Fullerenes: applications and generalizations

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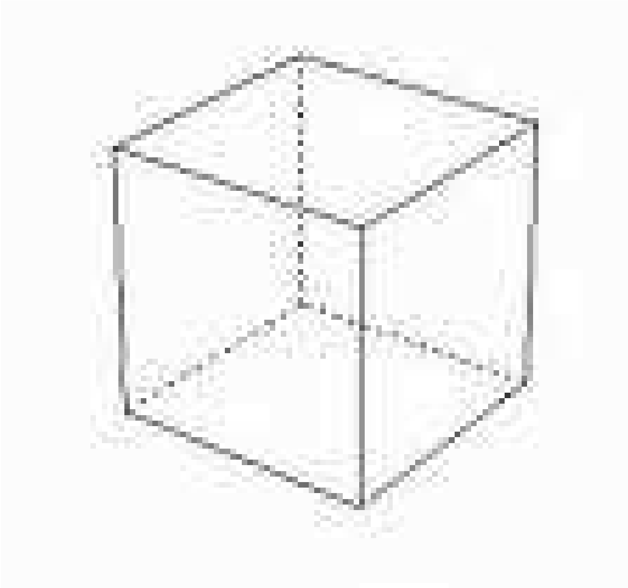
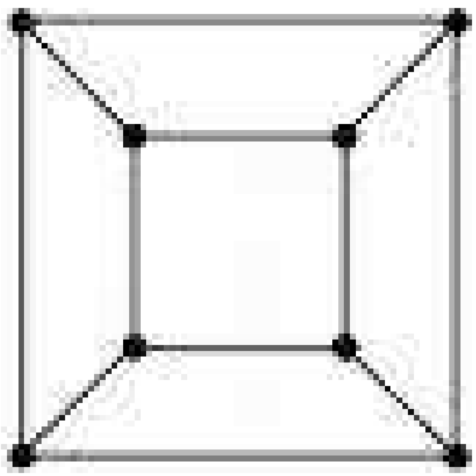
I. General setting

Polytopes and their faces

- A d-polytope: the convex hull of a finite subset of R^d.
- A face of P is the set $\{x \in P : f(x) = 0\}$ where f is linear non-negative function on P.

A face of dimension i is called i-face; for i=$0, 1, 2, d-2, d-1$ it is called, respectively, vertex, edge, face, ridge and facet.

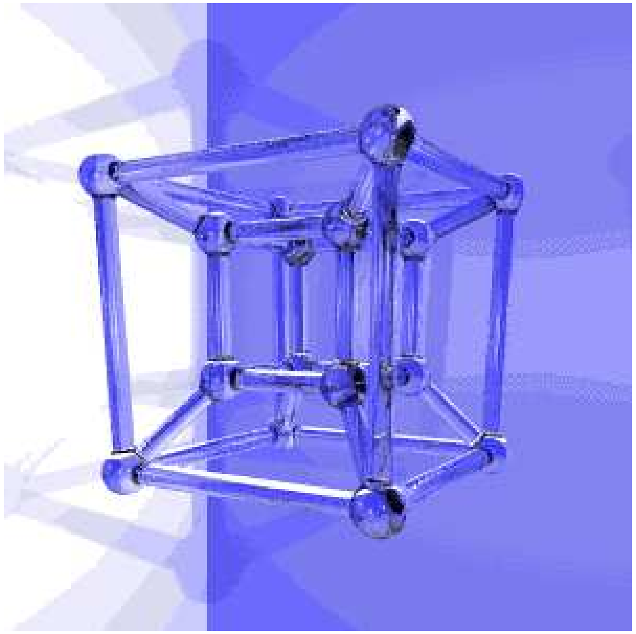




Skeleton of polytope

- The skeleton of polytope P is the graph $G(P)$ formed by vertices, with two vertices *adjacent* if they form an edge. d-polytopes P and P' are of the same combinatorial type if $G(P) \simeq G(P')$.
- The dual skeleton is the graph $G^*(P)$ formed by facets with two facets *adjacent* if their intersection is a ridge. (Poincaré) dual polytopes P and P^* on sphere S^{d-1}: $G^*(P) = G(P^*)$.
- Steinitz's theorem: a graph is the skeleton of a 3-polytope if and only if it is planar and 3-connected, i.e., removing any two edges keep it connected.

4-cube



Regular d-polytopes:
self-dual d-simplex $G(\alpha_d) = K_{d+1}$,
d-cube $G(\gamma_d) = H_d = (K_2)^d$ and
its dual d-cross-polytope $G(\beta_d) = K_{2d} - dK_2$.

Euler formula

f-vector of d-polytope: $(f_0, \dots, f_{d-1}, f_d = 1)$ where f_j is the number of i-faces. Euler characteristic equation for a map on oriented $(d-1)$-surface of genus g:

$\chi = \sum_{j=0}^{d-1} (-1)^j f_j = 2(1-g)$.

For a polyhedron (3-polytope on S^2), it is $f_0 - f_1 + f_2 = 2$.
p-vector: $(p_3, \dots)$ where p_i is number of i-gonal faces.
v-vector: $(v_3, \dots)$ where v_i is number of i-valent vertices.
So, $f_0 = \sum_{i \geq 3} v_i$, $f_2 = \sum_{i \geq 3} p_i$ and $2f_1 = \sum_{i \geq 3} i v_i = \sum_{i \geq 3} i p_i$.

$$\sum_{i \geq 3} (6-i) p_i + \sum_{i \geq 3} (3-i) v_i = 12.$$

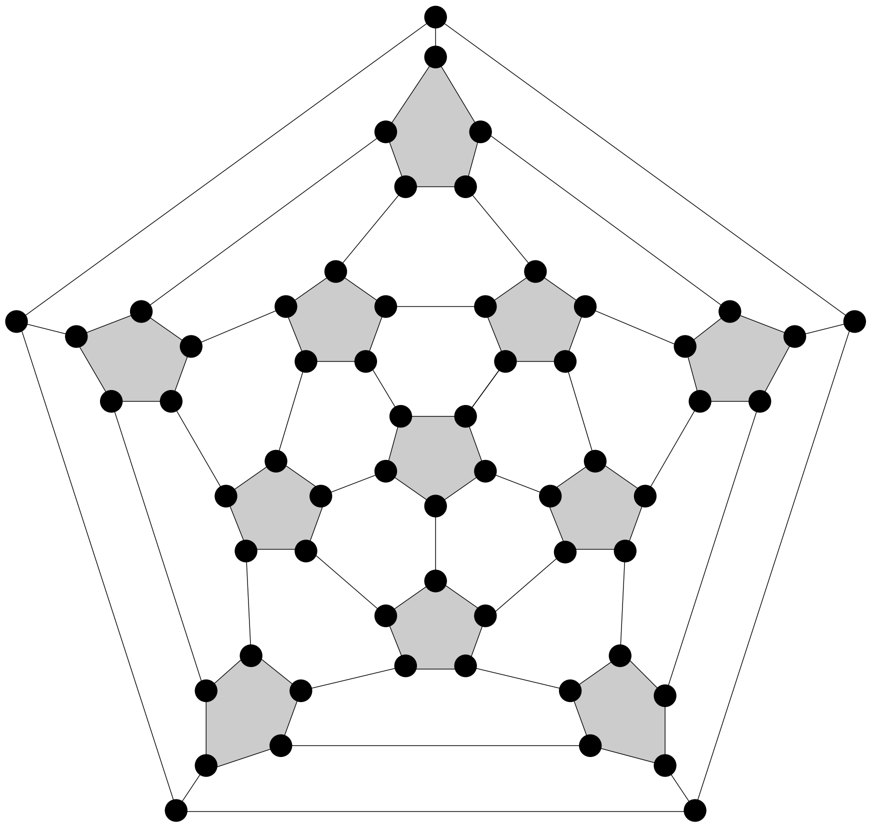
A fullerene polyhedron has $v_i \neq 0$ only for $i = 3$ and $p_i \neq 0$ only for $i = 5, 6$. So, $(6-5)p_5 = p_5 = 12$.

Definition of fullerene

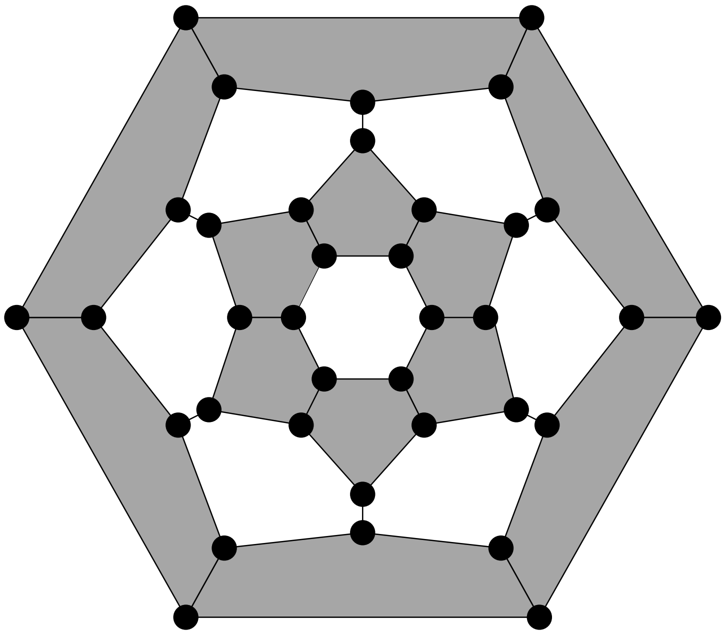
A fullerene F_n is a simple (i.e., 3-valent) polyhedron (putative carbon molecule) whose n vertices (carbon atoms) are arranged in 12 pentagons and $(\frac{n}{2} - 10)$ hexagons. The $\frac{3}{2}n$ edges correspond to carbon-carbon bonds.

- F_n exist for all even $n \geq 20$ except $n = 22$.
- $1, 1, 1, 2, 5 \ldots, 1812, \ldots 214127713, \ldots$ isomers F_n, for $n = 20, 24, 26, 28, 30 \ldots, 60, \ldots, 200, \ldots$.
- Thurston,1998, implies: no. of F_n grows as n^9.
- $C_{60}(I_h)$, $C_{80}(I_h)$ are only icosahedral (i.e., with highest symmetry I_h or I) fullerenes with $n \leq 80$ vertices.
- preferable fullerenes, C_n, satisfy isolated pentagon rule, but Beavers et al, August 2006, produced buckyegg: C_{84} (and Tb_3N inside) with 2 adjacent pentagons.

Examples

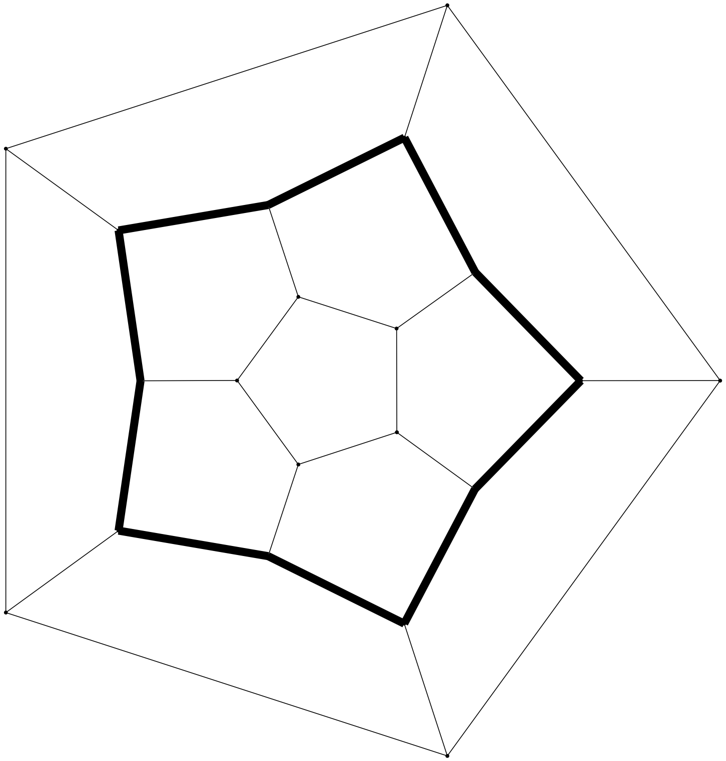


buckminsterfullerene $C_{60}(I_h)$
truncated icosahedron,
soccer ball

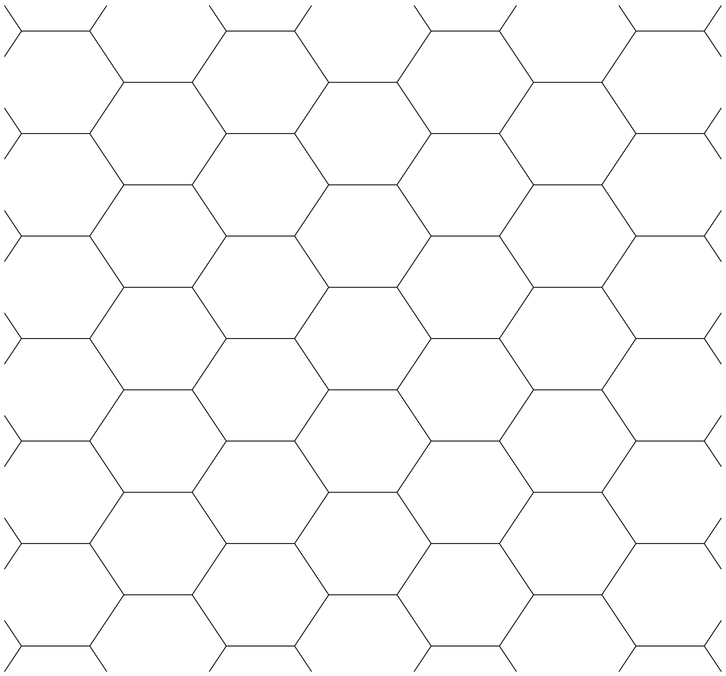


$F_{36}(D_{6h})$
elongated hexagonal barrel
$F_{24}(D_{6d})$

The range of fullerenes



Dodecahedron $F_{20}(I_h)$:
the smallest fullerene



Graphite lattice (6^3) as F_∞:
the "largest fullerene"

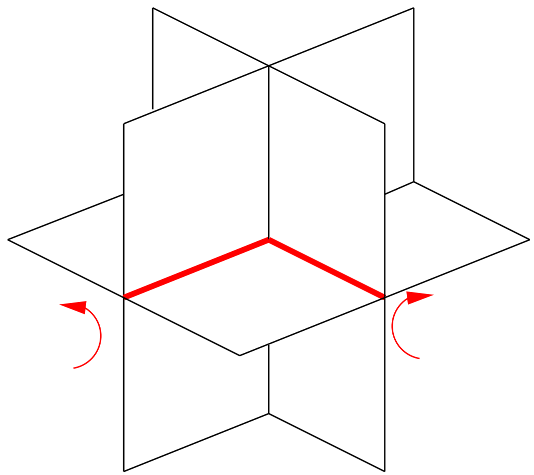
Finite isometry groups

All finite groups of isometries of 3-space are classified. In Schoenflies notations:

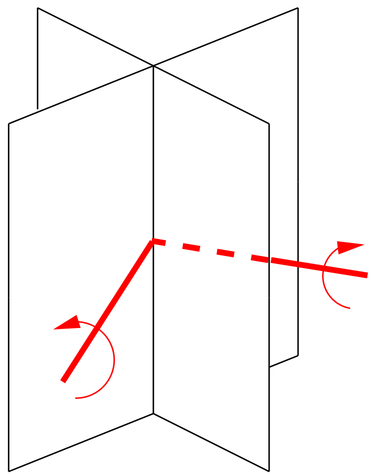
- C_1 is the trivial group
- C_s is the group generated by a plane reflexion
- $C_i = \{I_3, -I_3\}$ is the inversion group
- C_m is the group generated by a rotation of order m of axis Δ
- C_{mv} ($\simeq$ dihedral group) is the group formed by C_m and m reflexion containing Δ
- $C_{mh} = C_m \times C_s$ is the group generated by C_m and the symmetry by the plane orthogonal to Δ
- S_N is the group of order N generated by an antirotation

Finite isometry groups

- D_m ($\simeq$ dihedral group) is the group formed of C_m and m rotations of order 2 with axis orthogonal to Δ
- D_{mh} is the group generated by D_m and a plane symmetry orthogonal to Δ
- D_{md} is the group generated by D_m and m symmetry planes containing Δ and which does not contain axis of order 2



D_{2h}



D_{2d}

Finite isometry groups

- $I_h = H_3 \simeq Alt_5 \times C_2$ is the group of isometries of the regular Dodecahedron
- $I \simeq Alt_5$ is the group of rotations of the regular Dodecahedron
- $O_h = B_3$ is the group of isometries of the regular Cube
- $O \simeq Sym(4)$ is the group of rotations of the regular Cube
- $T_d = A_3 \simeq Sym(4)$ is the group of isometries of the regular Tetrahedron
- $T \simeq Alt(4)$ is the group of rotations of the regular Tetrahedron
- $T_h = T \cup -T$

Point groups

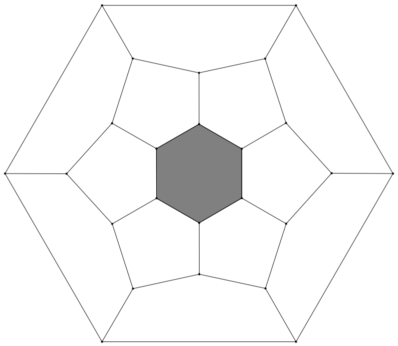
(point group) $Isom(P) \subset Aut(G(P))$ (combinatorial group)

Theorem *(Mani, 1971)*
Given a 3-connected planar graph G, there exist a 3-polytope P, whose group of isometries is isomorphic to $Aut(G)$ and $G(P) = G$.

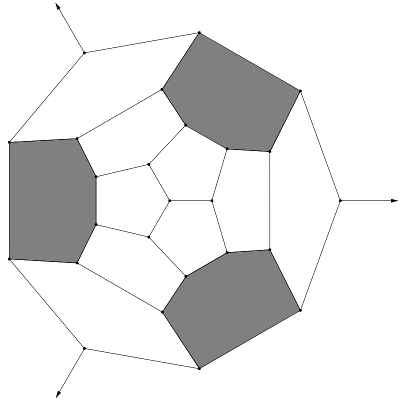
All groups for fullerenes (Fowler et al) are:

1. C_1, C_s, C_i
2. C_2, C_{2v}, C_{2h}, S_4 and C_3, C_{3v}, C_{3h}, S_6
3. D_2, D_{2h}, D_{2d} and D_3, D_{3h}, D_{3d}
4. D_5, D_{5h}, D_{5d} and D_6, D_{6h}, D_{6d}
5. T, T_d, T_h and I, I_h

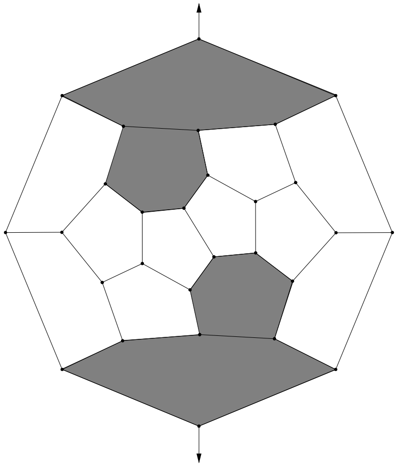
Small fullerenes



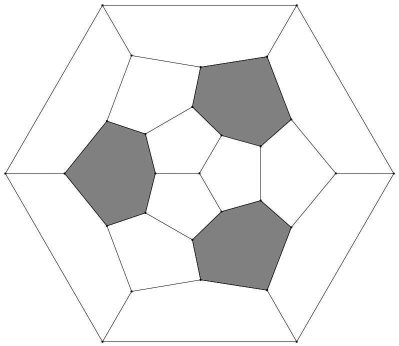
24, D_{6d}



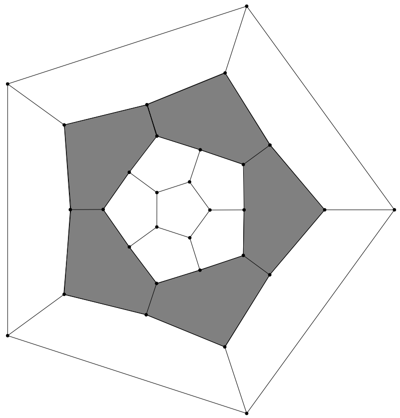
26, D_{3h}



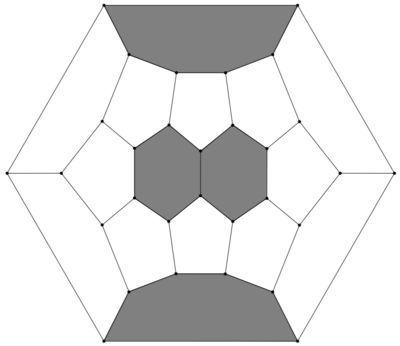
28, D_2



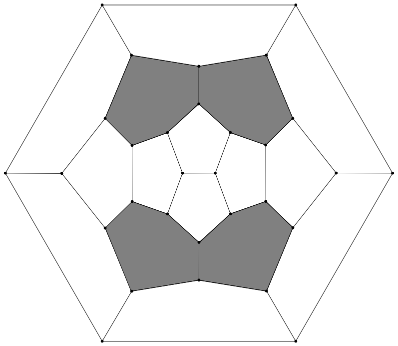
28, T_d



30, D_{5h}

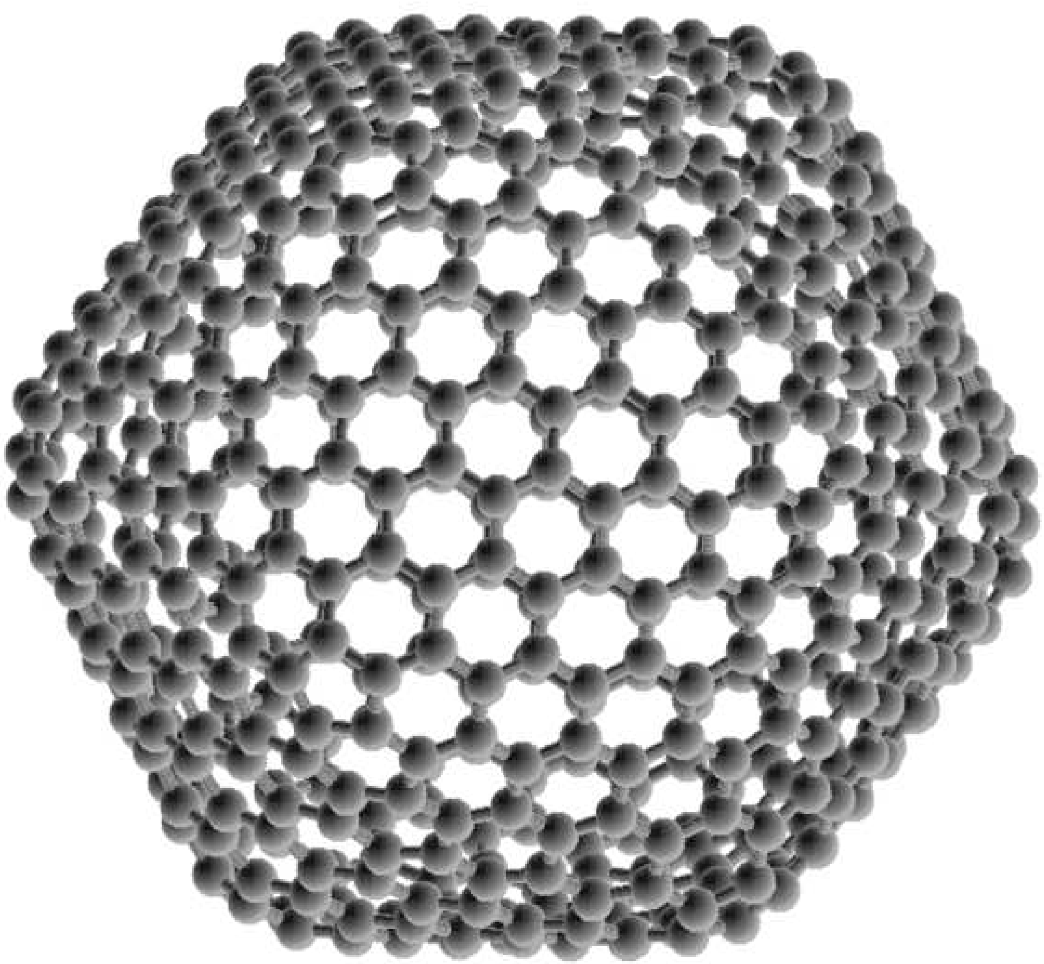


30, C_{2v}



30, D_{2v}

A C_{540}



What nature wants?

Fullerenes or their duals appear in Architecture and nanoworld:

- Biology: virus capsids and clathrine coated vesicles
- Organic (i.e., carbon) Chemistry
- also: (energy) minimizers in Thomson problem (for n unit charged particles on sphere) and Skyrme problem (for given baryonic number of nucleons);
  maximizers, in Tammes problem, of minimum distance between n points on sphere

Which, among simple polyhedra with given number of faces, are the “best” approximation of sphere?

Conjecture: FULLERENES

Graver's superfullerenes

- Almost all optimizers for Thomson and Tammes problems, in the range $25 \leq n \leq 125$ are fullerenes.
- For $n > 125$, appear 7-gonal faces;
  for $n > 300$: almost always.
- However, J.Graver, 2005: in all large optimizers, the 5- and 7-gonal faces occurs in 12 distinct clusters, corresponding to a unique underlying fullerene.

Skyrmions and fullerenes

Conjecture (Battye-Sutcliffe, 1997):
any minimal energy Skyrmion (baryonic density isosurface for single soliton solution) with baryonic number (the number of nucleons) $B \geq 7$ is a fullerene F_{4B-8}.

Conjecture (true for $B < 107$; open from $(b, a) = (1, 4)$):
there exist icosahedral fullerene as a minimal energy Skyrmion for any $B = 5(a^2 + ab + b^2) + 2$ with integers $0 \leq b < a$, $gcd(a, b) = 1$ (not any icosahedral Skyrmion has minimal energy).

Skyrme model (1962) is a Lagrangian approximating QCD (a gauge theory based on $SU(3)$ group). Skyrmions are special topological solitons used to model baryons.

Isoperimetric problem for polyhedra

Lhuilier 1782, Steiner 1842, Lindelöf 1869, Steinitz 1927, Goldberg 1933, Fejes Tóth 1948, Pólya 1954

- Polyhedron of greatest volume V with a given number of faces and a given surface S?
- Polyhedron of least volume with a given number of faces circumscribed around the unit sphere?
- Maximize Isoperimetric Quotient for solids. Schwarz,1890:
  $IQ = 36\pi\frac{V^2}{S^3} \leq 1$ (with equality only for sphere)
- In Biology: the ratio $\frac{V}{S}$ (=$\frac{r}{3}$ for spherical animal of radius r) affects heat gain/loss, nutritient/gas transport into body cells and organism support on its legs.

Isoperimetric problem for polyhedra

polyhedron	$IQ(P)$	upper bound
Tetrahedron	$\frac{\pi}{6\sqrt{3}} \simeq 0.302$	$\frac{\pi}{6\sqrt{3}}$
Cube	$\frac{\pi}{6} \simeq 0.524$	$\frac{\pi}{6}$
Octahedron	$\frac{\pi}{3\sqrt{3}} \simeq 0.605$	$\simeq 0.637$
Dodecahedron	$\frac{\pi\tau^{7/2}}{3.5^{5/4}} \simeq 0.755$	$\frac{\pi\tau^{7/2}}{3.5^{5/4}}$
Icosahedron	$\frac{\pi\tau^{4}}{15\sqrt{3}} \simeq 0.829$	$\simeq 0.851$

IQ of Platonic solids

($\tau = \frac{1+\sqrt{5}}{2}$: *golden mean*)

Conjecture (Steiner 1842):
Each of the 5 Platonic solids has maximal IQ among all isomorphic to it (i.e., with same skeleton) polyhedra (still open for the Icosahedron)

Classical isoperimetric inequality

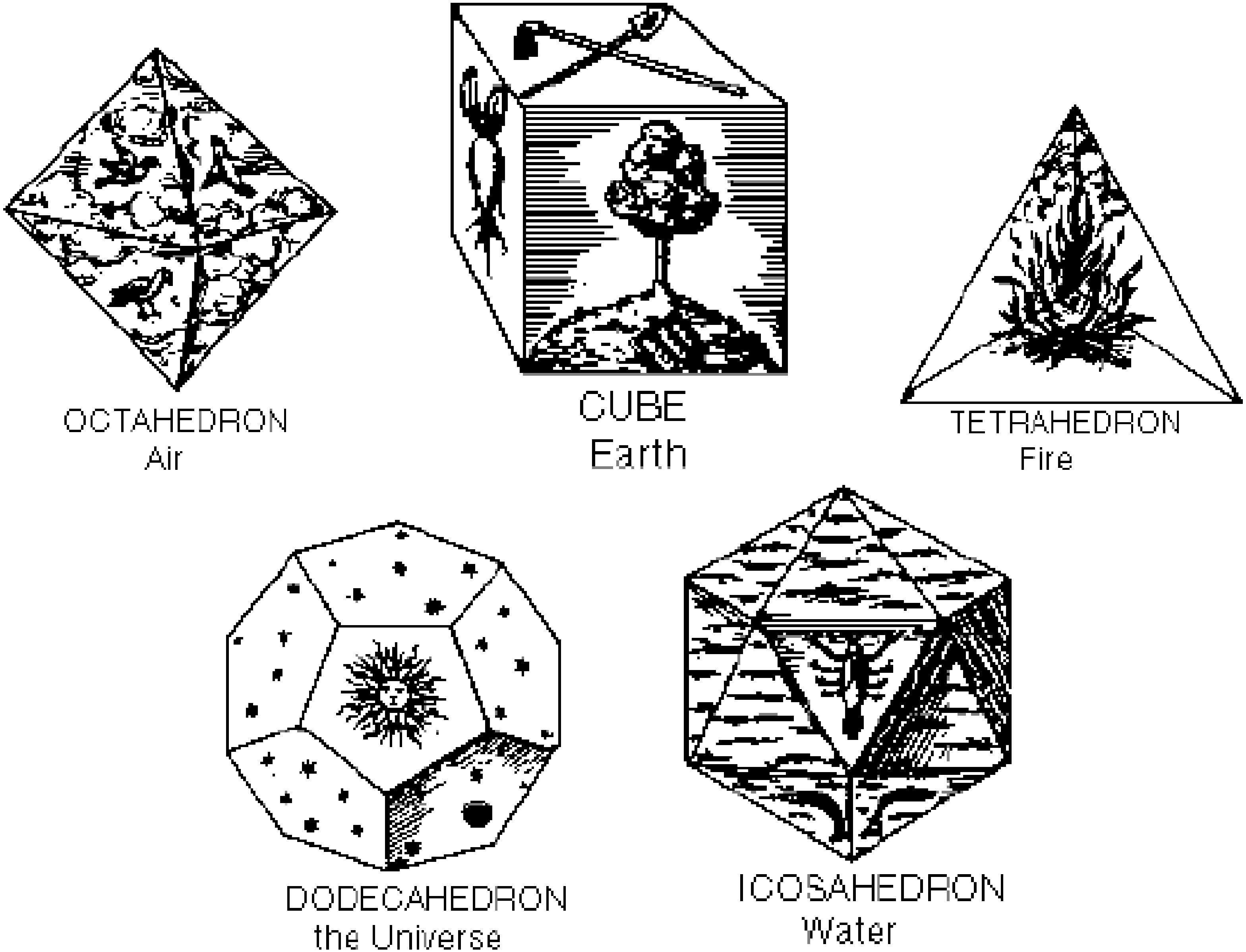
If a domain $D \subset E^n$ has volume V and bounded by hypersurface of $(n-1)$-dimensional area A, then Lyusternik, 1935:

$$IQ(D) = \frac{n^n \omega_n V^{n-1}}{A^n} \leq 1$$

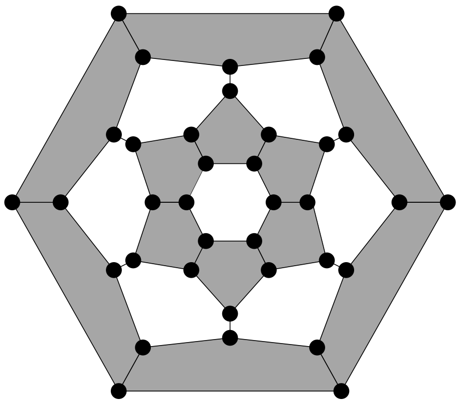
with equality only for unit sphere S^n; its volume is $\omega_n = \frac{2\pi^{\frac{n}{2}}}{n\Gamma(\frac{n}{2})}$, where Euler's Gamma function is

$$\Gamma(\frac{n}{2}) = \begin{cases} (\frac{n}{2})! & \text{for even } n \\ \sqrt{\pi}\frac{(n-2)!!}{2^{\frac{n-2}{2}}} & \text{for odd } n \end{cases}$$

Five Platonic solids



Goldberg Conjecture



20 faces: $IQ(Icosahedron) < IQ(F_{36}) \simeq 0.848$

Conjecture (Goldberg 1933):
The polyhedron with $m \geq 12$ facets with maximal IQ is a fullerene (called "medial polyhedron" by Goldberg)

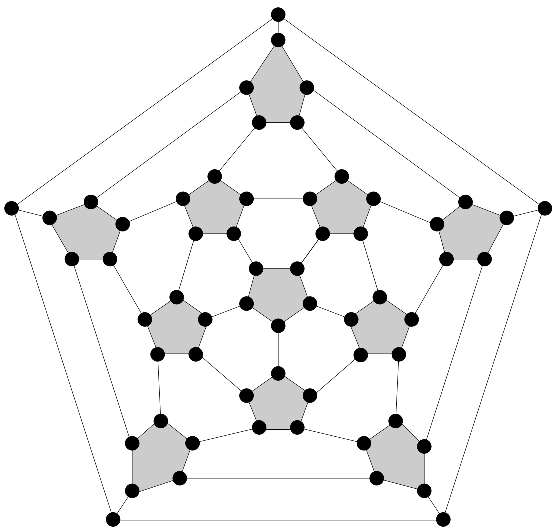
polyhedron	$IQ(P)$	upper bound
Dodecahedron $F_{20}(I_h)$	$\frac{\pi\tau^{7/2}}{3.5^{5/4}} \simeq 0.755$	$\frac{\pi\tau^{7/2}}{3.5^{5/4}}$
Truncated icosahedron $C_{60}(I_h)$	$\simeq 0.9058$	$\simeq 0.9065$
Chamfered dodecahed. $C_{80}(I_h)$	$\simeq 0.928$	$\simeq 0.929$
Sphere	1	1

II. Icosahedral fullerenes

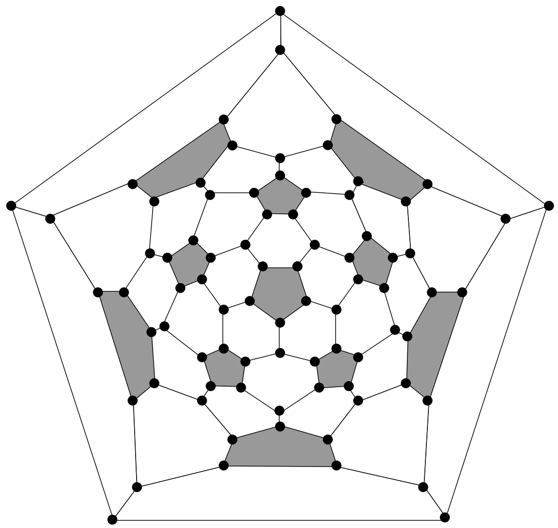
Icosahedral fullerenes

Call icosahedral any fullerene with symmetry I_h or I

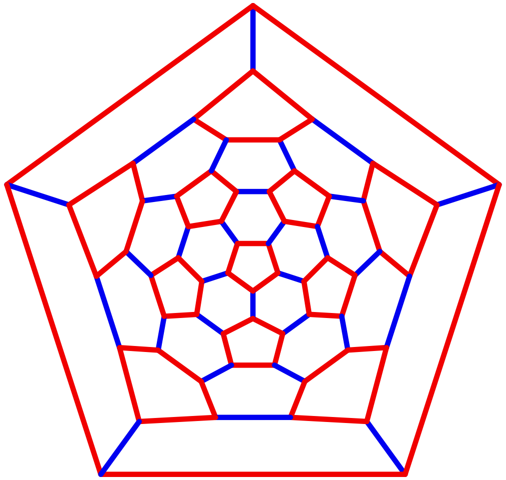
- All icosahedral fullerenes are preferable, except $F_{20}(I_h)$
- $n = 20T$, where $T = a^2 + ab + b^2$ (triangulation number) with $0 \leq b \leq a$.
- I_h for $a = b \neq 0$ or $b = 0$ (extended icosahedral group); I for $0<b<a$ (proper icos. group); T=7,13,21,31,43,57...



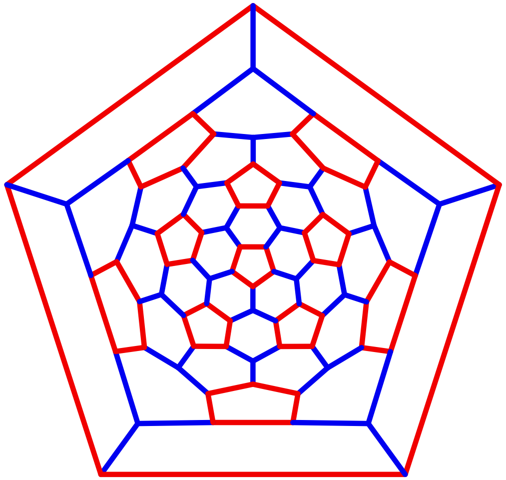
$C_{60}(I_h)$=$(1,1)$-dodecahedron
truncated icosahedron



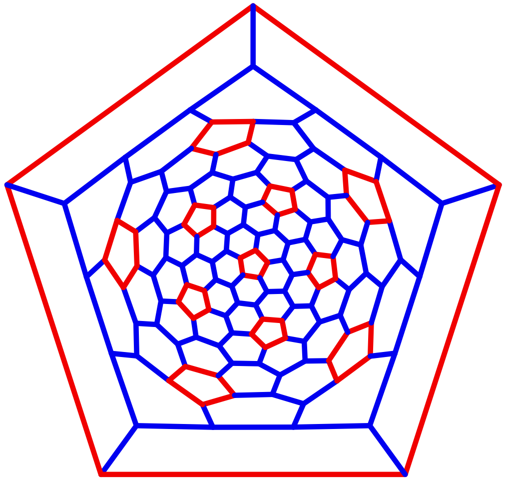
$C_{80}(I_h)$=$(2,0)$-dodecahedron
chamfered dodecahedron



$C_{60}(I_h)$: $(1,1)$-dodecahedron



$C_{80}(I_h)$: $(2,0)$-dodecahedron



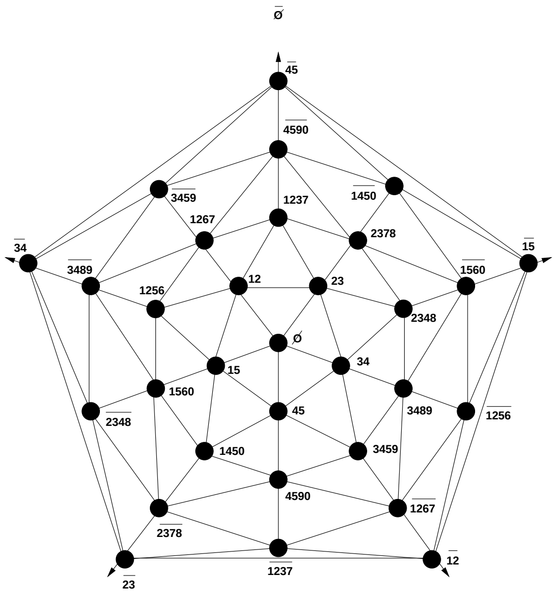
$C_{140}(I)$: $(2,1)$-dodecahedron

From 1998, $C_{80}(I_h)$ appeared in Organic Chemistry in some endohedral derivatives as $La_2@C_{80}$, etc.

