Symmetry of Fulleroids

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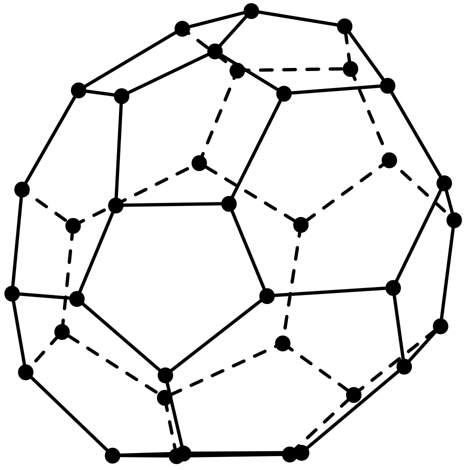
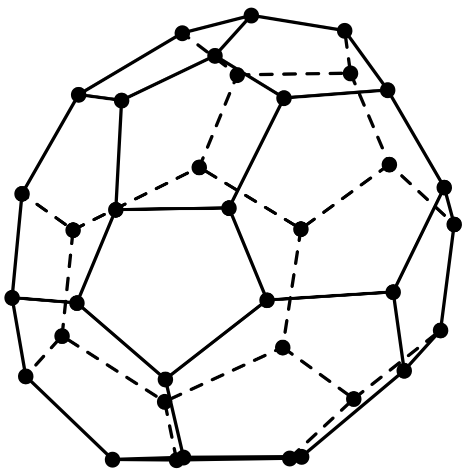
Fullerenes and Fullerene Graphs

- *Fullerene* is a 3-regular (or cubic) carbon molecule, where atoms are arranged in pentagons and hexagons.



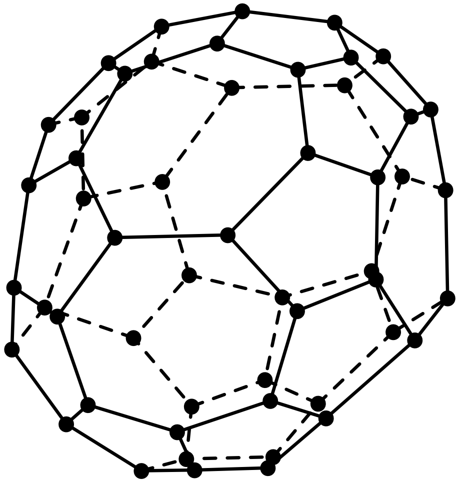
Fullerenes and Fullerene Graphs

- *Fullerene* is a 3-regular (or cubic) carbon molecule, where atoms are arranged in pentagons and hexagons.
- *Fullerene graph* is a planar, 3-regular and 3-connected graph, twelve of whose faces are pentagons and any remaining faces are hexagons.



Fulleroids

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



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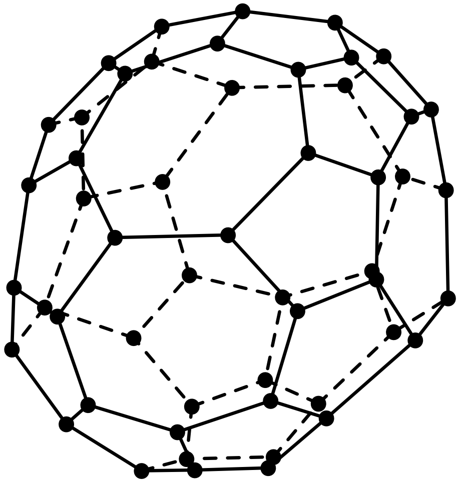

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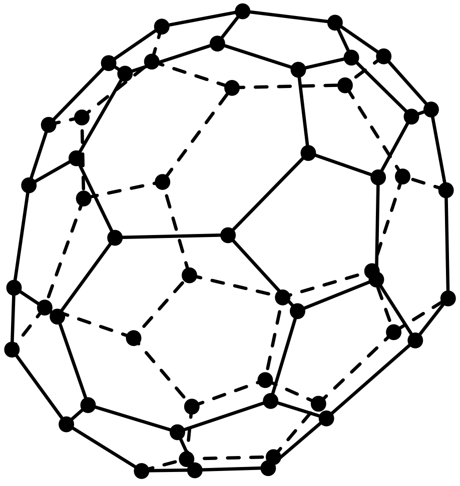
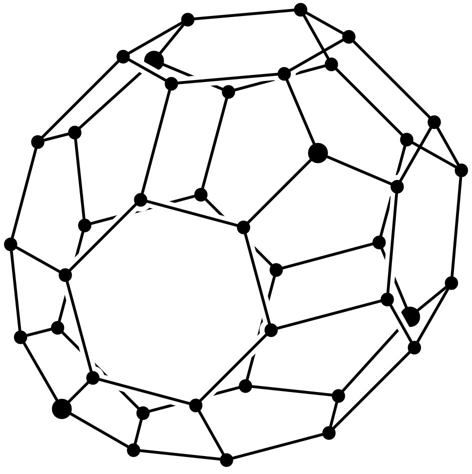


