Fullerenes and Fulleroids

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- There are two well-known forms of carbon: diamond and graphite.
  In diamond all atoms are 4-valent and form a 3-dimensional grid.
  In graphite all atoms are 3-valent. They form flat sheets with hexagonal structure.

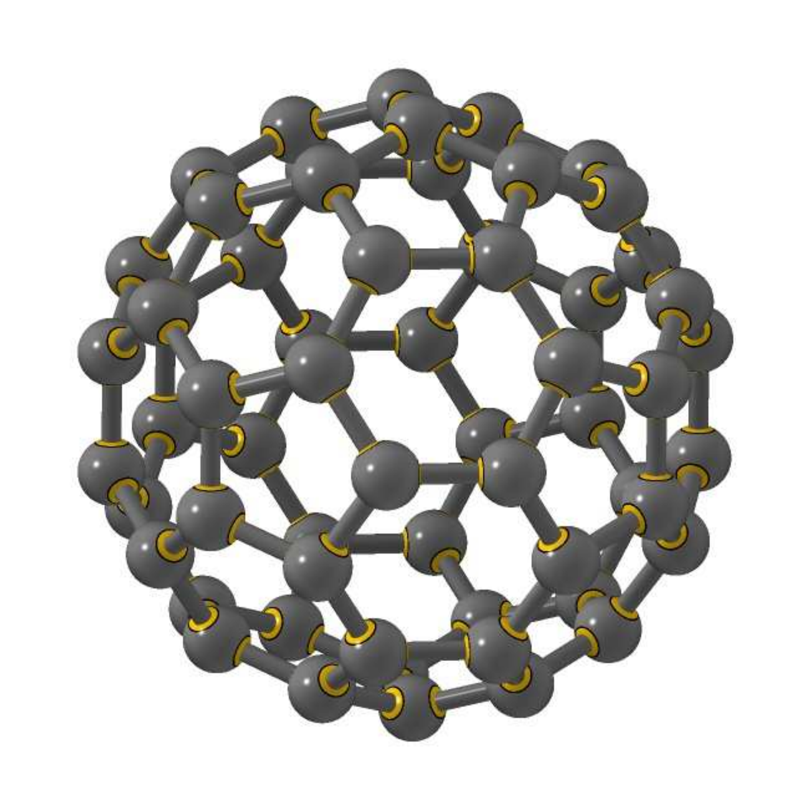
How did it begin?

In 80s, certain experiments predicted the existence of molecules with the exact mass of sixty or seventy or more carbon atoms. In 1985, Harold Kroto (then of the University of Sussex, now of Florida State University), James R. Heath, Sean O'Brien, Robert Curl and Richard Smalley, from Rice University, discovered C_{60}, and shortly after came to discover the fullerenes.

Kroto, Curl, and Smalley were awarded the 1996 Nobel Prize in Chemistry for their roles in the discovery of this class of compounds.