Icosadeltahedra

Call icosadeltahedron the dual of an icosahedral fullerene $C^*_{20T}(I_h)$ or $C^*_{20T}(I)$

- Geodesic domes: B.Fuller, patent 1954
- Capsids of viruses: Caspar and Klug, Nobel prize 1982



Dual $C^*_{60}(I_h)$, $(a, b) = (1, 1)$
pentakis-dodecahedron

GRAVIATION (Esher 1952)
omnicapped dodecahedron

Icosadeltahedra in Architecture

(a, b)	Fullerene	Geodesic dome
$(1, 0)$	$F_{20}^*(I_h)$	One of Salvador Dali houses
$(1, 1)$	$C_{60}^*(I_h)$	Artic Institute, Baffin Island
$(3, 0)$	$C_{180}^*(I_h)$	Bachelor officers quarters, US Air Force, Korea
$(2, 2)$	$C_{240}^*(I_h)$	U.S.S. Leyte
$(4, 0)$	$C_{320}^*(I_h)$	Geodesic Sphere, Mt Washington, New Hampshire
$(5, 0)$	$C_{500}^*(I_h)$	US pavilion, Kabul Afghanistan
$(6, 0)$	$C_{720}^*(I_h)$	Radome, Artic dEW
$(8, 8)$	$C_{3840}^*(I_h)$	Lawrence, Long Island
$(16, 0)$	$C_{5120}^*(I_h)$	US pavilion, Expo 67, Montreal
$(18, 0)$	$C_{6480}^*(I_h)$	Géode du Musée des Sciences, La Villete, Paris
$(18, 0)$	$C_{6480}^*(I_h)$	Union Tank Car, Baton Rouge, Louisiana

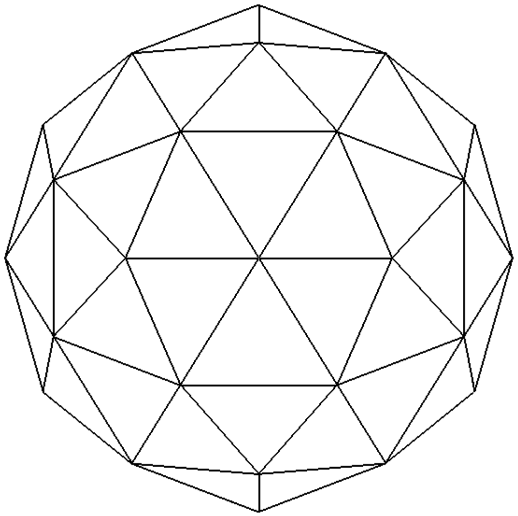
$b = 0$ Alternate, $b = a$ Triacon and $a + b$ Frequency (distance of two 5-valent neighbors) are Buckminster Fullers's terms

Geodesic Domes

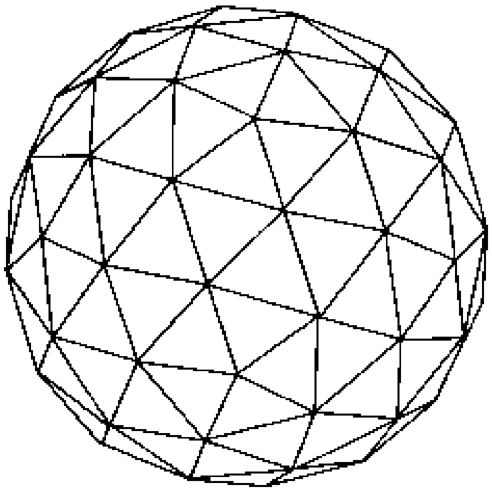
US pavilion, World Expo 1967, Montreal

Spaceship Earth, Disney World's Epcot, Florida

Icosadeltahedra C_n^* with $a = 2$



$C^*_{80}(I_h)$, (a, b)=$(2, 0)$



$C^*_{140}(I)$, (a, b)=$(2, 1)$

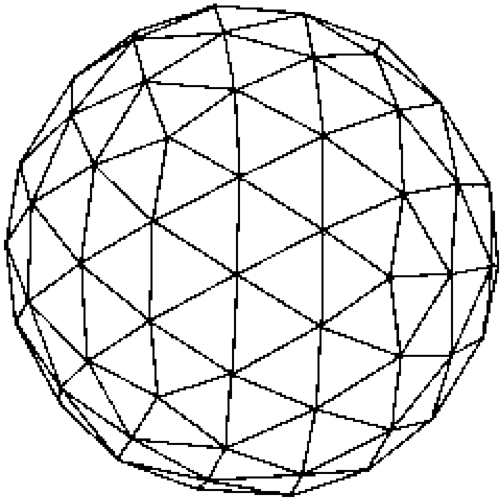
Icosadeltahedra $C^*_{20\times 4^t}(I_h)$ (i.e., $(a, b) = (2^t, 0)$) with $t \leq 4$ are used as schemes for directional sampling in Diffusion MRI (Magnetic Resonance Imaging) for scanning brain space more uniformly along many directions (so, avoiding sampling direction biases).

$C_{60}(I_h)$ in leather

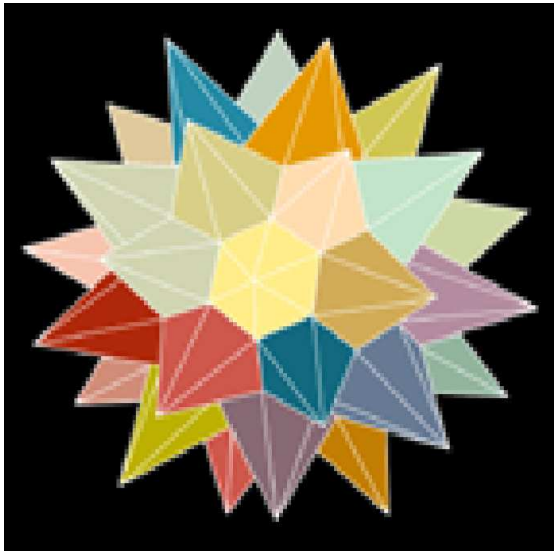
Telstar ball, official match ball
for 1970 and 1974 FIFA World Cup

$C_{60}(I_h)$ is also the state molecule of Texas.

The leapfrog of $C_{60}(I_h)$

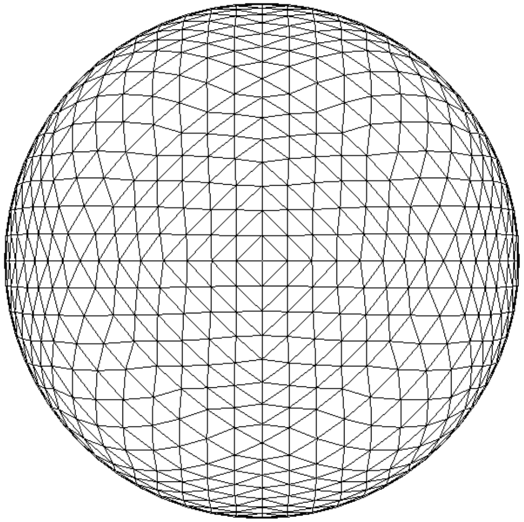


$C^*_{180}(I_h)$, $(a, b) = (3, 0)$



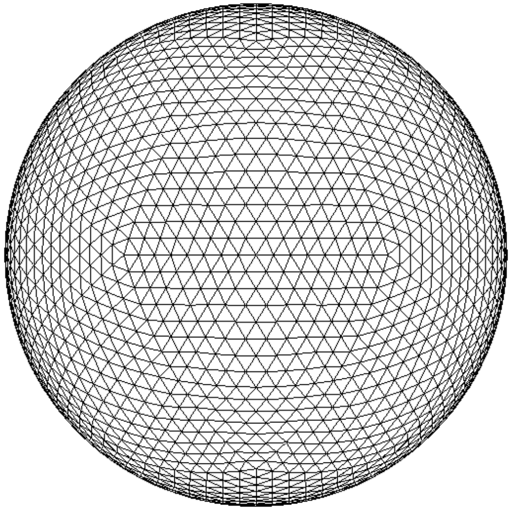
$C^*_{180}(I_h)$ as omnicapped buckminsterfullerene C_{60}

Triangulations, spherical wavelets



Dual 4-chamfered cube

$(a, b) = (2^4 = 16, 0)$, O_h



Dual 4-cham. dodecahedron

C^*_{5120}, $(a, b) = (2^4 = 16, 0)$, I_h

Used in Computer Graphics and Topography of Earth

III. Fullerenes in Chemistry and Biology

Fullerenes in Chemistry

Carbon C and, possibly, silicium Si are only 4-valent elements producing homoatomic long stable chains or nets

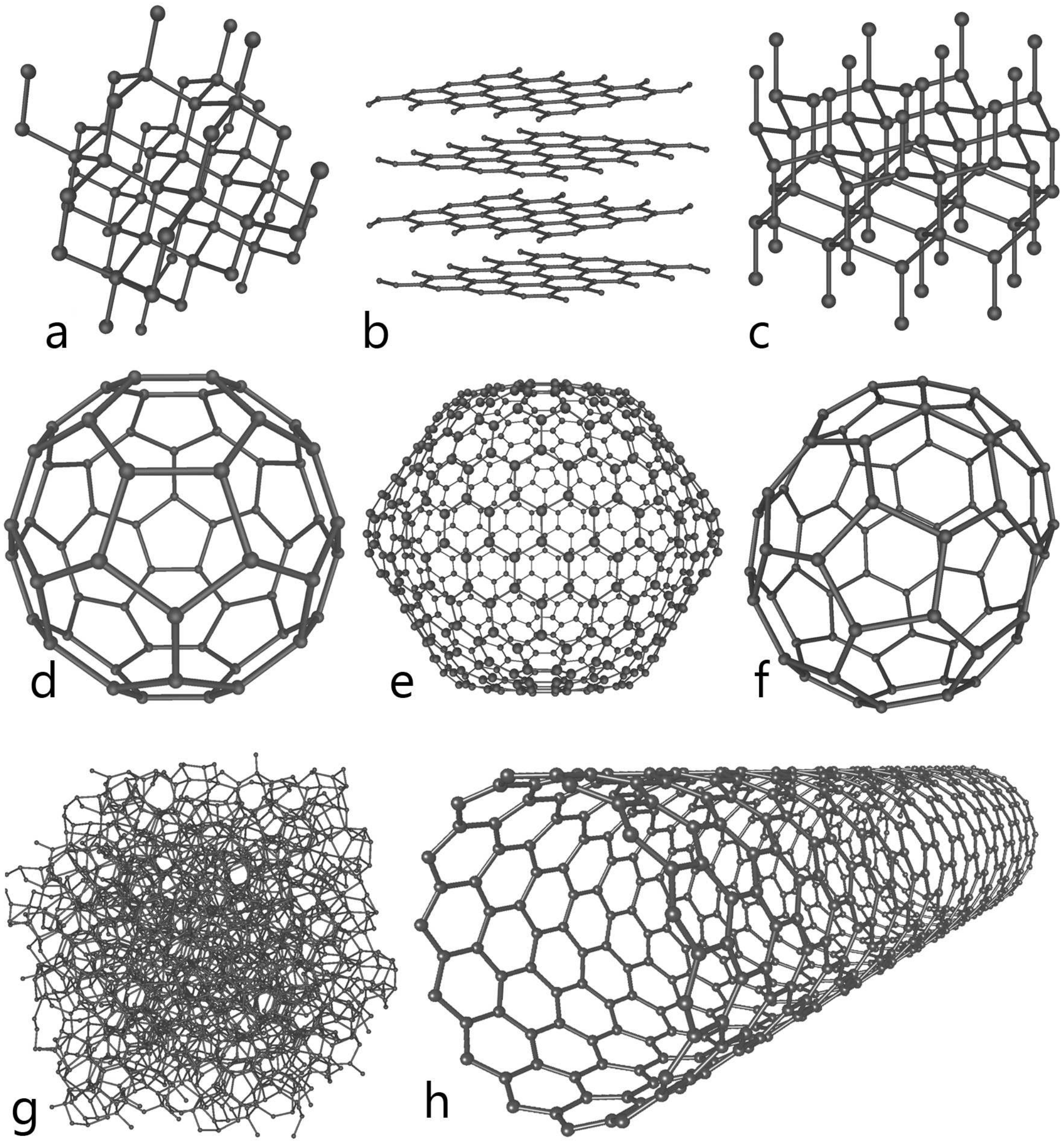
- Graphite sheet: bi-lattice (6^3), Voronoi partition of the hexagonal lattice (A_2), “infinite fullerene”
- Diamond packing: bi-lattice D-complex, α_3-centering of the lattice f.c.c.=A_3
- Fullerenes: 1985 (Kroto, Curl, Smalley): Cayley A_5, $C_{60}(I_h)$, tr. icosahedon, football; Nobel prize 1996 but Ozawa (in japanese): 1984. “Cheap” C_{60}: 1990. 1991 (Iijima): nanotubes (coaxial cylinders).
  Also isolated chemically by now: C_{70}, C_{76}, C_{78}, C_{82}, C_{84}.
  If > 100 carbon atoms, they go in concentric layers;
  if < 20, cage opens for high temperature.
  Full. alloys, stereo org. chemistry, carbon: semi-metal.

Allotropes of carbon

- Diamond: cryst.tetrahedral, electro-isolating, hard, transparent. Rarely > 50 carats, unique $> 800ct$: Cullinan $3106ct = 621g$. Kuchner: diamond planets?
- Hexagonal diamond (lonsdaleite): cryst.hex., very rare; 1967, in shock-fused graphite from several meteorites
- ANDR (aggregated diamond nanorods): 2005, Bayreuth University; hardest known substance
- Graphite: cryst.hexagonal, soft, opaque, el. conducting 2004: **Graphene**, 2dim. carbon, most expensive in 2008
- Amorphous carbon (no long-range pattern): synthetic; coal and soot are almost such
- Fullerenes: 1985, spherical; only soluble carbon form
- Nanotubes: 1991, cylindric, few nm wide, upto few mm; nanobudes: 2007, nanotubes combined with fullerenes

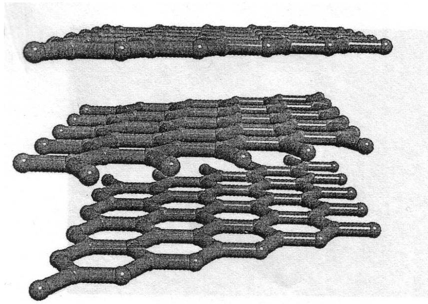
Allotropes of carbon: pictures

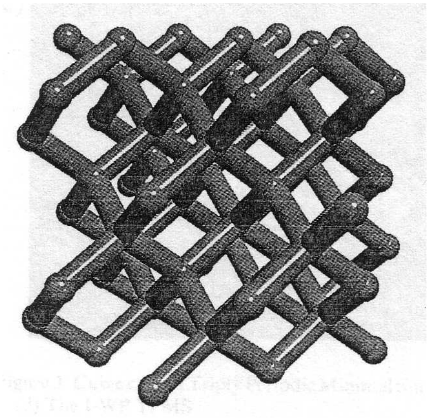
a) Diamond b) Graphite c) Lonsdaleite d) C_{60} (e) C_{540} f) C_{70}
g) Amorphous carbon h) single-walled carbon nanotube



Other allotropes of carbon

- Carbon nanofoam: 1997, clusters of about 4000 atoms linked in graphite-like sheets with some 7-gons (negatively curved), ferromagnetic
- Glassy carbon: 1967; carbyne: linear Acetilic Carbon
- ? White graphite (chaoite): cryst.hexagonal; 1968, in shock-fused graphite from Ries crater, Bavaria
- ? Carbon(VI); ? metallic carbon; ?
? Prismane C_8, bicapped $Prism_3$

graphite: 

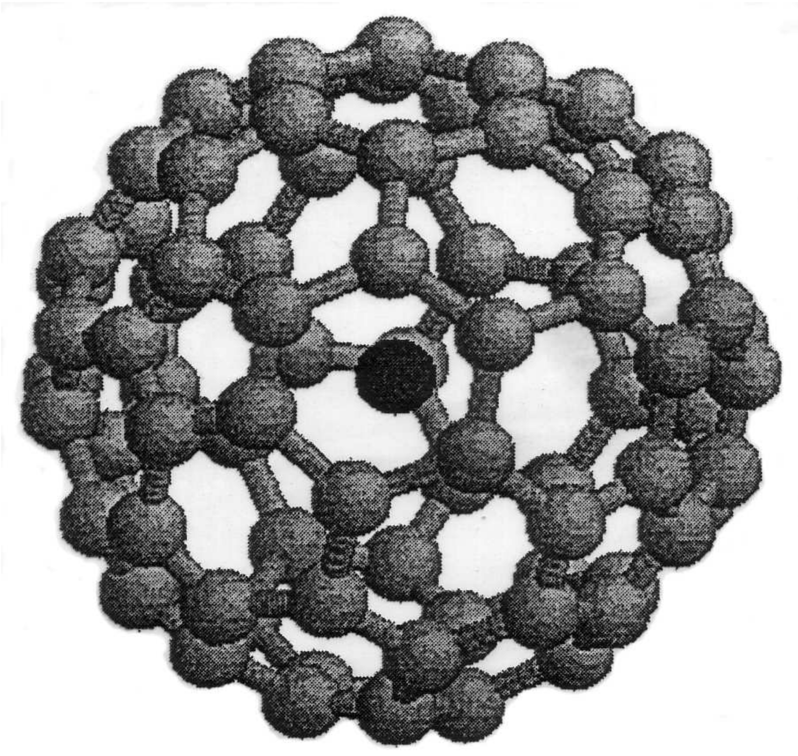
diamond: 

Carbon and Anthropic Principle

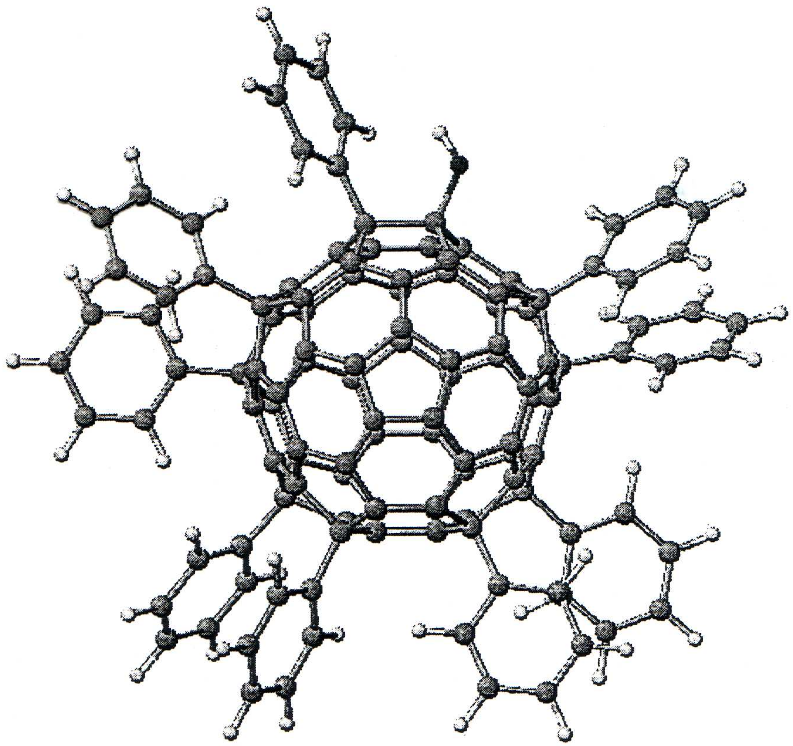
- Nucleus of lightest elements H, He, Li, Be (and Boron?) were produced in seconds after Big Bang, in part, by scenario: Deuterium H^2, H^3, He^3, He^4, H, Li^7.
  If week nuclear force was slightly stonger, 100% hydrogen Univers; if weaker, 100% helium Univers.
- Billion years later, by atom fusion under high t^0 in stars

  $$3He^4 \longrightarrow C^{12}$$

  (12 *nucleons*, i.e., protons/neutrons), then Ni, O, Fe etc.
- "Happy coincidence": energy level of C $\simeq$ the energies of 3 He; so, reaction was possible/probable.
- Without carbon, no other heavy elements and life could not appear. C: 18.5% of human (0.03% Universe) weight.

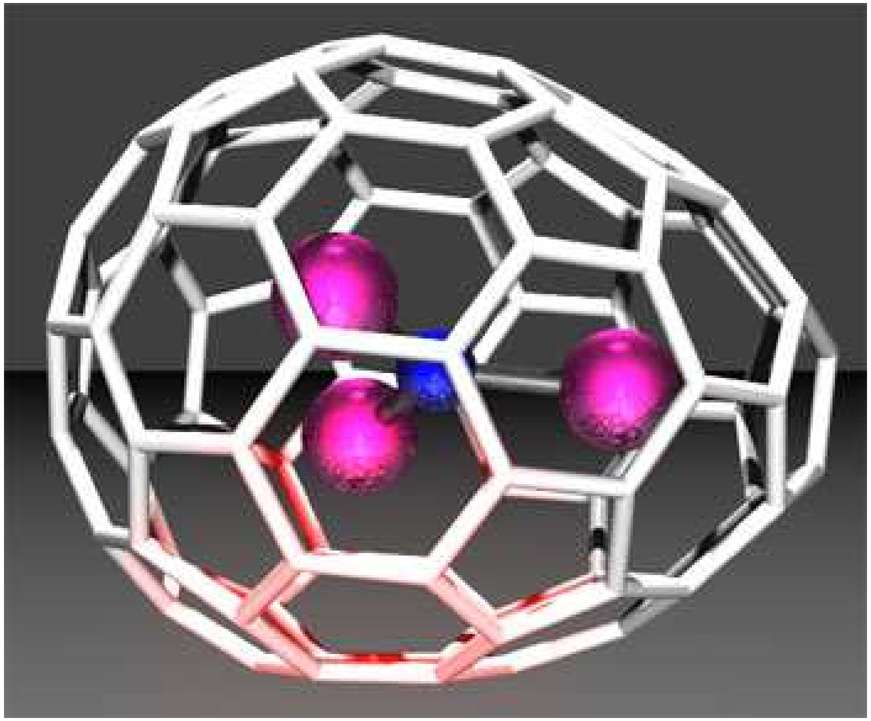


LaC_{82}
first Endohedral Fullerene compound



$C_{10}Ph_9OH$
Exohedral Fullerene compound (first with a single hydroxy group attached)

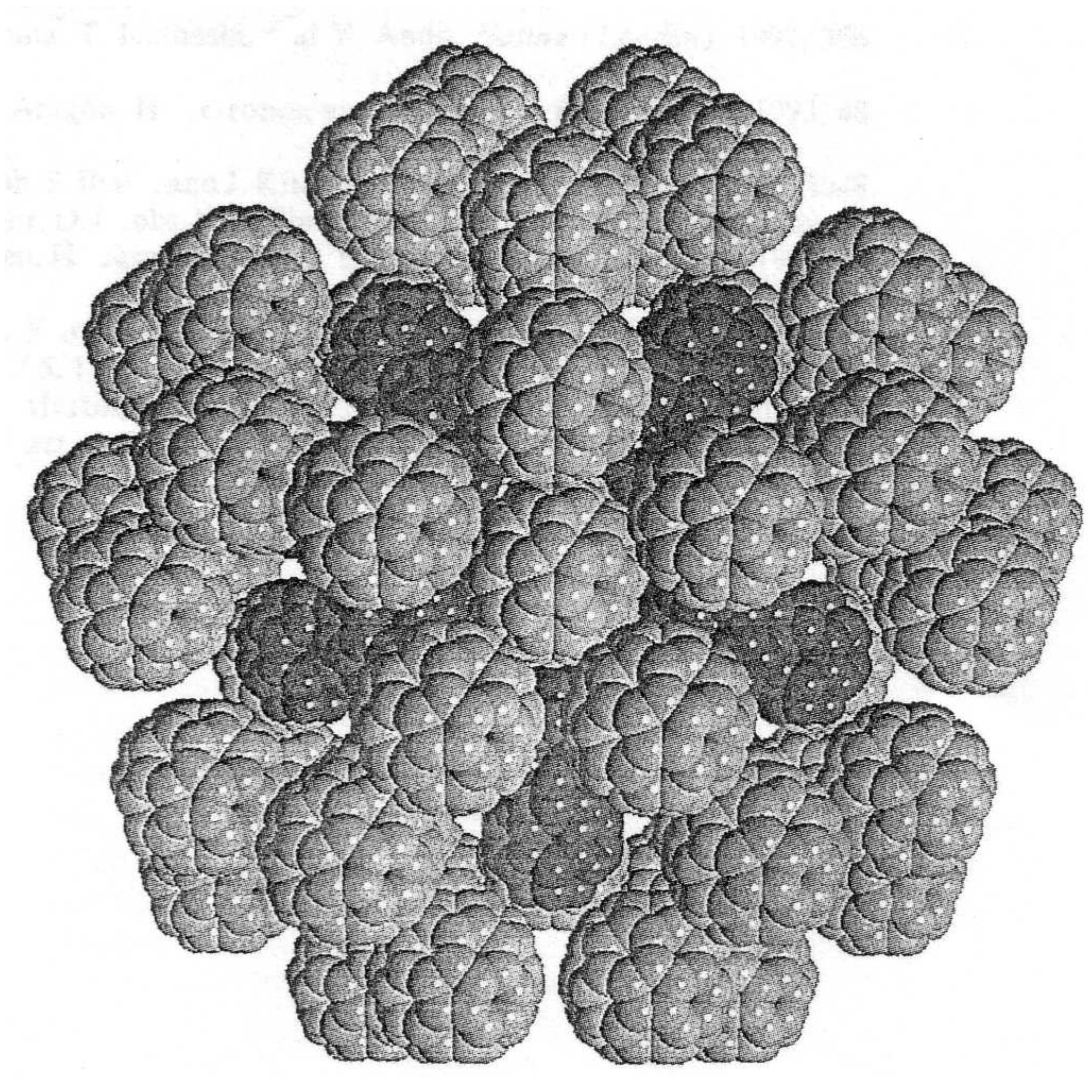
First non-preferable fullerene compound



$Tb_3N@C_{84}$ with a molecule of triterbium nitride inside

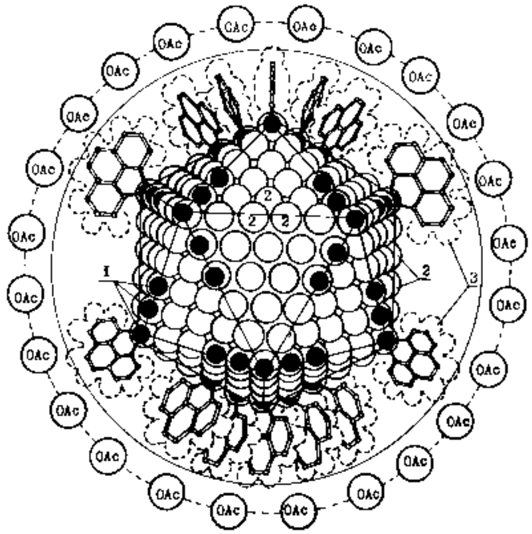
Beavers et al, 2006: above "buckyegg".
Unique pair of adjacent pentagons makes the pointy end.
One Tb atom is nestled within the fold of this pair.

Terrones quasicrystalline cluster



In silico: from C_{60} and $F_{40}(T_d)$; cf. 2 atoms in quasicrystals

Onion-like metallic clusters



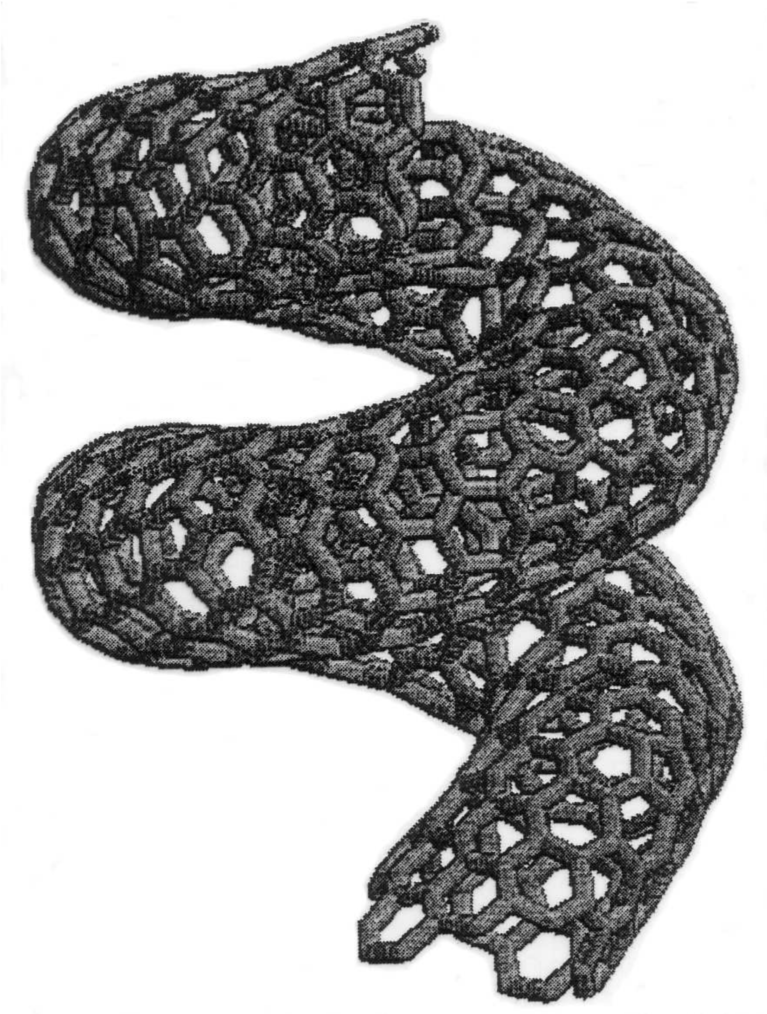
Palladium icosahedral 5-cluster

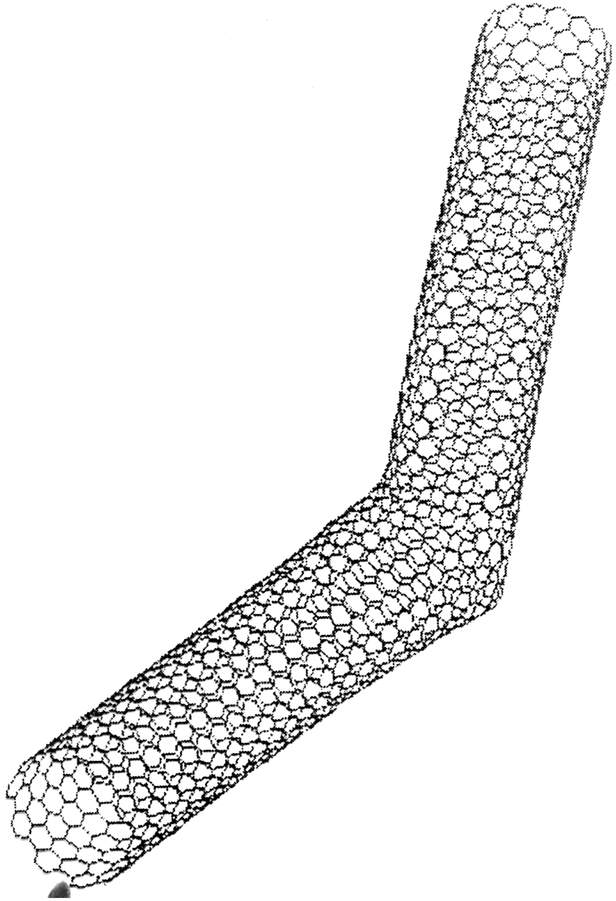
$Pd_{561}L_{60}(O_2)_{180}(OAc)_{180}$

α	Outer shell	Total # of atoms	# Metallic cluster
1	$C^*_{20}(I_h)$	13	$[Au_{13}(PMe_2Ph)_{10}Cl_2]^{3+}$
2	$RhomDode^*_{80}(O_h)$	55	$Au_{55}(PPh_3)_{12}Cl_6$
4	$RhomDode^*_{320}(O_h)$	309	$Pt_{309}(Phen_{36}O_{30\pm10})$
5	$C^*_{500}(I_h)$	561	$Pd_{561}L_{60}(O_2)_{180}(OAc)_{180}$

Icosahedral and cuboctahedral metallic clusters

Nanotubes and Nanotechnology





Helical graphite Deformed graphite tube

Nested tubes (concentric cylinders) of rolled graphite; use(?): for composites and “nanowires”

Applications of nanotubes/fullerenes

Fullerenes are heat-resistant and dissolve at room t^0. There are thousands of patents for their commercial applications Main areas of applications (but still too expensive) are:

- El. conductivity of alcali-doped C_{60}: insulator K_2C_{60} but superconductors K_3C_{60} at $18K$ and Rb_3C_{60} at $30K$ (however, it is still too low transition T_c)
- Catalists for hydrocarbon upgrading (of heavy oils, methane into higher HC, termal stability of fuels etc.)
- Pharmaceceuticals: protease inhibitor since derivatives of C_{60} are highly hydrophobic and antioxydant (they soak cell-damaging free radicals)
- Superstrong materials, nanowires?
- Now/soon: buckyfilms, sharper scanning microscope

Nanotubes/fullerenes: hottest sci. topics

Ranking (by Hirsch-Banks h-b index) of most popular in 2006 scientific fields in Physics:
Carbon nanotubes 12.85,
nanowires 8.75,
quantum dots 7.84,
fullerenes 7.78,
giant magnetoresistance 6.82,
M-theory 6.58, quantum computation 5.21, ...

Chem. compounds ranking: C_{60} 5.2, gallium nitride 2.1, ...

h-index of a topic, compound or a scholar is the highest number T of published articles on this topic, compound or by this scholar that have each received $\geq T$ citations.
h-b index of a topic or compound is h-index divided by the number of years that papers on it have been published.

Chemical context

- Crystals: from basic units by symm. operations, incl. translations, excl. order 5 rotations ("cryst. restriction"). Units: from few (inorganic) to thousands (proteins).
- Other very symmetric mineral structures: quasicrystals, fullerenes and like, icosahedral packings (no translations but rotations of order 5).
- Fullerene-type polyhedral structures (polyhedra, nanotubes, cones, saddles, $\dots$) were first observed with carbon. But also inorganic ones were considered: boron nitrides, tungsten, disulphide, allumosilicates and, possibly, fluorides and chlorides.
  May 2006, Wang-Zeng-al.: first metal hollow cages $Au_n = F^*_{2n-4}$ $(16 \leq n \leq 18)$. F^*_{28} is the smallest; the gold clusters are flat if $n < 16$ and compact (solid) if $n > 18$.

Stability of fullerenes

Stability of a molecule: minimal total energy, i.e.,

- I-energy and
- the strain in the 6-system.

Hückel theory of I-electronic structure: every eigenvalue λ of the adjacency matrix of the graph corresponds to an orbital of energy $\alpha + \lambda\beta$, where
α is the Coulomb parameter (same for all sites) and
β is the resonance parameter (same for all bonds).
The best I-structure: same number of positive and negative eigenvalues.

Fullerene Kekule structure

- Perfect matching (or 1-factor) of a graph is a set of disjoint edges covering all vertices. A Kekule structure of an organic compound is a perfect matching of its carbon skeleton, showing the locations of double bonds.
- A set H of disjoint 6-gons of a fullerene F is a resonant pattern if, for a perfect matching M of F, any 6-gon in H is M**-alternating** (its edges are alternatively in and off M).
- Fries number of F is maximal number of M-alternating hexagons over all perfect matchings M;
Clar number is maximal size of its resonant pattern.
- A fullerene is k-resonant if any $i \leq k$ disjoint hexagons form a resonant pattern. Any fullerene is 1-resonant; **conjecture**: any preferable fulerene is 2-resonant. Zhang et al, 2007: all 3-resonant fullerenes: $C_{60}(I_h)$ and a F_{4m} for $m = 5, 6, 7, 8, 9, 9, 10, 12$. All 9 are k-resonant for $k \geq 3$.

Life fractions

- life: DNA and RNA (cells)
- $1/2$-life: DNA or RNA (cell parasites: viruses)
- “naked” RNA, no protein (satellite viruses, viroids)
- DNA, no protein (plasmids, nanotech, “junk” DNA, ...)
- no life: no DNA, nor RNA (only proteins, incl. prions)

	Atom	DNA	Cryo-EM	Prion	Virus capsides
size	$\simeq 0.25$	$\simeq 2$	$\simeq 5$	11	$20 - 50 - 100 - 400$
nm					SV40, HIV, Mimi

- Viruses: 4th domain (Acytota)?
  But crystals also self-assembly spontaneously.
- Viral eukaryogenesis hypothesis (Bell, 2001).

Icosahedral viruses

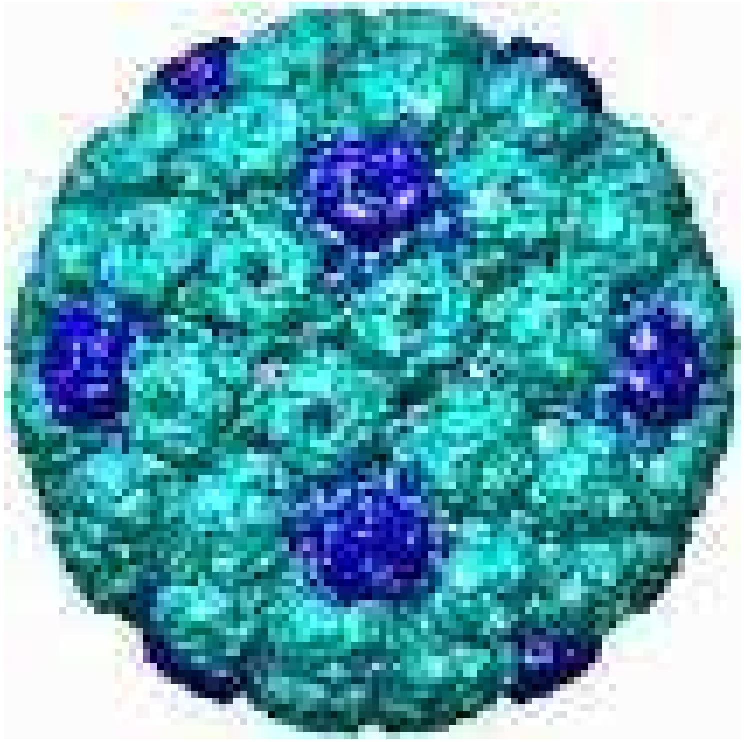
- Virus: virion, then (rarely) cell parasite.
- Watson and Crick, 1956:
  "viruses are either spheres or rods". In fact, all, except most complex (as brick-like pox virus) and enveloped (as conic HIV) are helical or ($\approx \frac{1}{2}$ of all) icosahedral.
- Virion: protein shell (capsid) enclosing genome (RNA or DNA) with $3 - 911$ protein-coding genes.
- Shere-like capsid has $60T$ protein subunits, but EM resolves only clusters (capsomers), incl. 12 pentamers (5 bonds) and 6-mers; plus, sometimes, 2- and 3-mers.
- Bonds are flexible: $\simeq 5^0$ deviation from mean direction. Self-assembly: slight but regular changes in bonding.