- only pentagons and hexagons $\Rightarrow$ fullerenes
- only pentagons and n-gons $\Rightarrow (5, n)$-fulleroids

Symmetry of convex polyhedra

rotations, reflections, point inversion. . .



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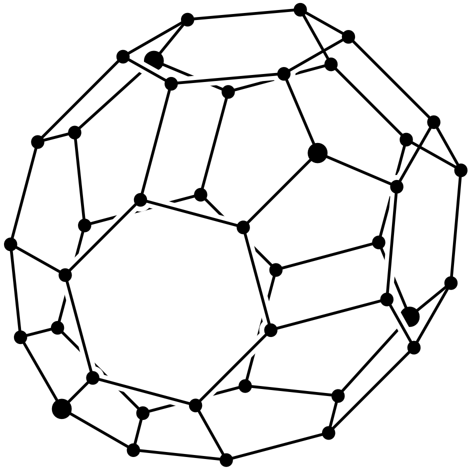

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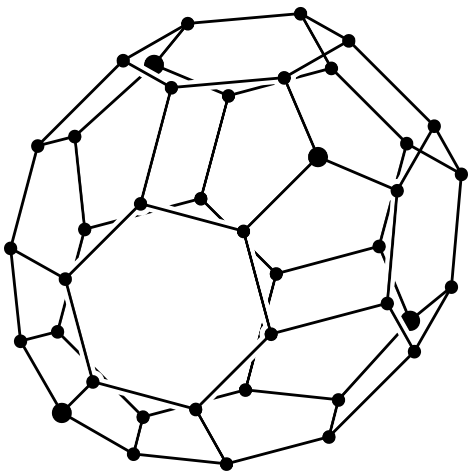
Possible symmetry groups:



- 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: $\mathscr{C}_s$, $\mathscr{C}_i$, $\mathscr{C}_1$

Symmetry of fullerenes

Fowler and al. (1993): Possible symmetry: only 28 out of 36 groups

Babić, Klein and Sah (1993): All fullerenes with up to 70 vertices classified according to the symmetry group

Fowler and Manolopoulos (1995): Symmetry of all fullerenes with up to 100 vertices; the smallest Γ-fullerene for each symmetry group Γ; the smallest Γ-fullerene without adjacent pentagons for each symmetry group Γ

Graver (2001): Catalogue of all fullerenes with ten or more symmetries

Icosahedral fulleroids

Dress and Brinkmann (1996): The smallest $\mathscr{I}_h(5,7)$ and $\mathscr{I}(5,7)$-fulleroids are unique

Delgado Friedrichs and Deza (2000): $\mathscr{I}_h(5,n)$-fulleroids for $n = 8$, 9, 10, 12, 14 and 15

Jendrol' and Trenkler (2001): $\mathscr{I}(5,n)$-fulleroids for all $n \geq 8$

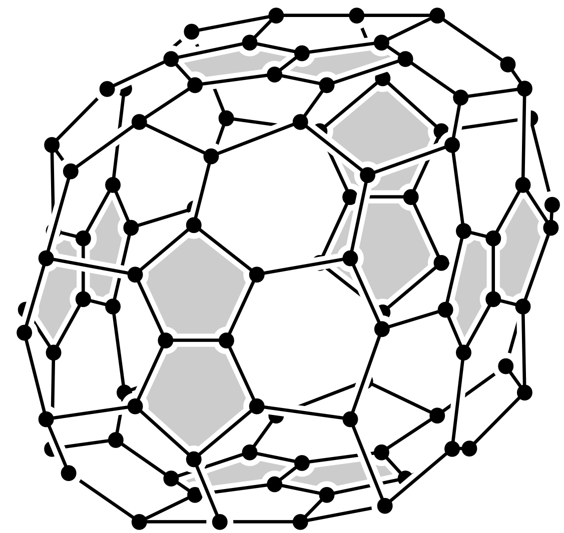
K.:$\mathscr{I}(5,n)$-fulleroids for all $n \geq 7$