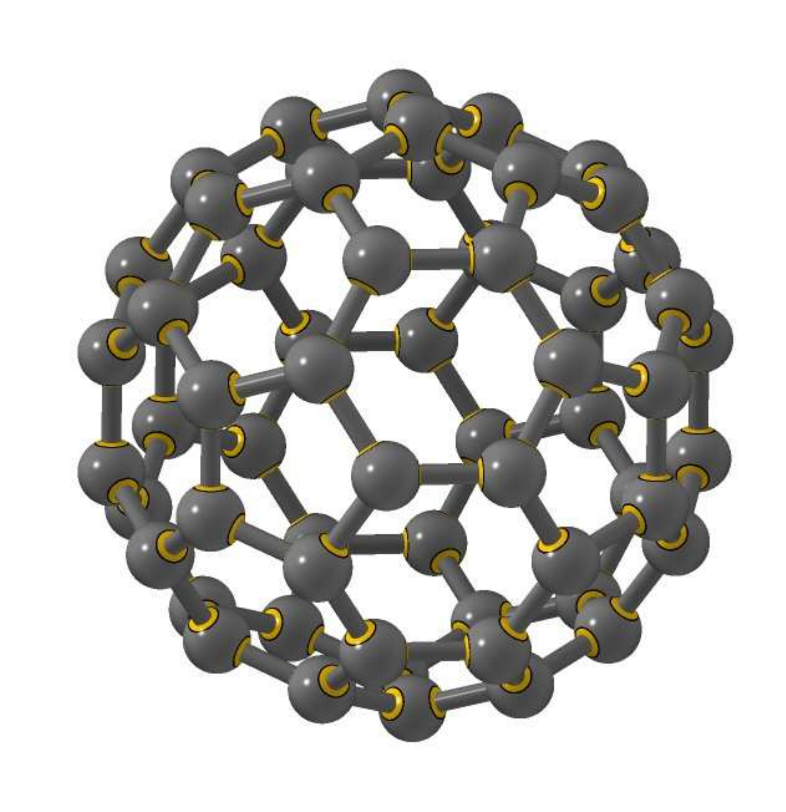
The buckyball C_{60}

The most common and the most known fullerene is the Buckminsterfullerene C_{60}. It is the smallest fullerene in which no two pentagons share an edge. It was named after Richard Buckminster Fuller, a noted architect who popularized the geodesic dome. Later the name got shortened to buckyball.



The buckyball C_{60}

The structure of C_{60} is a truncated icosahedron. It resembles a round soccer ball of the type made of hexagons and pentagons.
The pattern of soccer ball with white hexagons and black pentagons appeared first in 70s. In that times no one suspected it could be a model for a carbon molecule...

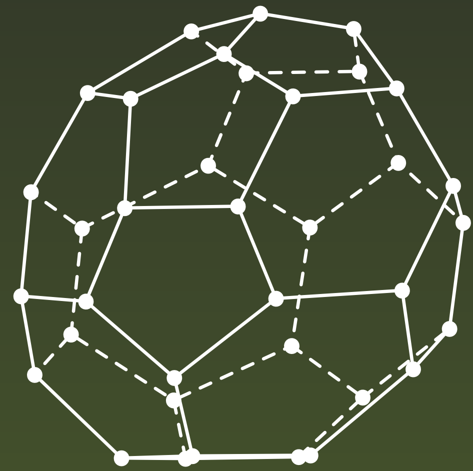


The buckyball C_{60}

A truncated icosahedron and a soccer ball

Fullerene graphs

- *Fullerene graph* is a planar, 3-regular and 3-connected graph, the faces of which are only pentagons and hexagons.



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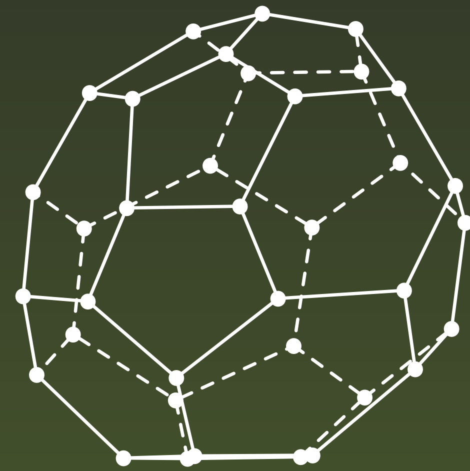
- Steinitz's Theorem: A graph G is polytopal (e.g. isomorphic to the graph of a convex polyhedron) if and only if G is planar and 3-connected.



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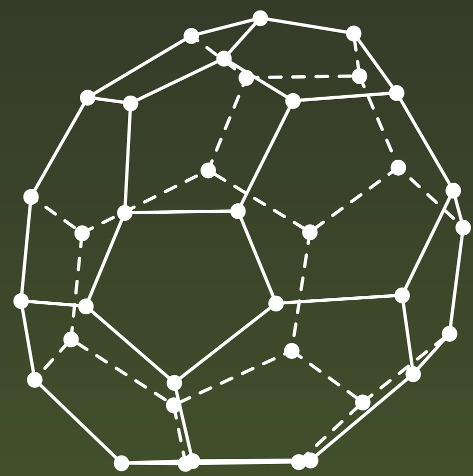
- Steinitz's Theorem: A graph G is polytopal (e.g. isomorphic to the graph of a convex polyhedron) if and only if G is planar and 3-connected.
- Whitney's Theorem: Planar 3-connected (polytopal) graphs can be embedded in the plane essentially only one way.