- Caspar- Klug (quasi-equivalence) principle: virion minimizes by organizing capsomers in min. number T of locations with non-eqv. bonding. Also, icosah. group generates max. enclosed volume for given subunit size. But origin, termodynamics and kinetics of this self-assembly is unclear. Modern computers cannot evaluate capsid free energy by all-atom simulations.)
- So, capsomers are $10T + 2$ vertices of icosadeltahedron C^*_{20T}, $T = a^2 + ab + b^2$ (triangulation number). It is symmetry of capsid , not general shape (with spikes).
- Lower pseudo-equivalence when 2-, 3-mers appear and/or different protein type in different locations.
- Hippocrates: disease = icosahedra (water) body excess

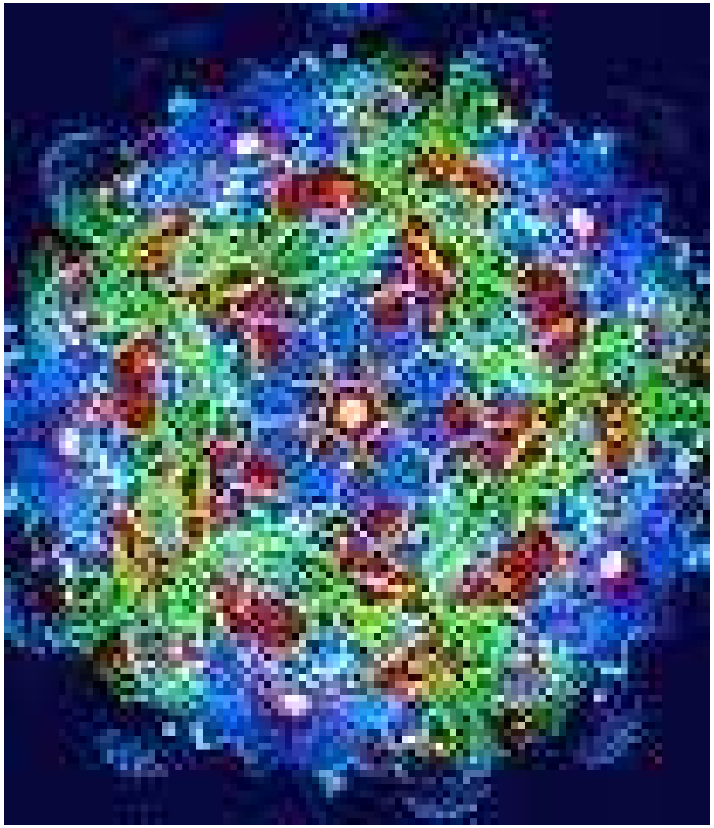
Capsids of icosahedral viruses

(a, b)	$T = a^2 + ab + b^2$	Fullerene	Examples of viruses
$(1, 0)$	1	$F^*_{20}(I_h)$	*B19 parvovirus, cowpea mosaic virus*
$(1, 1)$	3	$C^*_{60}(I_h)$	*picornavirus, turnip yellow mosaic virus*
$(2, 0)$	4	$C^*_{80}(I_h)$	*human hepatitis B, Semliki Forest virus*
$(2, 1)$	$7l$	$C^*_{140}(I)_{laevo}$	*HK97, rabbit papilloma virus,* Λ*-like viruses*
$(1, 2)$	$7d$	$C^*_{140}(I)_{dextro}$	*polyoma (human wart) virus, SV40*
$(3, 1)$	$13l$	$C^*_{260}(I)_{laevo}$	*rotavirus*
$(1, 3)$	$13d$	$C^*_{260}(I)_{dextro}$	*infectious bursal disease virus*
$(4, 0)$	16	$C^*_{320}(I_h)$	*herpes virus, varicella*
$(5, 0)$	25	$C^*_{500}(I_h)$	*adenovirus, phage PRD1*
$(3, 3)$	27	$C^*_{540}(I)_h$	*pseudomonas phage phiKZ*
$(6, 0)$	36	$C^*_{720}(I_h)$	*infectious canine hepatitis virus, HTLV1*
$(7, 7)$	147	$C^*_{2940}(I_h)$	*Chilo iridescent iridovirus* (outer shell)
$(7, 8)$	$169d$	$C^*_{3380}(I)_{dextro}$	*Algal chlorella virus PBCV1* (outer shell)
$(7, 10)$	$219d?$	$C^*_{4380}(I)$	*Algal virus PpV01*

Examples

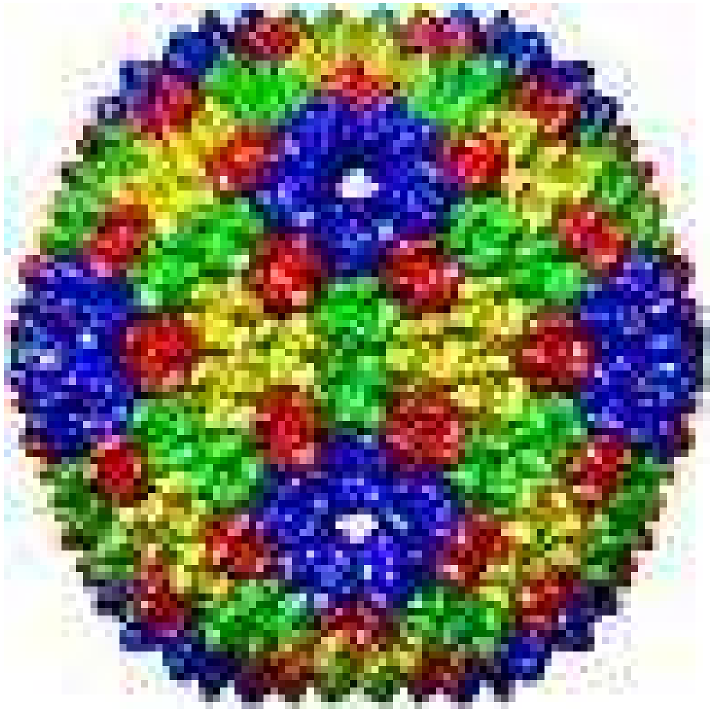


Satellite, $T = 1$, of TMV, helical Tobacco Mosaic virus 1st discovered (Ivanovski, 1892), 1st seen (1930, EM)

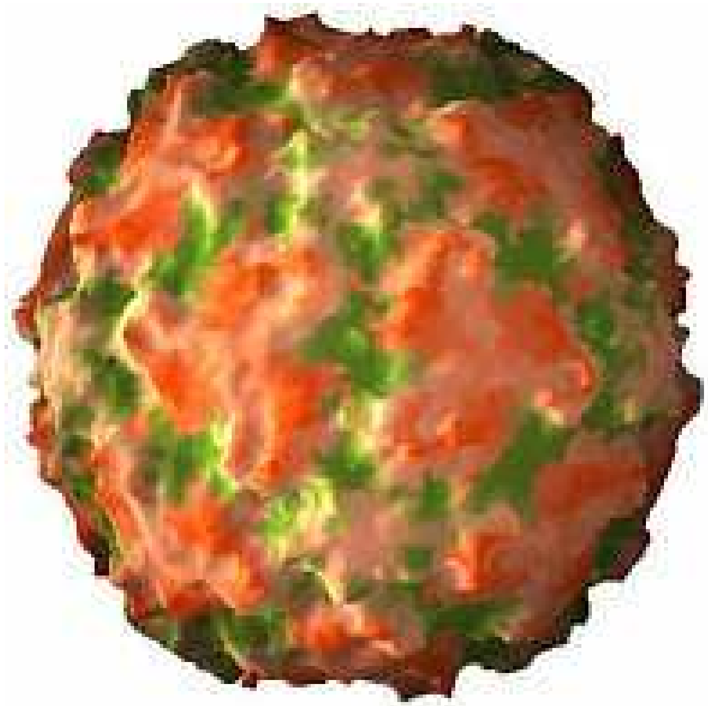


Foot-and-Mouth virus, $T = 3$

Viruses with (pseudo) $T = 3$

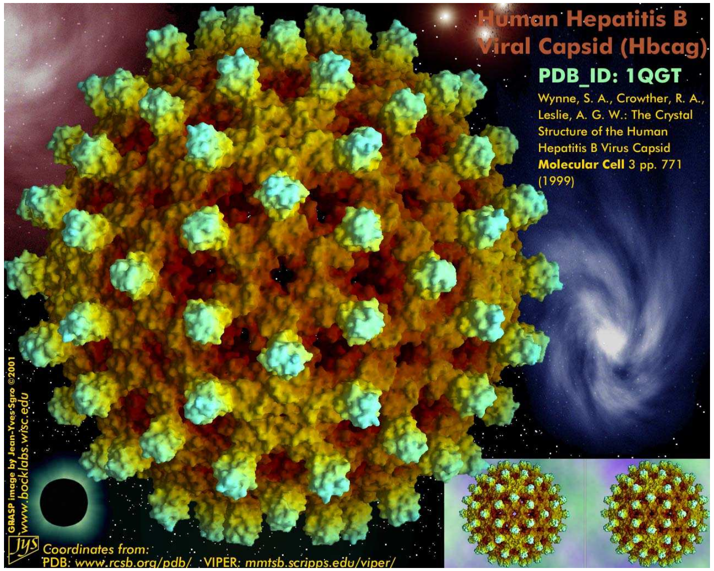


Poliovirus
(polyomyelitis)

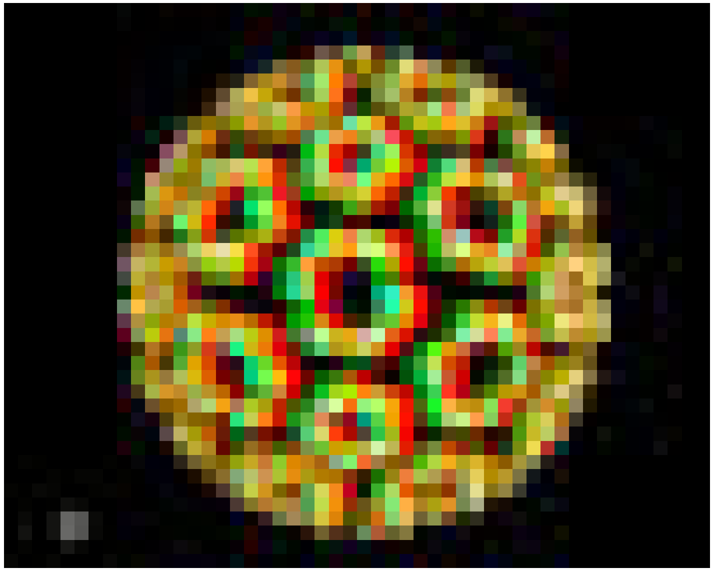


Human Rhinovirus
(cold)

Viruses with $T = 4$

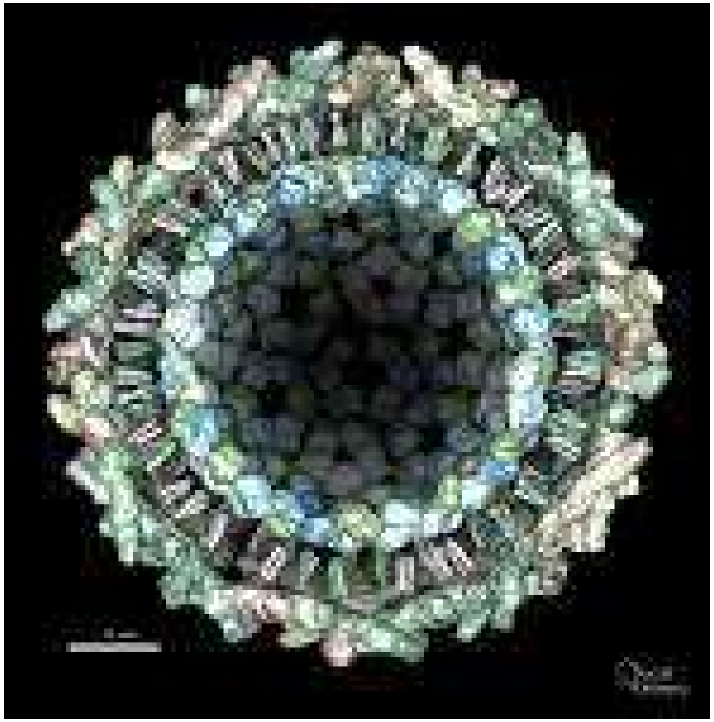


Human hepatitis B

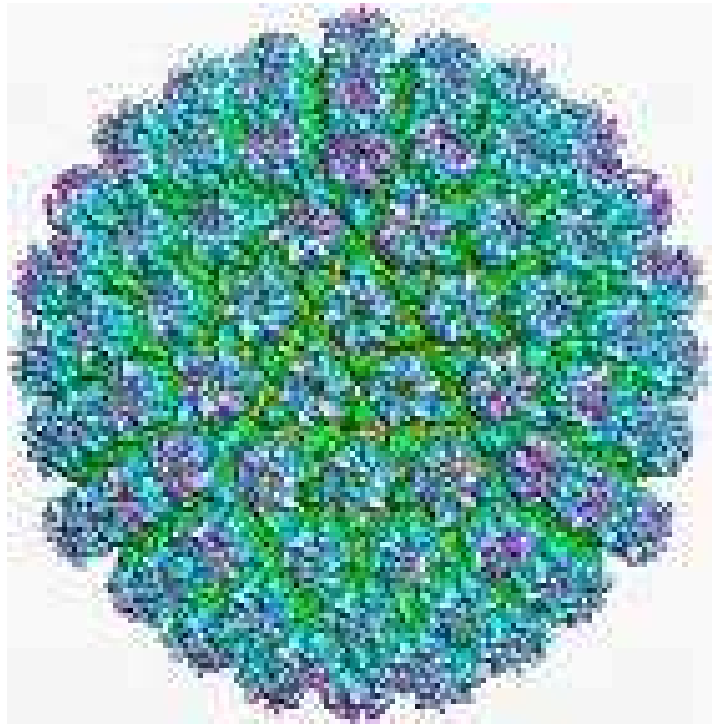


Semliki Forest virus

More $T = a^2$ viruses



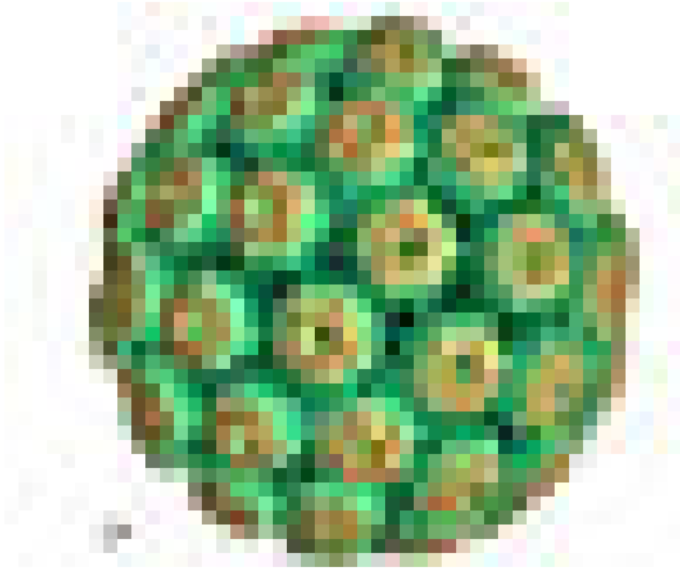
Sindbis virus,
$T = 4$



Herpes virus,
$T = 16$

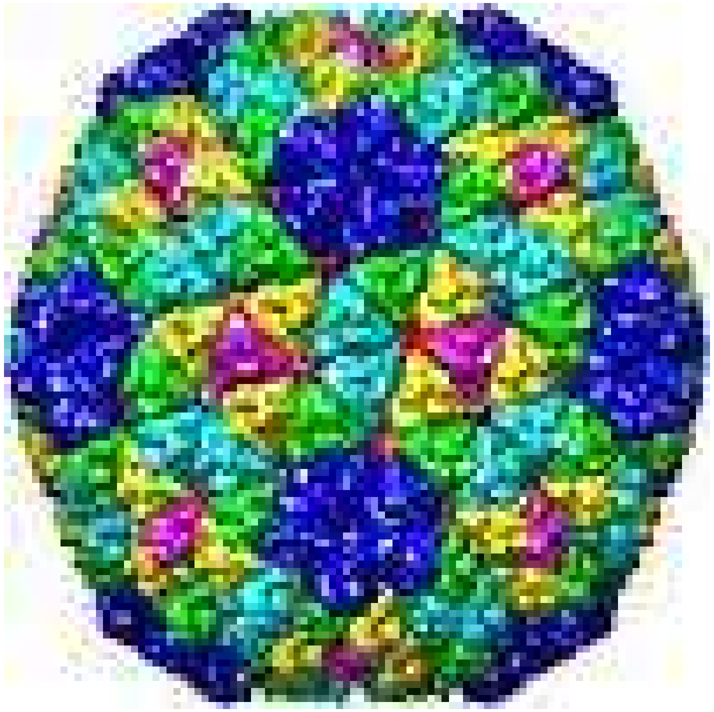
Human and simian papilloma viruses

Polyoma virus,
$T = 7d$

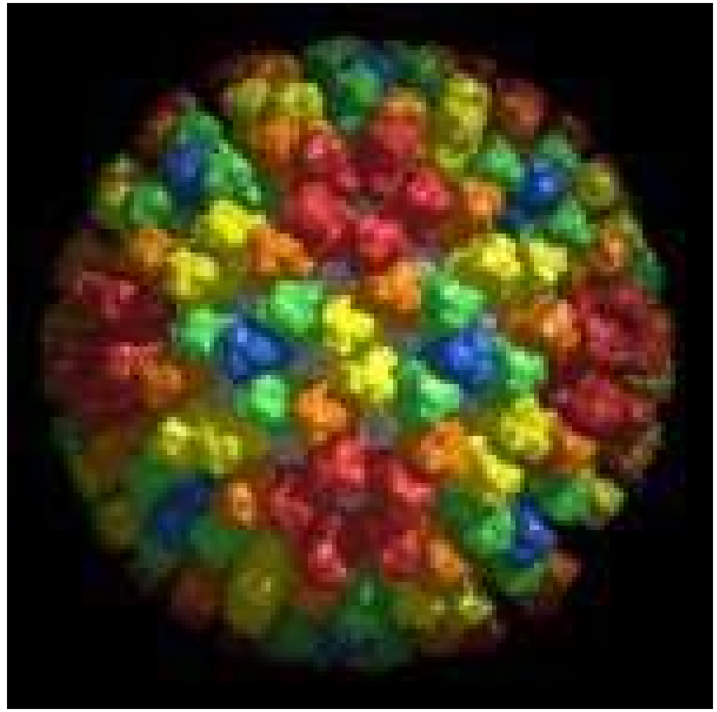


Simian virus 40,
$T = 7d$

Viruses with $T = 13$

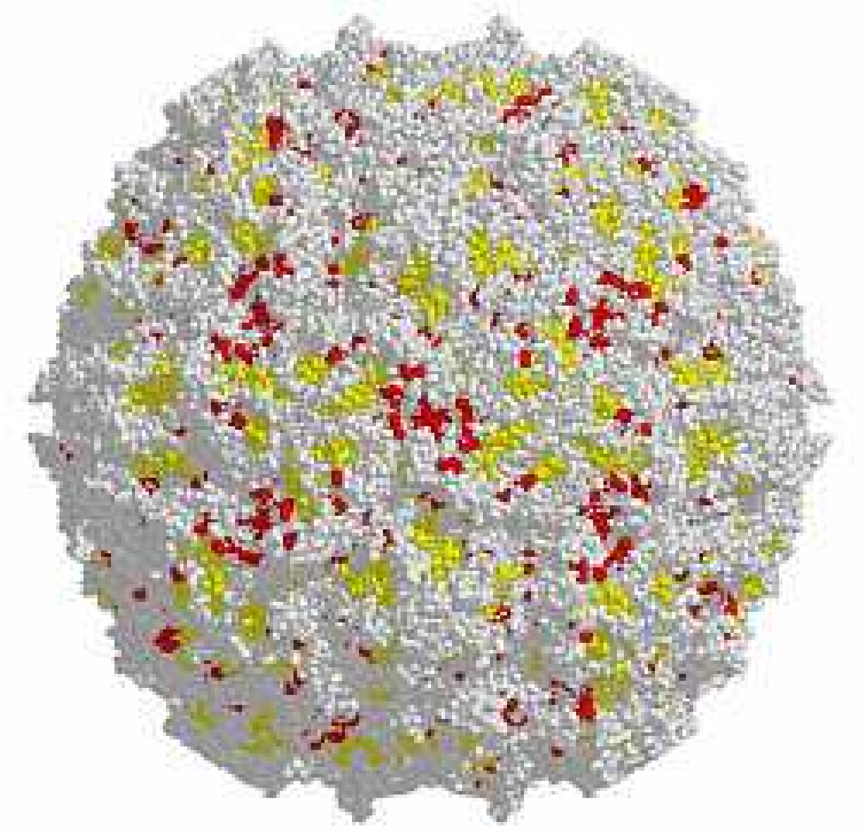


Rice dwarf virus

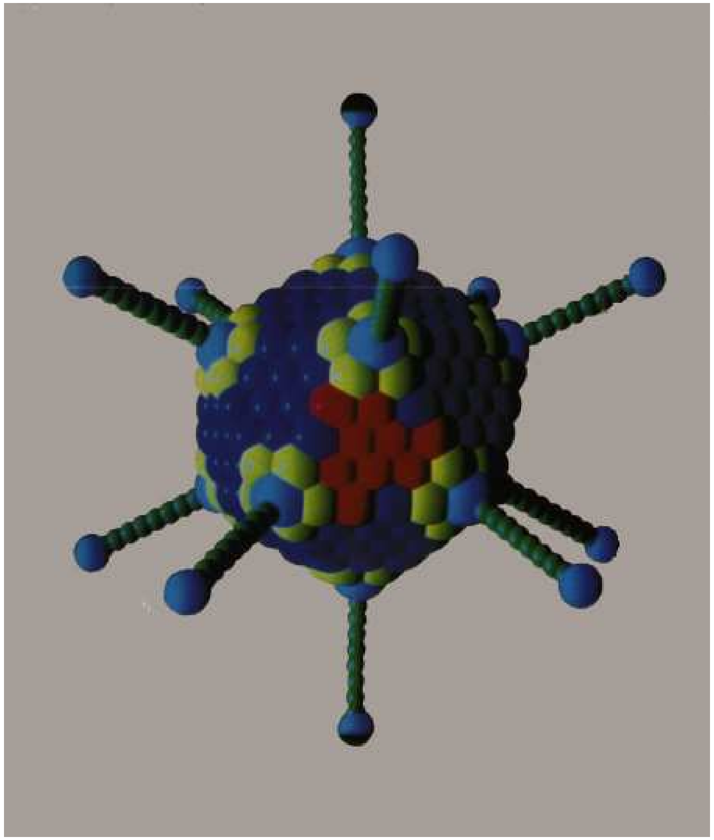


Bluetongue virus

Viruses with $T = 25$

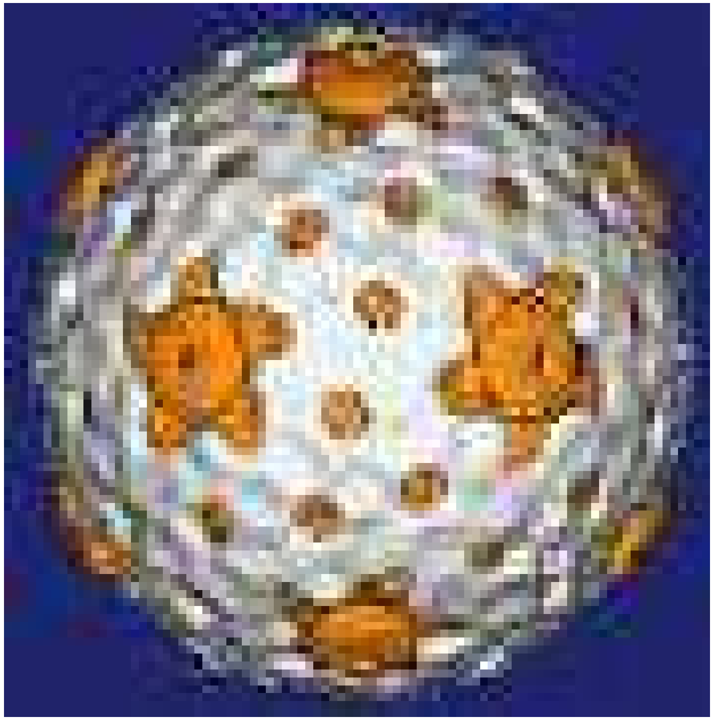


PRD1 virus

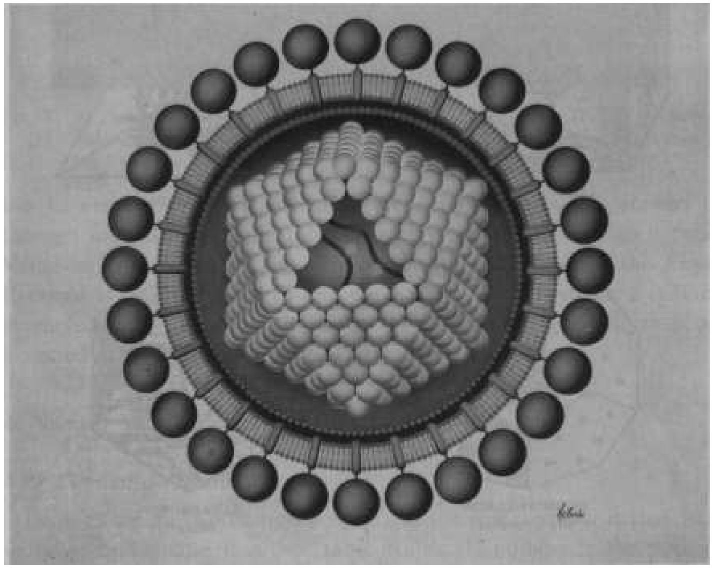


Adenovirus (with its spikes)

More I_h-viruses

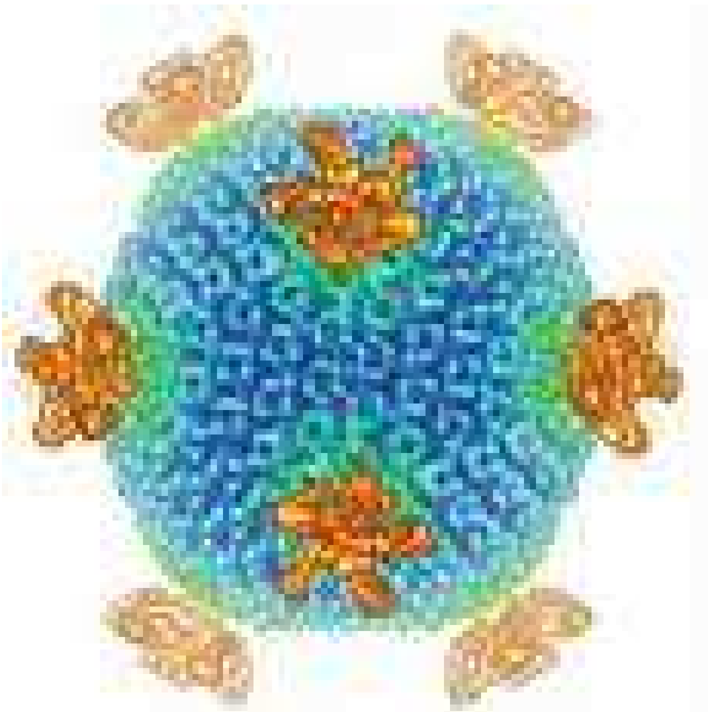


Pseudomonas phage phiKZ,
$T = 27$

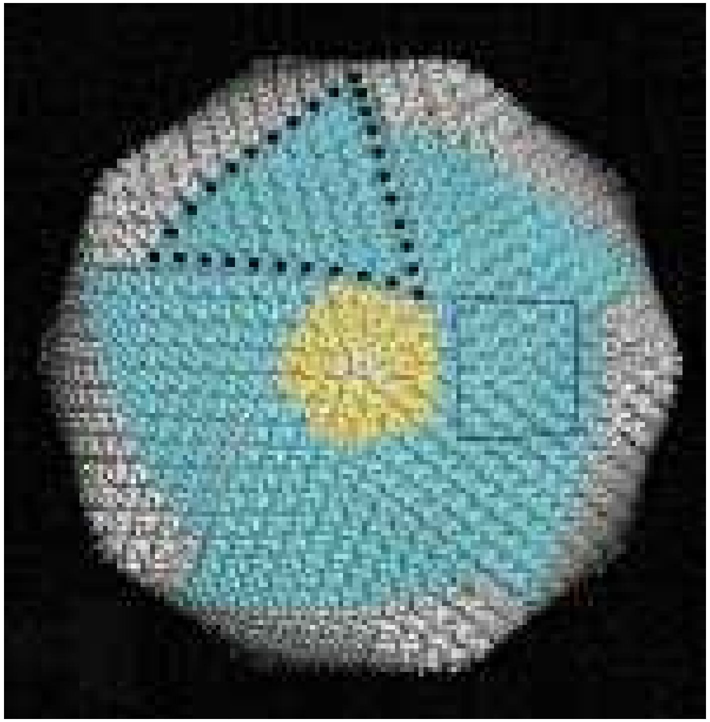


HTLV1 virus,
$T = 36$

Special viruses



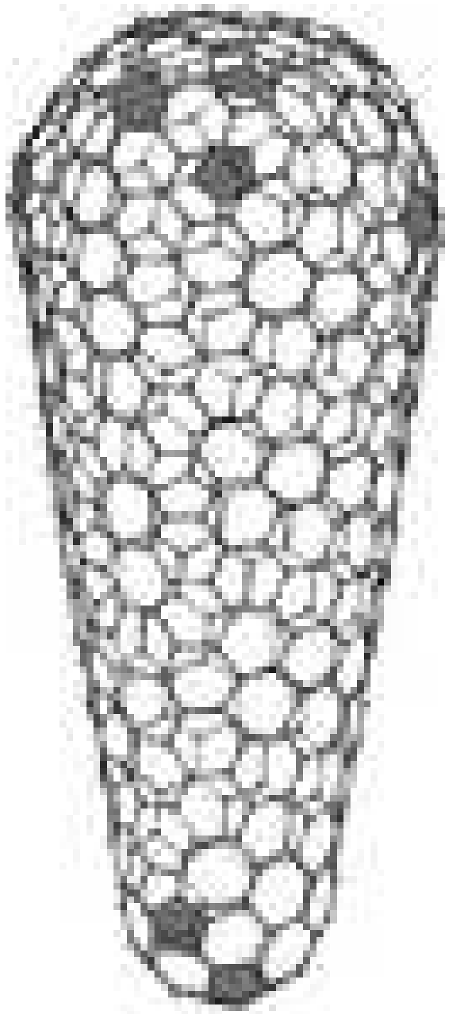
Archeal virus STIV, $T = 31$



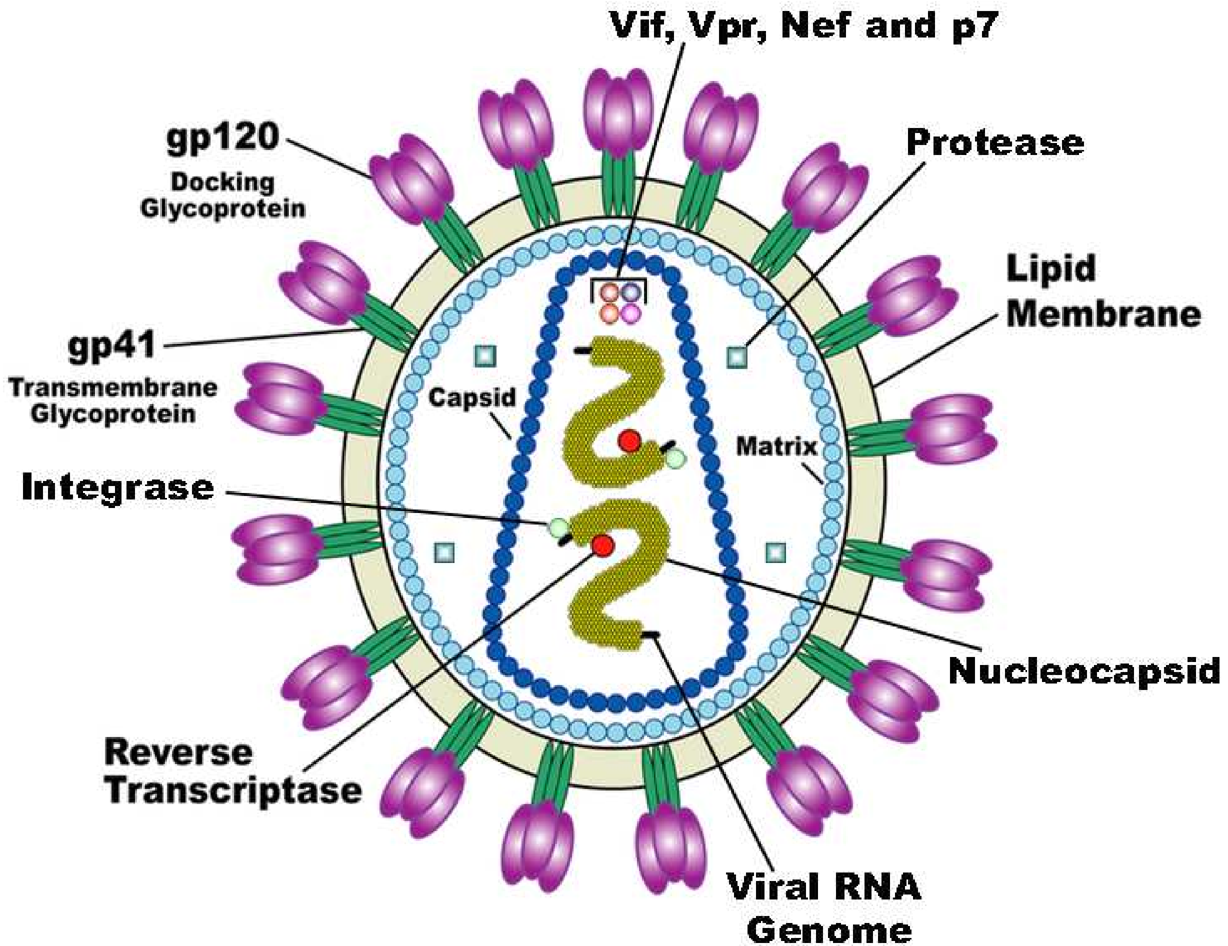
Algal chlorella virus PBCV1 (4th: $\simeq 331.000$ bp), $T = 169$

- Sericesthis iridescent virus, $T = 7^2 + 49 + 7^2 = 147$?
- Tipula iridescent virus, $T = 12^2 + 12 + 1^2 = 157$?

HIV conic fullerene

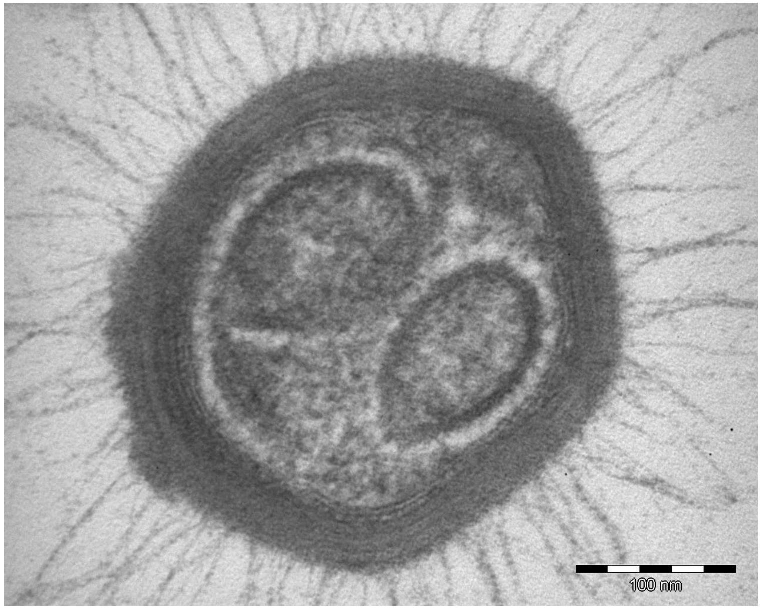


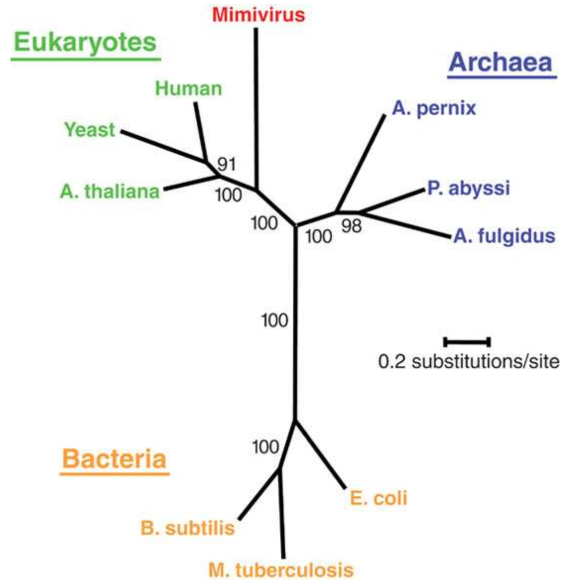
Capsid core



Shape (spikes): $T \simeq 71$?

Mimivirus and other giants





Largest (400nm), >150 (bacteria *Micoplasma genitalium*), $\frac{1}{30}$ of its host *Acanthamoeba Polyphaga* (record: $\frac{1}{10}$). Largest genome: $1.181.404$ bp; 911 protein-coding genes >182 (bacterium *Carsonella ruddii*). Icosahedral: $T = 1179$

Giant DNA viruses (giruses): if >300 genes, >250nm. Ex-"cells-parasiting cells" as smallest bacteria do now?

Viruses: big picture

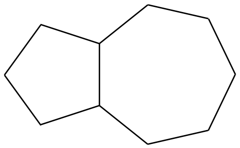
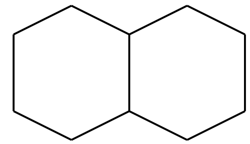
- $1mm^3$ of seawater has $\simeq 10$ million viruses; all seagoing viruses $\simeq 270$ million tons (more 20 x weight of whales).
- Main defense of multi-cellulars, sexual reproduction, is not effective (in cost, risk, speed) but arising mutations give chances against viruses. Wiped out: <10 viruses.
- Origin: ancestors or vestiges of cells, or gene mutation. Or evolved in prebiotic “RNA world" together with cellular forms from self-replicating molecules?
- Viral eukaryogenesis hypothesis (Bell, 2001): nucleus of eukaryotic cell evolved from endosymbiosis event: a girus took control of a *micoplasma* (i.e. without wall) bacterial or archeal cell but, instead of replicating and destroying it, became its ”nucleus”.
- 5-8 $\%$ of human genome: endogeneous retroviruses; In November 2006, Phoenix, 5 Mya old, was resurrected.