Octahedral fulleroids

Jendrol' and K. (to appear): Let $n \geq 7$. Then $\mathscr{O}_h(5, n)$-fulleroids exist if and only if
(i) $n \equiv 0 \pmod{60}$ or
(ii) $n \equiv 0 \pmod{4}$ and $n \not\equiv 0 \pmod{5}$.
K.: Analogous claim for the group $\mathscr{O}$.

Tetrahedral fulleroids

K. (to appear): Let $n \geq 6$. Then $\mathscr{T}_d(5,n)$-fulleroids exist if and only if $n \not\equiv 5 \pmod{10}$. $\mathscr{T}(5,n)$- and $\mathscr{T}_h(5,n)$-fulleroids exist for all $n \geq 6$.



Other symmetry types I.

The groups Γ, for which $\Gamma(5, n)$-fulleroids exist for all $n \geq 6$: $\mathcal{D}_{5d}$, $\mathcal{D}_{3d}$, $\mathcal{D}_{2h}$, $\mathcal{D}_{5}$, $\mathcal{D}_{3}$, $\mathcal{D}_{2}$, $\mathcal{S}_{6}$, $\mathcal{C}_{3v}$, $\mathcal{C}_{2v}$, $\mathcal{C}_{2h}$, $\mathcal{C}_{3}$, $\mathcal{C}_{2}$, $\mathcal{C}_{s}$, $\mathcal{C}_{i}$, $\mathcal{C}_{1}$.

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The groups Γ, for which $\Gamma(5, n)$-fulleroids exist for all $n \geq 7$, but not for $n = 6$: $\mathscr{S}_{10}$, $\mathscr{C}_{5v}$, $\mathscr{C}_5$.

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$\mathscr{D}_{5h}(5,n)$-fulleroids exist if and only if $n \not\equiv 5, 10, 15, 20 \pmod{25}$.

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The groups Γ, for which $\Gamma(5,n)$-fulleroids exist if and only if $n \not\equiv 5, 10 \pmod{15}$: $\mathcal{D}_{3h}$, $\mathcal{C}_{3h}$.

$\mathcal{D}_{5h}(5,n)$-fulleroids exist if and only if $n \not\equiv 5, 10, 15, 20 \pmod{25}$.

$\mathcal{C}_{5h}(5,n)$-fulleroids exist if and only if $n \not\equiv 5, 10, 15, 20 \pmod{25}$ and $n \neq 6$.

Other symmetry types II.

The groups Γ, for which $\Gamma(5, n)$-fulleroids exist if and only if n is a multiple of a number m ($m = 4$ or $m \geq 6$): $\mathscr{D}_{md}$, $\mathscr{D}_m$, $\mathscr{S}_{2m}$, $\mathscr{C}_{mv}$, $\mathscr{C}_m$.

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The groups Γ, for which there is one more case of nonexistence in addition – if m is divisible by 5, then $\Gamma(5,n)$-fulleroids exist if and only if n is a multiple of $5m$: $\mathscr{D}_{mh}$, $\mathscr{C}_{mh}$.

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One more exception: There are no fullerenes with $\mathscr{S}_{12}$, $\mathscr{C}_{6v}$, $\mathscr{C}_{6h}$, nor $\mathscr{C}_{6}$ symmetry.

Proving nonexistence

All the cases of nonexistence are either the fullerenes case, or the case of fulleroids with multi-pentagonal faces.

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K.: 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.

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K.: 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.

Proving nonexistence

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. Therefore, there is no cubic convex polyhedron such that the sizes of all its faces are odd multiples of five with the symmetry group $\mathscr{S}_4$, $\mathscr{D}_{2d}$, or $\mathscr{T}_d$.