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Euler's formula:

$$\begin{aligned} v + f_5 + f_6 &= 2 + e \\ 6v + 6f_5 + 6f_6 &= 12 + 4e + 2e \\ f_5 &= 12 \end{aligned}$$

thus the number of pentagons in a fullerene graph is exactly 12.

Fullerene graphs

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The number of (non-isomorphic) fullerene graphs with n vertices for some even numbers n:

20	22	24	26	28	30	40	60	80	100
1	0	1	1	2	3	40	1812	31924	285913

[P. W. Fowler, D. E. Manolopoulos: Atlas of Fullerenes]

Perfect matchings in fullerene graphs

A perfect matching in a graph is a set of pairwise non-adjacent edges of G which covers all vertices of G. A perfect matching is in chemistry called a *Kekulé structure*. The more perfect matchings the fullerene graph has, the more stable the fullerene molecule is supposed to be.

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4 Colour Theorem: Any planar cubic graph is decomposable into 3 perfect matchings.

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Every fullerene graph with p vertices contains at least $\frac{p}{4} + 2$ different perfect matchings.

Perfect matchings in fullerene graphs

Graph G is *bicritical* if $G - u - v$ contains a perfect matching for every pair of distinct vertices of G.

Graph G is *cyclically k-edge-connected* if G cannot be separated onto two components, each containing a cycle, by deletion of fewer then k edges.

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[T. Došlić] Every fullerene graph is cyclically 4-edge connected.

Perfect matchings in fullerene graphs

[T. Došlić] Every fullerene graph is cyclically 5-edge connected.

Symmetry of fullerenes

The presence of symmetry elements in a fullerene molecule can have important consequences on its various chemical and physical properties. It is important to know the possible symmetries of fullerene structures if the structure of higher fullerene is to be discovered and proved.
Given a fullerene, one can look for *symmetry objects* such as mirror planes and rotational axes.
The reflections, rotations and other *symmetries* altogether form the *symmetry group*.

Symmetry of convex polyhedra

Possible symmetry groups
(*point groups*):

- icosahedral: $\mathscr{I}_h$, $\mathscr{I}$
- octahedral: $\mathscr{O}_h$, $\mathscr{O}$
- tetrahedral: $\mathscr{T}_h$, $\mathscr{T}_d$, $\mathscr{T}$
- cylindrical: $\mathscr{D}_{nh}$, $\mathscr{D}_{nd}$, $\mathscr{D}_n$ $(n \geq 2)$
- skewed: $\mathscr{S}_{2n}$, $\mathscr{C}_{nh}$ $(n \geq 2)$
- pyramidal: $\mathscr{C}_{nv}$, $\mathscr{C}_n$ $(n \geq 2)$
- low symmetry: $\mathscr{C}_s$, $\mathscr{C}_i$, $\mathscr{C}_1$

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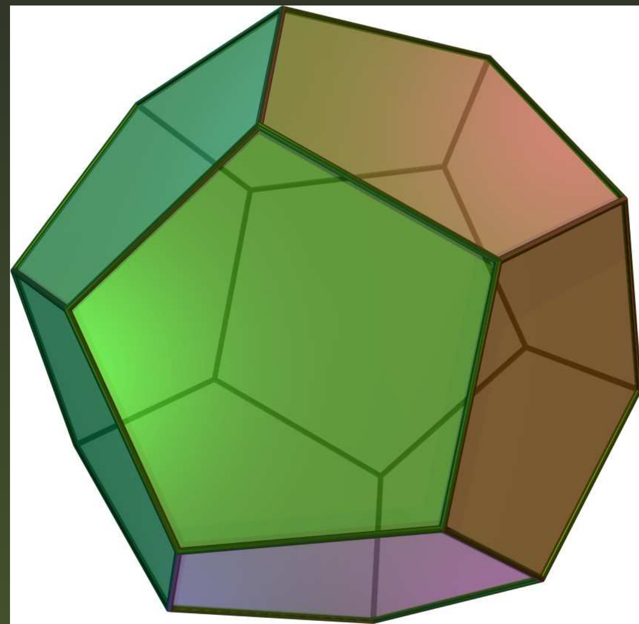