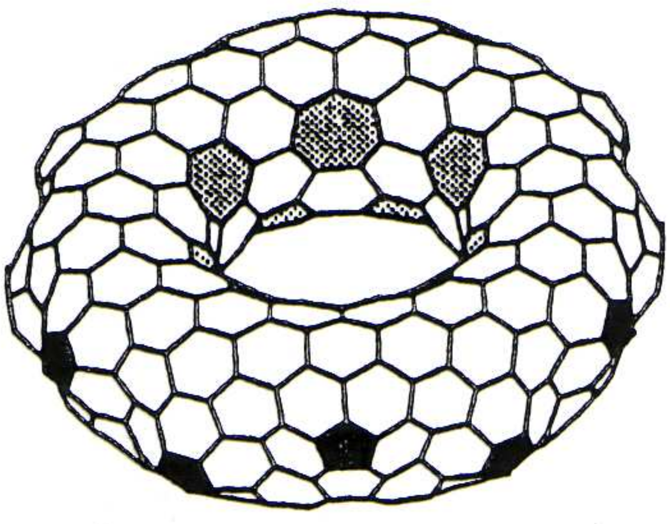
IV. Some fullerene-like 3-valent maps

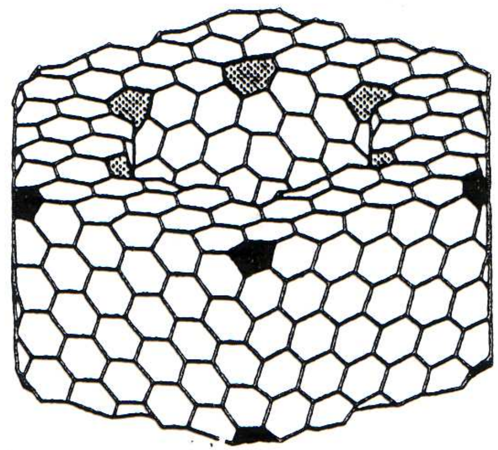
Useful fullerene-like 3-valent maps

Mathematical Chemistry use following fullerene-like maps:

- Polyhedra (p_5, p_6, p_n) for $n = 4$, 7 or 8 ($v_{min} = 14$, 30, 34)
  Aulonia hexagona (E. Haeckel 1887): plankton skeleton
- Azulenoids (p_5, p_7) on torus $g = 1$; so, $p_5 = p_7$

azulen  is an isomer $C_{10}H_8$ of naftalen 

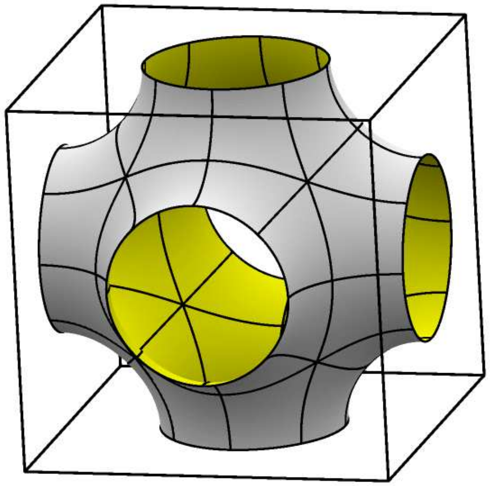




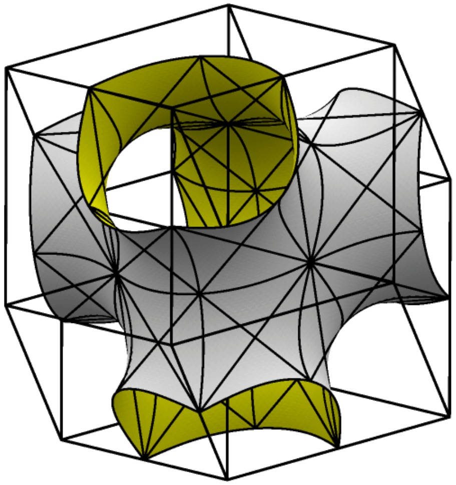
$(p_5, p_6, p_7) = (12, 142, 12)$,
$v = 432$, D_{6d}

Schwarzits

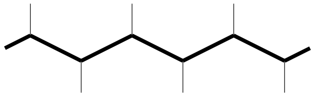
Schwarzits (p_6, p_7, p_8) on minimal surfaces of constant negative curvature ($g \geq 3$). We consider case $g = 3$:



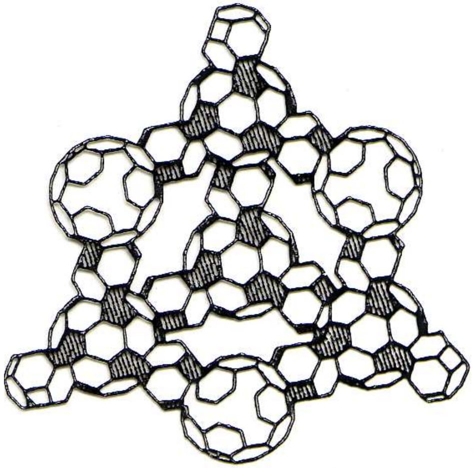
Schwarz P-surface



Schwarz D-surface

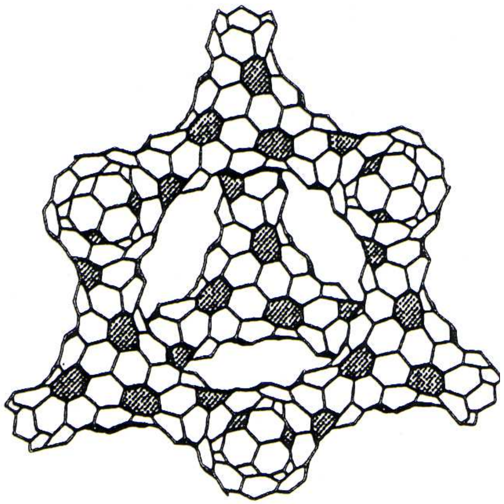
- Take a 3-valent map of genus 3 and cut it along zigzags  and paste it to form D- or P-surface.
- One needs 3 non-intersecting zigzags. For example, Klein regular map 7^3 has 5 types of such triples; $D56$.

$(6,7)$-surfaces

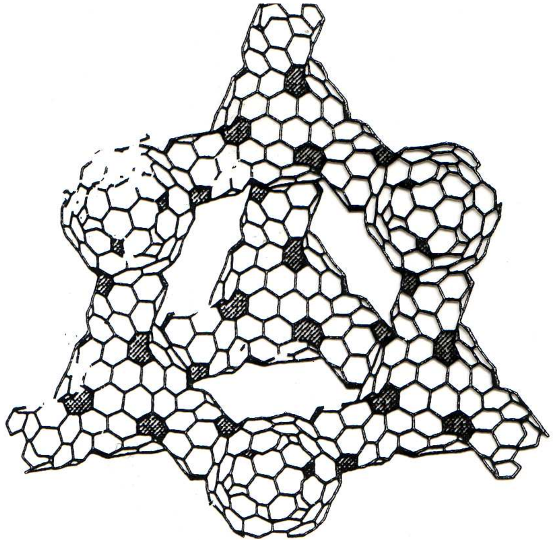


$(1,1)$

$D168$: putative carbon, 1992, (Vanderbilt-Tersoff)



$(0,2)$



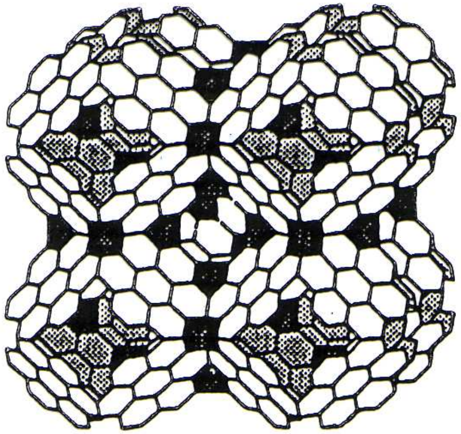
$(1,2)$

$(p_6, p_7 = 24)$, $v = 2p_6 + 56 = 56(p^2 + pq + q^2)$

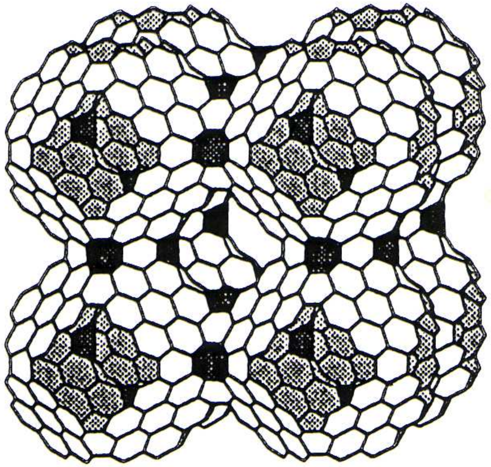
Unit cell of $(1,0)$ has $p_6 = 0, v = 56$: Klein regular map (7^3).

$D56$, $D168$ and $(6,7)$-surfaces are analogs of $F_{20}(I_h)$, $F_{60}(I_h)$ and icosahedral fullerenes.

$(6,8)$-surfaces

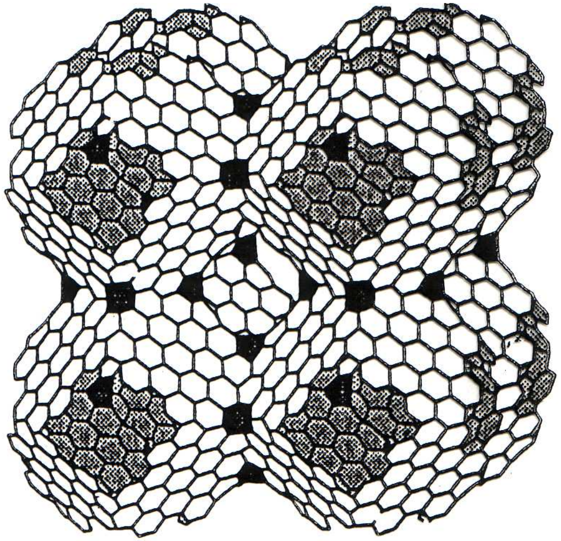


$(1,1)$



$(0,2)$

$P192$, $p_6 = 80$



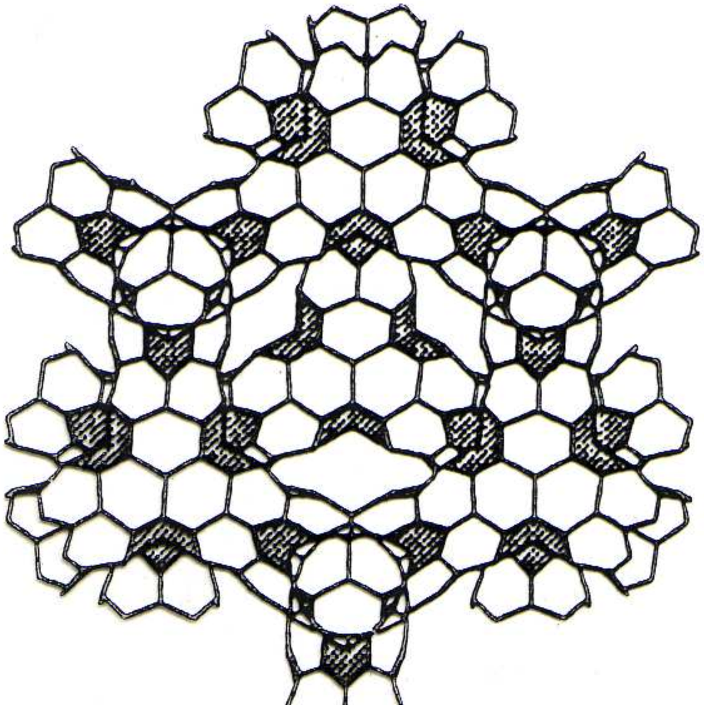
$(1,2)$

$(p_6, p_8 = 12)$, $v = 2p_6 + 32 = 48(p^2 + pq + q^2)$

Starting with $(1,0)$: $P48$ with $p_6 = 8$

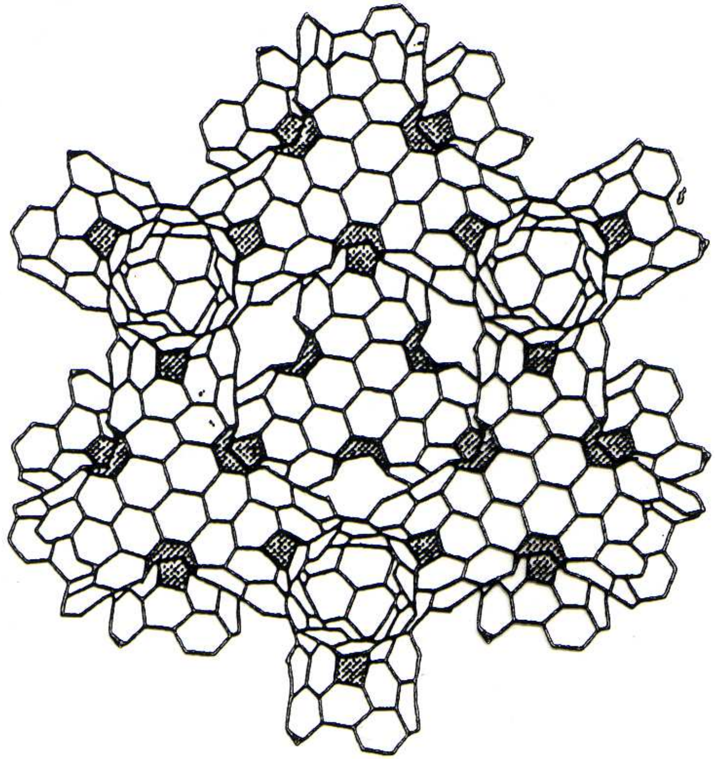
while unit cell with $p_6 = 0$ is $P32$ - Dyck regular map (8^3)

More $(6,8)$-surfaces



$(0,2)$

$v = 120$, $p_6 = 44$



$(1,2)$

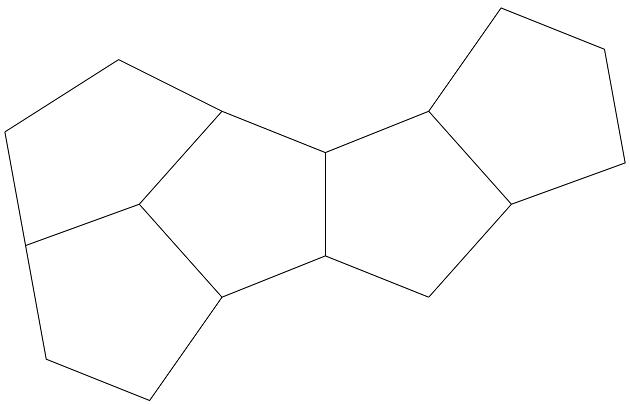
$(p_6, p_8 = 12)$, $v = 2p_6 + 32 = 30(p^2 + pq + q^2)$

Unit cell of $p_6 = 0$: $P32$ - Dyck regular map (8^3)

Polycycles

A finite (p, q)-polycycle is a plane 2-connected finite graph, such that :

- all interior faces are (combinatorial) p-gons,
- all interior vertices are of degree q,
- all boundary vertices are of degree in $[2, q]$.



a $(5, 3)$-polycycle

Examples of $(p, 3)$-polycycles

- $p = 3 : 3^3, 3^3 - v, 3^3 - e$;
- $p = 4 : 4^3, 4^3 - v, 4^3 - e$, and
  $P_2 \times A$ with $A = P_{n \geq 1}$, $P_{\mathbb{N}}$, $P_{\mathbb{Z}}$
- Continuum for any $p \geq 5$.
  But 39 proper $(5, 3)$-polycycles,
  i.e., partial subgraphs of Dodecahedron
- $p = 6$: polyhexes=benzenoids

Theorem
(i) Planar graphs admit at most one realization as $(p, 3)$-polycycle
(ii) any unproper $(p, 3)$-polycycle is a $(p, 3)$-helicene (homomorphism into the plane tiling $\{p^3\}$ by regular p-gons)

Icosahedral fulleroids (with Delgado)

3-valent polyhedra with $p = (p_5, p_{n>6})$ and icosahedral symmetry (I or I_h); so, $v = 20 + 2p_n(n-5)$ vertices.

face orbit size	60	30	20	12
number of orbits	any	≤ 1	≤ 1	1
face degrees $5, n$	any	$3t$	$2t$	$5t$

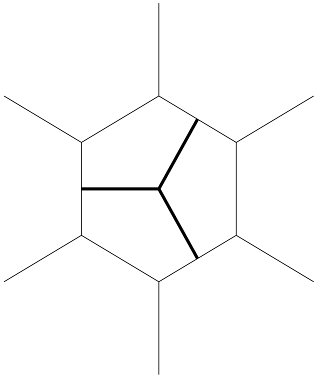
$A_{n,k} : (p_5, p_n) = (12 + 60k, \frac{60k}{n-6})$ with $k \geq 1$, $n > 6$,

$B_{n,k} : (p_5, p_n) = (60k, 12\frac{5k-1}{n-6})$ with $k \geq 1$, $n = 5t > 5$.

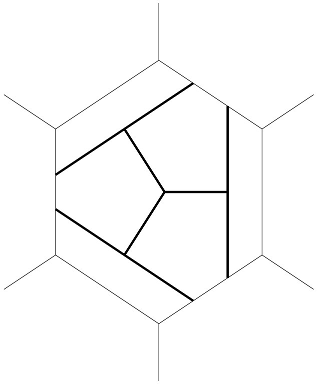
Also: infinite series for $n = 7$ generalizing $A_{7,1}b$ and $n = 8$; obtained from $(2k+1, 0)$-dodecahedron by decorations (partial operations T_1 and T_2, respectively).

Jendrol-Trenkler (2001): for any integers $n \geq 8$ and $m \geq 1$, there exists an $I(5, n)$-fulleroid with $p_n = 60m$.

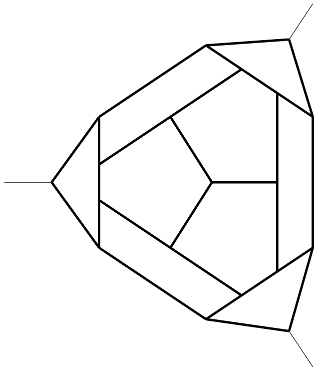
Decoration operations producing 5-gons



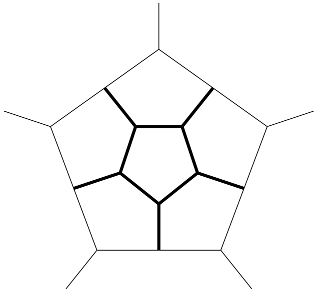
Triacon T_1



Triacon T_2



Triacon T_3



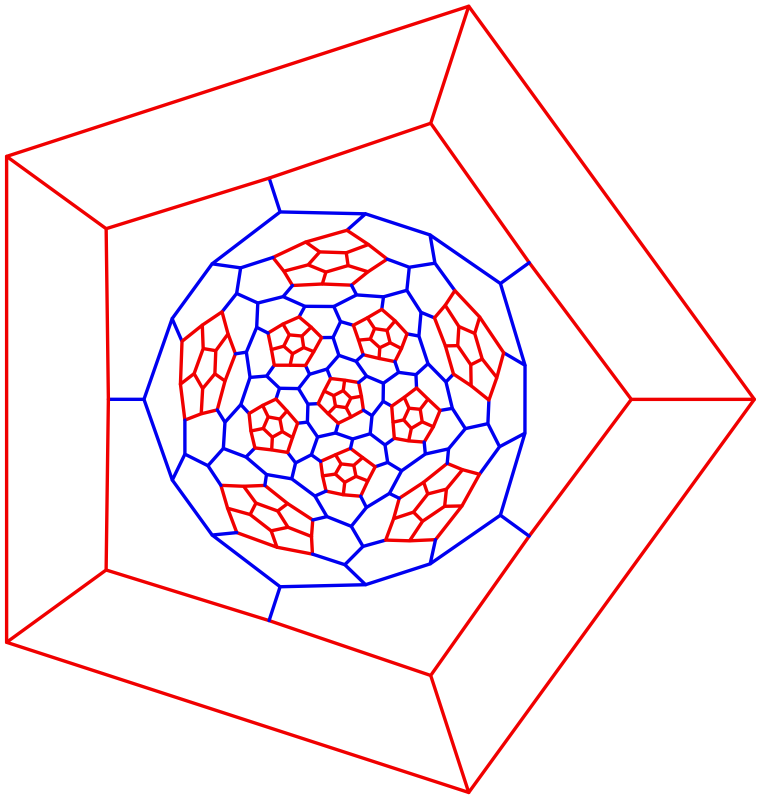
Pentacon P

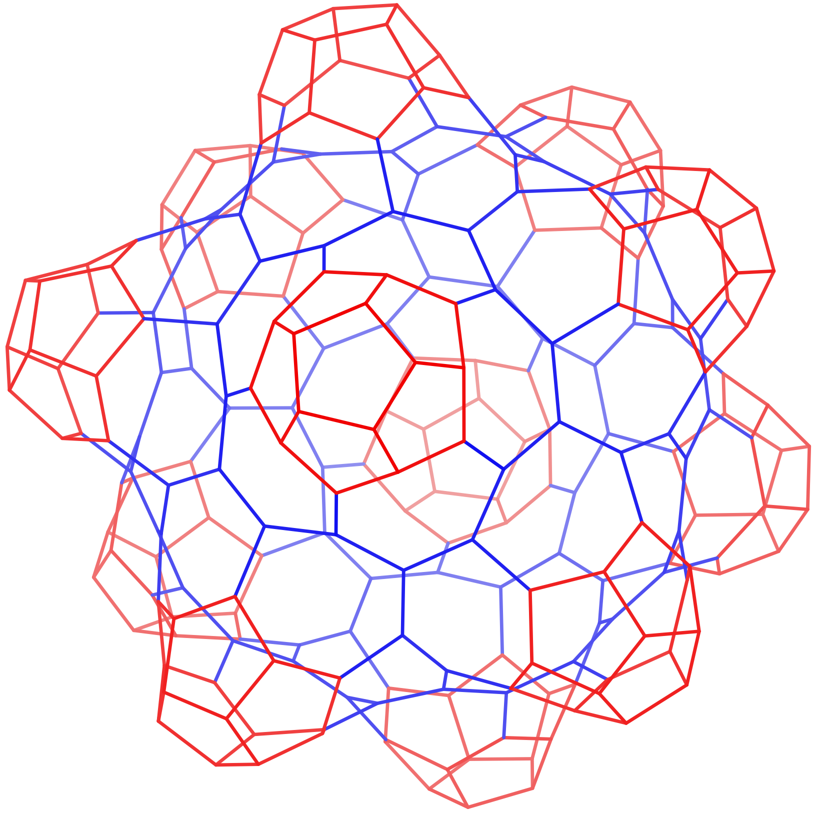
I-fulleroids

	p_5	$n; p_n$	v	# of	Sym
$A_{7,1}$	72	$7, 60$	260	2	I
$A_{8,1}$	72	$8, 30$	200	1	I_h
$A_{9,1}$	72	$9, 20$	180	1	I_h
$B_{10,1}$	60	$10, 12$	140	1	I_h
$A_{11,5}$	312	$11, 60$	740	$?$	
$A_{12,2}$	132	$12, 20$	300	$-$	
$A_{12,3}$	192	$12, 30$	440	1	I_h
$A_{13,7}$	432	$13, 60$	980	$?$	
$A_{14,4}$	252	$14, 30$	560	1	I_h
$B_{15,2}$	120	$15, 12$	260	1	I_h

Above $(5, n)$-spheres: unique for their p-vector (p_5, p_n), $n > 7$

1st smallest icosahedral $(5,7)$-spheres

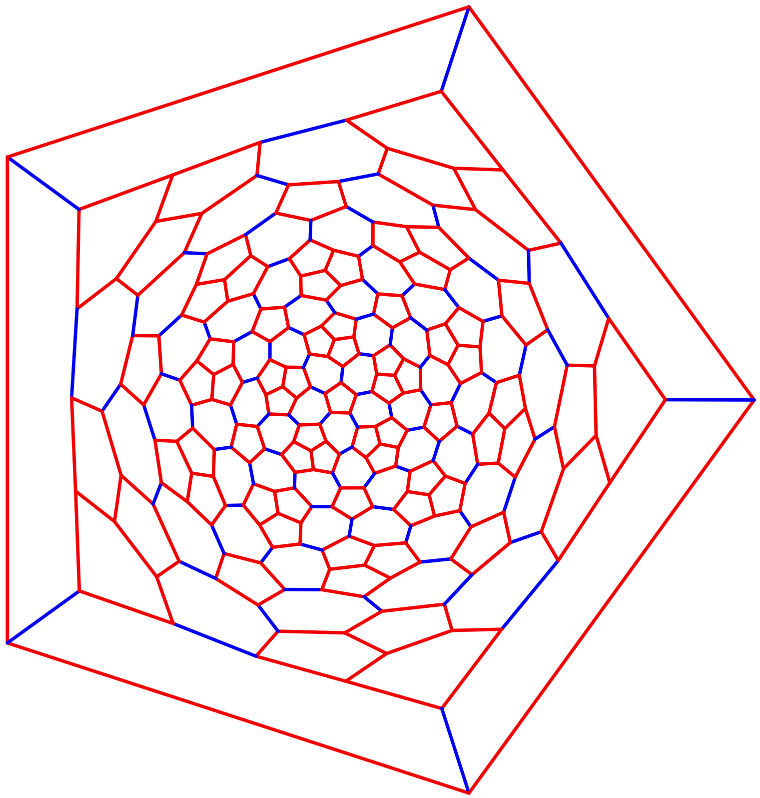


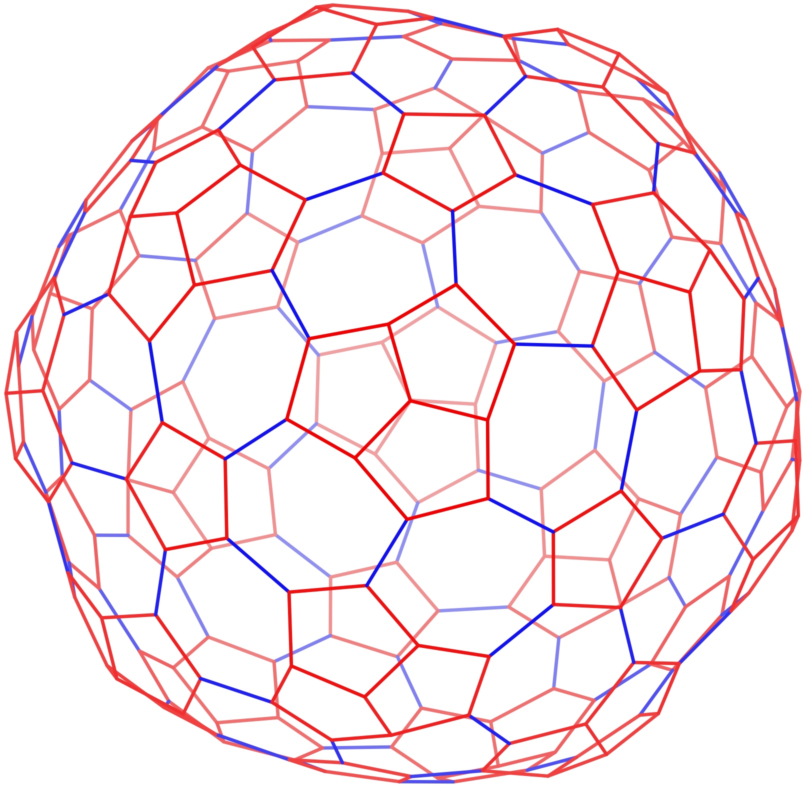


$F_{5,7}(I)a = P(C_{140}(I))$; $v = 260$

Dress-Brinkmann (1996) 1st Phantasmagorical Fulleroid

2nd smallest icosahedral $(5,7)$-spheres

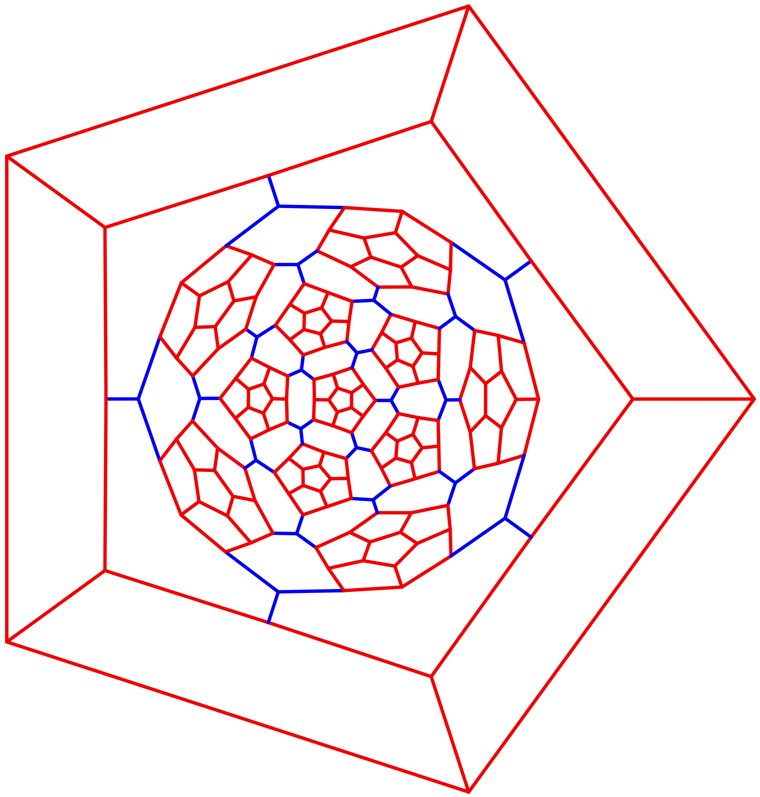


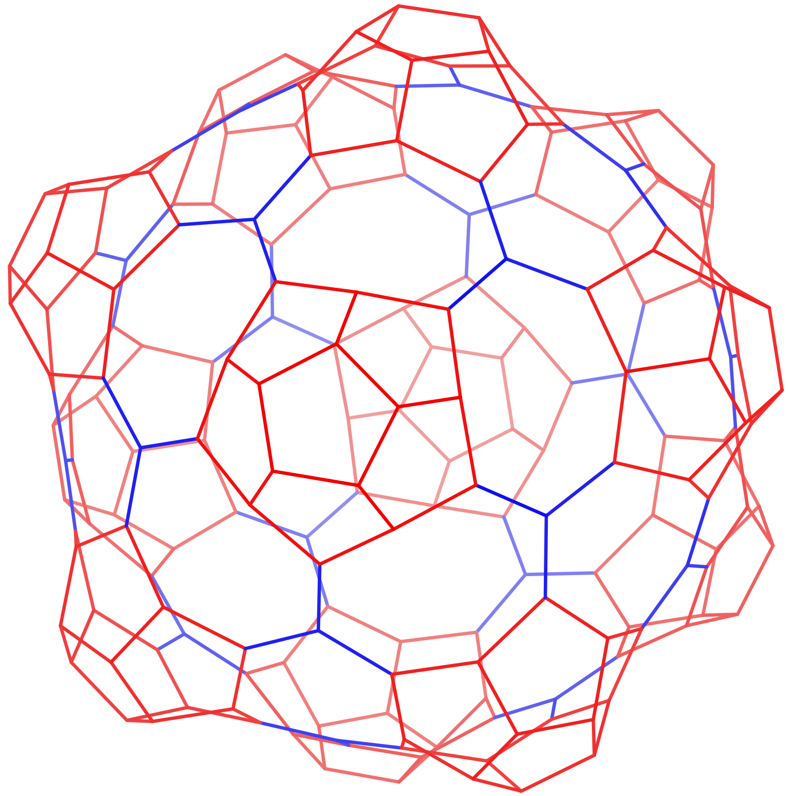


$F_{5,7}(I)b = T_1(C_{180}(I_h))$; $v = 260$

Dress-Brinkmann (1996) 2nd Phantasmagorical Fulleroid

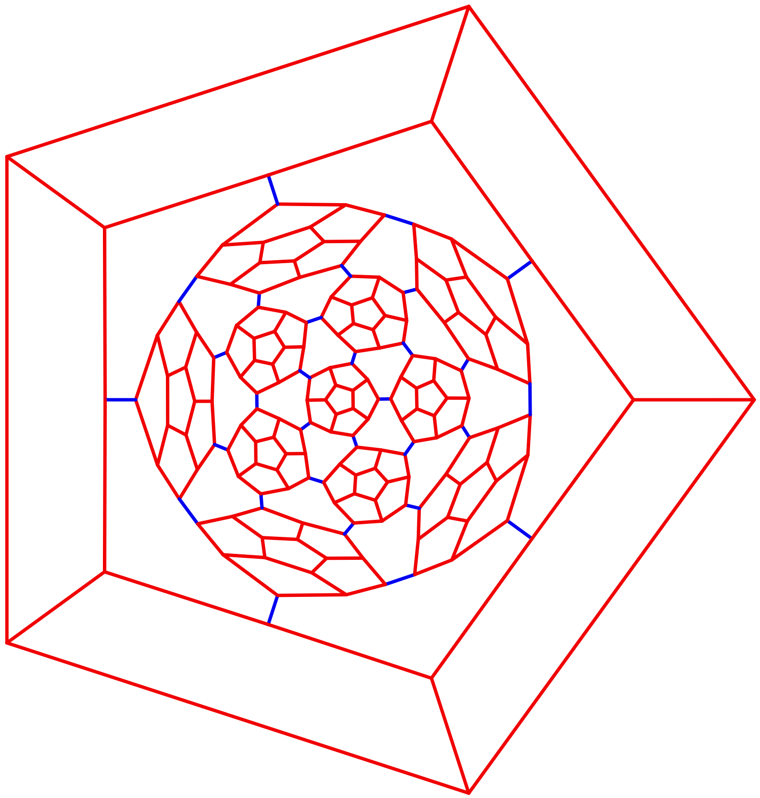
The smallest icosahedral $(5,8)$-sphere

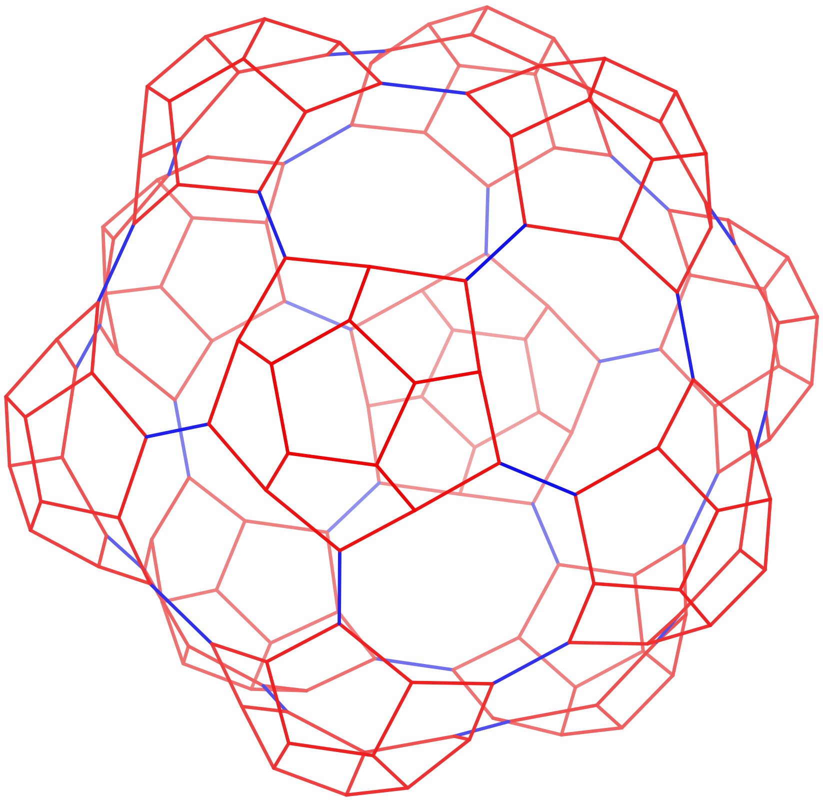




$F_{5,8}(I_h) = P(C_{80}(I_h))$; $v = 200$

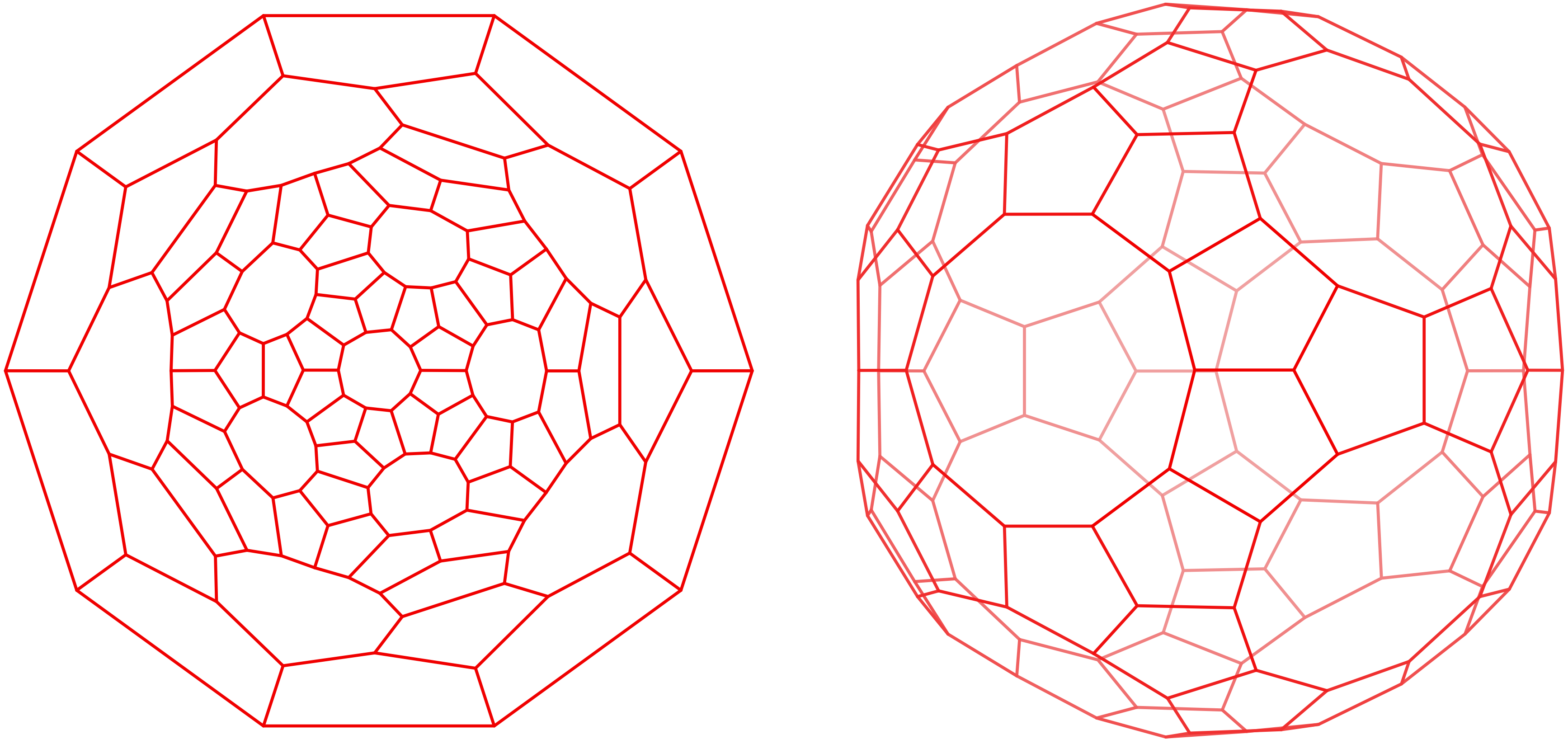
The smallest icosahedral $(5,9)$-sphere





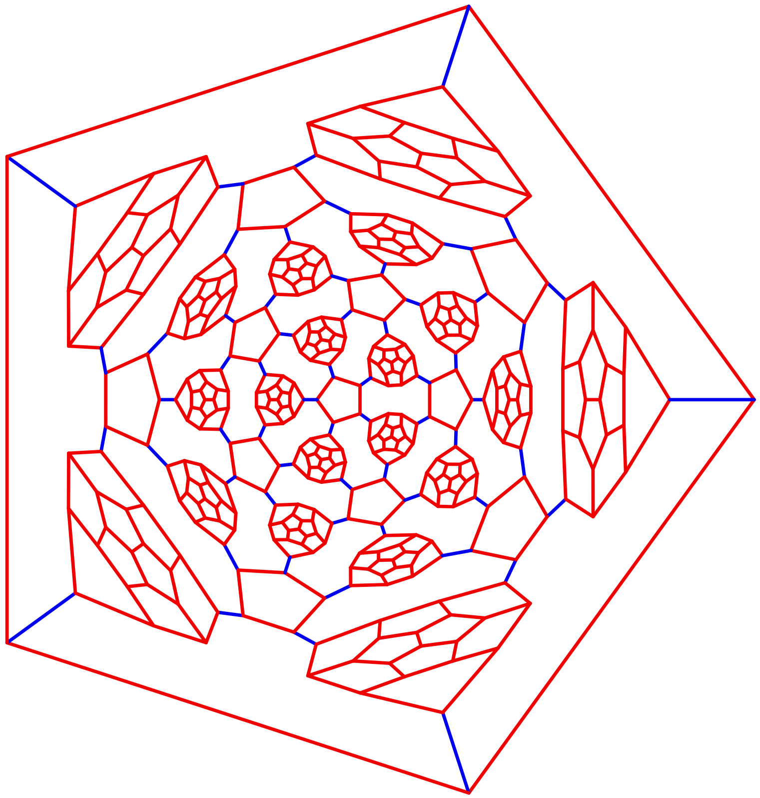
$F_{5,9}(I_h) = P(C_{60}(I_h))$; $v = 180$