Proving nonexistence

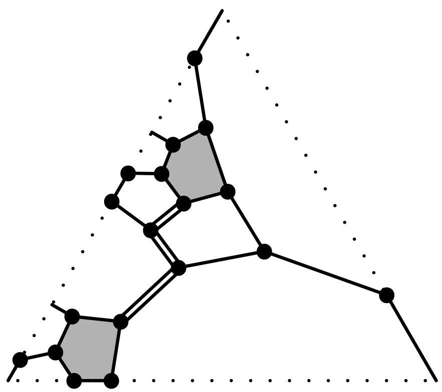
Let P be a cubic convex polyhedron such that all its faces are multi-pentagons and none of the face sizes is divisible by three. Then the symmetry group $\Gamma(P)$ does not contain the group $\mathscr{C}_{3h}$ as a subgroup. Therefore, there is no cubic convex polyhedron P such that all its faces are multi-pentagons, none of the face sizes is divisible by three, and the symmetry group of P is $\mathscr{C}_{3h}$ or $\mathscr{D}_{3h}$.

Proving nonexistence

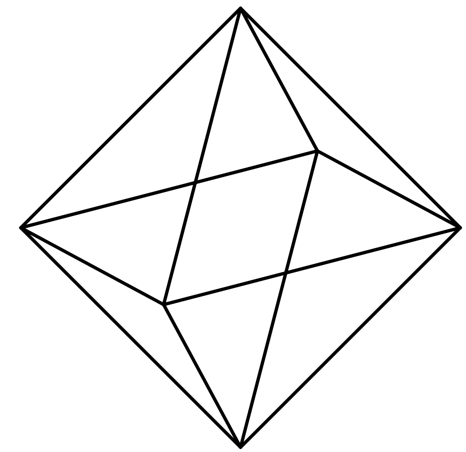
Let P be a cubic convex polyhedron such that all its faces are multi-pentagons and none of the face sizes is divisible by 25. Then the symmetry group $\Gamma(P)$ does not contain the group $\mathscr{C}_{5h}$ as a subgroup. Therefore, there is no cubic convex polyhedron P such that all its faces are multi-pentagons, none of the face sizes is divisible by 25, and the symmetry group of P is $\mathscr{C}_{5h}$ or $\mathscr{D}_{5h}$.

Examples

construction of a graph of a $\mathscr{D}_{2h}(5,9)$-fulleroid:



$\longrightarrow$



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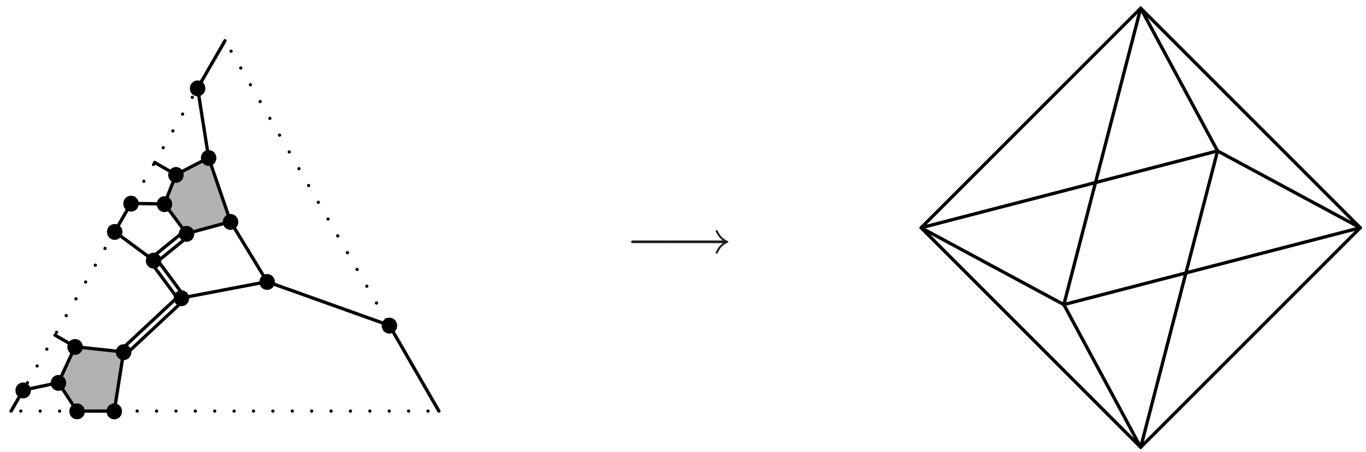
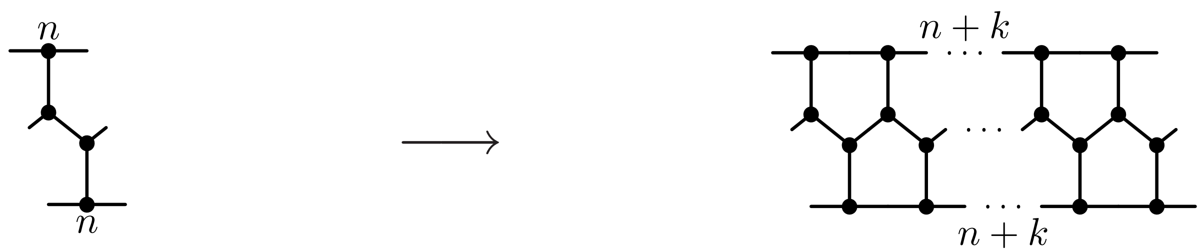