The regular dodecahedron has $\mathscr{I}_h$ symmetry

Local symmetry

In fullerene graphs, all vertices are 3-valent and all faces are pentagons or hexagons. Therefore, any symmetry axis must be of 2-fold, 3-fold, 5-fold or 6-fold rotational symmetry. This restriction reduces the list of possible symmetry groups of fullerenes to 36 groups:

- icosahedral: $\mathscr{I}_h$, $\mathscr{I}$
- tetrahedral: $\mathscr{T}_h$, $\mathscr{T}_d$, $\mathscr{T}$
- cylindrical: $\mathscr{D}_{6h}$, $\mathscr{D}_{6d}$, $\mathscr{D}_6$, $\mathscr{D}_{5h}$, $\mathscr{D}_{5d}$, $\mathscr{D}_5$, $\mathscr{D}_{3h}$, $\mathscr{D}_{3d}$, $\mathscr{D}_3$, $\mathscr{D}_{2h}$, $\mathscr{D}_{2d}$, $\mathscr{D}_2$
- skewed: $\mathscr{S}_{12}$, $\mathscr{C}_{6h}$, $\mathscr{S}_{10}$, $\mathscr{C}_{5h}$, $\mathscr{S}_6$, $\mathscr{C}_{3h}$, $\mathscr{S}_4$, $\mathscr{C}_{2h}$
- pyramidal: $\mathscr{C}_{6v}$, $\mathscr{C}_6$, $\mathscr{C}_{5v}$, $\mathscr{C}_5$, $\mathscr{C}_{3v}$, $\mathscr{C}_3$, $\mathscr{C}_{2v}$, $\mathscr{C}_2$
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Local symmetry

[P. W. Fowler, D. E. Manolopoulos, D. B. Redmond, and R. P. Ryan] Whenever 5-fold or 6-fold rotational axis is present, a perpendicular 2-fold rotational axis is forced. This means that $\mathscr{C}_5$, $\mathscr{C}_{5v}$, $\mathscr{C}_{5h}$, and $\mathscr{S}_{10}$ symmetries occur only as subgroups of fivefold dihedral ($\mathscr{D}_{5h}$, $\mathscr{D}_{5d}$, $\mathscr{D}_5$), or icosahedral ($\mathscr{I}_h$, $\mathscr{I}$) groups; likewise $\mathscr{C}_6$, $\mathscr{C}_{6v}$, $\mathscr{C}_{6h}$ and $\mathscr{S}_{12}$ symmetries occur only as subgroups of sixfold dihedral groups ($\mathscr{D}_{6h}$, $\mathscr{D}_{6d}$, $\mathscr{D}_6$). The list of possible symmetries of fullerenes thus contains 28 groups.

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[Graver] Catalogue of all fullerenes with ten or more symmetries

