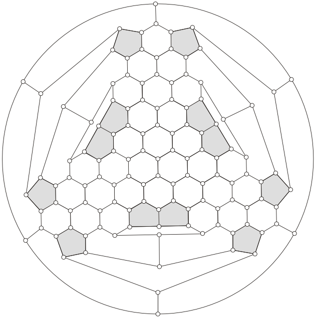
A fullerene of order 40 without a semiregular automorphism with the full automorphism group isomorphic to the cyclic group $\mathbb{Z}_3$.



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.



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 S_3.



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.

Thank you !