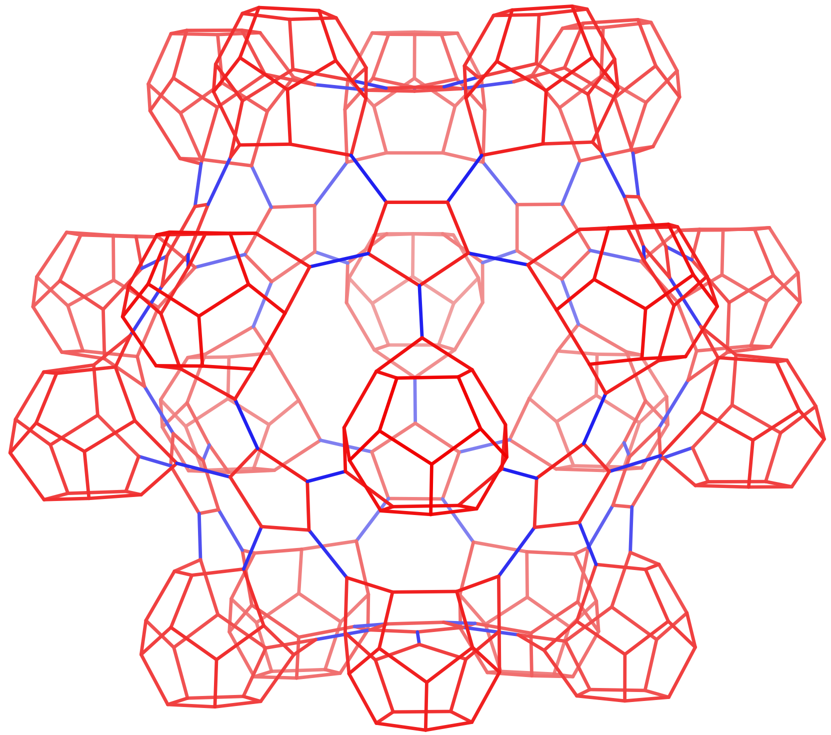
The smallest icosahedral $(5,10)$-sphere



$F_{5,10}(I_h) = T_1(C_{60}(I_h))$; $v = 140$

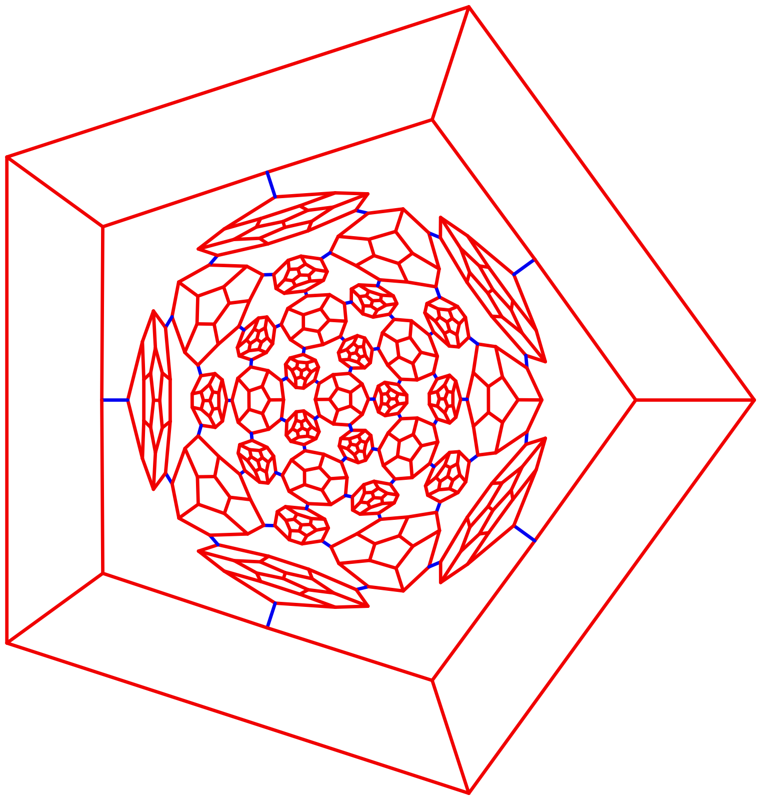
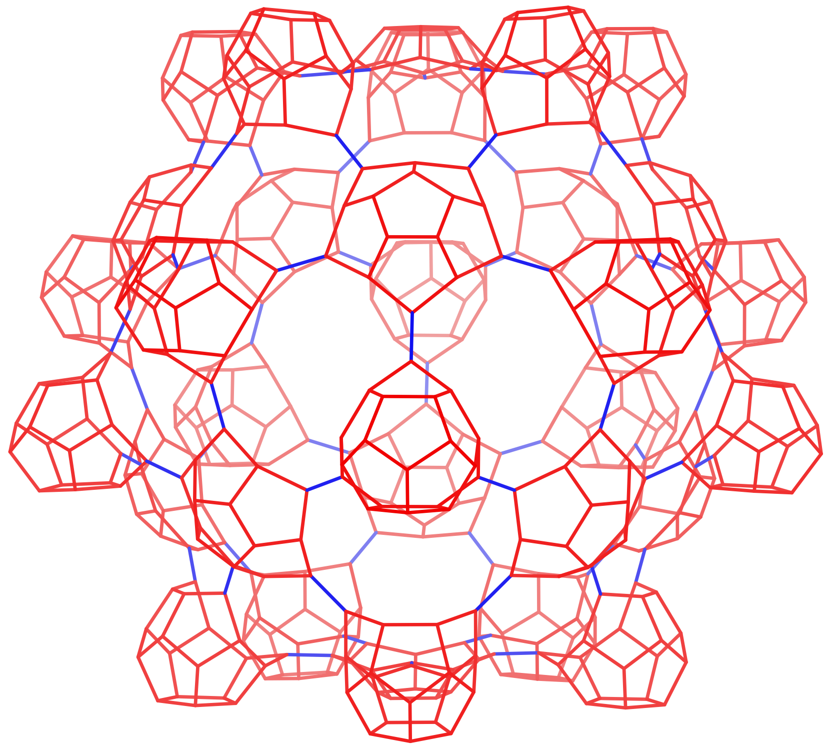
The smallest icosahedral $(5, 12)$-sphere





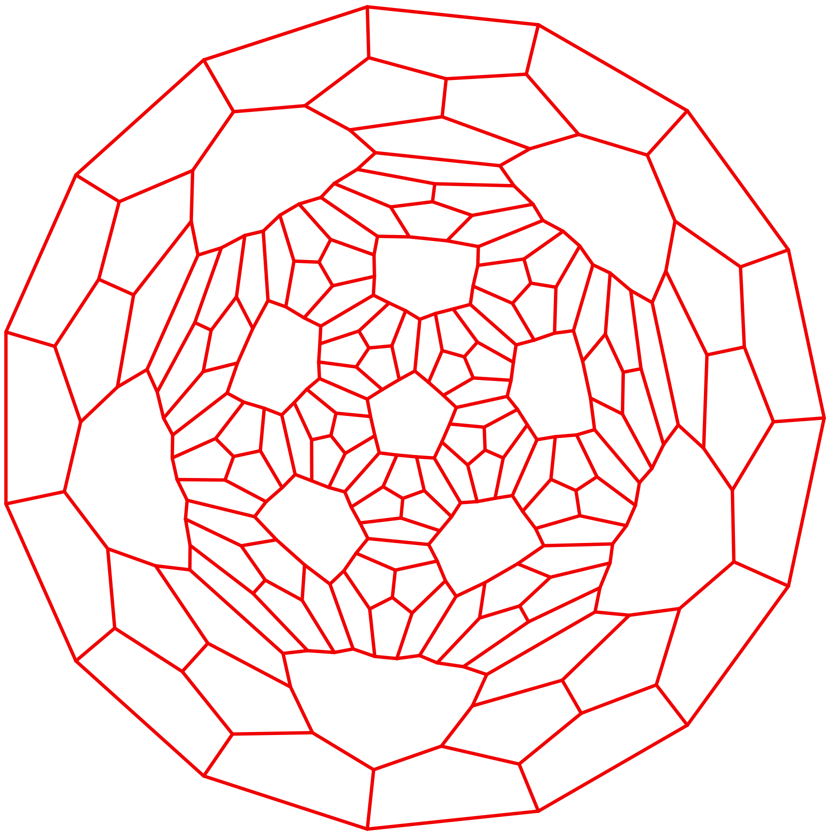
$$F_{5,12}(I_h) = T_3(C_{80}(I_h)); \; v = 440$$

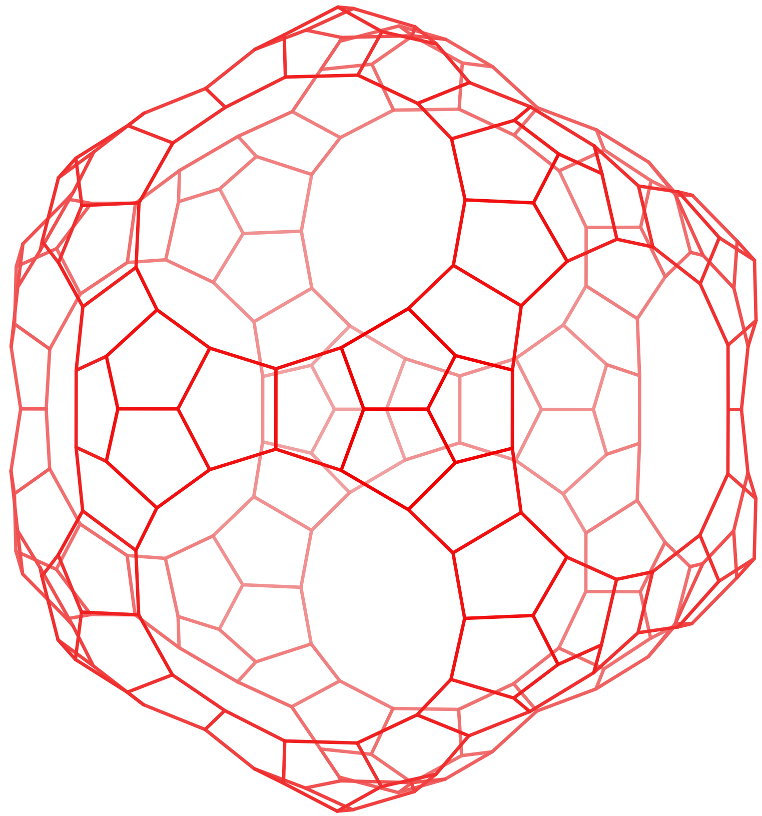
The smallest icosahedral $(5, 14)$-sphere

$$F_{5,14}(I_h) = P(F_{5,12}(I_h));\ v = 560$$

The smallest icosahedral $(5, 15)$-sphere



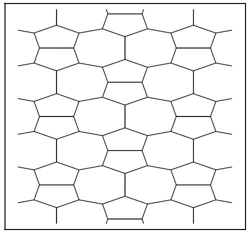
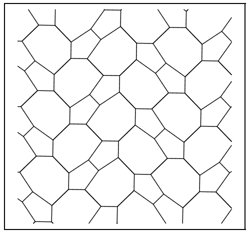
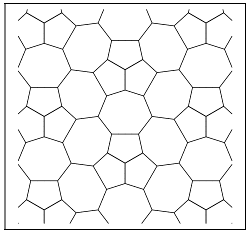
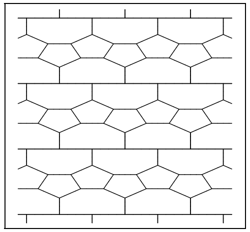
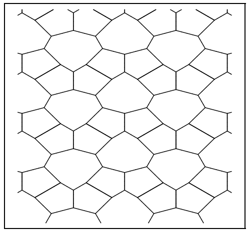
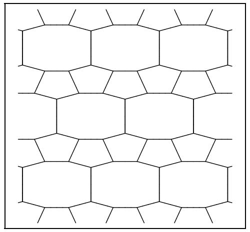
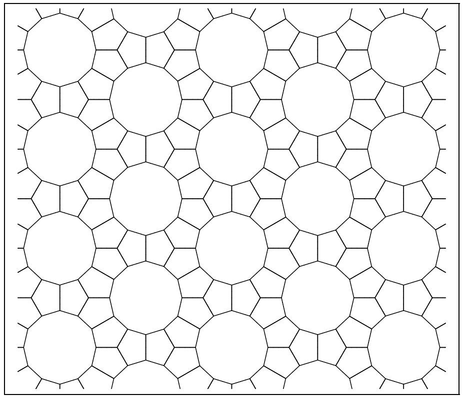


$F_{5,15}(I_h) = T_2(C_{60}(I_h))$; $v = 260$

G-fulleroids

- G-fulleroid: cubic polyhedron with $p = (p_5, p_n)$ and symmetry group G; so, $p_n = \frac{p_5 - 12}{n-6}$.
- Fowler et al., 1993: G-fulleroids with $n = 6$ (fullerenes) exist for 28 groups G.
- Kardos, 2007: G-fulleroids with $n = 7$ exists for 36 groups G; smallest for $G = I_h$ has 500 vertices.
  There are infinity of G-fulleroids for all $n \geq 7$ if and only if G is a subgroup of I_h; there are 22 types of such groups.
- Dress-Brinkmann, 1986: there are 2 smallest I-fulleroids with $n = 7$; they have 260 vertices.
- D-Delgado, 2000: 2 infinite series of I-fulleroids and smallest ones for $n = 8, 10, 12, 14, 15$.
- Jendrol-Trenkler, 2001: I-fulleroids for all $n \geq 8$.

All seven 2-isohedral $(5, n)$-planes

A $(5, n)$-plane is a 3-valent plane tiling by 5- and n-gons.
A plane tiling is 2-homohedral if its faces form 2 orbits under group of combinatorial automorphisms Aut.
It is 2-isohedral if, moreover, its symmetry group is isomorphic to Aut.

V. d-dimensional fullerenes (with Shtogrin)

d-fullerenes

$(d-1)$-dim. simple (d-valent) manifold (loc. homeomorphic to $\mathbb{R}^{d-1}$) compact connected, any 2-face is 5- or 6-gon.
So, any i-face, $3 \le i \le d$, is an polytopal i-fullerene.
So, $d = 2, 3, 4$ or 5 only since (Kalai, 1990) any 5-polytope has a 3- or 4-gonal 2-face.

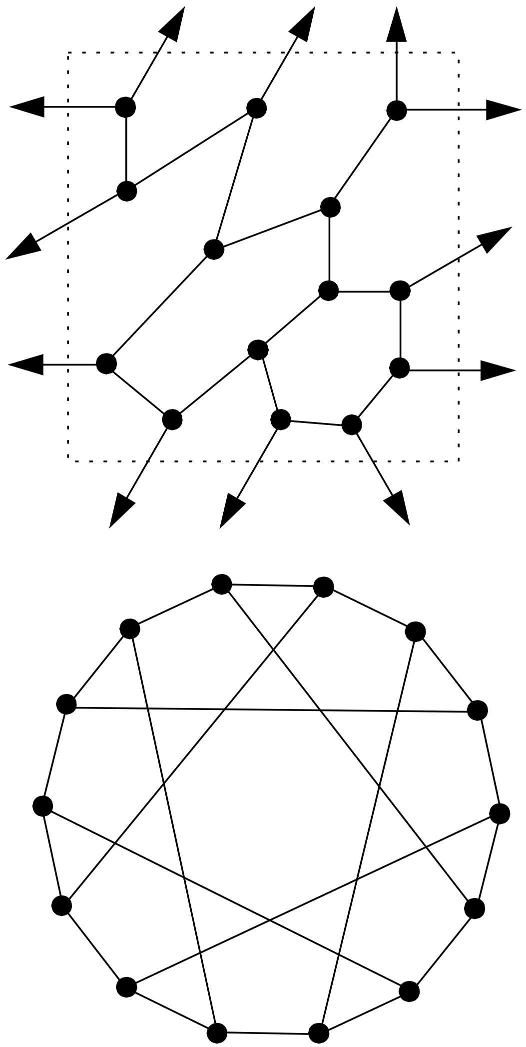
- All finite 3-fullerenes
- ∞: plane 3- and space 4-fullerenes
- 4 constructions of finite 4-fullerenes (all from 120-cell):
  - A (tubes of 120-cells) and B (coronas)
  - Inflation-decoration method (construction C, D)
- Quotient fullerenes; polyhexes
- 5-fullerenes from tiling of H^4 by 120-cell

All finite 3-fullerenes

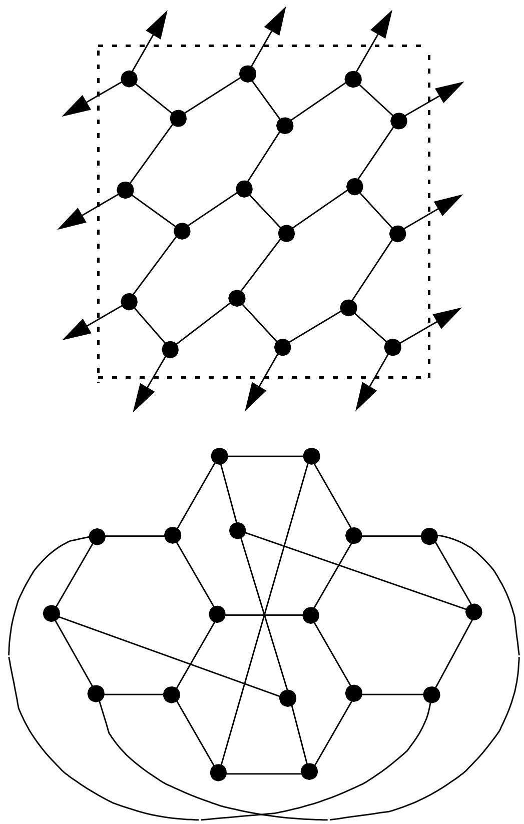
- Euler formula $\chi = v - e + p = \frac{p_5}{2} \geq 0$.
- But $\chi = \begin{cases} 2(1-g) & \text{if oriented} \\ 2-g & \text{if not} \end{cases}$
- Any 2-manifold is homeomorphic to S^2 with g (genus) handles (cyl.) if oriented or cross-caps (Möbius) if not.

g	0	$1(or.)$	$2(not\ or.)$	$1(not\ or.)$
surface	S^2	T^2	K^2	P^2
p_5	12	0	0	6
p_6	$\geq 0, \neq 1$	≥ 7	≥ 9	$\geq 0, \neq 1, 2$
3-fullerene	usual sph.	polyhex	polyhex	projective

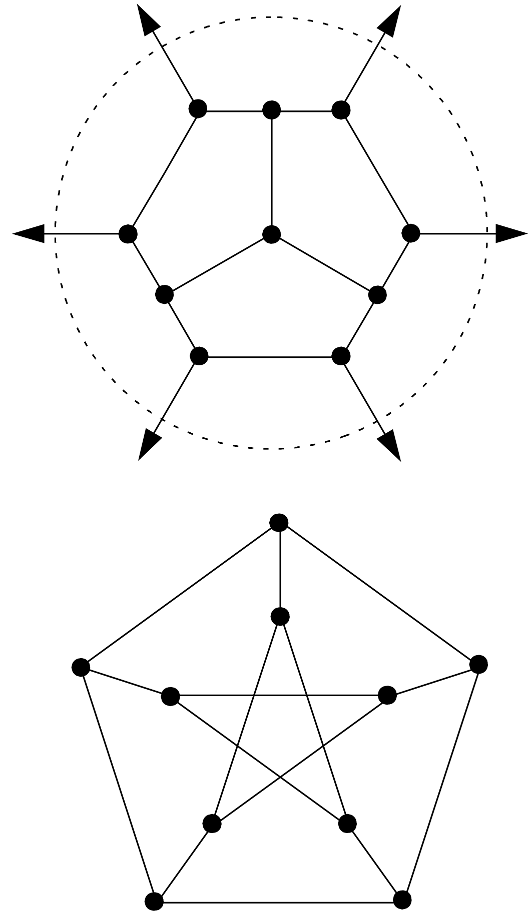
Smallest non-spherical finite 3-fullerenes



Toric fullerene



Klein bottle fullerene



projective fullerene

Non-spherical finite 3-fullerenes

- Projective fullerenes are antipodal quotients of centrally symmetric spherical fullerenes, i.e. with symmetry C_i, C_{2h}, D_{2h}, D_{6h}, D_{3d}, D_{5d}, T_h, I_h. So, $v \equiv 0 \pmod 4$. Smallest CS fullerenes $F_{20}(I_h)$, $F_{32}(D_{3d})$, $F_{36}(D_{6h})$
- Toroidal fullerenes have $p_5 = 0$. They are described by Negami in terms of 3 parameters.
- Klein bottle fullerenes have $p_5 = 0$. They are obtained as quotient of toroidal ones by a fixed-point free involution reversing the orientation.

Plane fullerenes (infinite 3-fullerenes)

- Plane fullerene: a 3-valent tiling of E^2 by (combinatorial) 5- and 6-gons.
- If $p_5 = 0$, then it is the graphite $\{6^3\} = F_\infty = 63$.
- **Theorem:** plane fullerenes have $p_5 \leq 6$ and $p_6 = \infty$.
- A.D. Alexandrov (1958): any metric on E^2 of non-negative curvature can be realized as a metric of convex surface on E^3.
  Consider plane metric such that all faces became regular in it. Its curvature is 0 on all interior points (faces, edges) and ≥ 0 on vertices.
  A convex surface is at most half S^2.

Space fullerenes (infinite 4-fullerene)

- 4 Frank-Kasper polyhedra (isolated-hexagon fullerenes): $F_{20}(I_h)$, $F_{24}(D_{6d})$, $F_{26}(D_{3h})$, $F_{28}(T_d)$
- FK space fullerene: a 4-valent 3-periodic tiling of E^3 by them; space fullerene: such tiling by any fullerenes.
- FK space fullerenes occur in:
  - tetrahedrally close-packed phases of metallic alloys.
  - Clathrates (compounds with 1 component, atomic or molecular, enclosed in framework of another), incl. Clathrate hydrates, where cells are solutes cavities, vertices are H_2O, edes are hydrogen bonds; Zeolites (hydrated microporous aluminosilicate minerals), where vertices are tetrahedra SiO_4 or $SiAlO_4$, cells are H_2O, edges are oxygen bridges.
  - Soap froths (foams, liquid crystals).

24 known primary FK space fullerenes

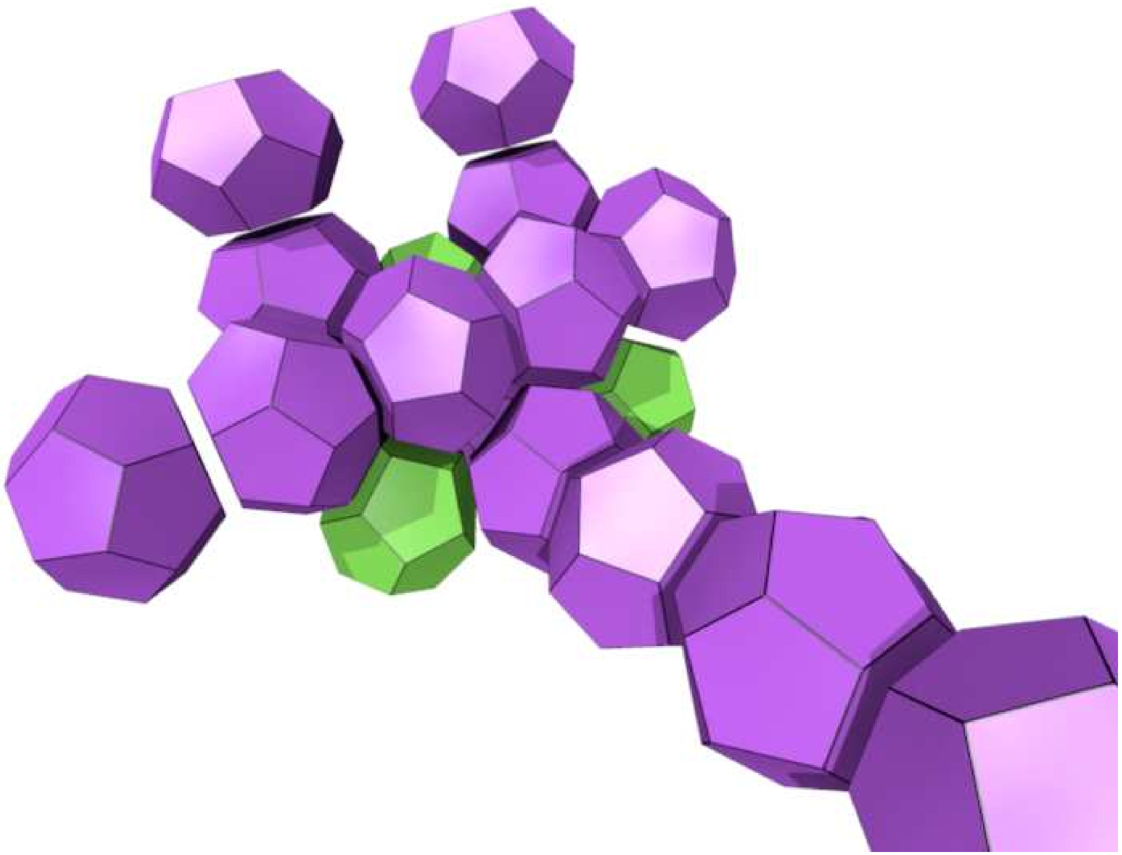
t.c.p.	clathrate, exp. alloy	sp. group	$\overline{f}$	F_{20}:F_{24}:F_{26}:F_{28}	N
A_{15}	type I, Cr_3Si	$Pm\overline{3}n$	13.50	1, 3, 0, 0	8
C_{15}	type II, $MgCu_2$	$Fd\overline{3}m$	13.(3)	2, 0, 0, 1	24
C_{14}	type V, $MgZn_2$	$P6_3/mmc$	13.(3)	2, 0, 0, 1	12
Z	type IV, Zr_4Al_3	$P6/mmm$	13.43	3, 2, 2, 0	7
σ	type III, $Cr_{46}Fe_{54}$	$P4_2/mnm$	13.47	5, 8, 2, 0	30
H	complex	$Cmmm$	13.47	5, 8, 2, 0	30
K	complex	$Pmmm$	13.46	14, 21,6,0	82
F	complex	$P6/mmm$	13.46	9, 13, 4, 0	52
J	complex	$Pmmm$	13.45	4, 5, 2, 0	22
ν	$Mn_{81.5}Si_{8.5}$	$Immm$	13.44	37, 40, 10, 6	186
δ	$MoNi$	$P2_12_12_1$	13.43	6, 5, 2, 1	56
P	$Mo_{42}Cr_{18}Ni_{40}$	$Pbnm$	13.43	6, 5, 2, 1	56

24 known primary FK space fullerenes

t.c.p.	exp. alloy	sp. group	$\overline{f}$	F_{20}:F_{24}:F_{26}:F_{28}	N
K	$Mn_{77}Fe_4Si_{19}$	$C2$	13.42	25,19, 4, 7	220
R	$Mo_{31}Co_{51}Cr_{18}$	$R\overline{3}$	13.40	27, 12, 6, 8	159
μ	W_6Fe_7	$R\overline{3}m$	13.38	7, 2, 2, 2	39
–	K_7Cs_6	$P6_3/mmc$	13.38	7, 2, 2, 2	26
$p\sigma$	$V_6(Fe,Si)_7$	$Pbam$	13.38	7, 2, 2, 2	26
M	$Nb_{48}Ni_{39}Al_{13}$	$Pnam$	13.38	7, 2, 2, 2	52
C	$V_2(Co,Si)_3$	$C2/m$	13.36	15, 2, 2, 6	50
I	$Vi_{41}Ni_{36}Si_{23}$	Cc	13.37	11, 2, 2, 4	228
T	$Mg_{32}(Zn,Al)_{49}$	$Im3$	13.36	49, 6, 6, 20	162
SM	$Mg_{32}(Zn,Al)_{49}$	$Pm\overline{3}n$	13.36	49, 9, 0, 23	162
X	$Mn_{45}Co_{40}Si_{15}$	$Pnmm$	13.35	23, 2, 2, 10	74
–	Mg_4Zn_7	$C2/m$	13.35	35, 2, 2, 16	110

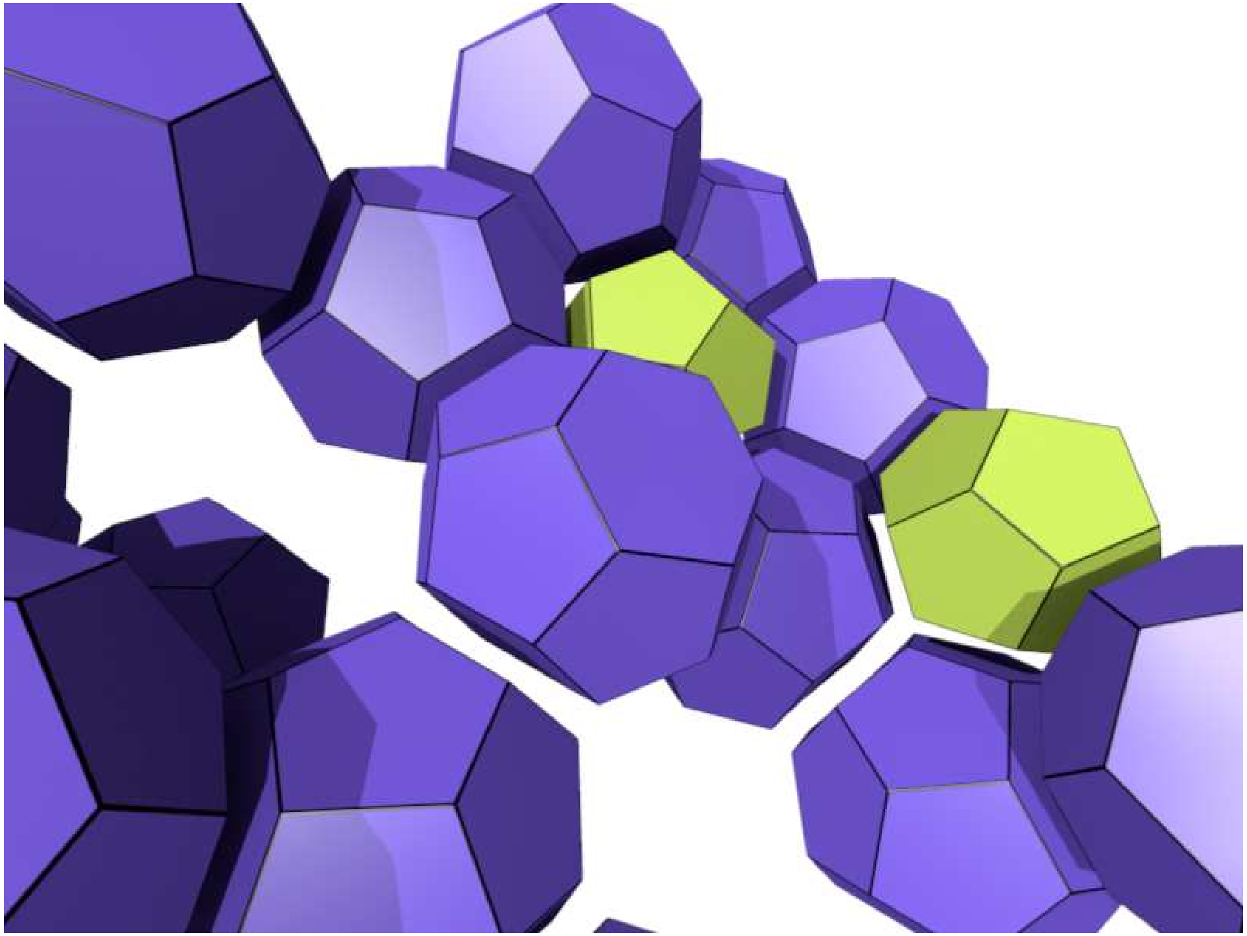
FK space fullerene A_{15} (β-W phase)

Gravicenters of cells F_{20} (atoms Si in Cr_3Si) form the bcc network A_3^*. Unique with its fractional composition $(1, 3, 0, 0)$. Oceanic methane hydrate (with type I, i.e., A_{15}) contains 500-2500 Gt carbon; cf. ~ 230 for other natural gas sources.



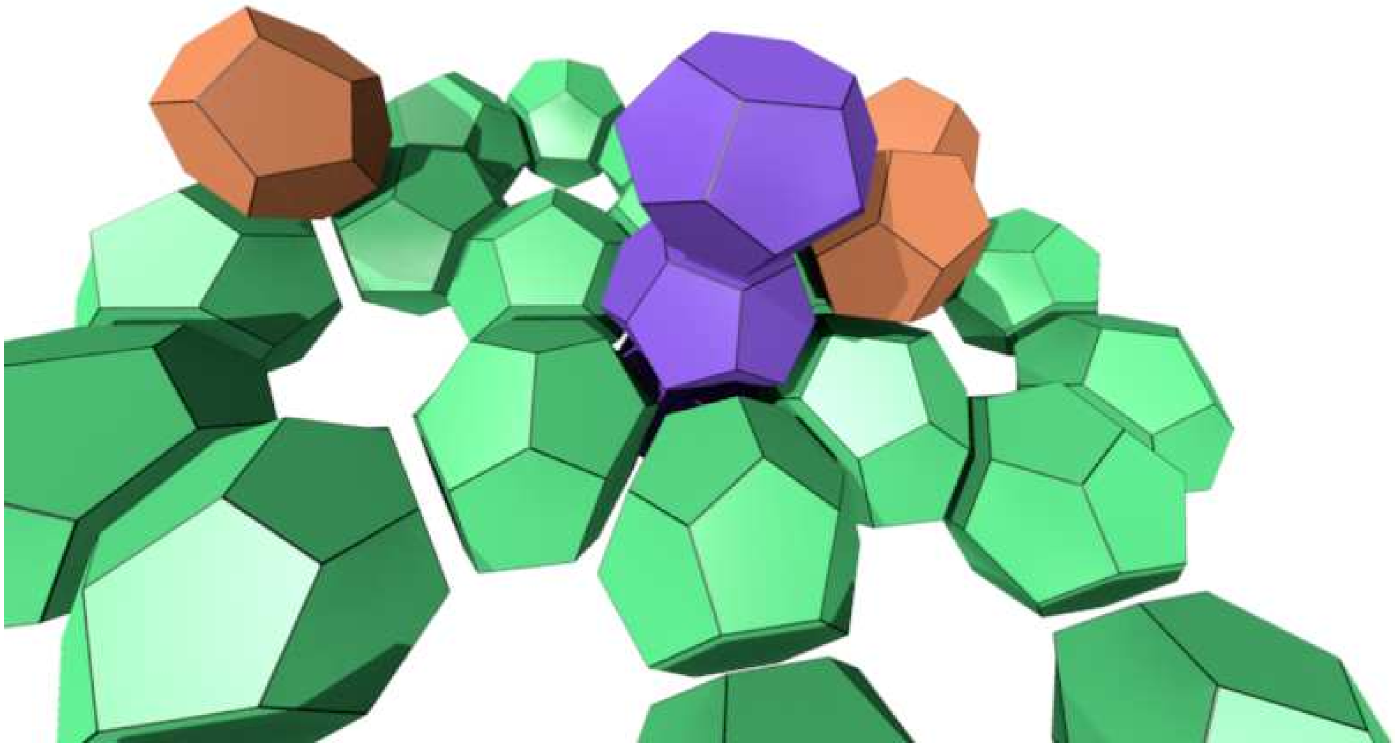
FK space fullerene C_{15}

Cubic N=24; gravicenters of cells F_{28} (atoms Mg in $MgCu_2$) form diamond network (centered A_3). Cf. $MgZn_2$ forming hexagonal N=12 variant C_{14} of diamond: lonsdaleite found in meteorites, 2nd in a continuum of $(2, 0, 0, 1)$-structures.



FK space fullerene Z

It is also not determined by its fract. composition $(3, 2, 2, 0)$.



Computer enumeration

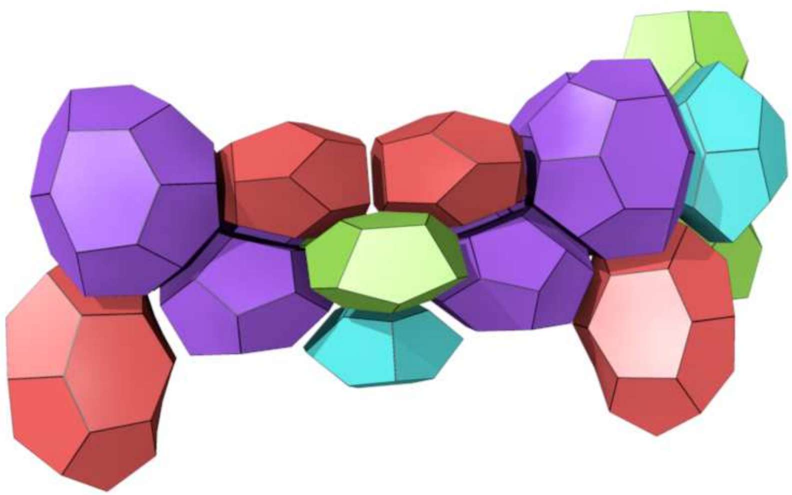
Dutour-Deza-Delgado, 2008, found 84 FK structures (incl. known: 10 and 3 stackings) with $N \leq 20$ fullerenes in reduced (i.e. by a Biberbach group) fundamental domain.