generating infinite series of examples:



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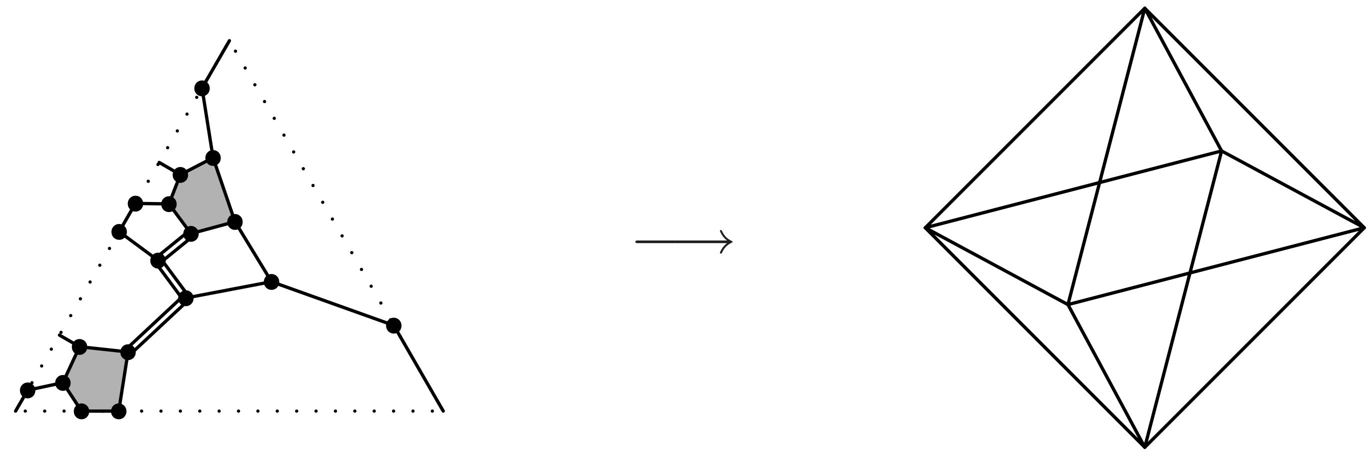
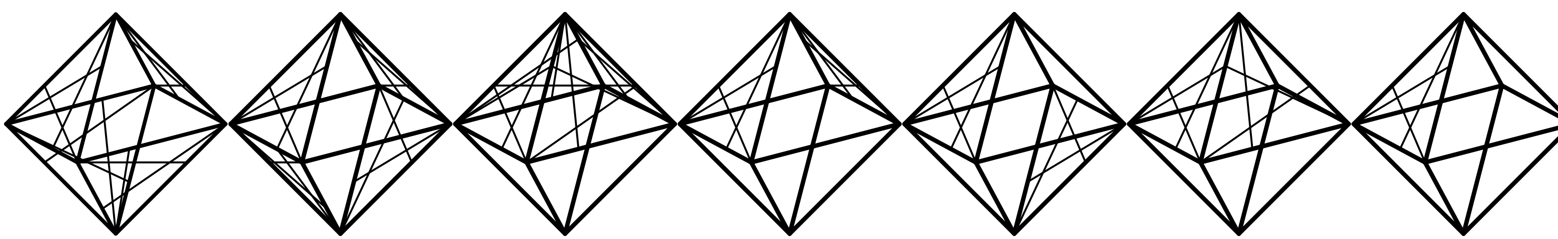


changing the symmetry group:



$\mathscr{D}_2$ $\mathscr{C}_{2h}$ $\mathscr{C}_{2v}$ $\mathscr{C}_2$ $\mathscr{C}_i$ $\mathscr{C}_s$ $\mathscr{C}_1$

Thank you for your attention!