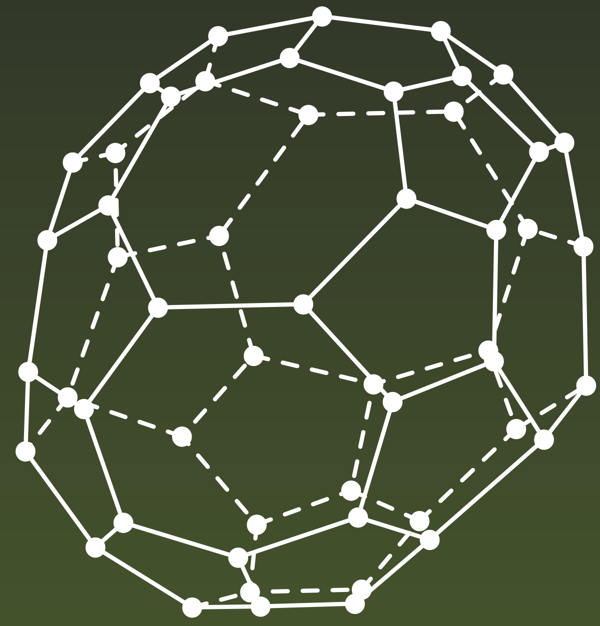
Symmetry of fullerenes

group	#1	#2	group	#1	#2	group	#1	#2
$\mathscr{I}_h$	20	60	$\mathscr{D}_5$	60	100	$\mathscr{C}_{3v}$	34	82
$\mathscr{I}$	140	140	$\mathscr{D}_{3h}$	26	74	$\mathscr{C}_3$	40	86
$\mathscr{T}_h$	92	116	$\mathscr{D}_{3d}$	32	84	$\mathscr{C}_{2h}$	48	108
$\mathscr{T}_d$	28	76	$\mathscr{D}_3$	32	78	$\mathscr{C}_{2v}$	30	78
$\mathscr{T}$	44	88	$\mathscr{D}_{2h}$	40	92	$\mathscr{C}_2$	32	82
$\mathscr{D}_{6h}$	36	84	$\mathscr{D}_{2d}$	36	84	$\mathscr{C}_s$	34	82
$\mathscr{D}_{6d}$	24	72	$\mathscr{D}_2$	28	76	$\mathscr{C}_i$	56	120
$\mathscr{D}_6$	72	120	$\mathscr{S}_6$	68	128	$\mathscr{C}_1$	36	84
$\mathscr{D}_{5h}$	30	70	$\mathscr{S}_4$	44	108			
$\mathscr{D}_{5d}$	40	80	$\mathscr{C}_{3h}$	62	116			

For each group Γ the number of vertices of the smallest Γ-fullerene (#1) and the number of vertice of the smallest Γ-fullerene without adjacent pentagons (#2) are listed.

Fulleroids

- *Fulleroid* is a cubic convex polyhedron with faces of size 5 or greater.



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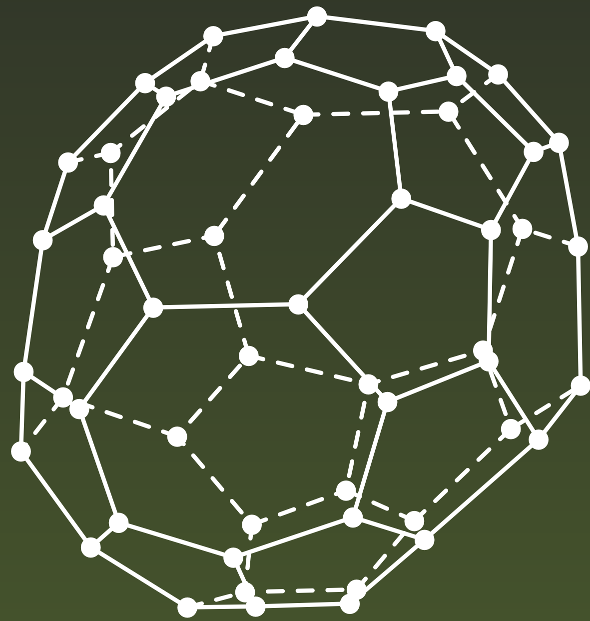

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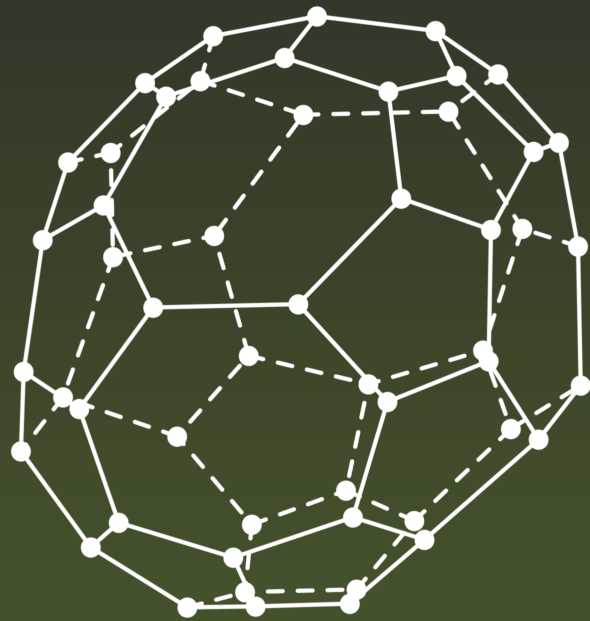
- only pentagons and hexagons $\Rightarrow$ fullerenes
- only pentagons and n-gons $\Rightarrow$ $(5, n)$-fulleroids