$\# 20$	$\# 24$	$\# 26$	$\# 28$	fraction	N(nr.of)	n(known structure)
4	5	2	0	known	11(1)	not J-complex
8	0	0	4	known	12(1)	24(C_{36})
7	2	2	2	known	13(5)	26($-$), 26($p\sigma$), 39(μ), not M
6	6	0	2	new	14(3)	-
6	5	2	1	known	14(6)	56(δ), not P
6	4	4	0	known	14(4)	7(Z)
7	4	2	2	conterexp.	15(1)	-
5	8	2	0	known	15(2)	30(σ), 30(H-complex)
9	2	2	3	new	16(1)	-
6	6	4	0	conterexp.	16(1)	-
4	12	0	0	known	16(1)	8(A_{15})
12	0	0	6	known	18(4)	12(C_{14}),24(C_{15}),36(6-*layer*),54(9-*layer*)

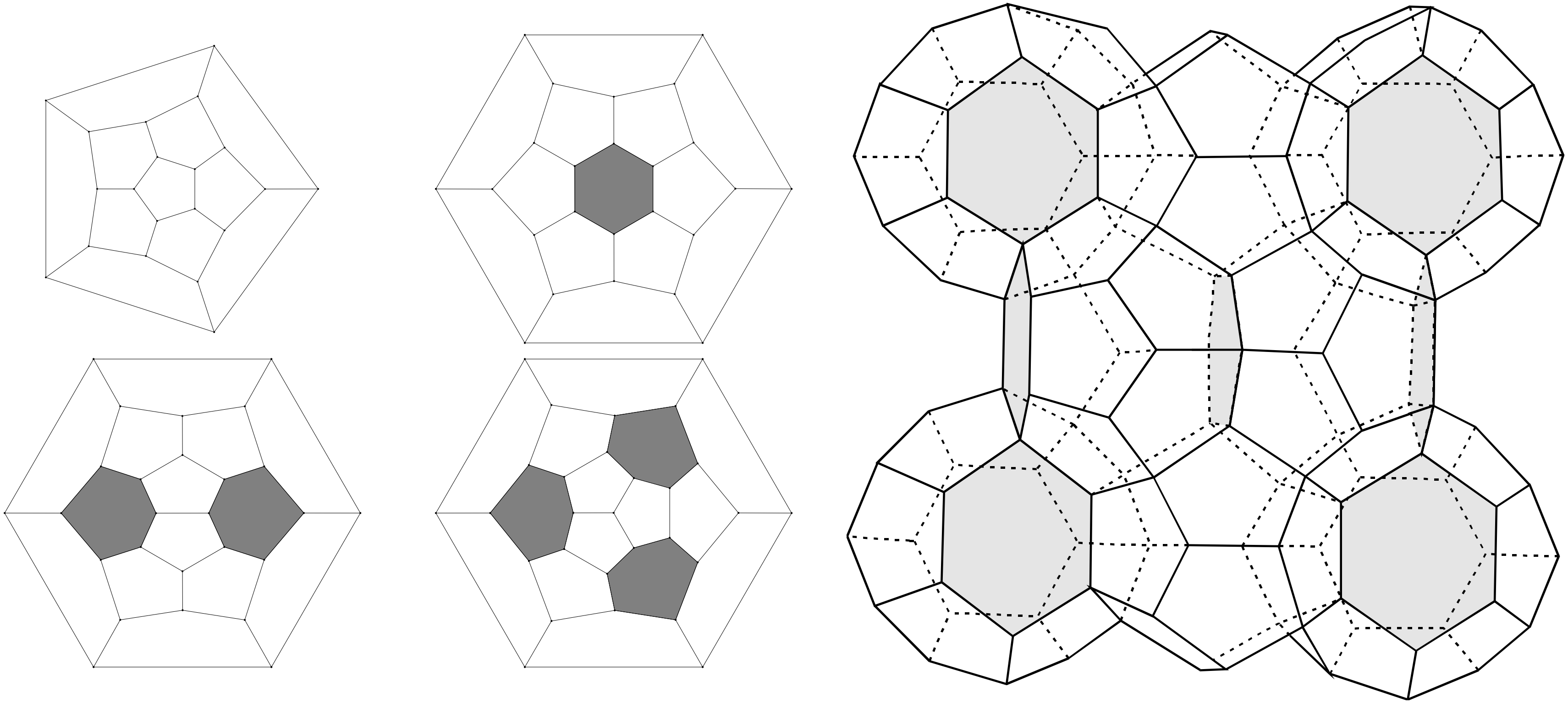
Conterexamples to 2 old conjectures

Any 4-vector, say, $(x_{20}, x_{24}, x_{26}, x_{28})$, is a linear combination $a_0(1,0,0,0)$+$a_1(1,3,0,0)A_{15}$+$a_2(3,2,2,0)$ Z+$a_3(2,0,0,1)C_{15}$ with $a_0 = x_{20}$- $\frac{x_{24}}{3}$-$\frac{7x_{26}}{6}$-$2x_{28}$ and a_1= $\frac{x_{24}-x_{26}}{3}$, a_2=$\frac{x_{26}}{2}$, a_3=x_{28}.

- Yarmolyuk-Krypyakevich, 1974: $a_0 = 0$ for FK fractions. So, $5.1 \leq \overline{q} \leq 5.(1)$, $13.(3) \leq \overline{f} \leq 13.5$; equalities iff C_{15}, A_{15}
- Conterexamples: $(7,4,2,2)$, $(6,6,4,0)$, $(6,8,4,0)$ (below). Mean face-sizes $\overline{q}$: ≈ 5.1089, $5.(1)$(A_{15}), ≈ 5.1148. Mean numbers of faces per cell $\overline{f}$: $13.4(6)$, 13.5($A15$), $13.(5)$ disproving Nelson-Spaepen, 1989: $\overline{q} \leq 5.(1)$, $\overline{f} \leq 13.5$.



Frank-Kasper polyhedra and A_{15}



Frank-Kasper polyhedra F_{20}, F_{24}, F_{26}, F_{28} with maximal symmetry I_h, D_{6d}, D_{3h}, T_d, respectively, are Voronoi cells surrounding atoms of a FK phase. Their duals: 12,14,15,18 coordination polyhedra. FK phase cells are almost regular tetrahedra; their edges, sharing 6 or 4 tetrahedra, are - or + disclination lines (defects) of local icosahedral order.

Special space fullerenes A_{15} and C_{15}

Those extremal space fullerenes A_{15}, C_{15} correspond to

- clathrate hydrates of type I,II;
- zeolite topologies MEP, MTN;
- clathrasils Melanophlogite, Dodecasil 3C;
- metallic alloys Cr_3Si (or β-tungsten W_3O), $MgCu_2$.

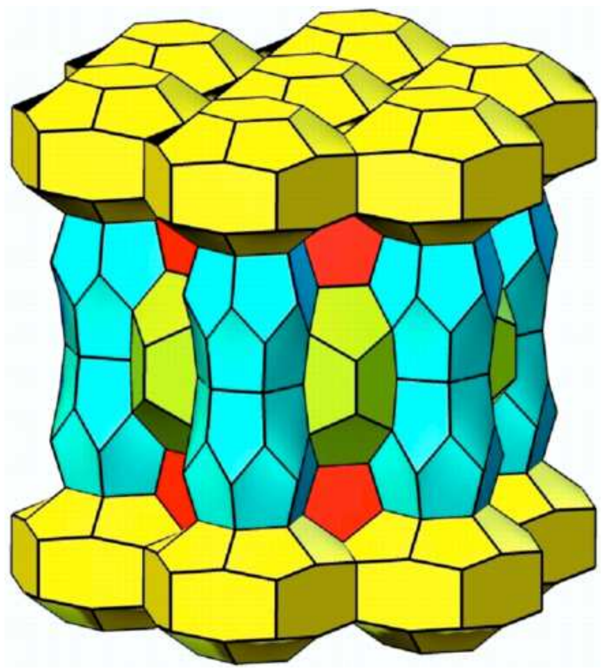
Their *unit cells* have, respectively, 46, 136 vertices and 8 (2 F_{20} and 6 F_{24}), 24 (16 F_{20} and 8 F_{28}) cells.

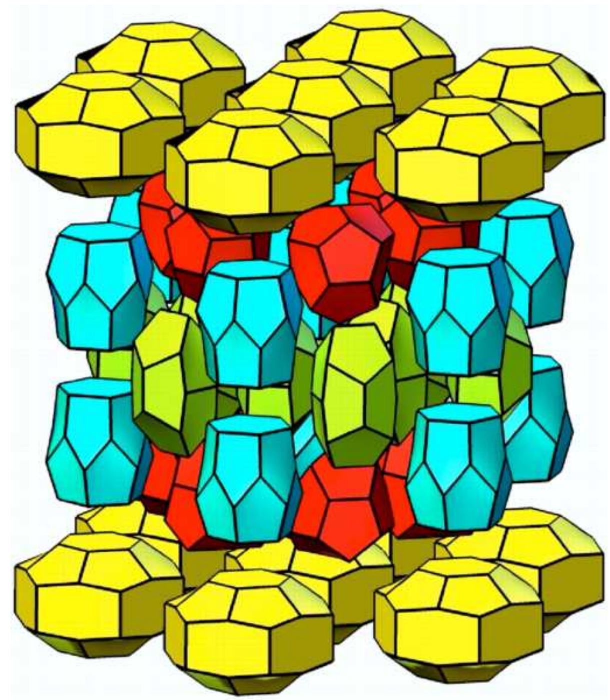
24 known FK structures have mean number $\overline{f}$ of faces per cell (mean coordination number) in $[13.(3)(C_{15}), 13.5(A_{15})]$ and their mean face-size is within $[5+\frac{1}{10}(C_{15}), 5+\frac{1}{9}(A_{15})]$.

Closer to impossible 5 or $\overline{f}=12$ (120-*cell*, $\mathbb{S}^3$-tiling by F_{20}) means lower energy. Minimal $\overline{f}$ for *simple* (3, 4 tiles at each edge, vertex) $\mathbb{E}^3$-tiling by a *simple* polyhedron is 14 (tr.oct).

Non-FK space fullerene: is it unique?

Deza-Shtogrin, 1999: unique known non-FK space fullerene, 4-valent 3-periodic tiling of E^3 by F_{20}, F_{24} and its elongation $F_{36}(D_{6h})$ in ratio $7:2:1$;
so, new record: mean face-size ≈ 5.091<5.1 (C_{15}) and $\overline{f}$=13.2<13.29 (Rivier-Aste, 1996, conj. min.) <13.(3) (C_{15}).

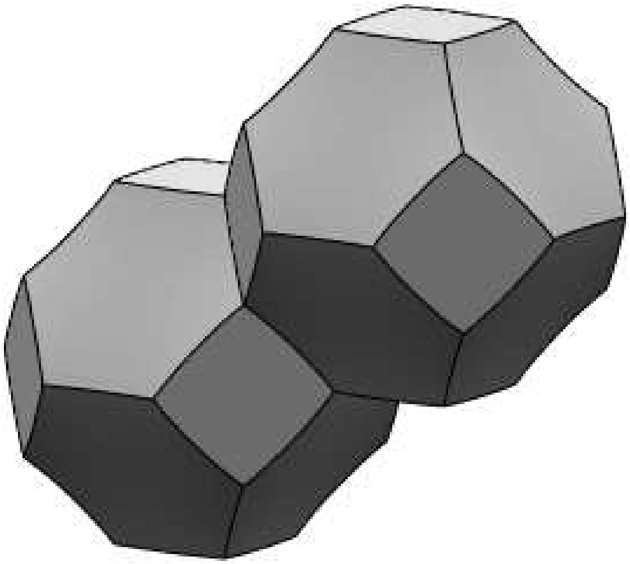




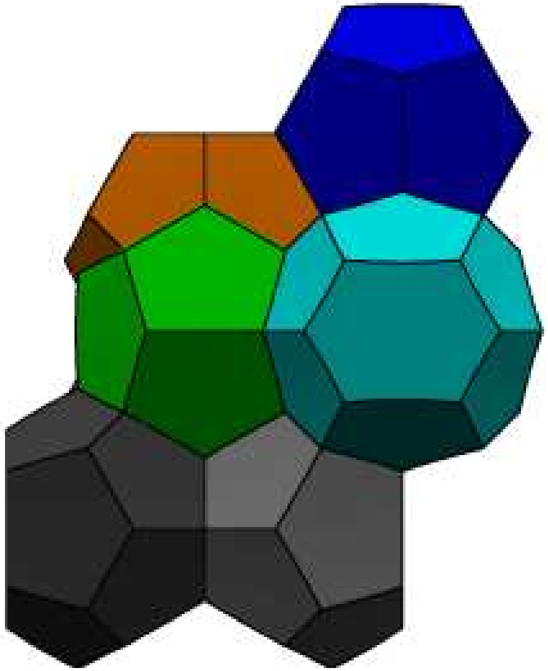
Delgado, O'Keeffe: all space fullerenes with ≤ 7 orbits of vertices are 4 FK (A_{15}, C_{15}, Z, C_{14}) and this one (3,3,5,7,7).

Weak Kelvin problem

Partition $\mathbb{E}^3$ into *equal volume* cells D of minimal surface area, i.e., with maximal $IQ(D) = \frac{36\pi V^2}{A^3}$ (lowest energy foam). Kelvin conjecture (about *congruent* cells) is still out.



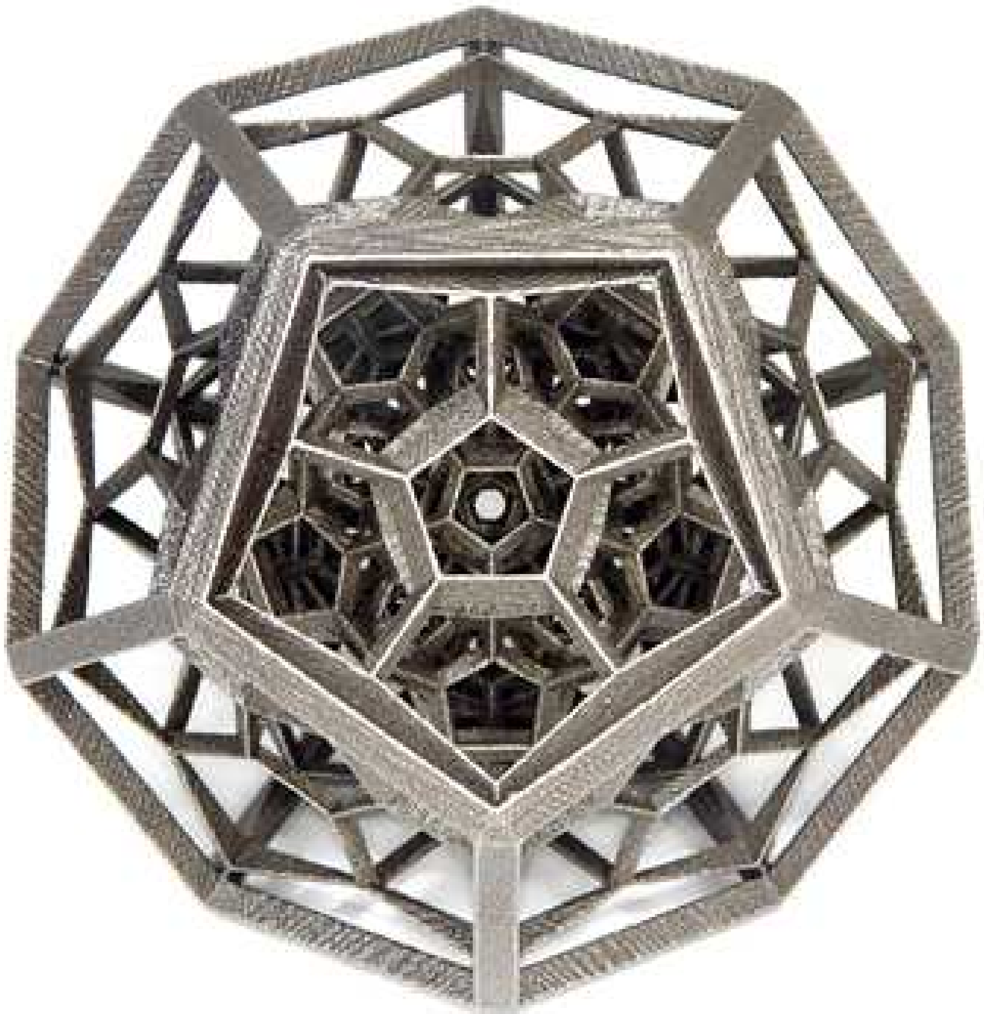
Lord Kelvin, 1887: bcc=A_3^*
IQ(curved tr.Oct.) ≈ 0.757
IQ(tr.Oct.) ≈ 0.753



Weaire-Phelan, 1994: A_{15}
IQ(unit cell) ≈ 0.764
2 curved F_{20} and 6 F_{24}

In $\mathbb{E}^2$, the best is (Ferguson-Hales) graphite $F_\infty = (6^3)$.

Projection of 120-cell in 3-space (G.Hart)



(533): 600 vertices, 120 dodecahedral facets, $|Aut| = 14400$

Regular (convex) polytopes

A regular polytope is a polytope, whose symmetry group acts transitively on its set of flags. The list consists of:

regular polytope	group
regular polygon P_n	$I_2(n)$
Icosahedron and Dodecahedron	H_3
120-cell and 600-cell	H_4
24-cell	F_4
γ_n(hypercube) and β_n(cross-polytope)	B_n
α_n(simplex)	A_n=$Sym(n+1)$

There are 3 regular tilings of Euclidean plane: $44 = \delta_2$, 36 and 63, and an infinity of regular tilings pq of hyperbolic plane. Here pq is shortened notation for (p^q).

2-dim. regular tilings and honeycombs

Columns and rows indicate **vertex figures** and **facets**, resp.
Blue are elliptic (spheric), red are parabolic (Euclidean).

	2	3	4	5	6	7	m	∞
2	22	23	24	25	26	27	2m	2∞
3	32	α_3	β_3	Ico	36	37	3m	3∞
4	42	γ_3	δ_2	45	46	47	4m	4∞
5	52	Do	54	55	56	57	5m	5∞
6	62	63	64	65	66	67	6m	6∞
7	72	73	74	75	76	77	7m	7∞
m	m2	m3	m4	m5	m6	m7	mm	$m\infty$
∞	$\infty 2$	$\infty 3$	$\infty 4$	$\infty 5$	$\infty 6$	$\infty 7$	∞m	$\infty\infty$

3-dim. regular tilings and honeycombs

	α_3	γ_3	β_3	Do	Ico	δ_2	63	36
α_3	α_4*		β_4*		600-			336
β_3		24-				344		
γ_3	γ_4*		δ_3*		435*			436*
Ico				353				
Do	**120-**		534		535			536
δ_2		443*				444*		
36							363	
63	**633***		634*		635*			636*

4-dim. regular tilings and honeycombs

	α_4	γ_4	β_4	24-	120-	600-	δ_3
α_4	α_5*		β_5*			3335	
β_4				$De(D_4)$			
γ_4	γ_5*		δ_4*			$4335*$	
24-		$Vo(D_4)$					3434
600-							
120-	**5333**		5334			5335	
δ_3				$4343*$			

Finite 4-fullerenes

- $\chi = f_0 - f_1 + f_2 - f_3 = 0$ for any finite closed 3-manifold, no useful equivalent of Euler formula.
- Prominent 4-fullerene: 120-cell.
  Conjecture: it is unique equifacetted 4-fullerene ($\simeq Do = F_{20}$)
- Pasini: there is no 4-fullerene facetted with $C_{60}(I_h)$ (4-football)
- Few types of putative facets: $\simeq F_{20}$, F_{24} (hexagonal barrel), F_{26}, $F_{28}(T_d)$, $F_{30}(D_{5h})$ (elongated Dodecahedron), $F_{32}(D_{3h})$, $F_{36}(D_{6h})$ (elongated F_{24})

∞: "greatest" polyhex is 633
(convex hull of vertices of 63, realized on a horosphere);
its fundamental domain is not compact but of finite volume

4 constructions of finite 4-fullerenes

		$\lvert V \rvert$	3-faces are $\simeq$ to
	120-cell*	600	$F_{20} = Do$
$\forall i \geq 1$	A_i^*	$560i + 40$	F_{20}, $F_{30}(D_{5h})$
$\forall 3 - full.F$	$B(F)$	$30v(F)$	F_{20}, F_{24}, F(two)
decoration	C(120-cell)	20600	F_{20}, F_{24}, $F_{28}(T_d)$
decoration	D(120-cell)	61600	F_{20}, F_{26}, $F_{32}(D_{3h})$

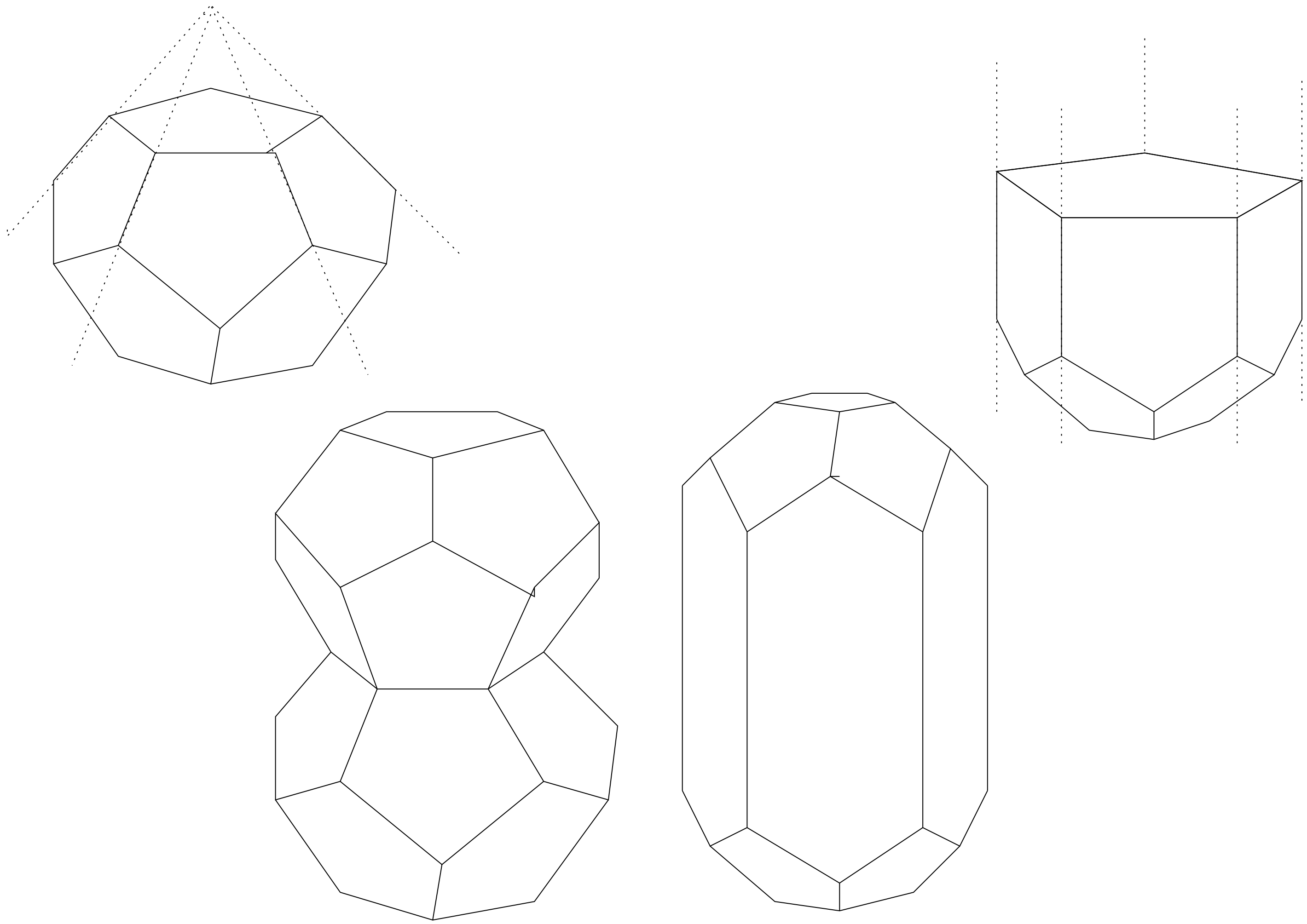
$*$ indicates that the construction creates a polytope; otherwise, the obtained fullerene is a 3-sphere.

A_i: tube of 120-cells

B: coronas of any simple tiling of $\mathbb{R}^2$ or H^2

C, D: any 4-fullerene decorations

Construction A of polytopal 4-fullerenes



Similarly, tubes of 120-cell's are obtained in $4D$

Inflation method

- Roughly: find out in simplicial d-polytope (a dual d-fullerene F^*) a suitable “large” $(d-1)$-simplex, containing an integer number t of “small” (fundamental) simplices.
- Constructions C, D: F^*=600-cell; $t = 20$, 60, respectively.
- The decoration of F^* comes by “barycentric homothety” (suitable projection of the “large” simplex on the new “small” one) as the orbit of new points under the symmetry group

All known 5-fullerenes

- Exp 1: 5333 (regular tiling of H^4 by 120-cell)
- Exp 2 (with 6-gons also): glue two 5333's on some 120-cells and delete their interiors. If it is done on only one 120-cell, it is $\mathbb{R} \times S^3$ (so, simply-connected)
- Exp 3: (finite 5-fullerene): quotient of 5333 by its symmetry group; it is a compact 4-manifold partitioned into a finite number of 120-cells
- Exp 3': glue above
- All known 5-fullerenes come as above

No polytopal 5-fullerene exist.

Quotient d-fullerenes

A. Selberg (1960), A. Borel (1963): if a discrete group of motions of a symmetric space has a compact fund. domain, then it has a torsion-free normal subgroup of finite index. So, quotient of a d-fullerene by such symmetry group is a finite d-fullerene.

Exp 1: Poincaré dodecahedral space

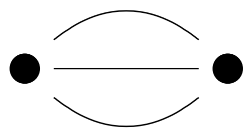
- quotient of 120-cell (on S^3) by the binary icosahedral group I_h of order 120; so, f-vector $(5, 10, 6, 1) = \frac{1}{120} f(120 - \text{cell})$
- It comes also from $F_{20} = Do$ by gluing of its opposite faces with $\frac{1}{10}$ right-handed rotation

Quot. of H^3 tiling: by F_{20}: $(1, 6, 6, p_5, 1)$ Seifert-Weber space and by F_{24}: $(24, 72, 48 + 8 = p_5 + p_6, 8)$ Löbell space

Polyhexes

Polyhexes on T^2, cylinder, its twist (Möbius surface) and K^2 are quotients of graphite 63 by discontinuous and fixed-point free group of isometries, generated by resp.:

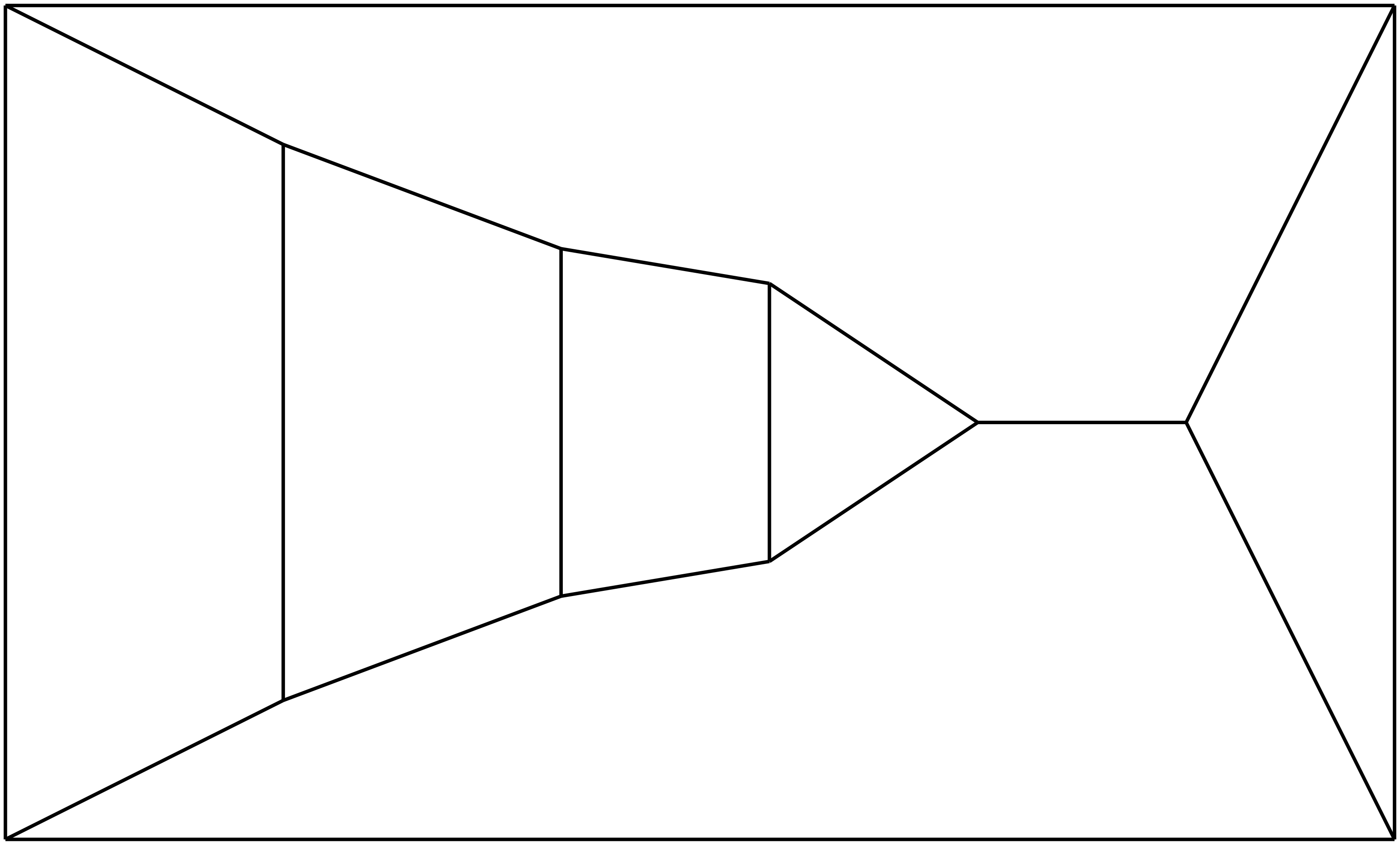
- 2 translations,
- a translation, a glide reflection
- a translation and a glide reflection.

The smallest polyhex has $p_6 = 1$:  on T^2.
The "greatest" polyhex is 633
(the convex hull of vertices of 63, realized on a horosphere); it is not compact (its fundamental domain is not compact), but cofinite (i.e., of finite volume) infinite 4-fullerene.

VI. Zigzags, railroads and knots in fullerenes (with Dutour and Fowler)

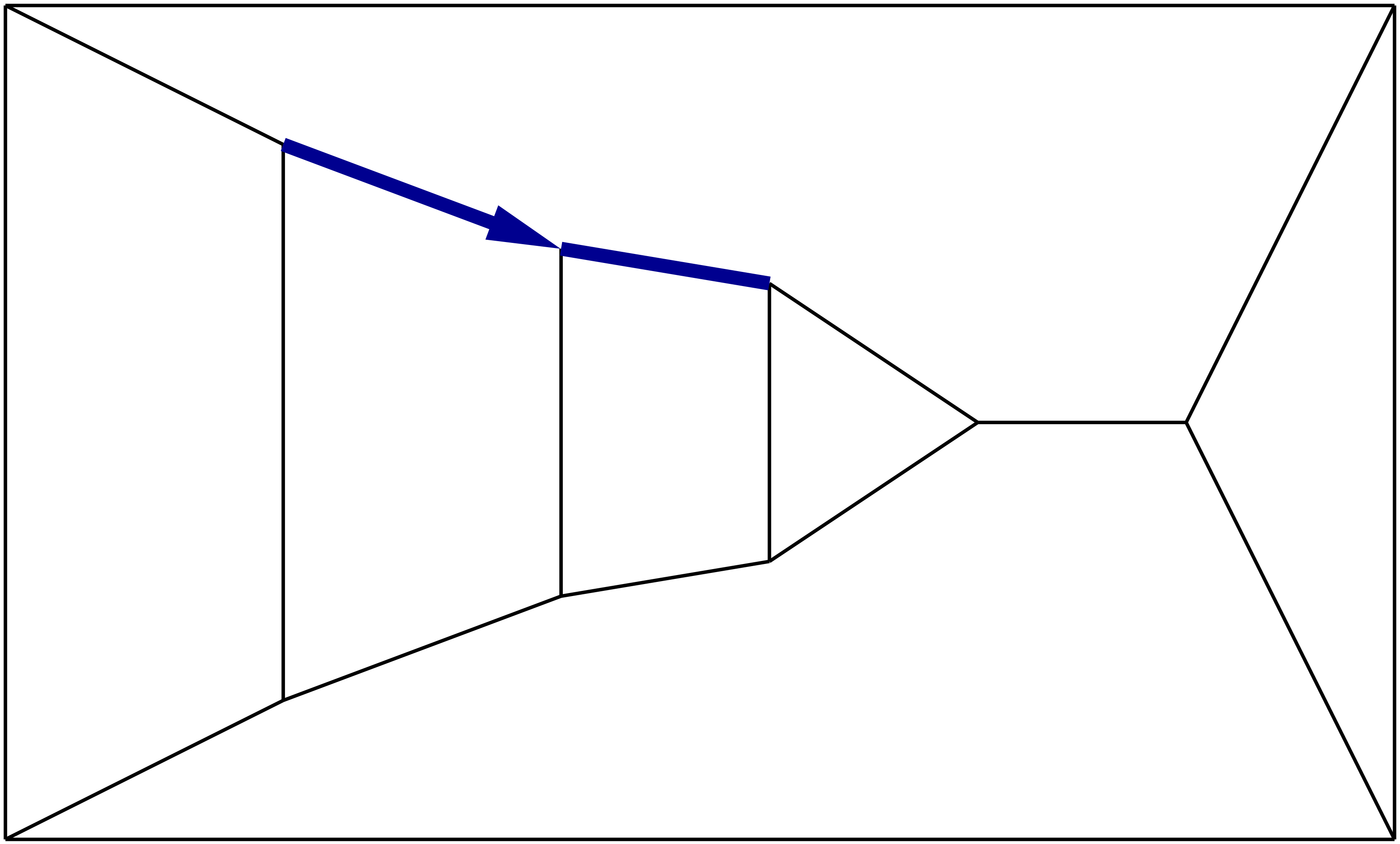
Zigzags

A plane graph G



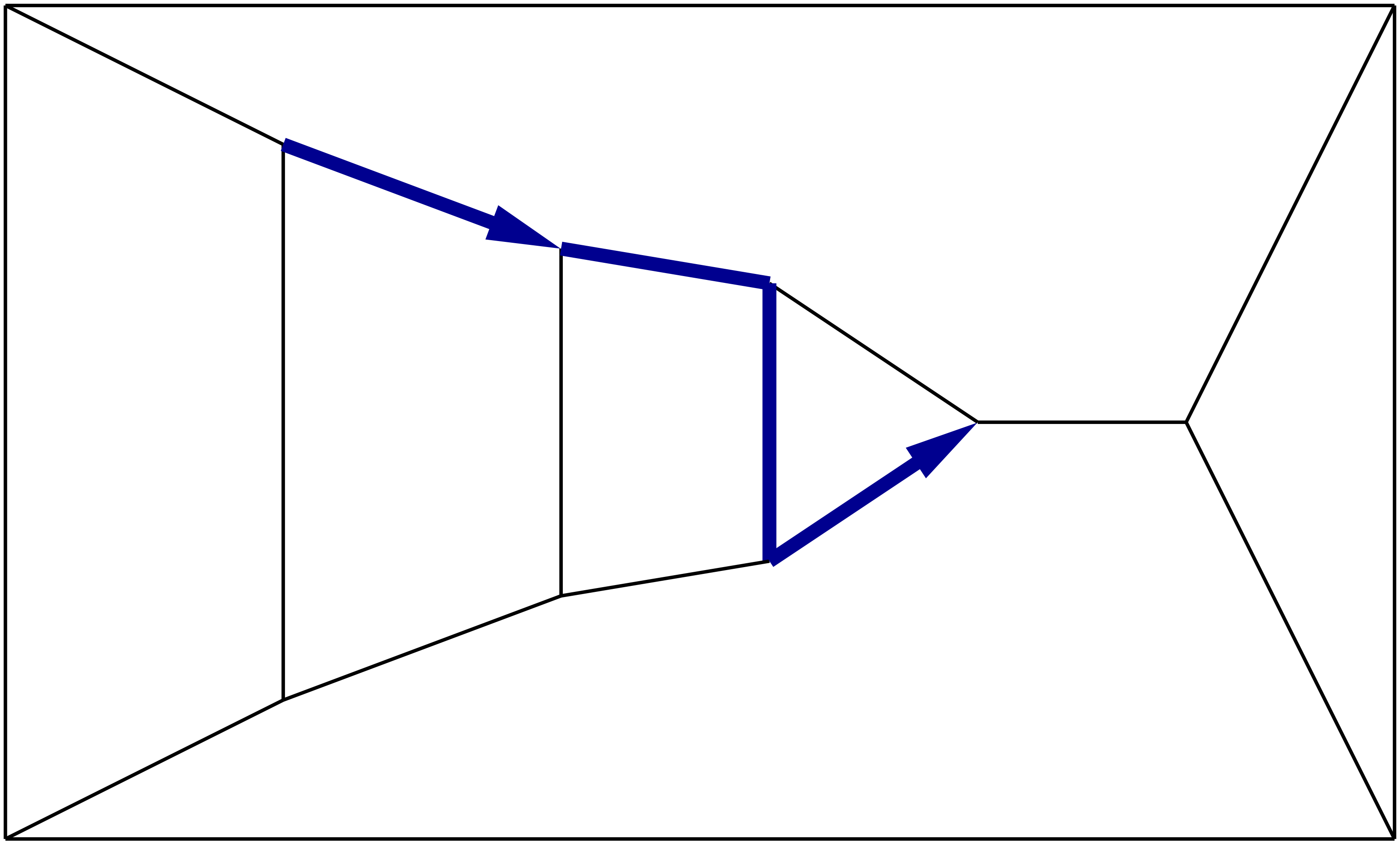
Zigzags

take two edges



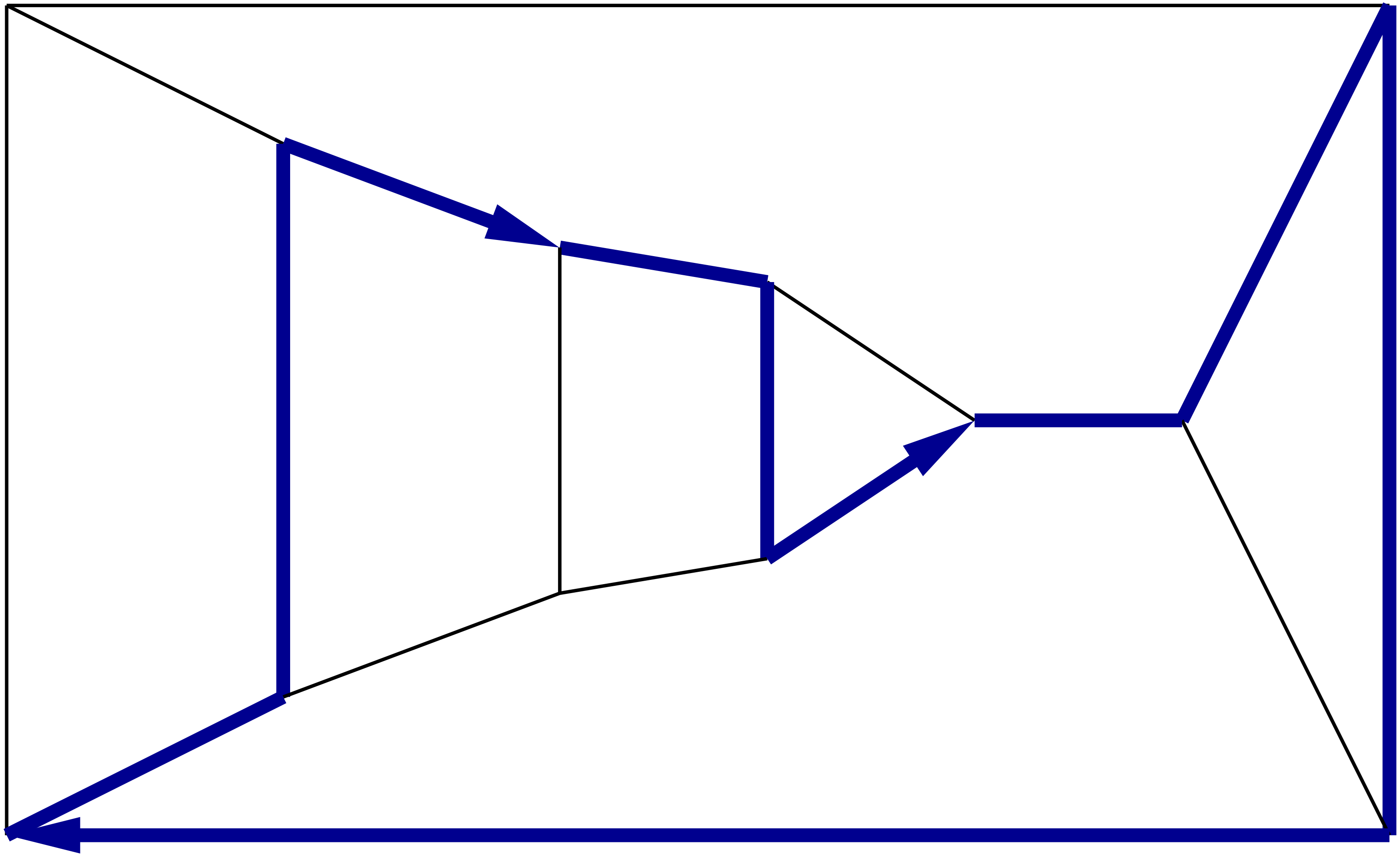
Zigzags

Continue it left−right alternatively ....



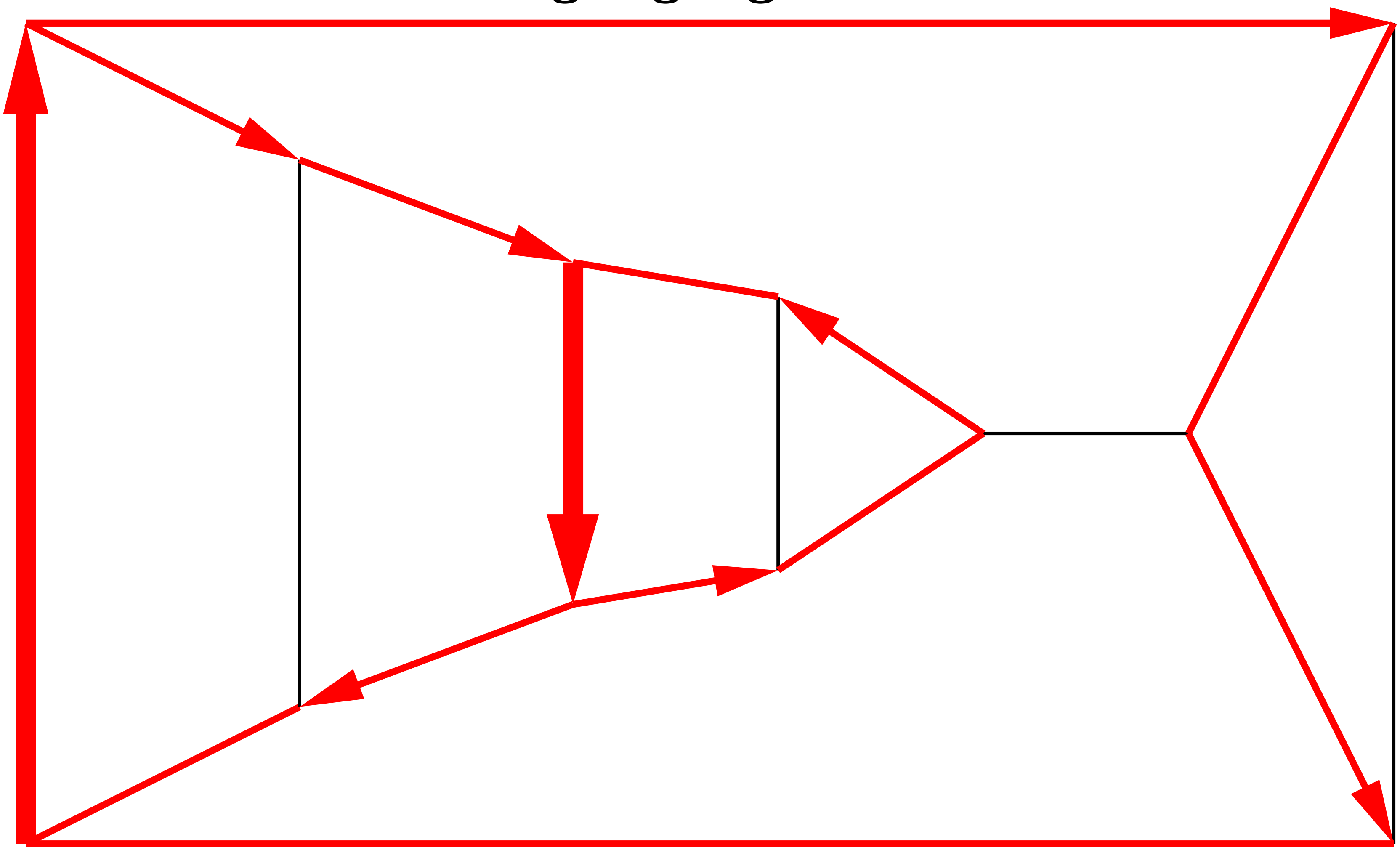
Zigzags

... until we come back.



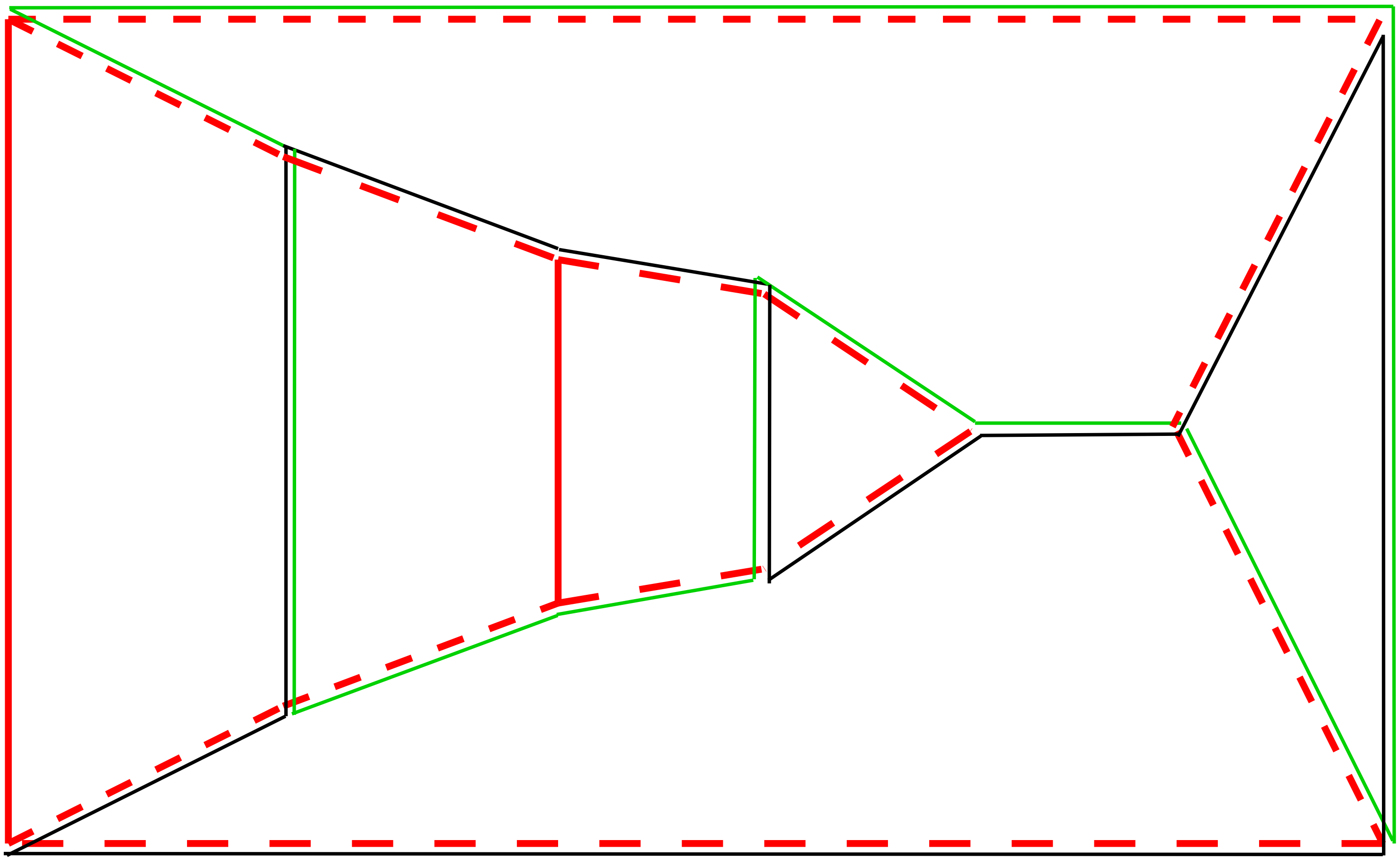
Zigzags

A self−intersecting zigzag



Zigzags

A double covering of 18 edges: 10+10+16



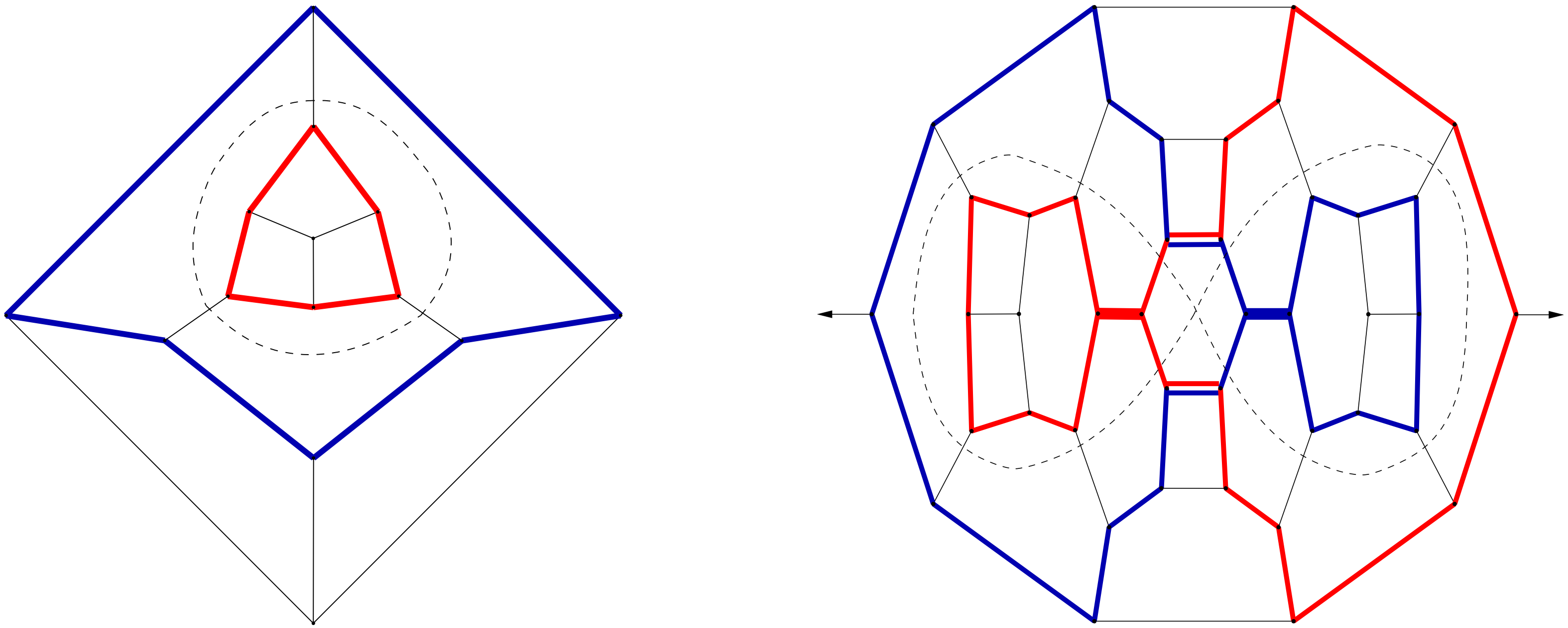
z−vector $z = 10^2, \ 16_{2,0}$

z-knotted fullerenes

- A zigzag in a 3-valent plane graph G is a circuit such that any 2, but not 3 edges belong to the same face.
- Zigzags can self-intersect in the same or opposite direction.
- Zigzags doubly cover edge-set of G.
- A graph is z-knotted if there is unique zigzag.
- What is proportion of z-knotted fullerenes among all F_n? Schaeffer and Zinn-Justin, 2004, implies: for any m, the proportion, among 3-valent n-vertex plane graphs of those having $\leq m$ zigzags goes to 0 with $n \to \infty$.
- **Conjecture**: all z-knotted fullerenes are chiral and their symmetries are all possible (among 28 groups for them) pure rotation groups: C_1, C_2, C_3, D_3, D_5.

Railroads

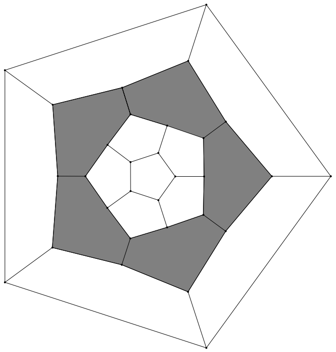
A railroad in a 3-valent plane graph is a circuit of hexagonal faces, such that any of them is adjacent to its neighbors on opposite faces. Any railroad is bordered by two zigzags.



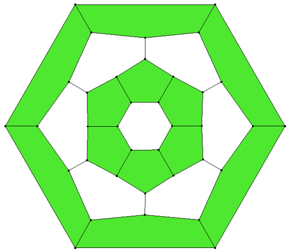
$4_{14}(D_{3h})$ $4_{42}(C_{2v})$

Railroads (as zigzags) can self-intersect (doubly or triply).
A 3-valent plane graph is tight if it has no railroad.

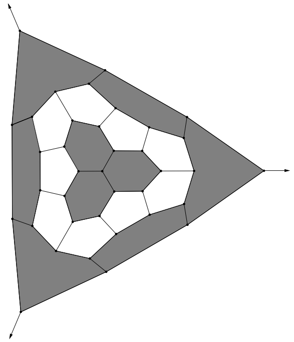
Some special fullerenes



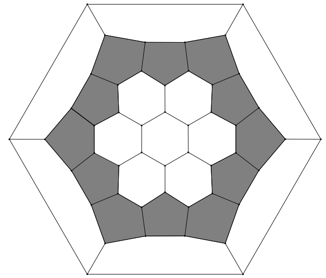
30, D_{5h}
all 6-gons
in railroad
(unique)



36,D_{6h}



38, C_{3v}
all 5-, 6-
in rings
(unique)



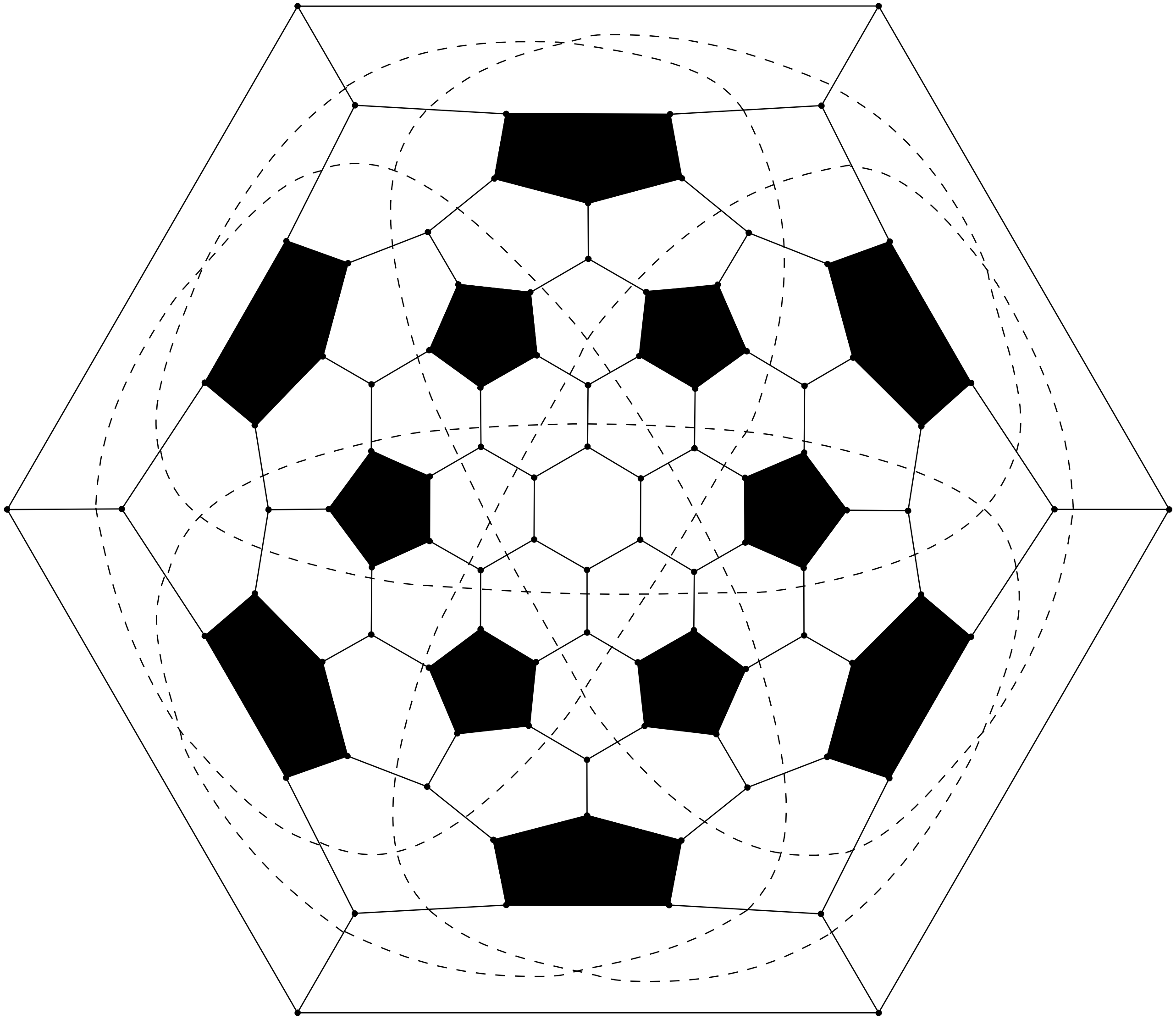
48, D_{6d}
all 5-gons
in alt. ring
(unique)

2nd one is the case $t = 1$ of infinite series $F_{24+12t}(D_{6d,h})$, which are only ones with 5-gons organized in two 6-rings.

It forms, with F_{20} and F_{24}, best known space fullerene tiling.

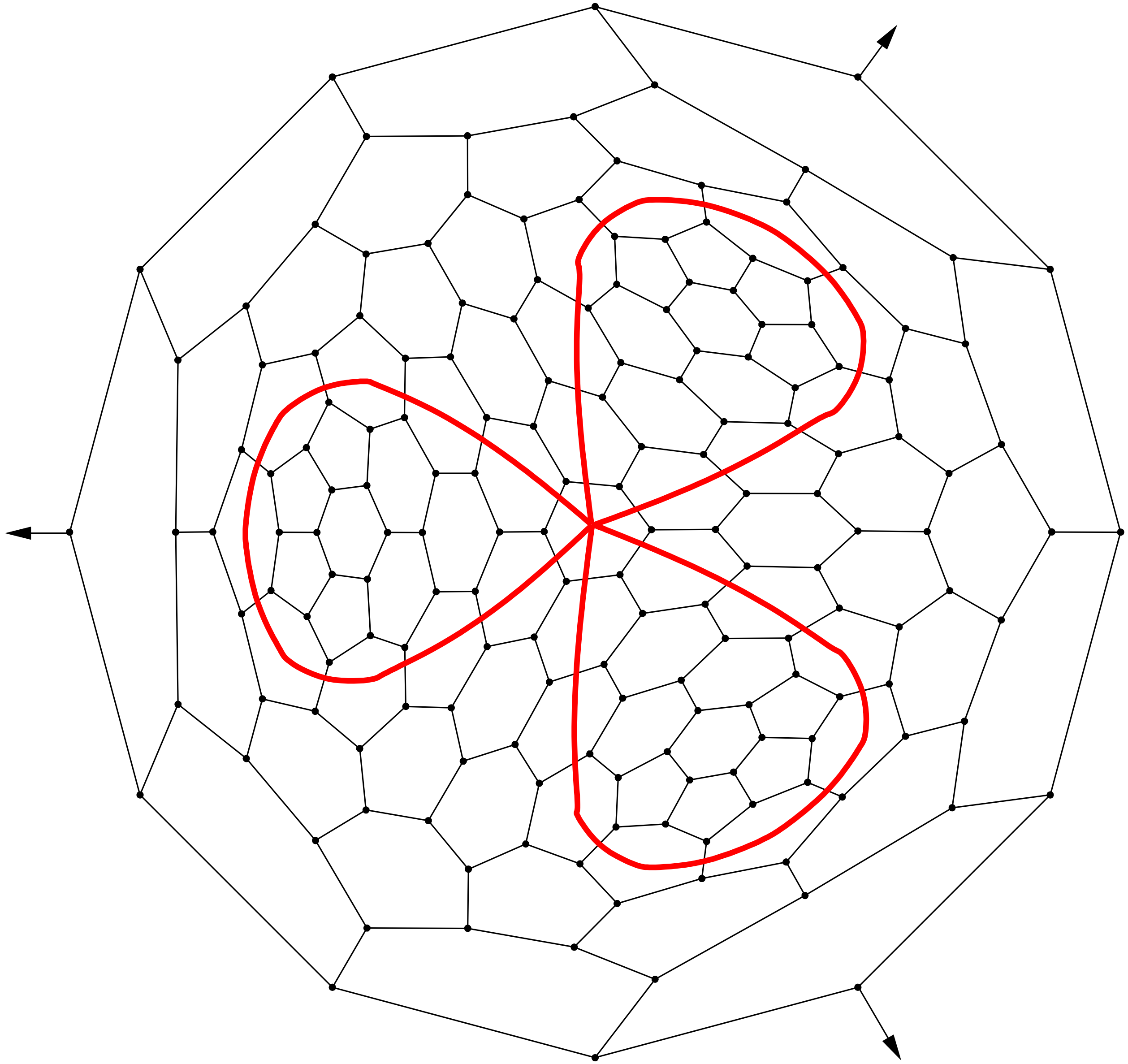
The skeleton of its dual is an isometric subgraph of $\frac{1}{2}H_8$.

First IPR fullerene with self-int. railroad



$F_{96}(D_{6d})$; realizes projection of Conway knot $(4 \times 6)^*$

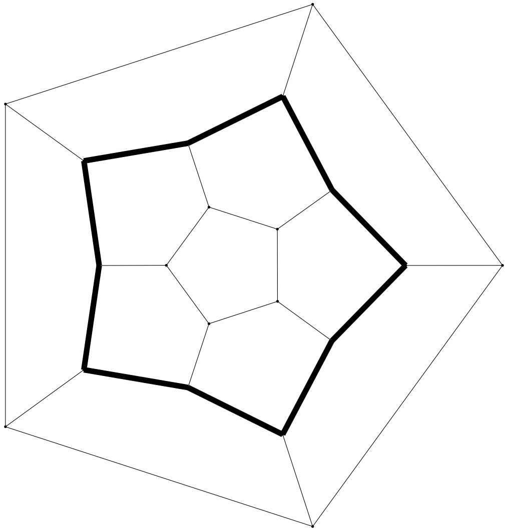
Triply intersecting railroad in $F_{172}(C_{3v})$



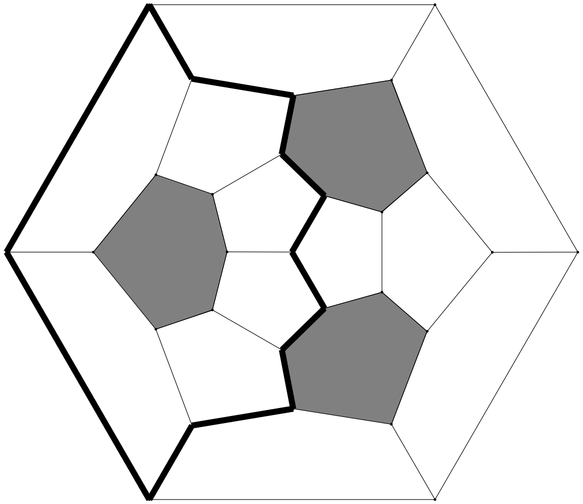
Tight fullerenes

- Tight fullerene is one without railroads, i.e., pairs of "parallel" zigzags.
- Clearly, any z-knotted fullerene (unique zigzag) is tight.
- $F_{140}(I)$ is tight with $z = 28^{15}$ (15 simple zigzags).
- **Conjecture**: any tight fullerene has ≤ 15 zigzags.
- **Conjecture**: All tight with simple zigzags are 9 known ones (holds for all F_n with $n \leq 200$).

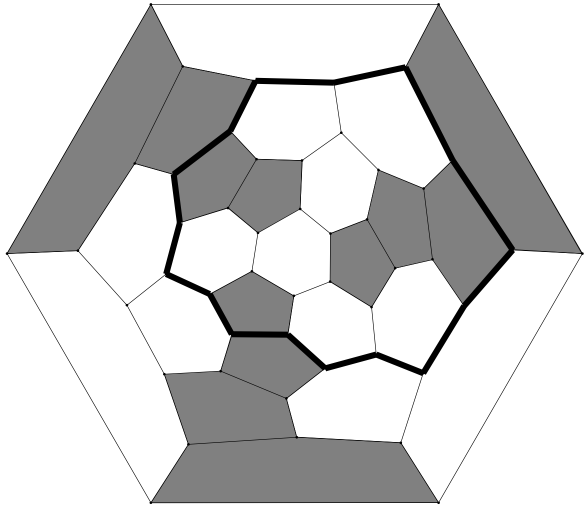
Tight F_n with simple zigzags



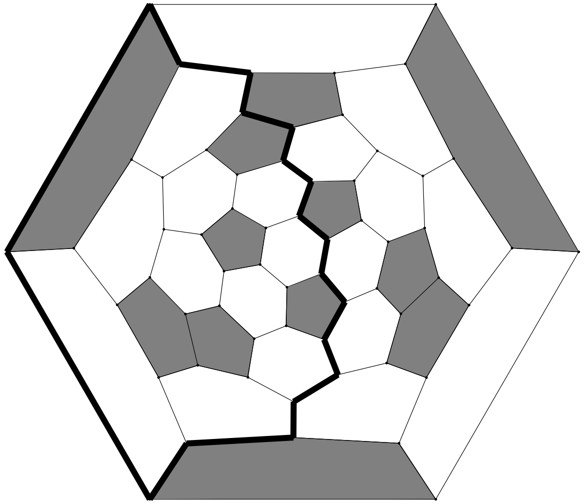
20 I_h, 20^6



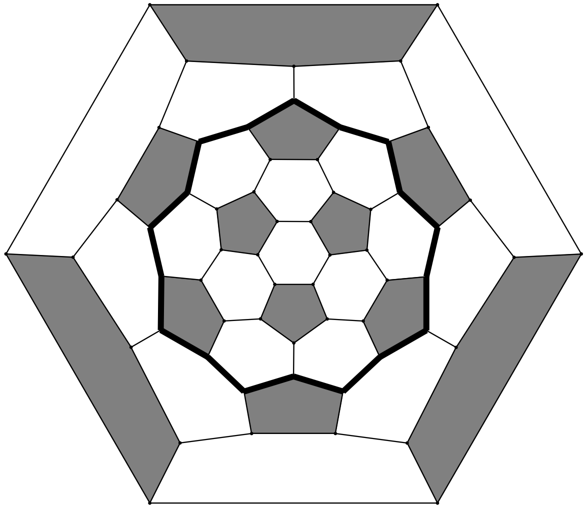
28 T_d, 12^7



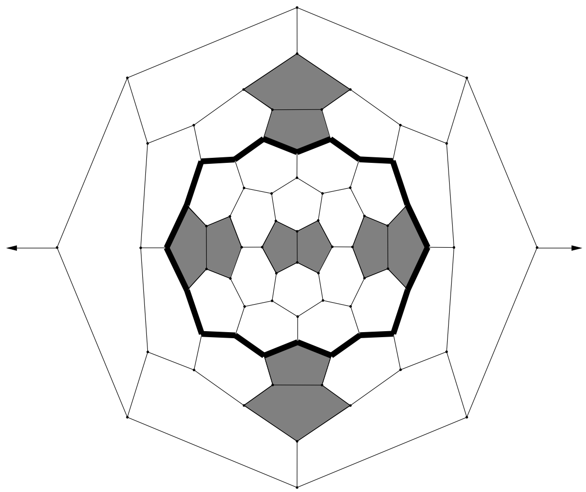
48 D_3, 16^9



60 D_3, 18^{10}

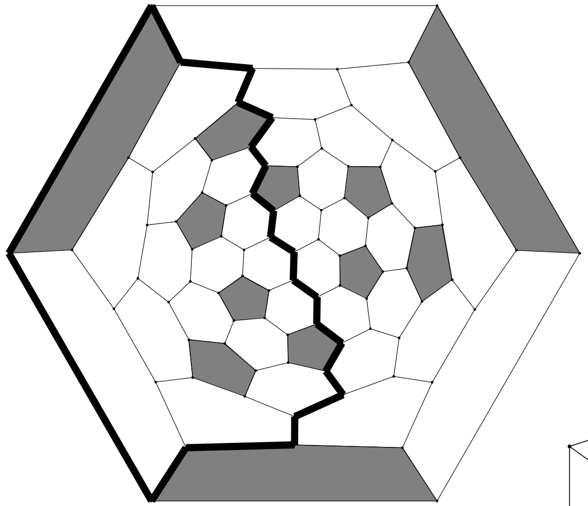


60 I_h, 18^{10}

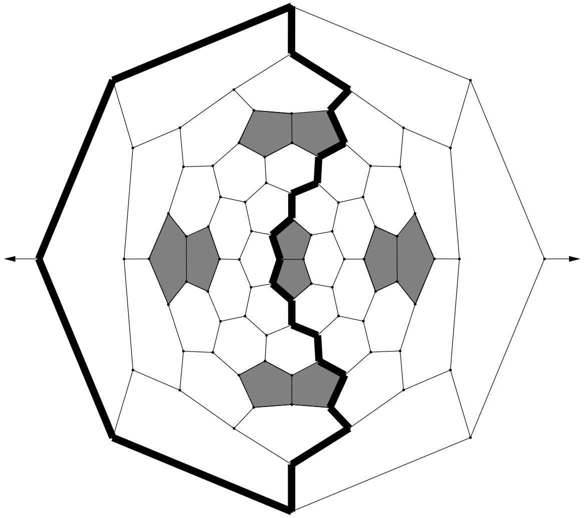


76 D_{2d}, $22^4, 20^7$

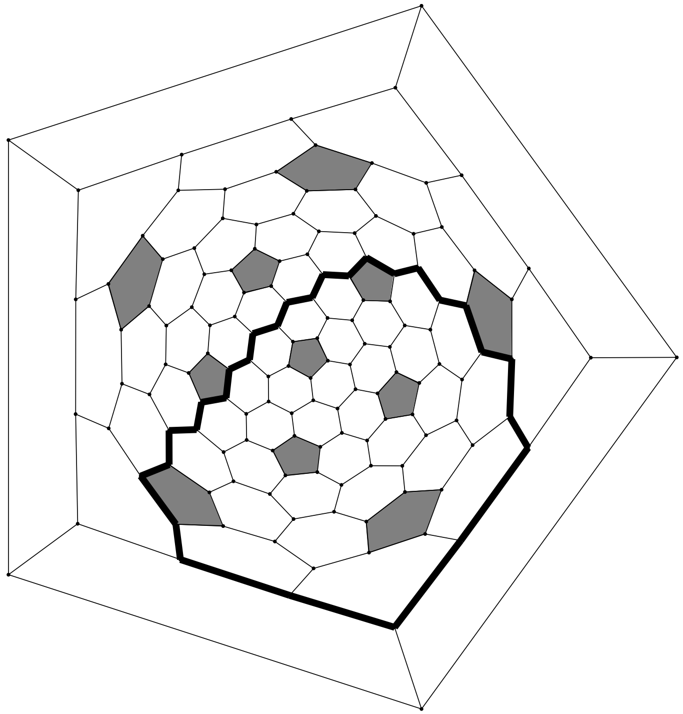
Tight F_n with simple zigzags



$88 \quad T,\ 22^{12}$



$92 \quad T_h,\ 24^6, 22^6$



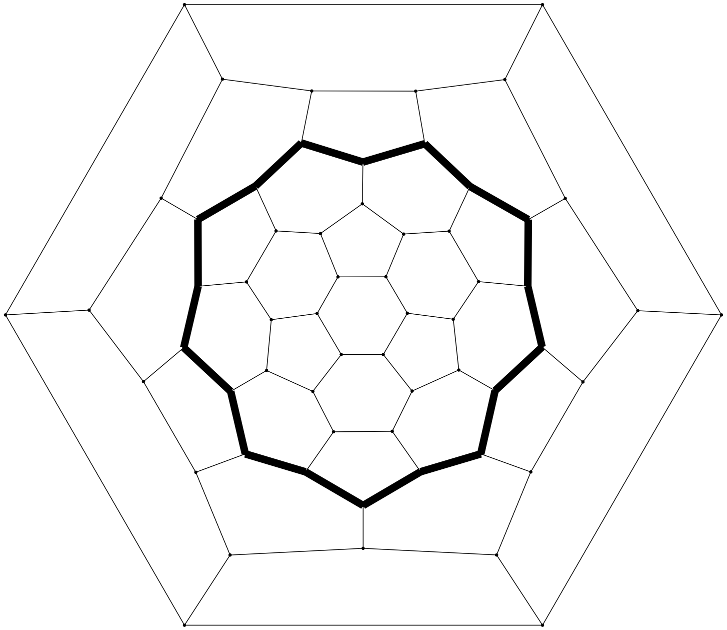
$140 \quad I,\ 28^{15}$

Tight F_n with only simple zigzags

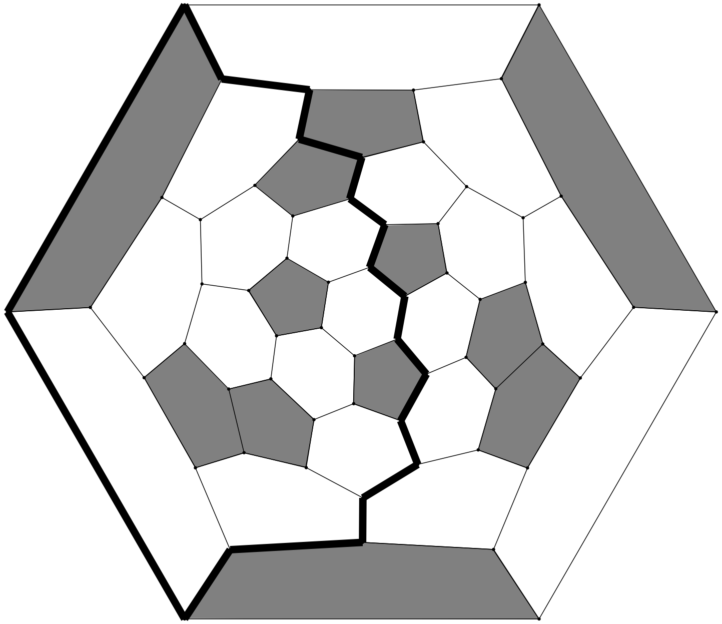
n	group	z-vector	orbit lengths	int. vector
20	I_h	10^6	6	2^5
28	T_d	12^7	3,4	2^6
48	D_3	16^9	3,3,3	2^8
60, IPR	I_h	18^{10}	10	2^9
60	D_3	18^{10}	1,3,6	2^9
76	D_{2d}	$22^4, 20^7$	1,2,4,4	$4, 2^9$ and 2^{10}
88, IPR	T	22^{12}	12	2^{11}
92	T_h	$22^6, 24^6$	6,6	2^{11} and $2^{10}, 4$
140, IPR	I	28^{15}	15	2^{14}

Conjecture: this list is complete (checked for $n \leq 200$).
It gives 7 Grünbaum arrangements of plane curves.

Two F_{60} with z-vector 18^{10}



$C_{60}(I_h)$



$F_{60}(D_3)$

This pair was first answer on a question in B.Grunbaum "Convex Polytopes" (Wiley, New York, 1967) about non-existance of simple polyhedra with the same p-vector but different zigzags.

z-uniform F_n with $n \leq 60$

n	isomer	orbit lengths	z-vector	int. vector
20	I_h:1	6	10^6	2^5
28	T_d:2	4,3	12^7	2^6
40	T_d:40	4	$30^4_{0,3}$	8^3
44	T:73	3	$44^3_{0,4}$	18^2
44	D_2:83	2	$66^2_{5,10}$	36
48	C_2:84	2	$72^2_{7,9}$	40
48	D_3:188	3,3,3	16^9	2^8
52	C_3:237	3	$52^3_{2,4}$	20^2
52	T:437	3	$52^3_{0,8}$	18^2
56	C_2:293	2	$84^2_{7,13}$	44
56	C_2:349	2	$84^2_{5,13}$	48
56	C_3:393	3	$56^3_{3,5}$	20^2
60	C_2:1193	2	$90^2_{7,13}$	50
60	D_2:1197	2	$90^2_{13,8}$	48
60	D_3:1803	6,3,1	18^{10}	2^9
60	I_h:1812	10	18^{10}	2^9

z-uniform IPR C_n with $n \leq 100$

n	isomer	orbit lengths	z-vector	int. vector
80	I_h:7	12	20^{12}	$0, 2^{10}$
84	T_d:20	6	$42^6_{0,1}$	8^5
84	D_{2d}:23	4,2	$42^6_{0,1}$	8^5
86	D_3:19	3	$86^3_{1,10}$	32^2
88	T:34	12	22^{12}	2^{11}
92	T:86	6	$46^6_{0,3}$	8^5
94	C_3:110	3	$94^3_{2,13}$	32^2
100	C_2:387	2	$150^2_{13,22}$	80
100	D_2:438	2	$150^2_{15,20}$	80
100	D_2:432	2	$150^2_{17,16}$	84
100	D_2:445	2	$150^2_{17,16}$	84

IPR means the absence of adjacent pentagonal faces;
IPR enhanced stability of putative fullerene molecule.

IPR z-knotted F_n with $n \leq 100$

n	signature	isomers
86	$43, 86^*$	C_2:2
90	$47, 88$	C_1:7
	$53, 82$	C_2:19
	$71, 64$	C_2:6
94	$47, 94^*$	C_1:60; C_2:26, 126
	$65, 76$	C_2:121
	$69, 72$	C_2:7
96	$49, 95$	C_1:65
	$53, 91$	C_1:7, 37, 63

98	$49, 98^*$	C_2:191, 194, 196
	$63, 84$	C_1:49
	$75, 72$	C_1:29
	$77, 70$	C_1:5; C_2:221
100	$51, 99$	C_1:371, 377; C_3:221
	$53, 97$	C_1:29, 113, 236
	$55, 95$	C_1:165
	$57, 93$	C_1:21
	$61, 89$	C_1:225
	$65, 85$	C_1:31, 234

The symbol * above means that fullerene forms a Kékule structure, i.e., edges of self-intersection of type I cover exactly once the vertex-set of the fullerene graph (in other words, they form a perfect matching of the graph).
All but one above have symmetry C_1, C_2.

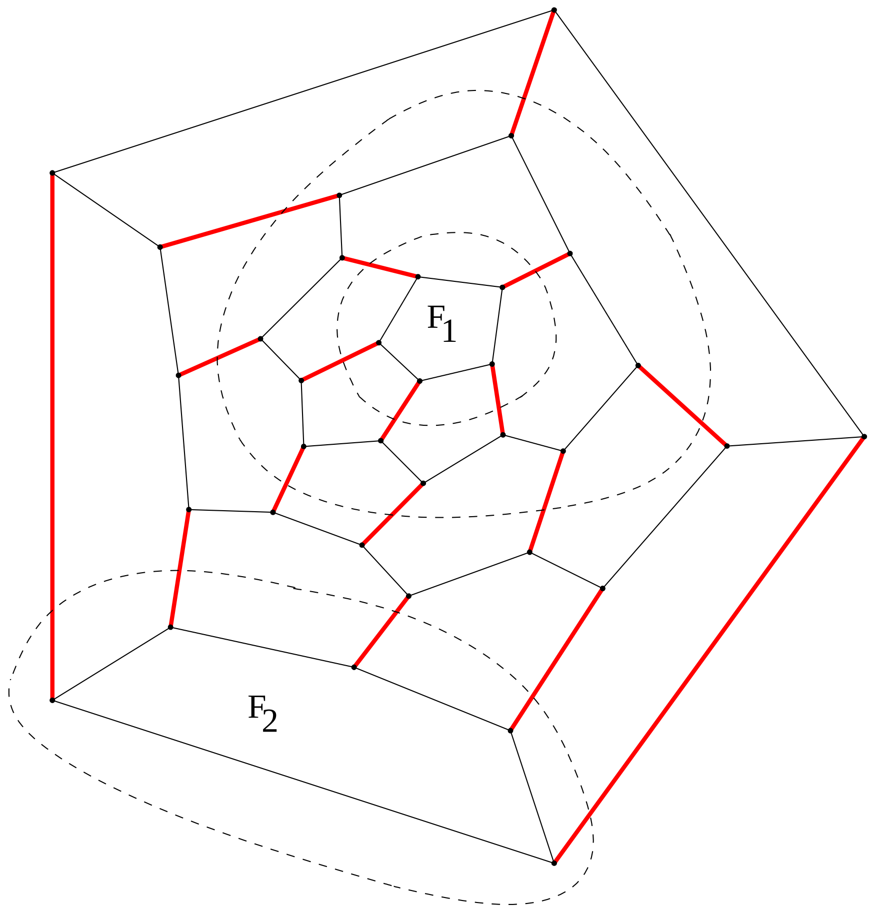
Perfect matching on fullerenes

Let G be a fullerene with one zigzag with self-intersection numbers (α_1, α_2). Here is the smallest one , $F_{34}(C_2)$. $\rightarrow\rightarrow$

(i) $\alpha_1 \geq \frac{n}{2}$. If $\alpha_1 = \frac{n}{2}$ then the edges of self-intersection of type I form a perfect matching PM

(ii) every face incident to 0 or 2 edges of PM

(iii) two faces, F_1 and F_2 are free of PM, PM is organized around them in concentric circles.

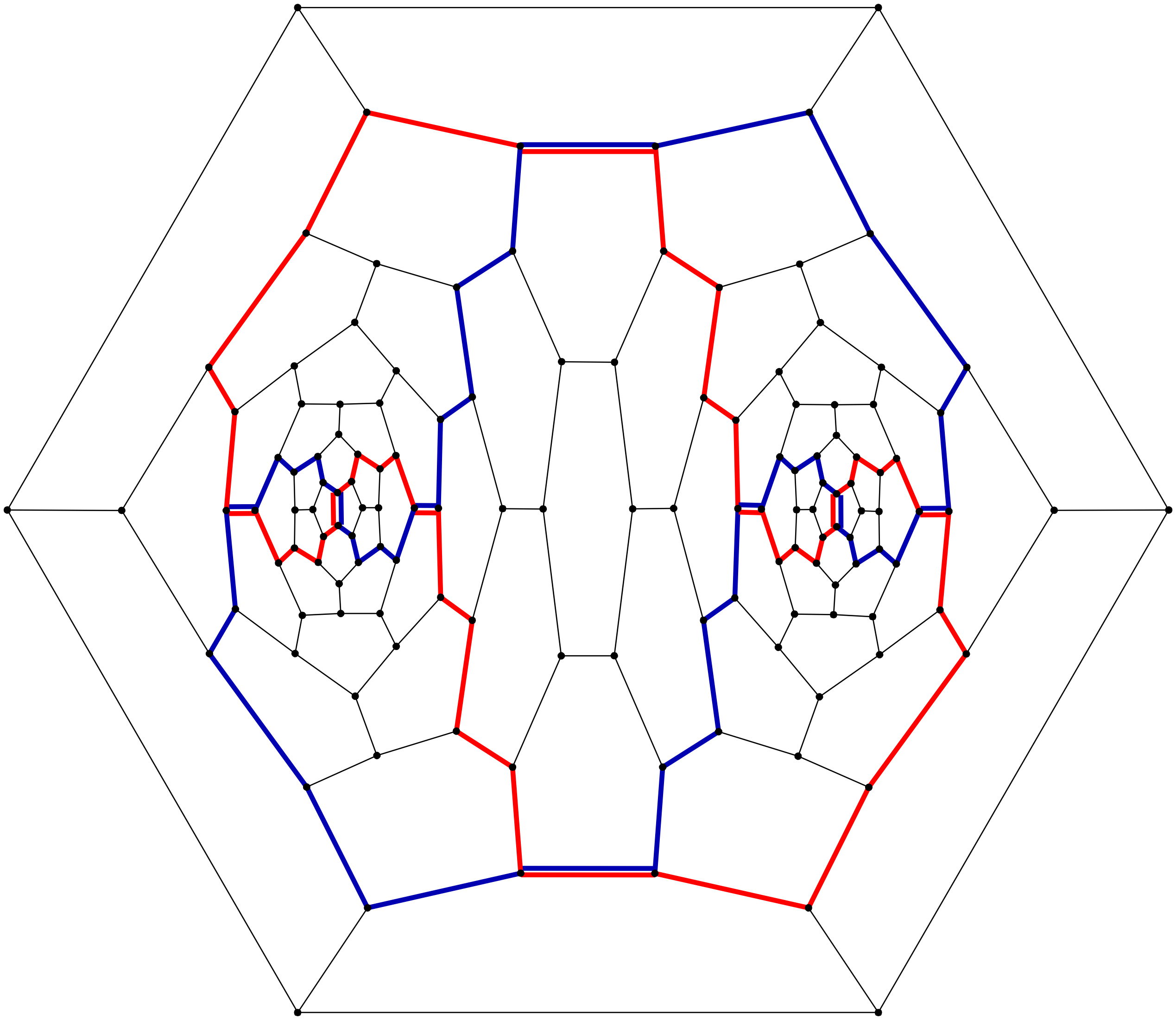


z-knotted fullerenes: statistics for $n \leq 74$

n	# of F_n	# of z-knotted
34	6	1
36	15	0
38	17	4
40	40	1
42	45	6
44	89	9
46	116	15
48	199	23
50	271	30
52	437	42
54	580	93
56	924	87
58	1205	186
60	1812	206
62	2385	341
64	3465	437
66	4478	567
68	6332	894
70	8149	1048
72	11190	1613
74	14246	1970

Proportion of z-knotted ones among all F_n looks stable.
For z-knotted among 3-valent $\leq n$-vertex plane graphs, it is 34% if $n = 24$ (99% of them are C_1) but goes to 0 if $n \to \infty$.

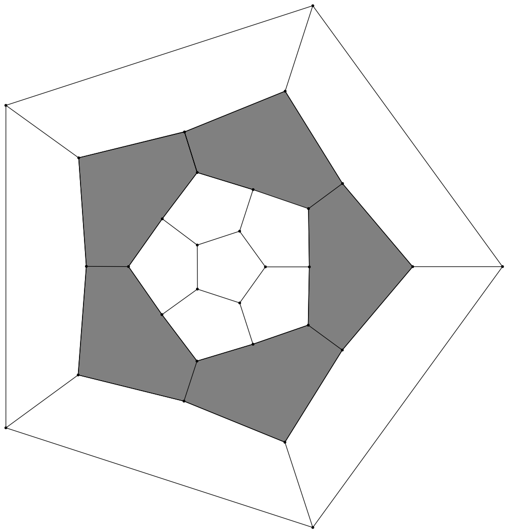
Intersection of zigzags



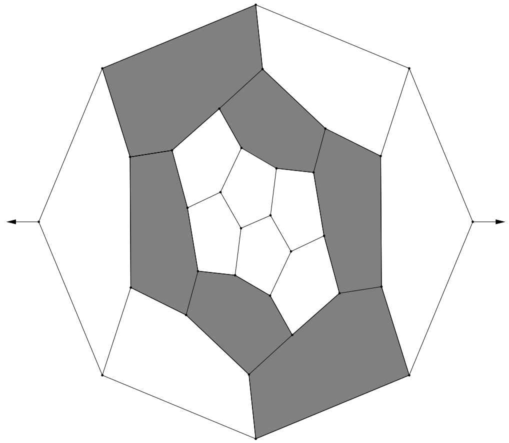
For any n, there is a fullerene F_{36n-8} with two simple zigzags having intersection $2n$; above $n = 4$.

VII. Ringed fullerenes (with Grishukhin)

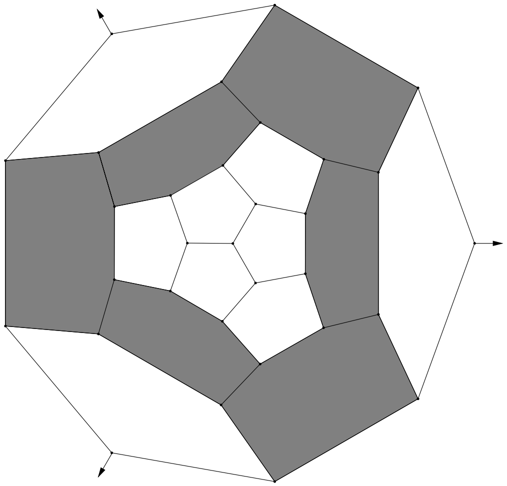
All fullerenes with hexagons in 1 ring



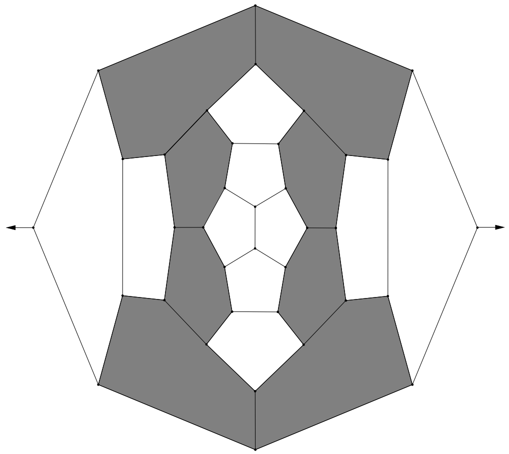
30, D_{5h}



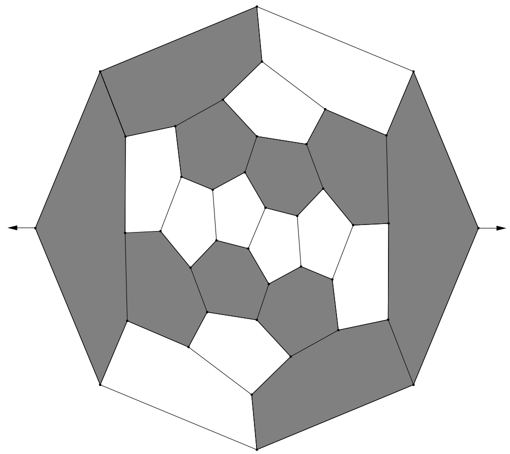
32, D_2



32, D_{3d}

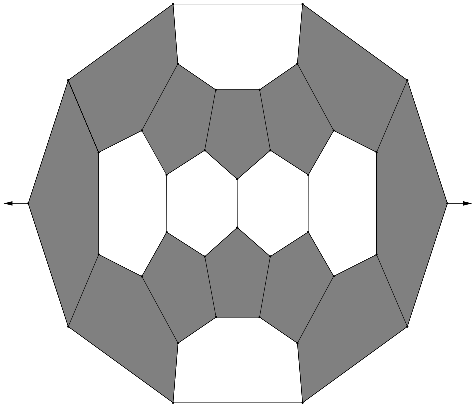


36, D_{2d}

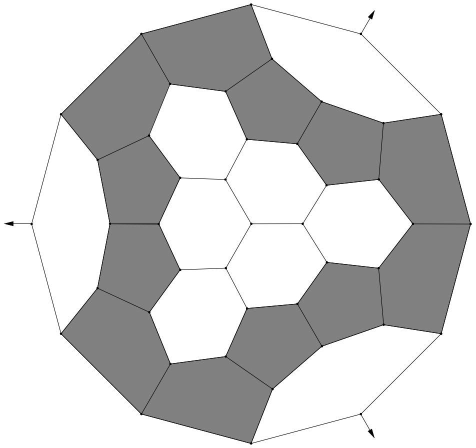


40, D_2

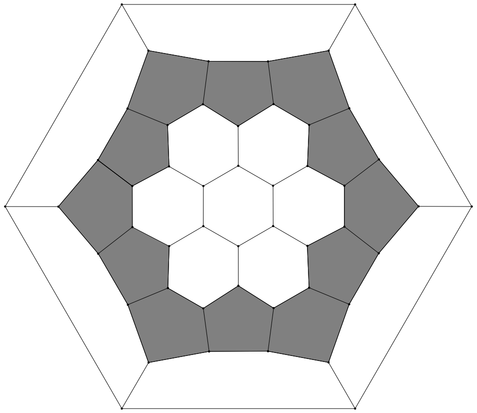
All fullerenes with pentagons in 1 ring



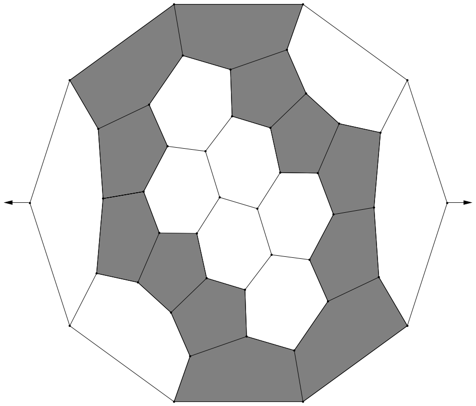
36, D_{2d}



44, D_{3d}

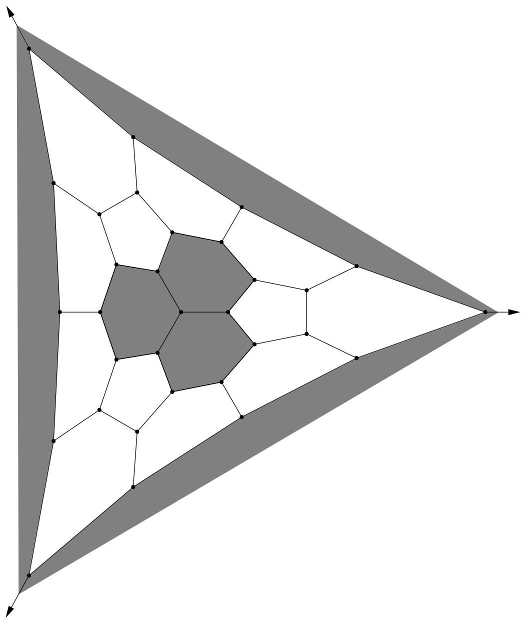


48, D_{6d}

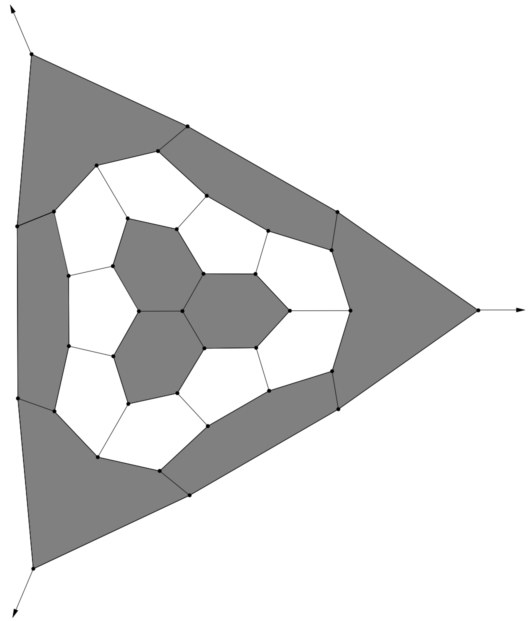


44, D_2

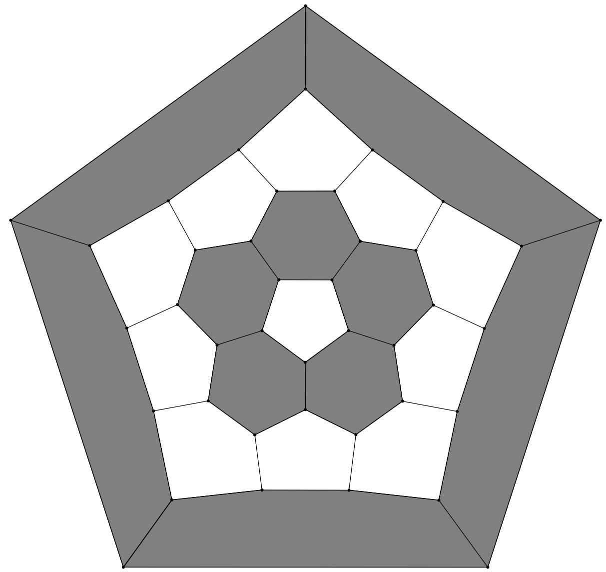
All fullerenes with hexagons in > 1 ring



32, D_{3h}

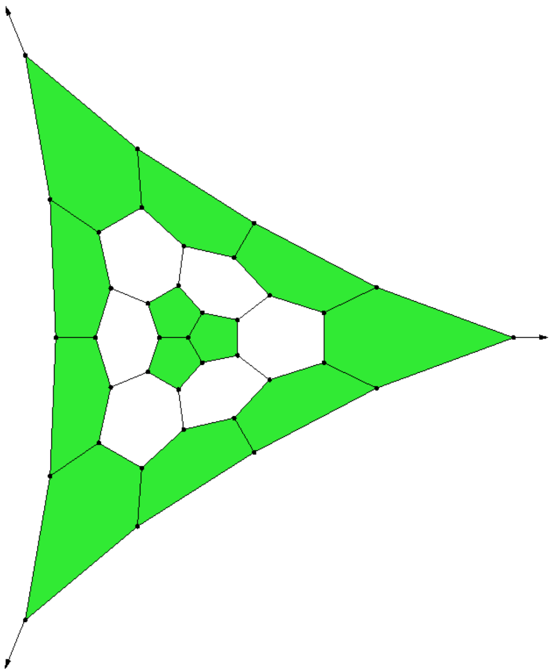


38, C_{3v}

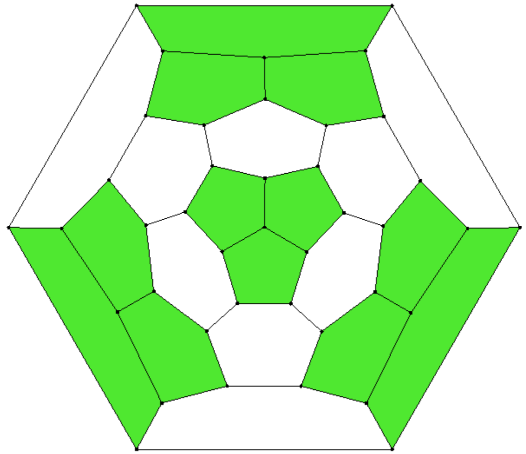


40, D_{5h}

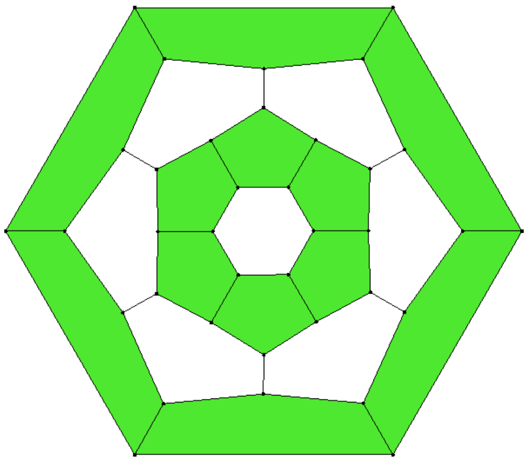
All fullerenes with pentagons in >1 ring



38, C_{3v}



infinite family:
4 triples in F_{4t},
$t \geq 10$, from
collapsed 3_{4t+8}



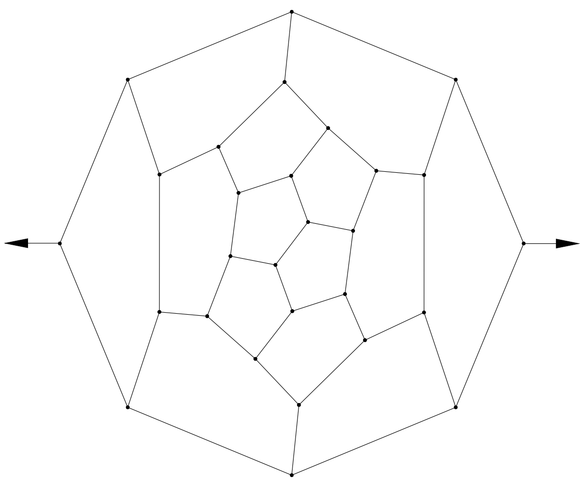
infinite family:
$F_{24+12t}(D_{6d})$,
$t \geq 1$,
D_{6h} if t odd
elongations of
hexagonal barrel

VIII. Face-regular fullerenes

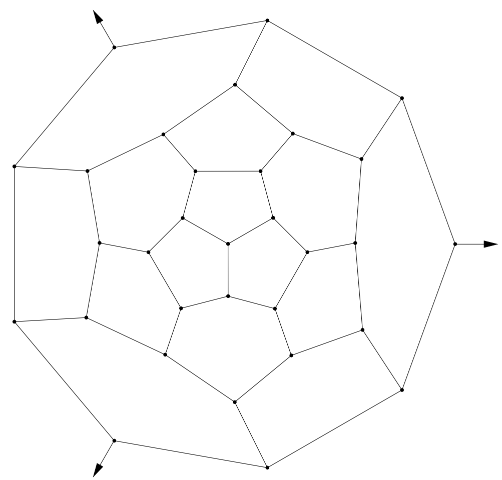
Face-regular fullerenes

A fullerene called $5R_i$ if every 5-gon has i exactly 5-gonal neighbors; it is called $6R_i$ if every 6-gon has exactly i 6-gonal neigbors.

i	0	1	2	3	4	5
# of $5R_i$	∞	∞	∞	2	1	1
# of $6R_i$	4	2	8	5	7	1



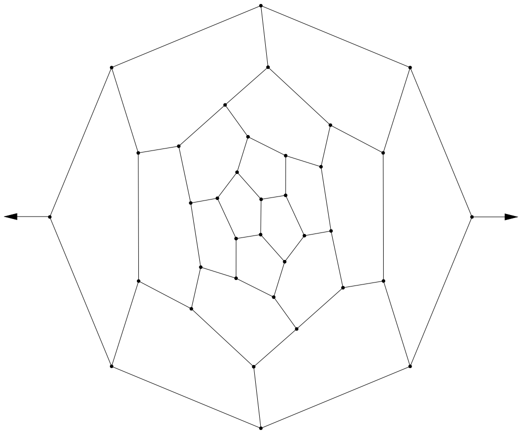
28, D_2



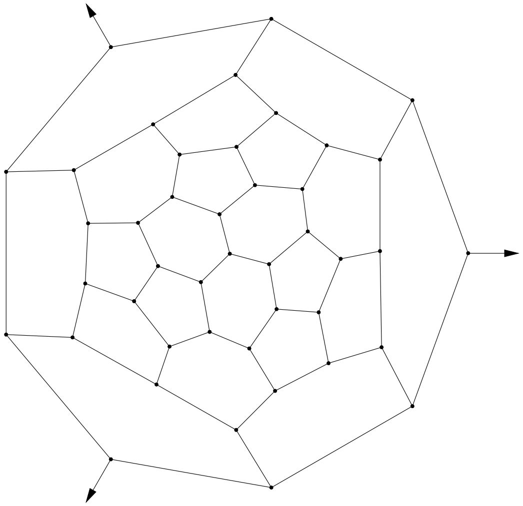
32, D_3

All fullerenes, which are $6R_1$

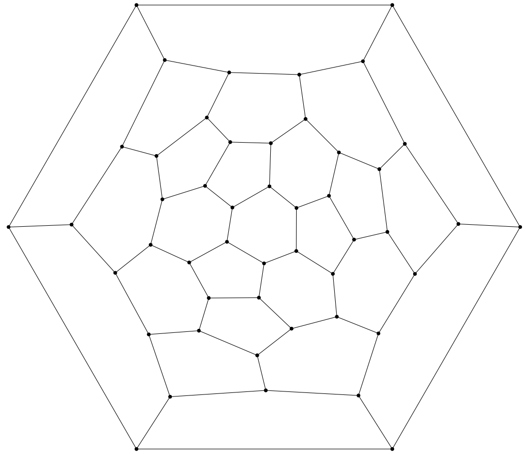
All fullerenes, which are $6R_3$



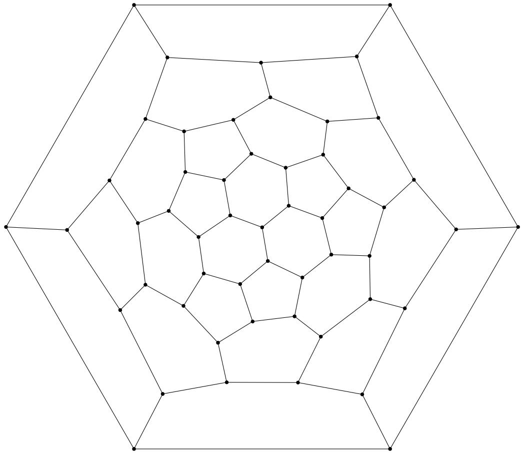
36, D_2



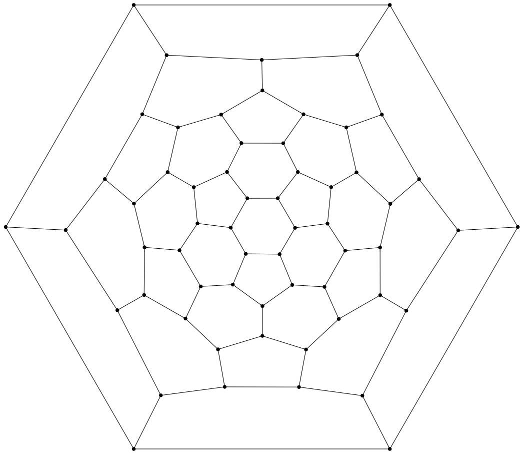
44, T (also $5R_2$)



48, D_3

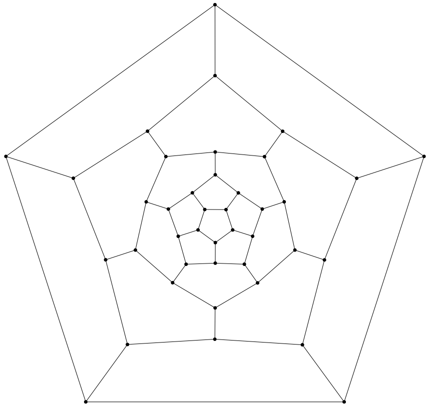


52, T (also $5R_1$)

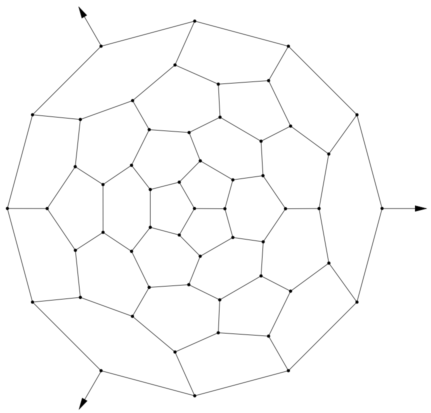


60, I_h (also $5R_0$)

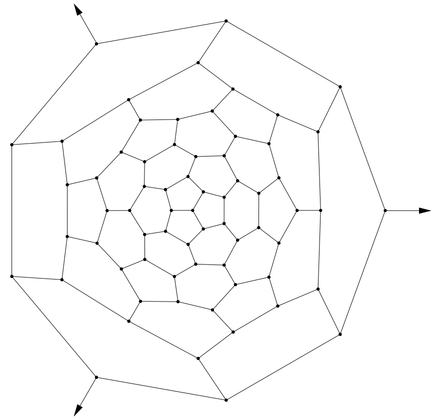
All fullerenes, which are $6R_4$



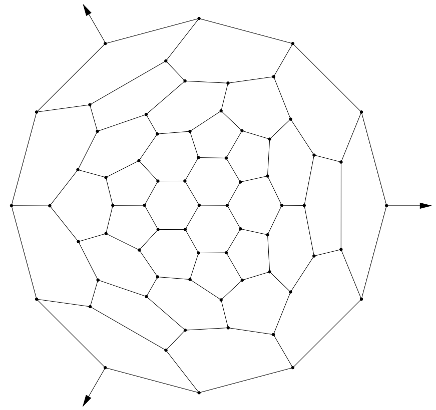
40, D_{5d}



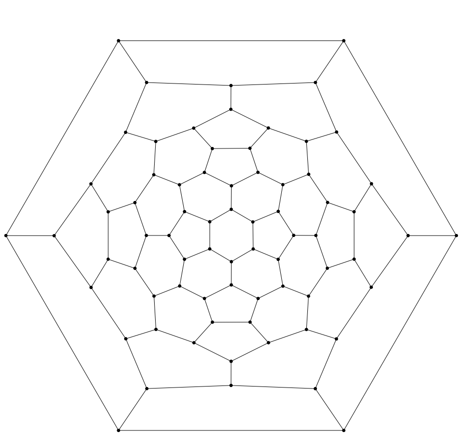
56, T_d
(also $5R_2$)



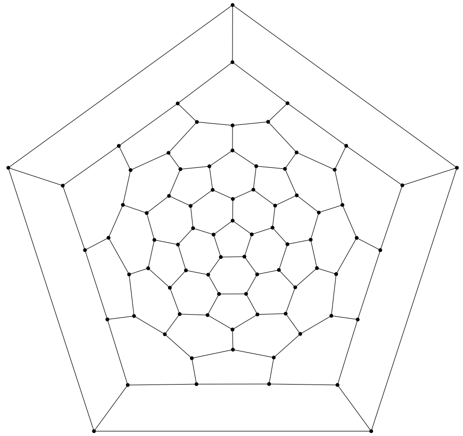
68, D_{3d}



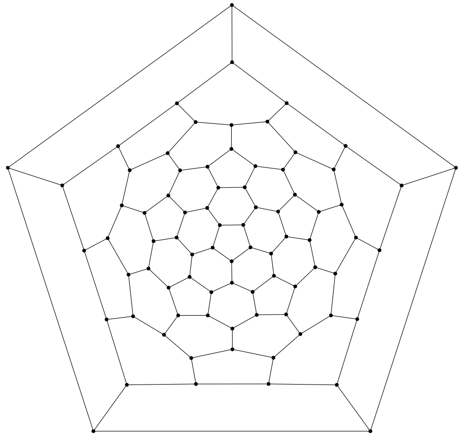
68, T_d
(also $5R_1$)



72, D_{2d}



80, D_{5h} (also $5R_0$)



80, I_h (also $5R_0$)

IX. Embedding of fullerenes

Fullerenes as isom. subgraphs of $\frac{1}{2}$-cubes

- All isometric embeddings of skeletons (with $(5R_i, 6R_j)$ of F_n), for I_h- or I-fullerenes or their duals, are:

$$F_{20}(I_h)(5,0) \to \tfrac{1}{2}H_{10} \qquad F_{20}^*(I_h)(5,0) \to \tfrac{1}{2}H_6$$
$$F_{60}^*(I_h)(0,3) \to \tfrac{1}{2}H_{10} \qquad F_{80}(I_h)(0,4) \to \tfrac{1}{2}H_{22}$$

- (Shpectorov-Marcusani, 2007: all others isometric F_n are 3 below (and number of isometric F_n^* is finite):

$$F_{26}(D_{3h})(-,0) \to \tfrac{1}{2}H_{12}$$
$$F_{40}(T_d)(2,-) \to \tfrac{1}{2}H_{15} \qquad F_{44}(T)(2,3) \to \tfrac{1}{2}H_{16}$$
$$F_{28}^*(T_d)(3,0) \to \tfrac{1}{2}H_7 \qquad F_{36}^*(D_{6h})(2,-) \to \tfrac{1}{2}H_8$$

- Also, for graphite lattice (infinite fullerene), it holds: (6^3)=$F_\infty(0,6) \to H_\infty, Z_3$ and (3^6)=$F_\infty^*(0,6) \to \frac{1}{2}H_\infty, \frac{1}{2}Z_3$.

Embeddable dual fullerenes in cells

The five above embeddable dual fullerenes F_n^* correspond exactly to five special (Katsura's "most uniform") partitions (5^3, $5^2.6$, 5.6^2, 6^3) of n vertices of F_n into 4 *types* by 3 gonalities (5- and 6-gonal) faces incident to each vertex.

- $F_{20}^*(I_h) \to \frac{1}{2}H_6$ corresponds to $(20,-,-,-)$
- $F_{28}^*(T_d) \to \frac{1}{2}H_7$ corresponds to $(4,24,-,-)$
- $F_{36}^*(D_{6h}) \to \frac{1}{2}H_8$ corresponds to $(-,24,12,-)$
- $F_{60}^*(I_h) \to \frac{1}{2}H_{10}$ corresponds to $(-,-,60,-)$
- $F_{\infty}^* \to \frac{1}{2}H_{\infty}$ corresponds to $(-,-,-,\infty)$

It turns out, that exactly above 5 fullerenes were identified as clatrin coated vesicles of eukaryote cells (the vitrified cell structures found during cryo-electronic microscopy).

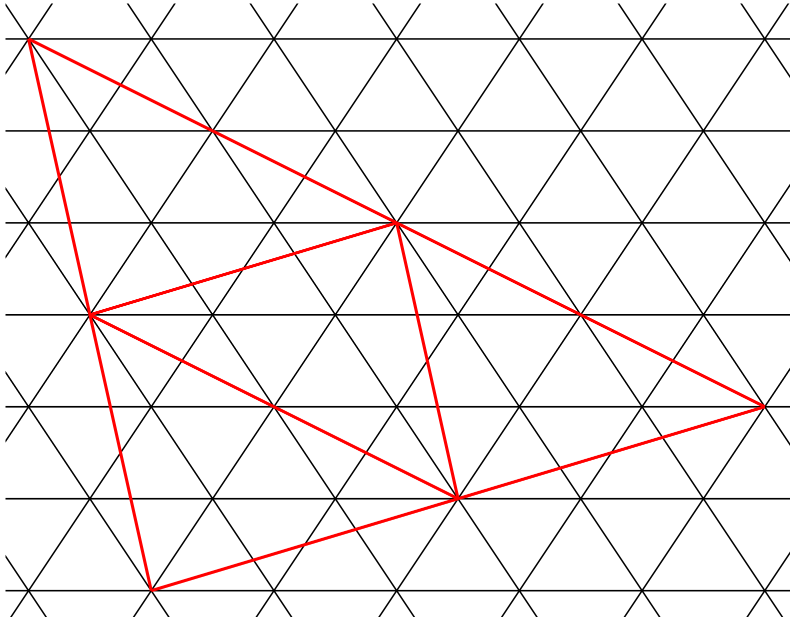
X. Parametrizing and generation of fullerenes

Parametrizing fullerenes

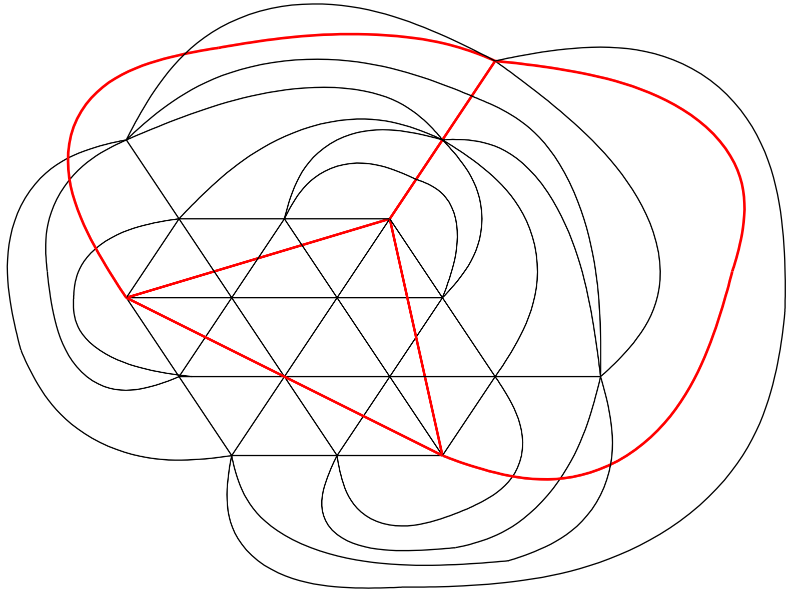
Idea: the hexagons are of zero curvature, it suffices to give relative positions of faces of non-zero curvature.

- Goldberg, 1937: all F_n of symmetry (I, I_h) are given by Goldberg-Coxeter construction $GC_{k,l}$.
- Fowler and al., 1988: all F_n of symmetry D_5, D_6 or T are described in terms of 4 integer parameters.
- Graver, 1999: all F_n can be encoded by 20 integer parameters.
- Thurston, 1998: all F_n are parametrized by 10 complex parameters.
- Sah (1994) Thurston's result implies that the number of fullerenes F_n is $\sim n^9$.

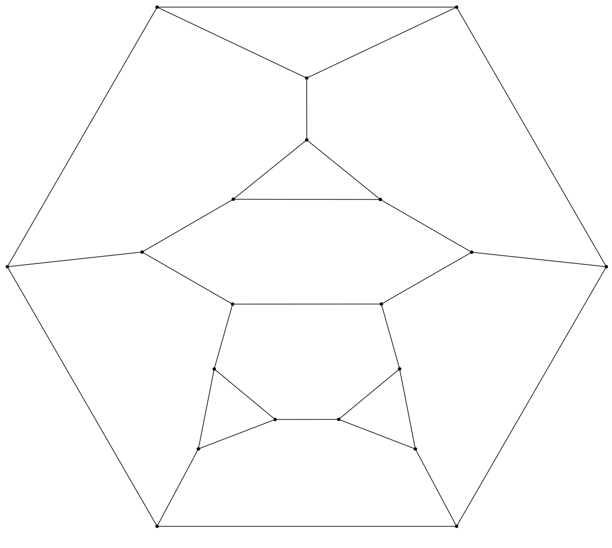
3-valent plane graph with $|F|$=3 or 6



4 triangles in $Z[\omega]$



The corresponding triangulation



Every such graph is obtained this way.

Generation of fullerenes

- Consider a fixed symmetry group and fullerenes having this group. In terms of complex parameters, we have

Group	$\#param.$	Group	$\#$	Group	$\#$
C_1	10	D_2	4	D_6	2
C_2	6	D_3	3	T	2
C_3	4	D_5	2	I	1

- For general fullerene (C_1) the best is to use fullgen (up to 180 vertices).
- For 1 parameter this is actually the Goldberg-Coxeter construction (up to 100000 vertices).
- For intermediate symmetry group, one can go farther by using the system of parameters (up to 1000 vertices).