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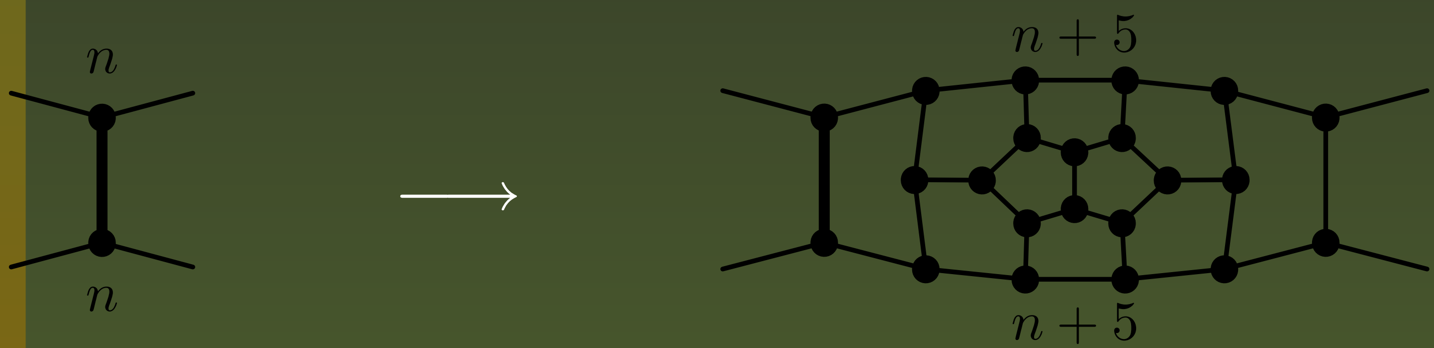
- Given a point group Γ, for which numbers n there exist $(5, n)$-fulleroids with the symmetry group Γ?
- If there are some $\Gamma(5, n)$-fulleroids for some group Γ and some number n, are there infinitely many of them?

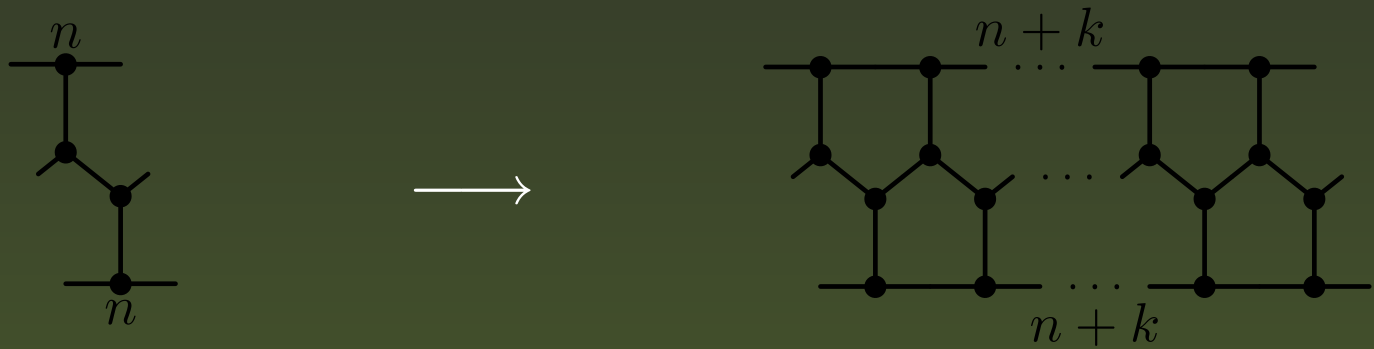
Construction of fulleroids

To create infinite series of examples of fulleroids, one can use several operations:
If two n-gons are connected by an edge, by inserting 10 pentagons they are changed to $(n+5)$-gons:



Construction of fulleroids

If two n-gons are separated by two faces, the size of them can be increased arbitrarily.



Construction of fulleroids

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 $n=7$ we need two additional pentagons if the operation is to be carried out again: