Fullerene Manifolds and Special Fullerenes

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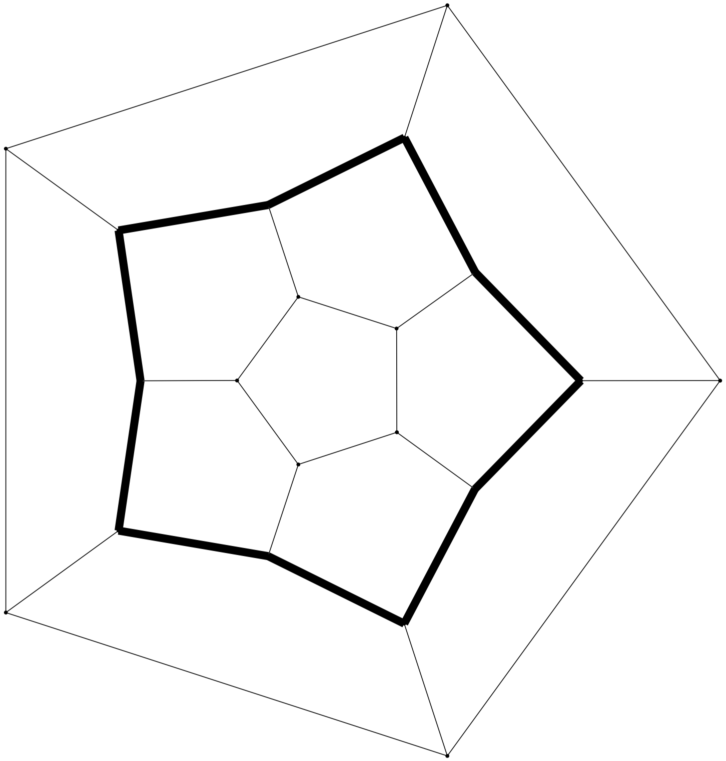
Definition of fullerene

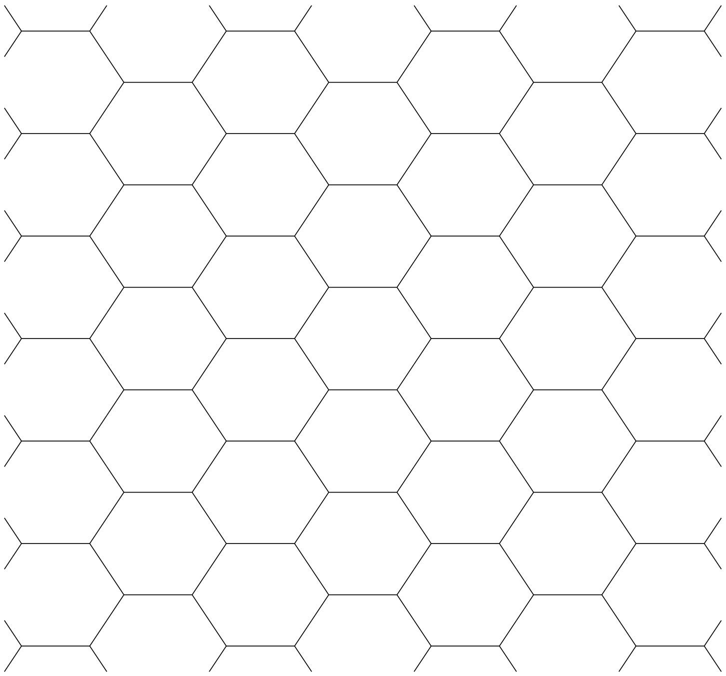
A fullerene F_v is a simple polyhedron whose v vertices are arranged in 12 pentagons and $(\frac{v}{2} - 10)$ hexagons.

- F_v exist for all even $v \geq 20$ except $v = 22$.
- $1, 1, 1, 2, 5 \dots, 1812, \dots 214127713, \dots$ isomers F_v, for $v = 20, 24, 26, 28, 30 \dots, 60, \dots, 200, \dots$.
- Thurston,1998, implies: number of F_v grows as v^9.
- $F_{60}(I_h)$, $F_{80}(I_h)$ are the only icosahedral (i.e., with highest possible symmetry I_h or I) fullerenes with $v \leq 80$ vertices.

The range of fullerenes

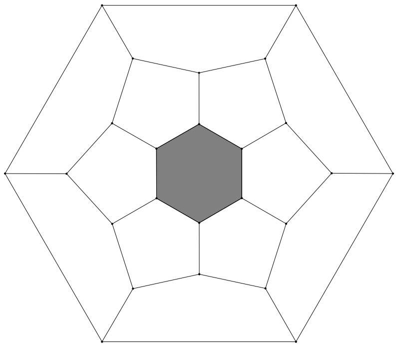


Dodecahedron $F_{20}(I_h)$:
the smallest fullerene

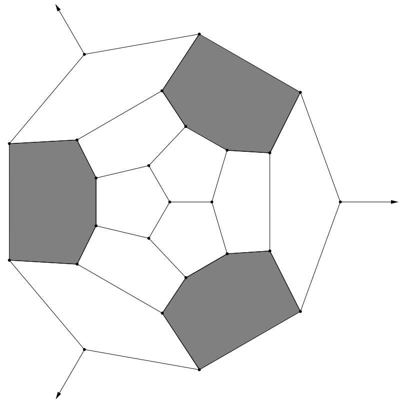


Graphite lattice (6^3) as F_∞:
the "largest fullerene"

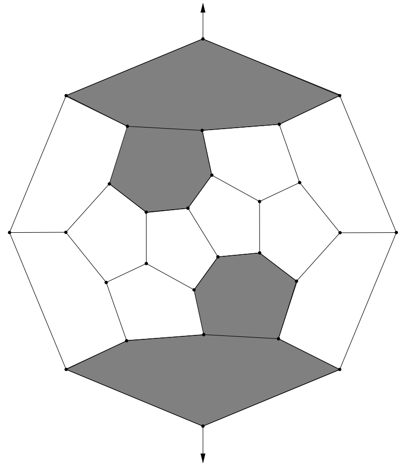
Small fullerenes



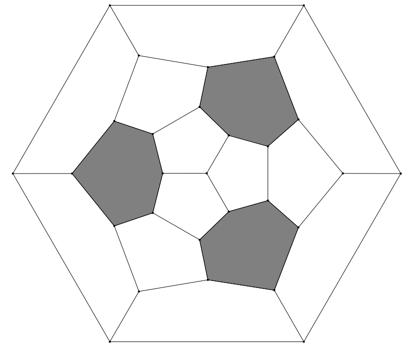
24, D_{6d}



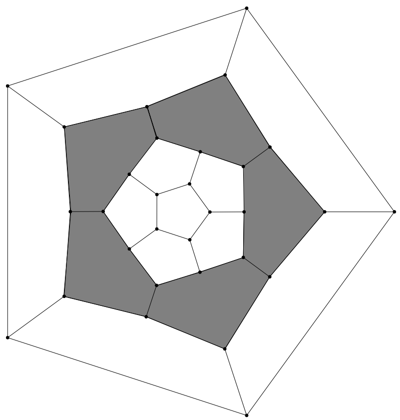
26, D_{3h}



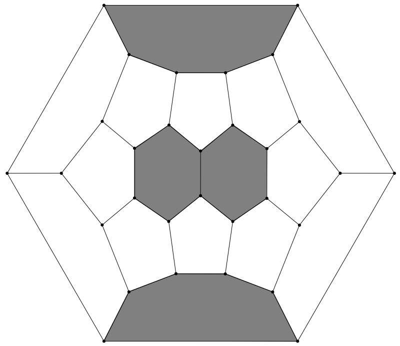
28, D_2



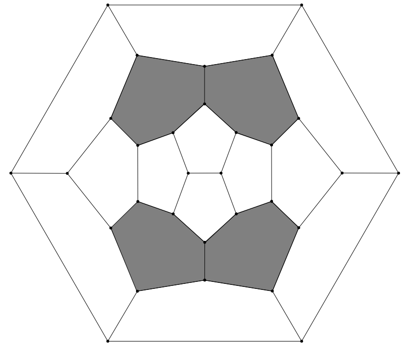
28, T_d



30, D_{5h}



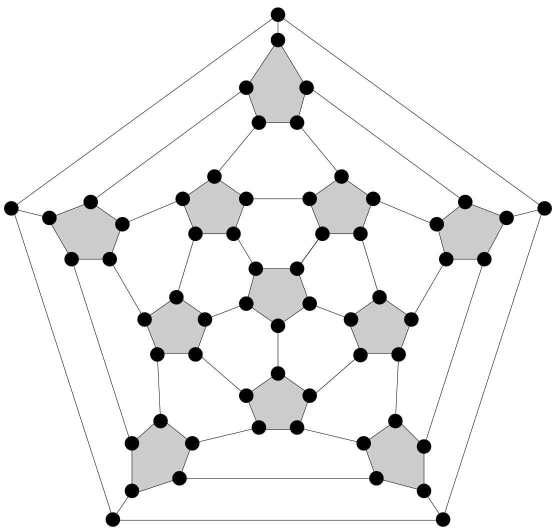
30, C_{2v}



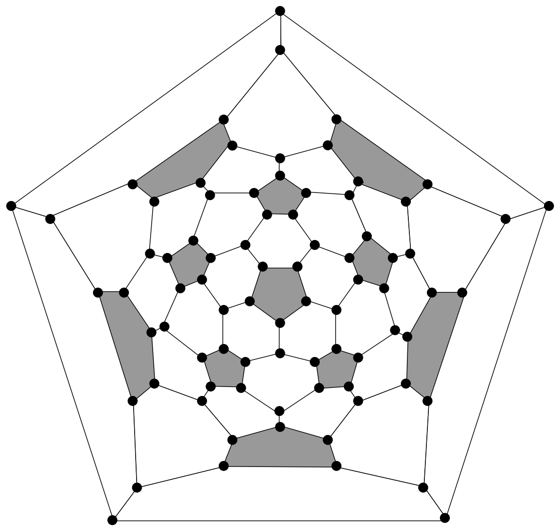
30, D_{2v}

Icosahedral fullerenes

- $v = 20T$, where $T = a^2 + ab + b^2$ (triangulation number) with $0 \leq b \leq a$; all come by construction $GC_{a,b}$.
- I_h (extended icosahedral group): for $a = b \neq 0$ or $b = 0$; I (proper icosahedral group): for $0 < b < a$.
- All except $F_{20}(I_h)$ are IPR (isolated pentagons).



$F_{60}(I_h)$=$(1,1)$-dodecahedron
Truncated Icosahedron



$F_{80}(I_h)$=$(2,0)$-dodecahedron
Chamfered Dodecahedron

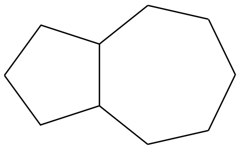
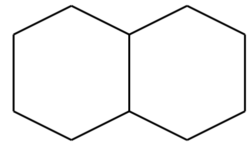
Parametrizing fullerenes

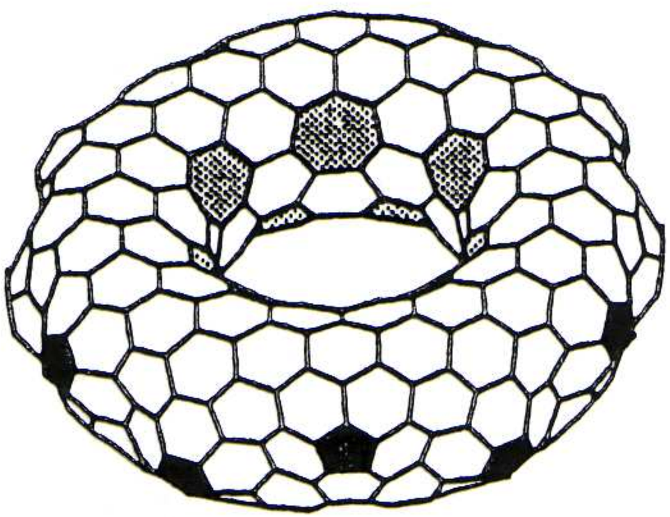
Since hexagons are of zero curvature, it suffices to give relative positions of faces of non-zero curvature.

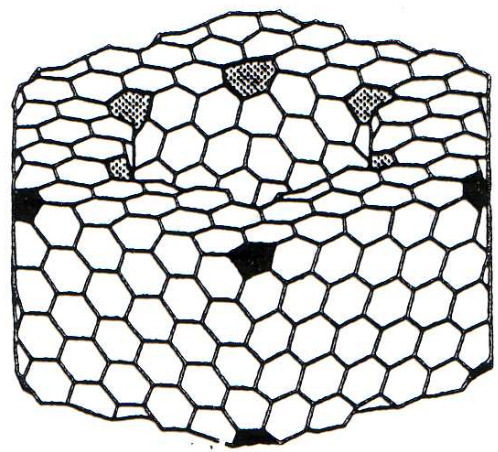
- Goldberg, 1937: all F_v of symmetry (I, I_h) are given by Goldberg-Coxeter construction $GC_{a,b}$.
- Fowler and al., 1988: all F_v of symmetry D_5, D_6 or T are described in terms of 4 integer parameters.
- Graver, 1999: all F_v can be encoded by 20 integer parameters.
- Thurston, 1998: all F_v are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

Useful fullerene-like 3-valent maps

- Polyhedra (p_5, p_6, p_n) for $n = 4$, 7 or 8 (math. chemistry)
- Azulenoids (p_5, p_7) on torus $g = 1$; so, $p_5 = p_7$

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





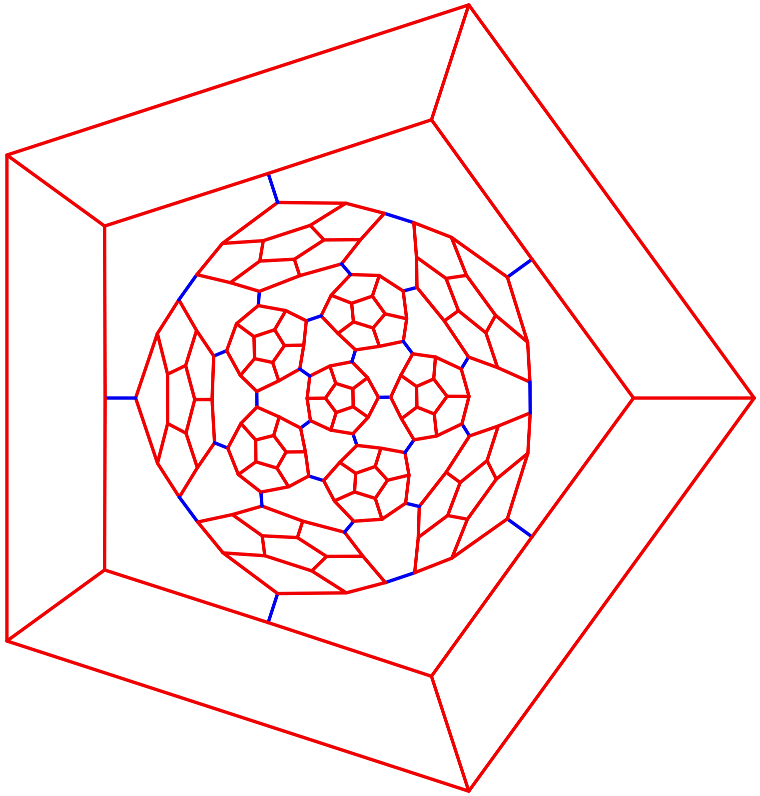
$$(p_5, p_6, p_7) = (12, 142, 12),$$
$$v = 432,\ D_{6d}$$

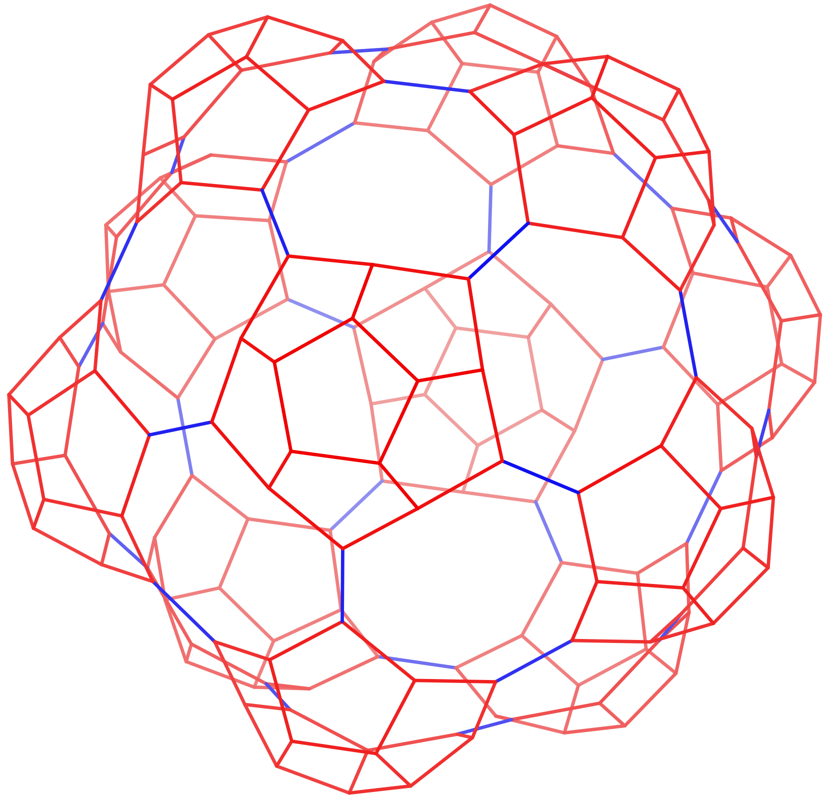
Fulleroids

- 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 $n \geq 8$.

The smallest I_h-fulleroid with $n = 9$

In general, n-fulleroid has $20 + 2p_n(n-5)$ vertices

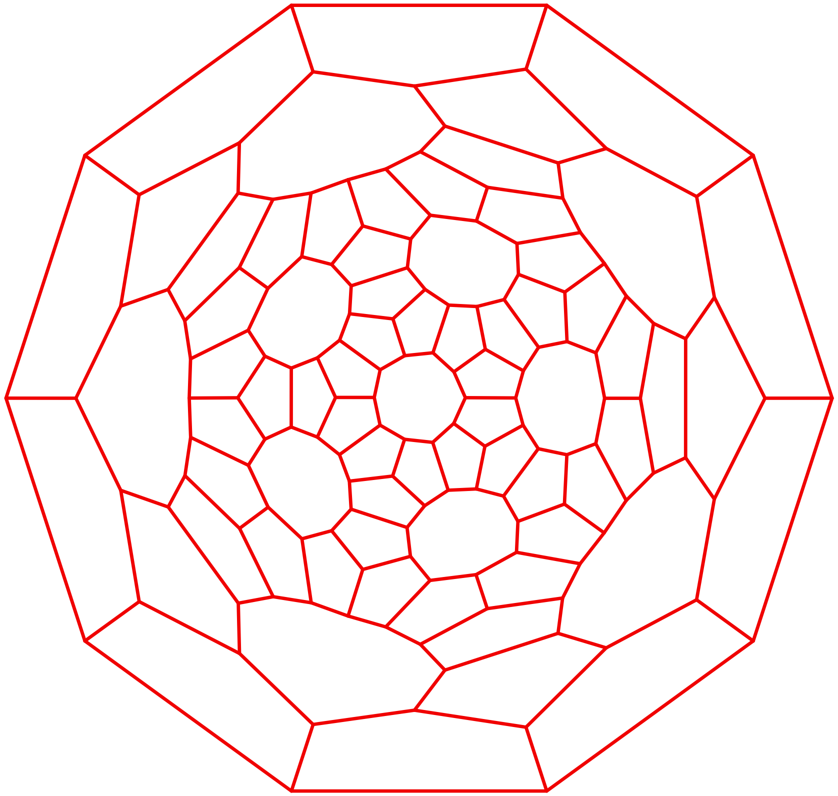


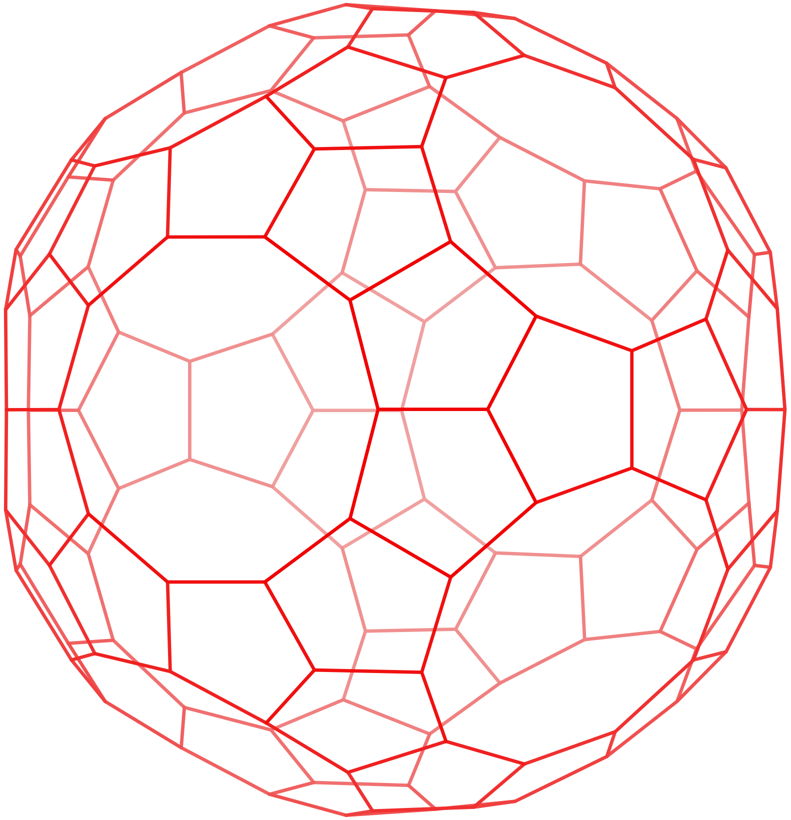


$F_{5,9}(I_h) = P(F_{60}(I_h))$ (pentacon of Truncated Icosahedron)

$v = 180$ and $p_5 = 72, p_9 = 20$

The smallest I_h-fulleroid with $n = 10$

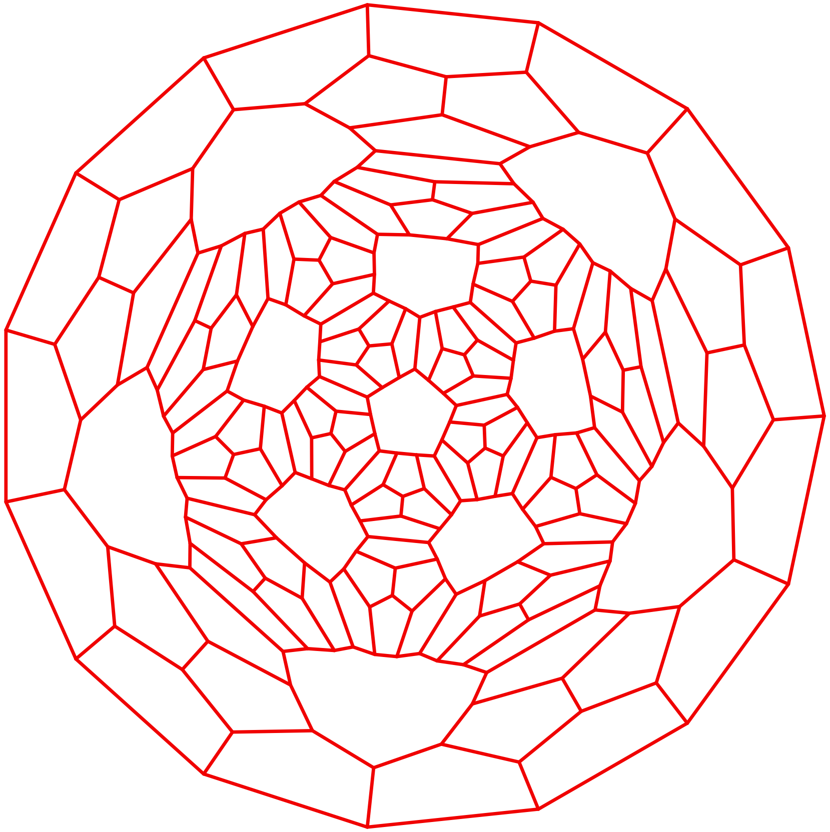


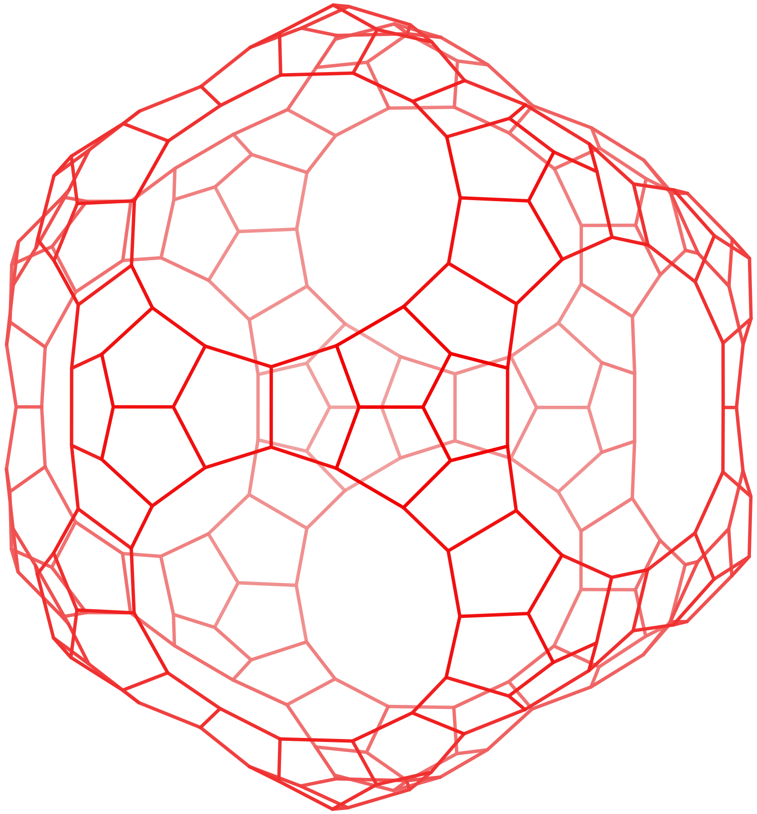


$F_{5,10}(I_h) = T_1(F_{60}(I_h))$ (triacon T_1 of Truncated Icosahedron)

$v = 140$ and $p_5 = 60, p_{10} = 12$

The smallest fulleroid with $n = 15$



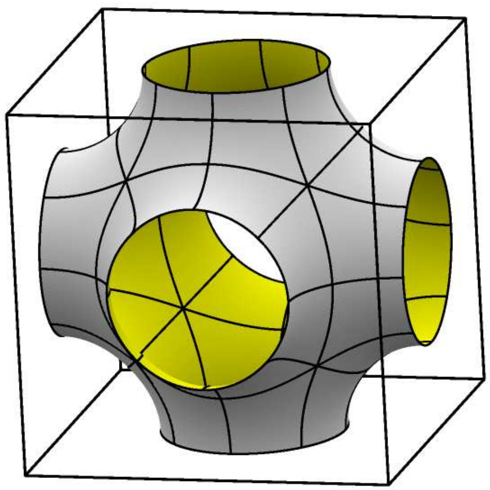


$F_{5,15}(I_h) = T_2(F_{60}(I_h))$ (triacon T_2 of Truncated Icosahedron)

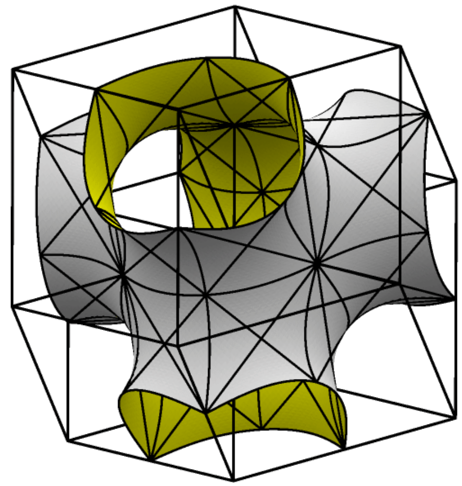
$v = 260$ and $p_5 = 120, p_{15} = 12$

Schwarzits

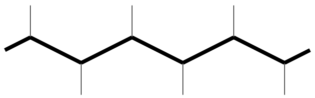
Schwarzits (p_6, p_7, p_8) on minimal surfaces of constant negative curvature ($g \geq 3$). We consider case $g = 3$:



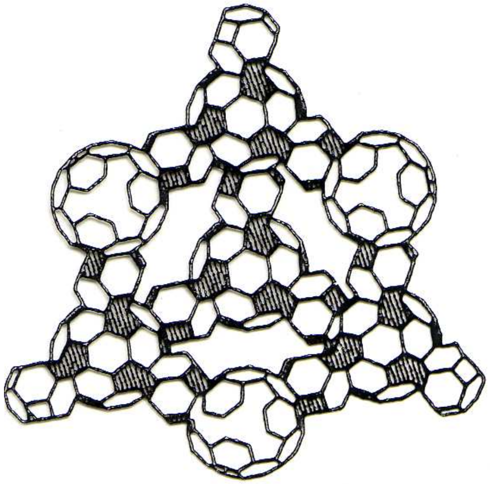
Schwarz P-surface



Schwarz D-surface

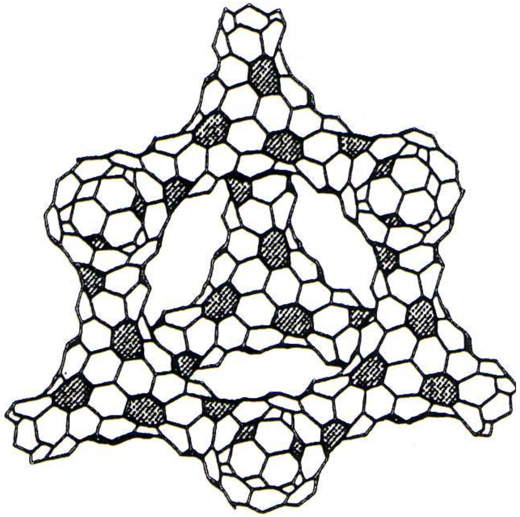
- Take a 3-valent map of genus 3 and cut it along zigzags  and paste it to form D- or P-surface.
- One needs 3 non-intersecting zigzags. For example, Klein regular map $D56 = (7^3)$ has 5 types of such triples

$(6,7)$-surfaces

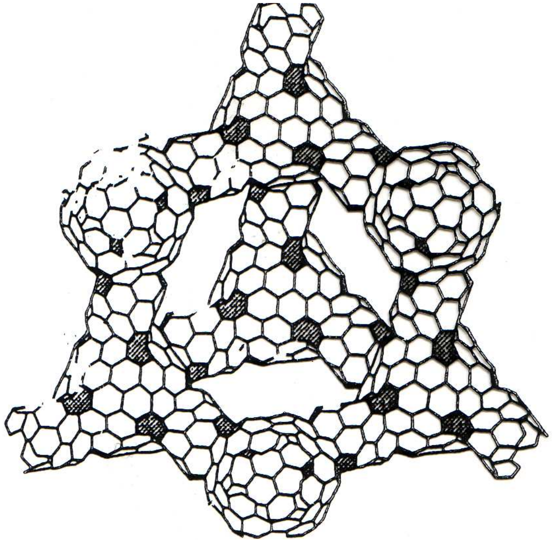


$(1,1)$

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



$(0,2)$



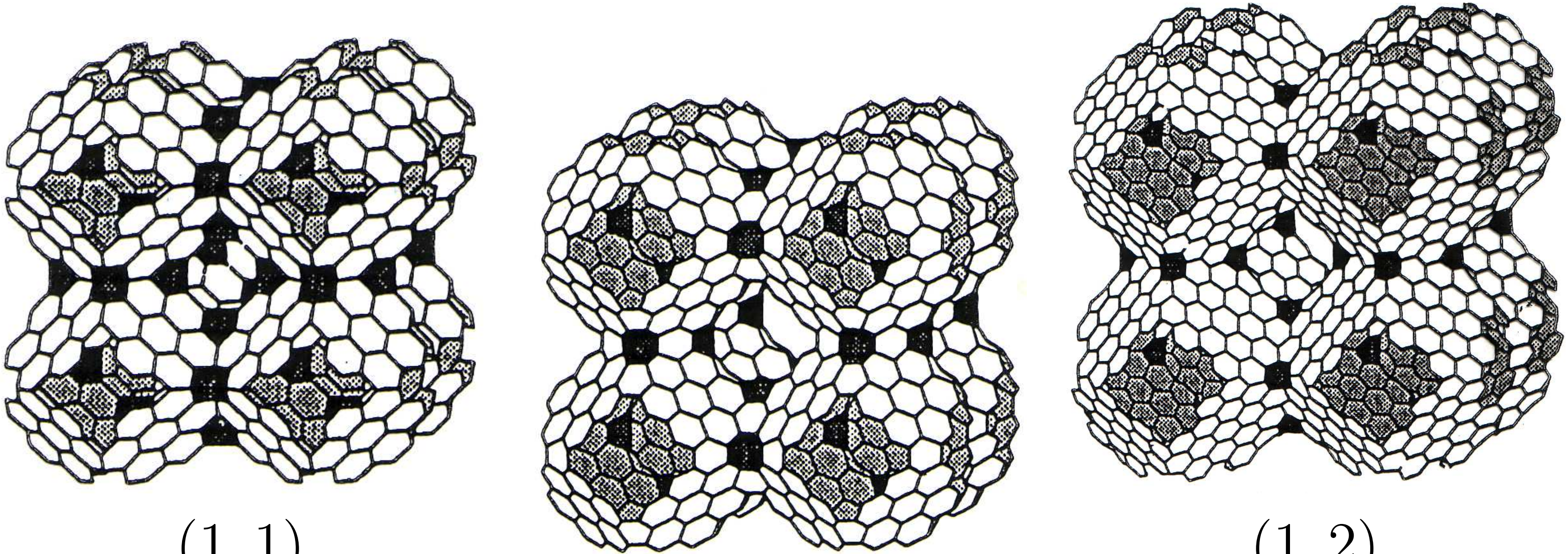
$(1,2)$

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

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



$(1,1)$ $(0,2)$ $(1,2)$

Unit cell with $p_6 = 0, p_8 = 12$: Dyck regular map $P32 = (8^3)$.

d-dimensional fullerenes

Fulerene manifolds

$(d-1)$-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, $3 \leq i \leq d$, 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.

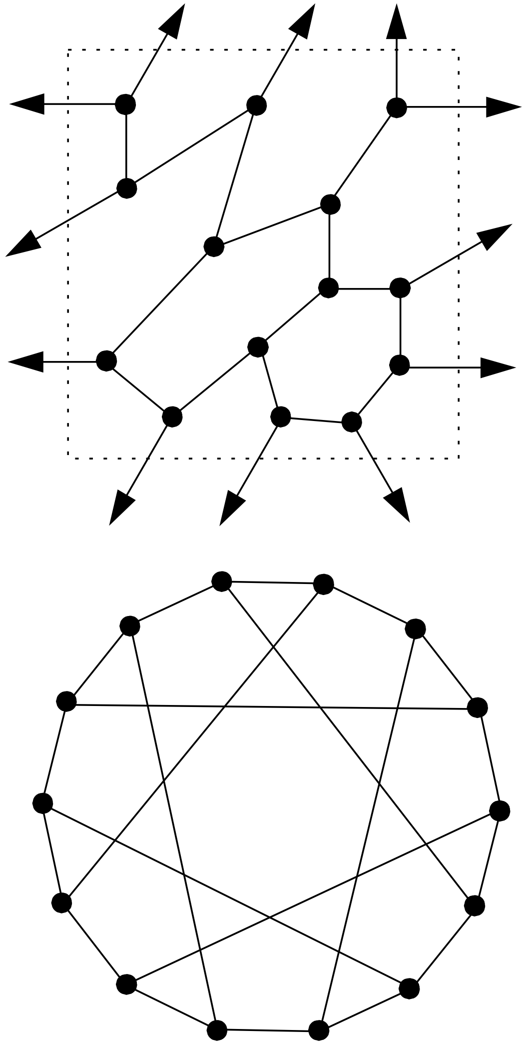
- All finite 3-fullerenes
- ∞: plane 3- and space 4-fullerenes
- 4 constructions of finite 4-fullerenes (all from 120-cell):
  - A (tubes of 120-cells) and B (coronas)
  - Inflation-decoration method (construction C, D)
- Quotient fullerenes; polyhexes
- 5-fullerenes from tiling of H^4 by 120-cell

All finite 3-fullerenes

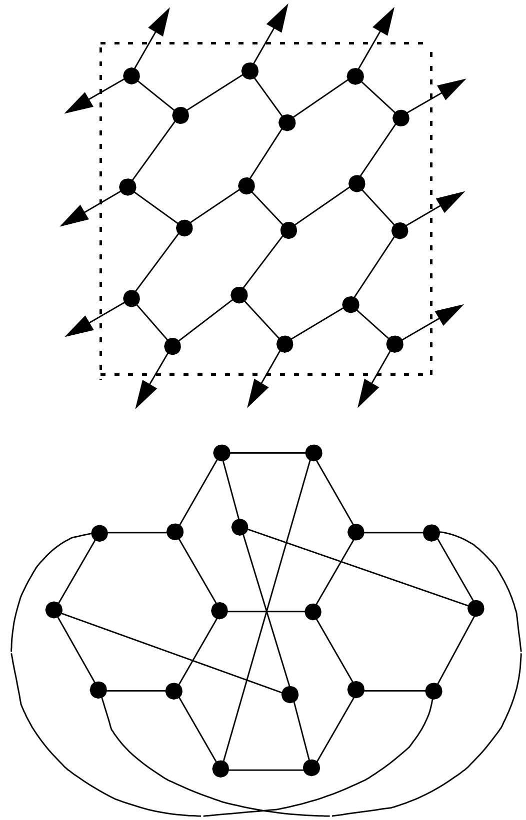
- Euler formula $\chi = v - e + p = \frac{p_5}{2} \geq 0$.
- But $\chi = \begin{cases} 2(1-g) & \text{if oriented} \\ 2-g & \text{if not} \end{cases}$
- Any 2-manifold is homeomorphic to S^2 with g (genus) handles (cyl.) if oriented or cross-caps (Möbius) if not.

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

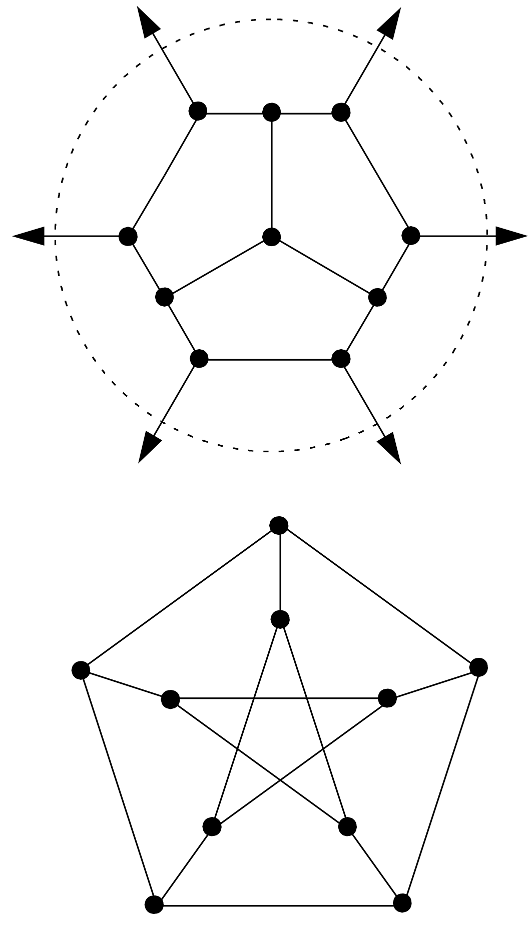
Smallest non-spherical finite 3-fullerenes



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)

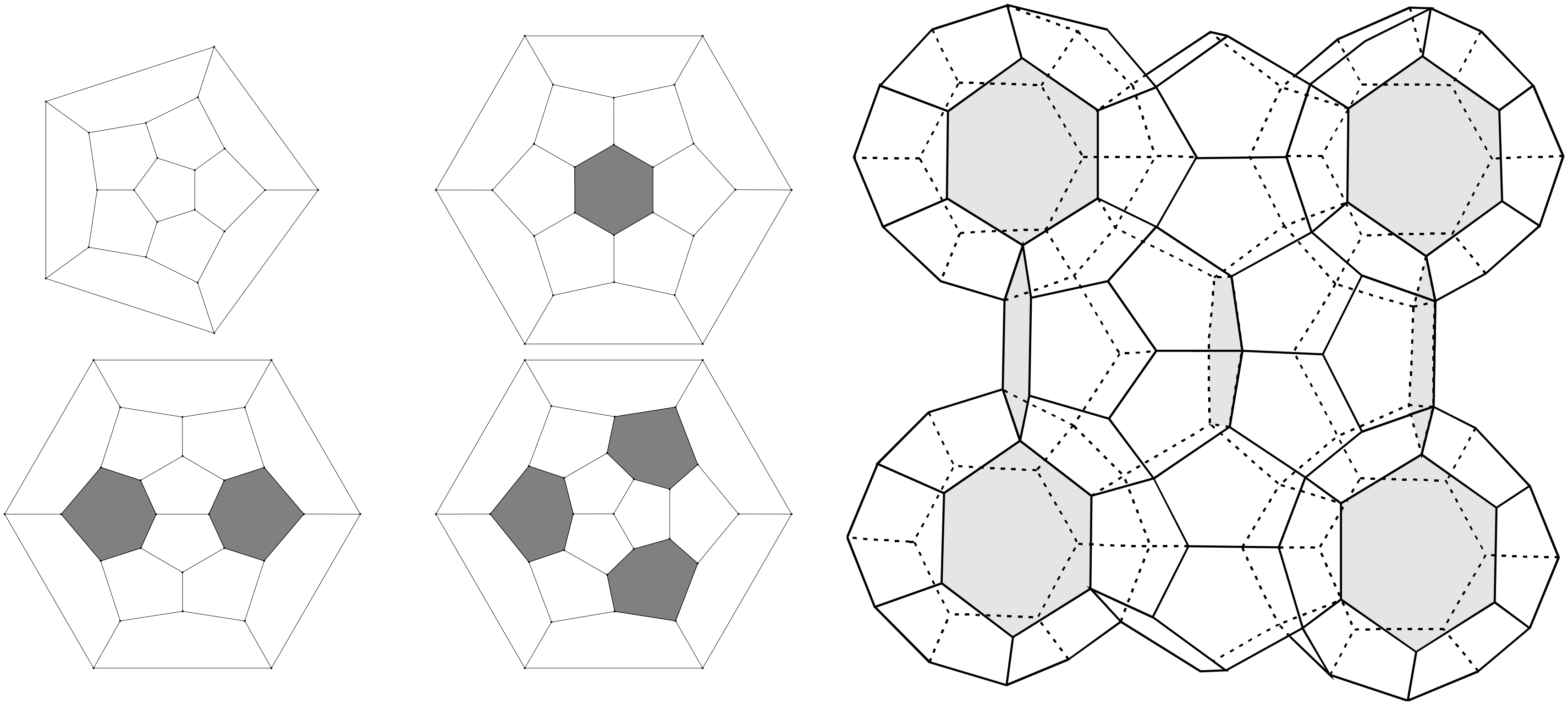
- 4 Frank-Kasper polyhedra (isolated-hexagon fullerenes): $F_{20}(I_h)$, $F_{24}(D_{6d})$, $F_{26}(D_{3h})$, $F_{28}(T_d)$
- FK space fullerene: a 4-valent tiling of E^3 by them. Space fullerene: a 4-valent tiling of E^3 by any fullerenes; Deza-Shtogrin, 1999: unique known non-FK example.
- FK space fullerenes occur in:
  - ordered tetrahedrally closed-packed phases of metallic alloys with cells being atoms. There are > 20 t.c.p. alloys (in addition to all quasicrystals)
  - soap froths (foams, liquid crystals)
  - hypothetical silicate (or zeolite) if vertices are tetrahedra SiO_4 (or $SiAlO_4$) and cells H_2O
  - better solution to the Kelvin problem

Main examples of FK space fullerenes

Also in clathrate "ice-like" hydrates: vertices are H_2O, hydrogen bonds, cells are sites of solutes (Cl, Br, ...).

t.c.p.	alloys	exp. clathrate	# 20	# 24	# 26	# 28
A_{15}	$Cr_3.Si$	I:$4Cl_2.7H_2O$	1	3	0	0
C_{15}	$MgCu_2$	II:$CHCl_3.17H_2O$	2	0	0	1
Z	Zr_4Al_3	III:$Br_2.86H_2O$	3	2	2	0
σ	$Cr_{46}.Fe_{54}$		5	8	2	0
μ	Mo_6Co_7		7	2	2	2
δ	$MoNi$		6	5	2	1
C	$V_2(Co, Si)_3$		15	2	2	6
T	$Mg_{32}(Zn, Al)_{49}$	T_I(Bergman)	49	6	6	20
SM		T_P(Sadoc-Mossieri)	49	9	0	26

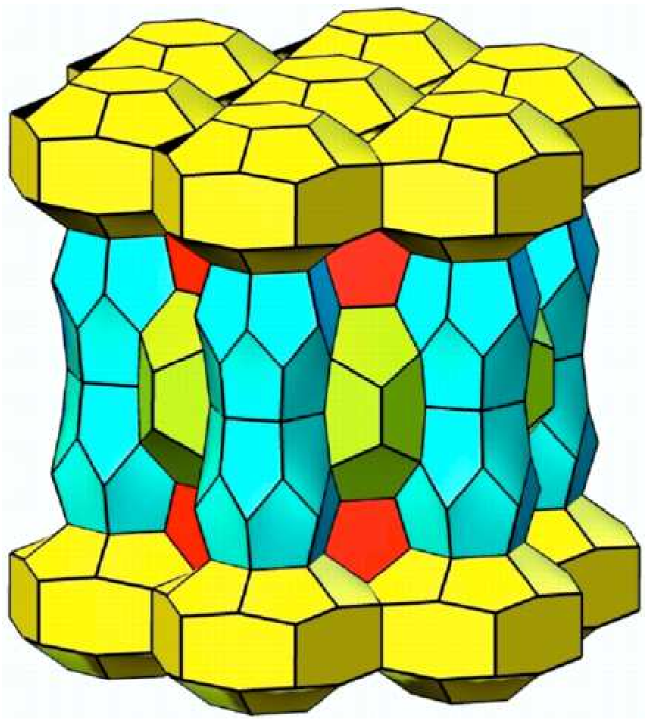
Frank-Kasper polyhedra and A_{15}

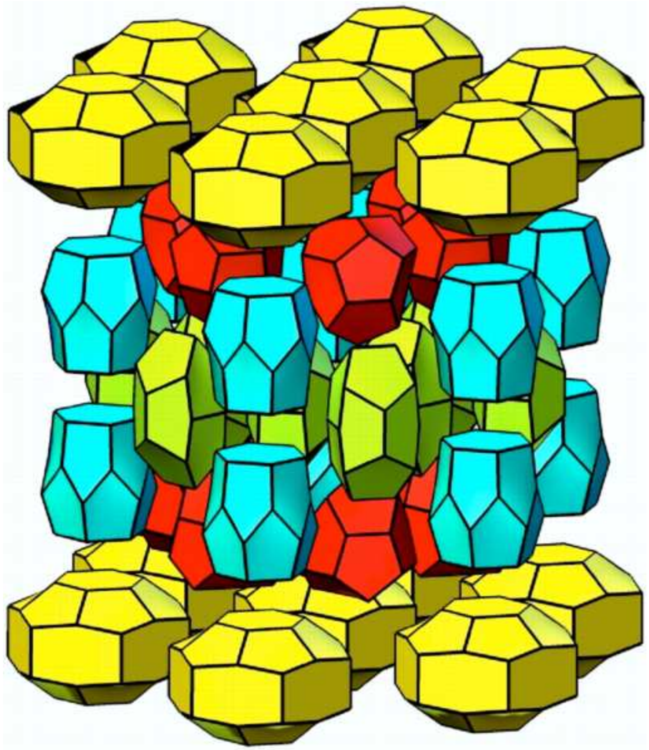


Mean face-size of all known space FK fullerenes is in $[5+\frac{1}{10}(C_{15}), 5+\frac{1}{9}(A_{15})]$. Closer to impossible 5 (120-cell on 3-sphere) means energetically competitive with diamond.

Non-FK space fullerene: is it unique?

The only known which is not by F_{20}, F_{24}, F_{26} and $F_{28}(T_d)$.
By F_{20}, F_{24} and its elongation $F_{36}(D_{6h})$ in ratio $7:2:1$;
so, best known mean face-size $5.091 < 5.1(C_{15})$.

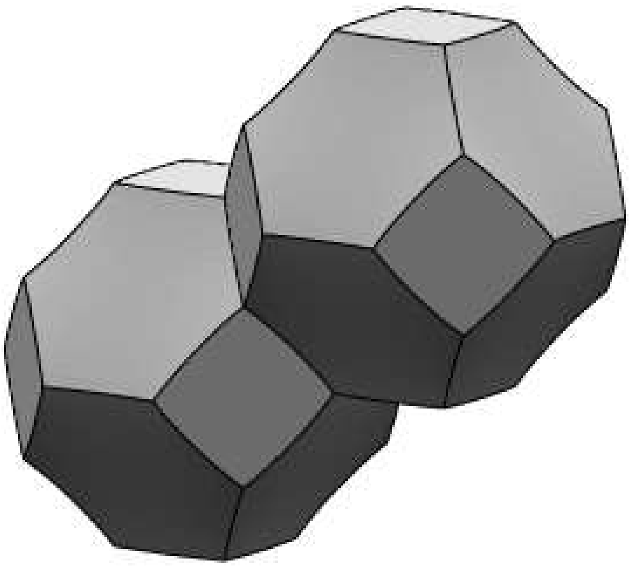




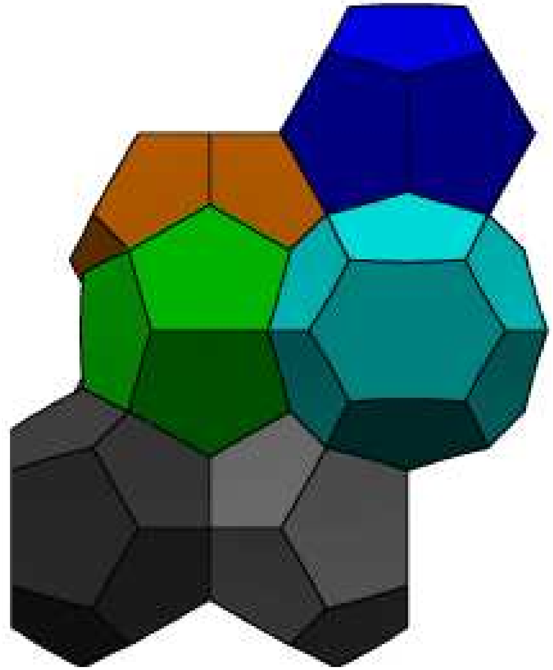
All space fullerenes with at most 7 kinds of vertices:
A_{15}, C_{15}, Z, σ and this one (Delgado, O'Keeffe; 3,3,5,7,7).

Kelvin problem

Partition E^3 into cells D of equal volume and minimal surface, i.e., with maximal $IQ(D) = \frac{36\pi V^2}{A^3}$.



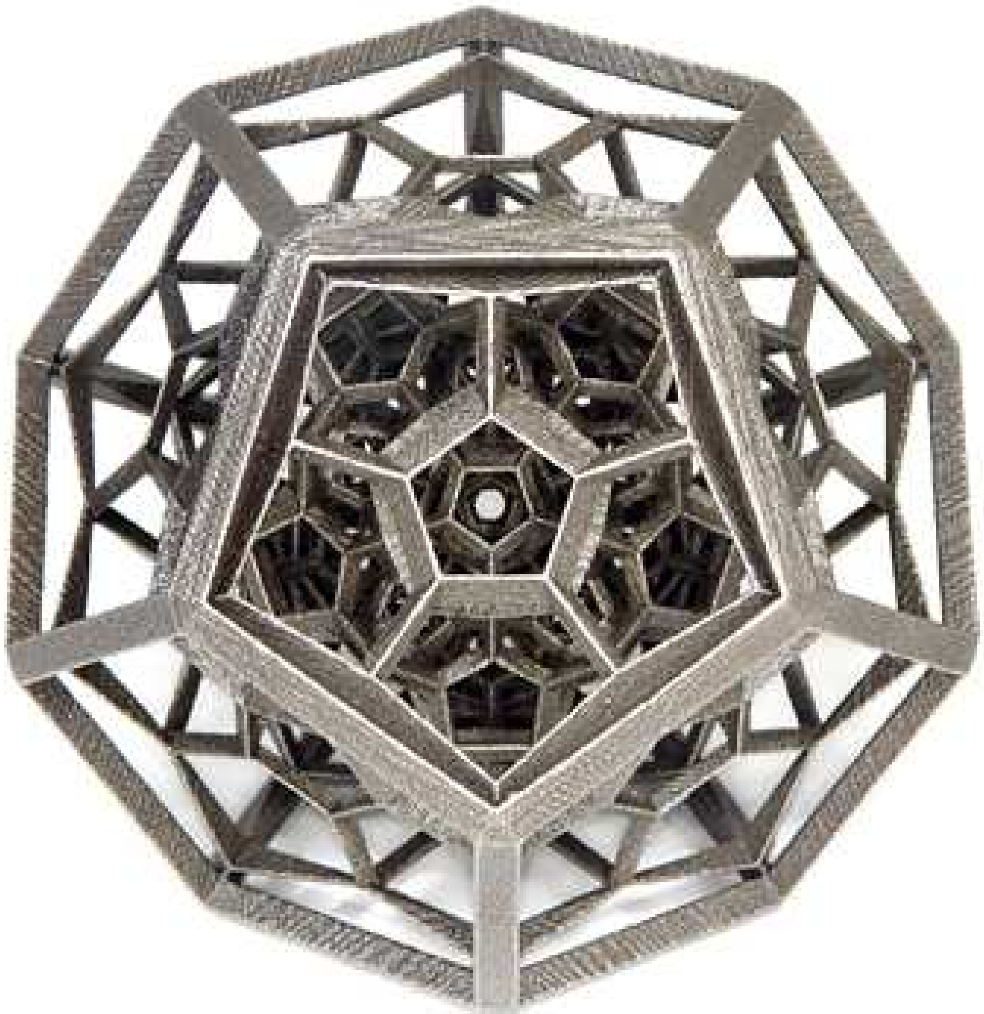
Lord Kelvin, 1887
IQ(curved tr.Oct.) ≈ 0.757
IQ(tr.Oct.) ≈ 0.753



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

In 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}, $F_{32}(D_{3h})$

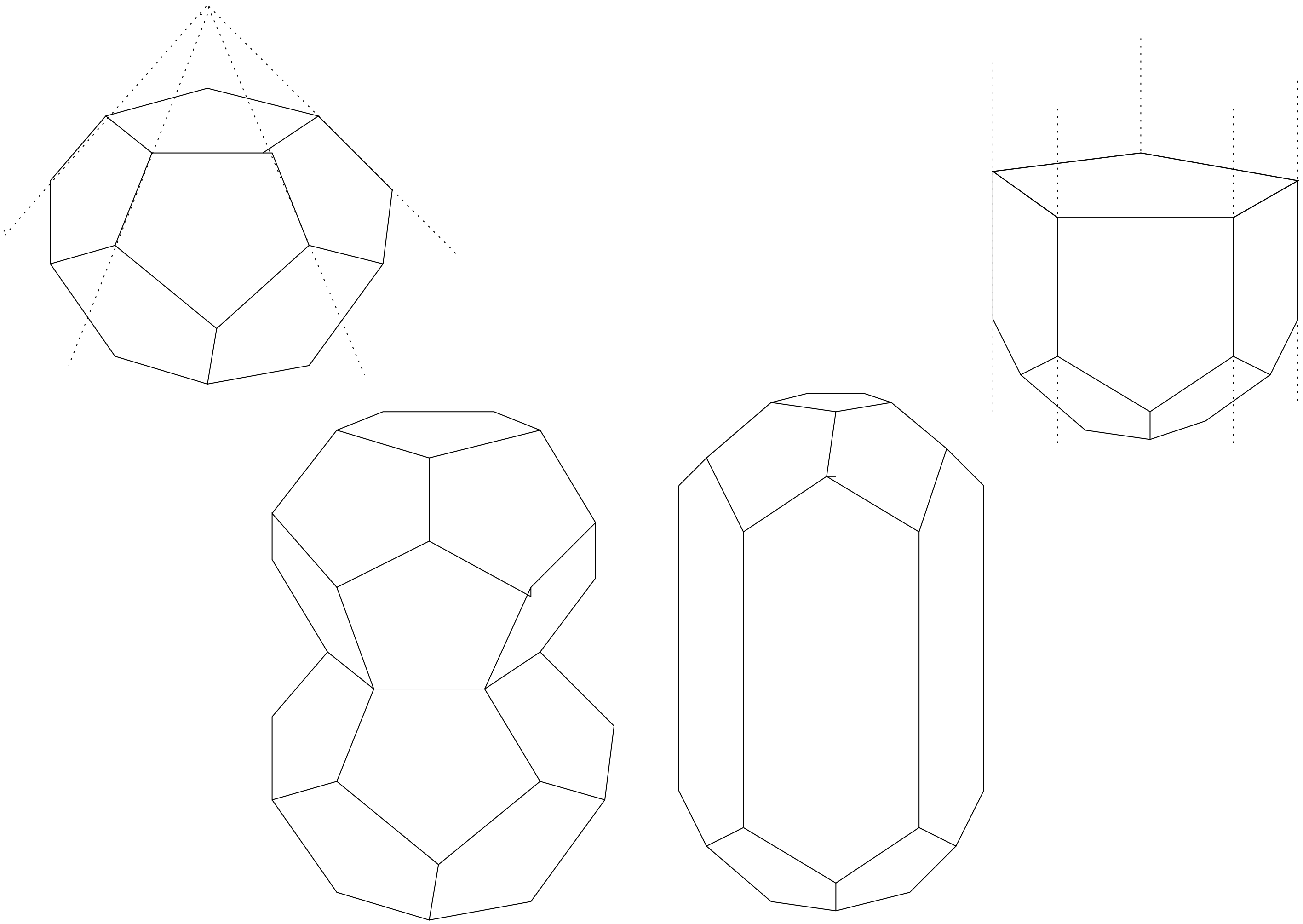
$*$ indicates that the construction creates a polytope; otherwise, the obtained fullerene is a 3-sphere.

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

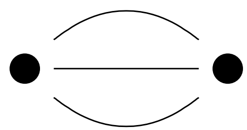
- quotient of 120-cell (on S^3) by the binary icosahedral group I_h of order 120; so, f-vector $(5, 10, 6, 1) = \frac{1}{120} f(120 - \text{cell})$
- It comes also from $F_{20} = Do$ by gluing of its opposite faces with $\frac{1}{10}$ right-handed rotation

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.:

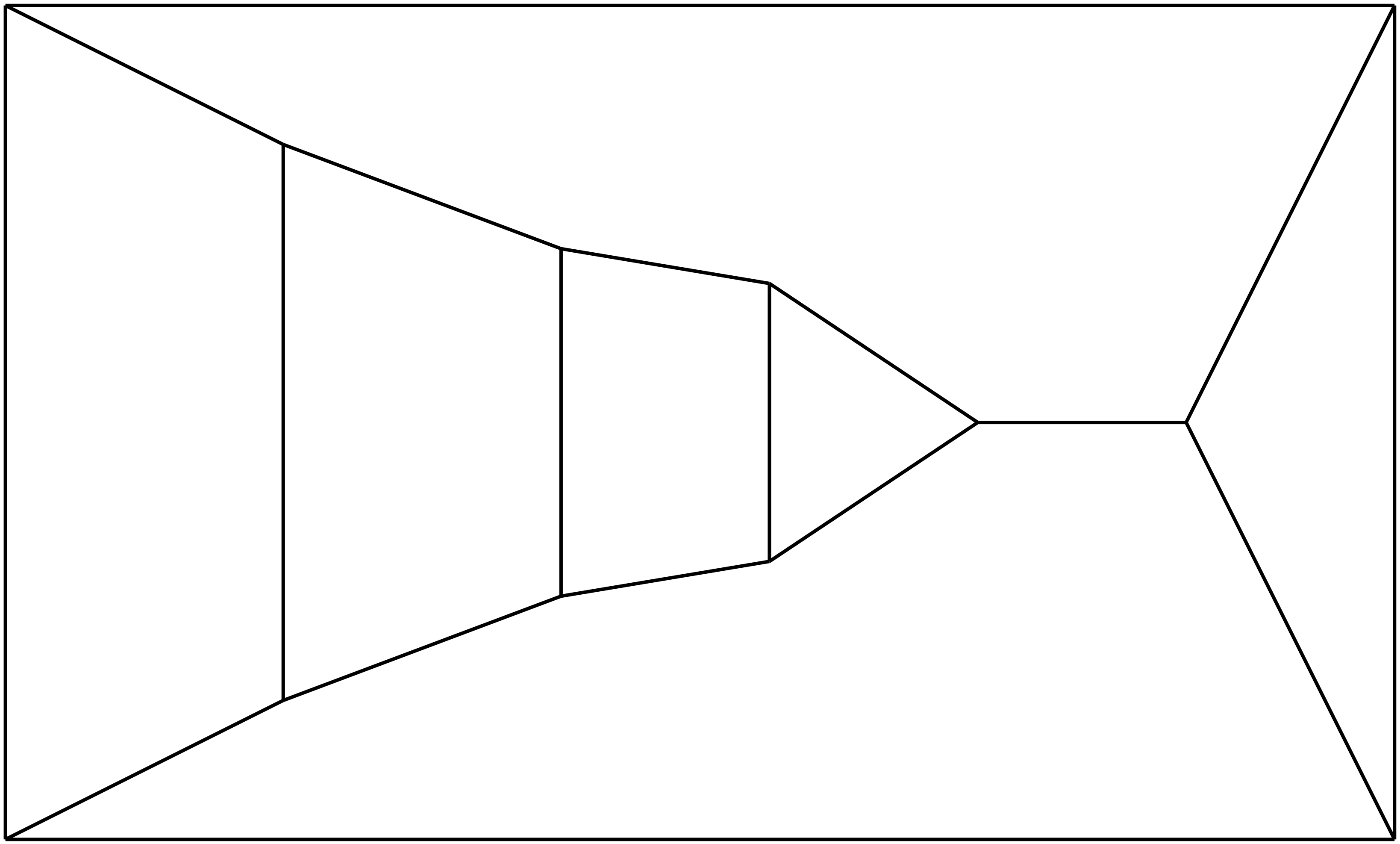
- 2 translations,
- a translation, a glide reflection
- a translation and a glide reflection.

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.

Zigzags, railroads and knots in fullerenes

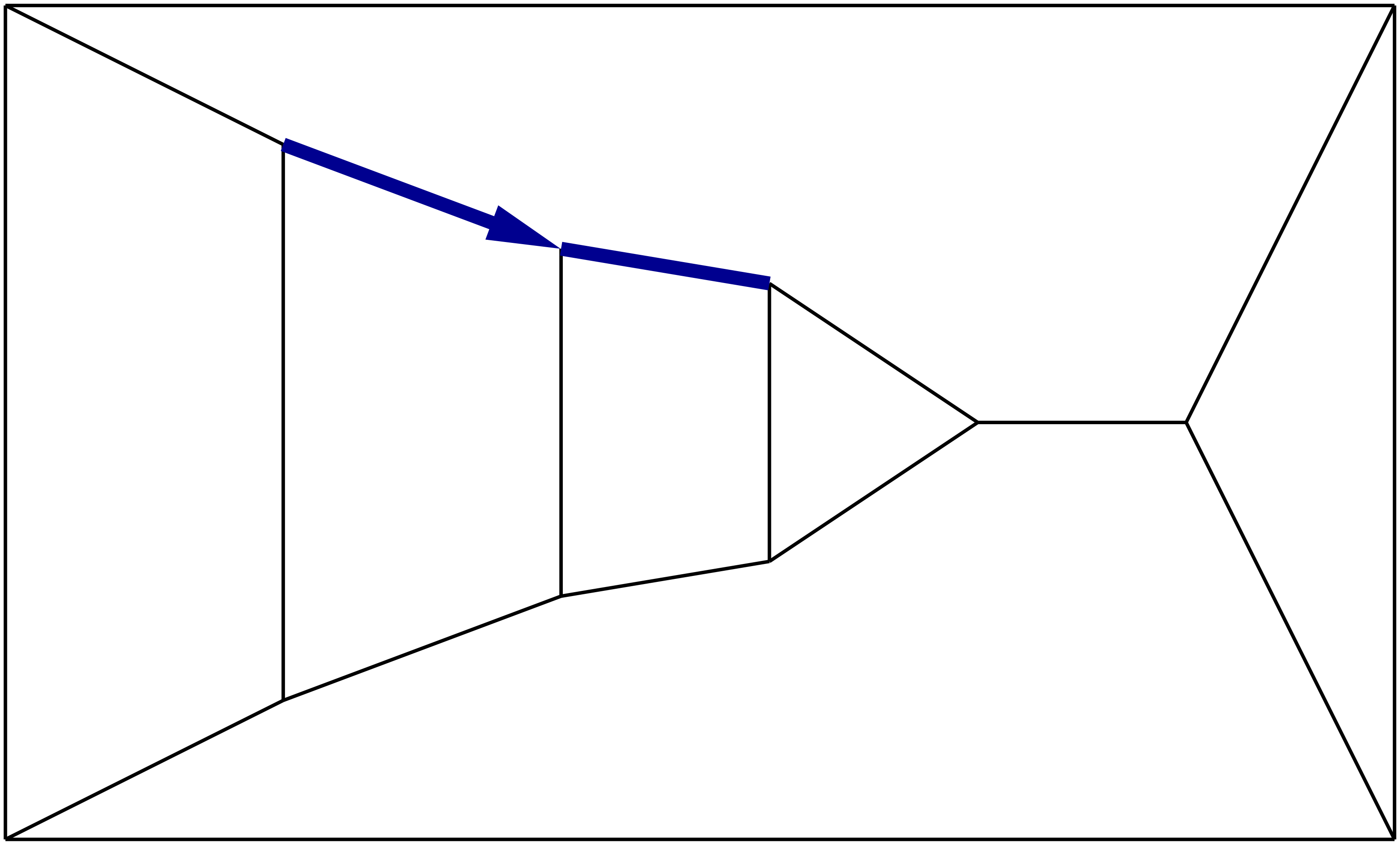
Zigzags

A plane graph G



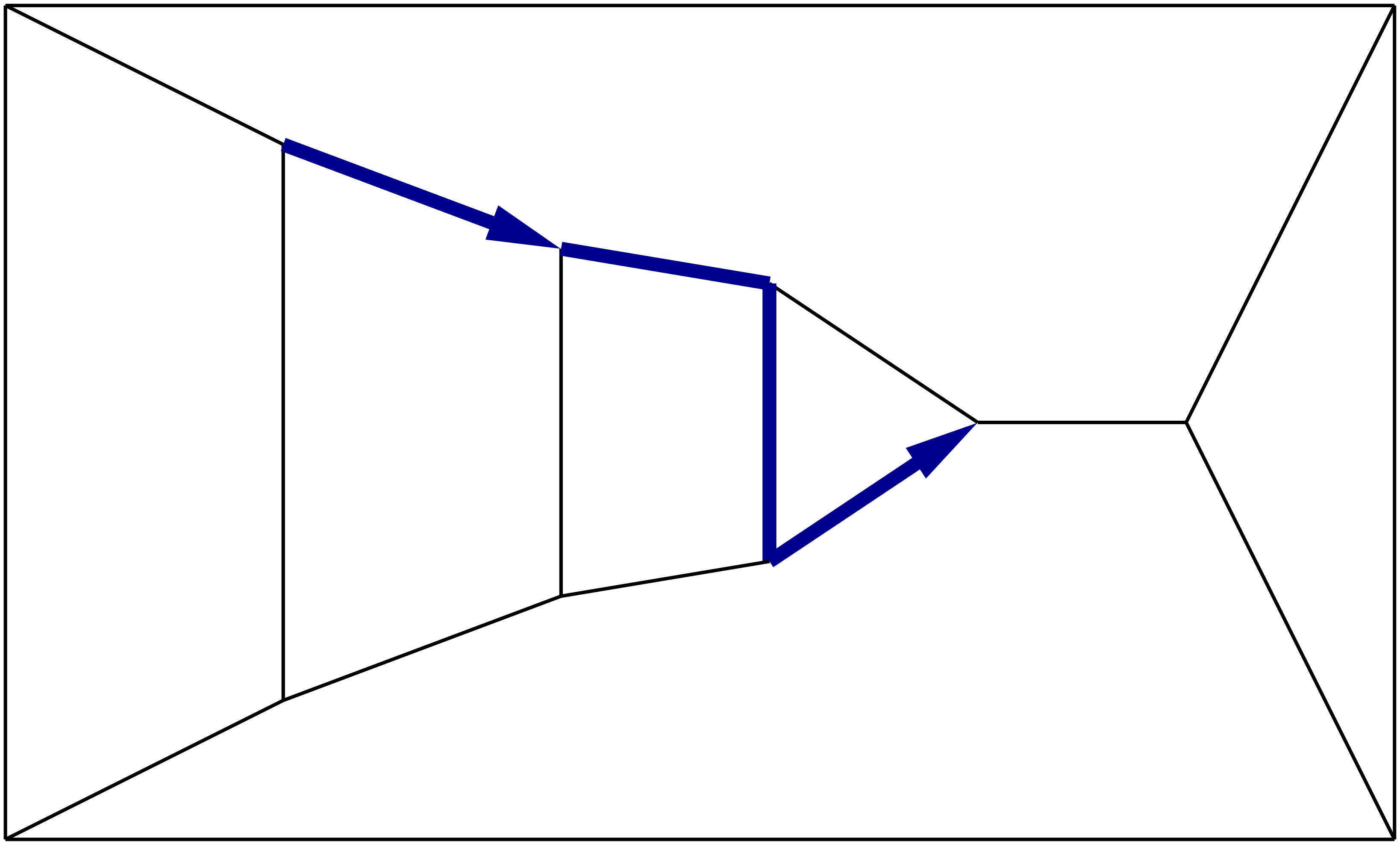
Zigzags

take two edges



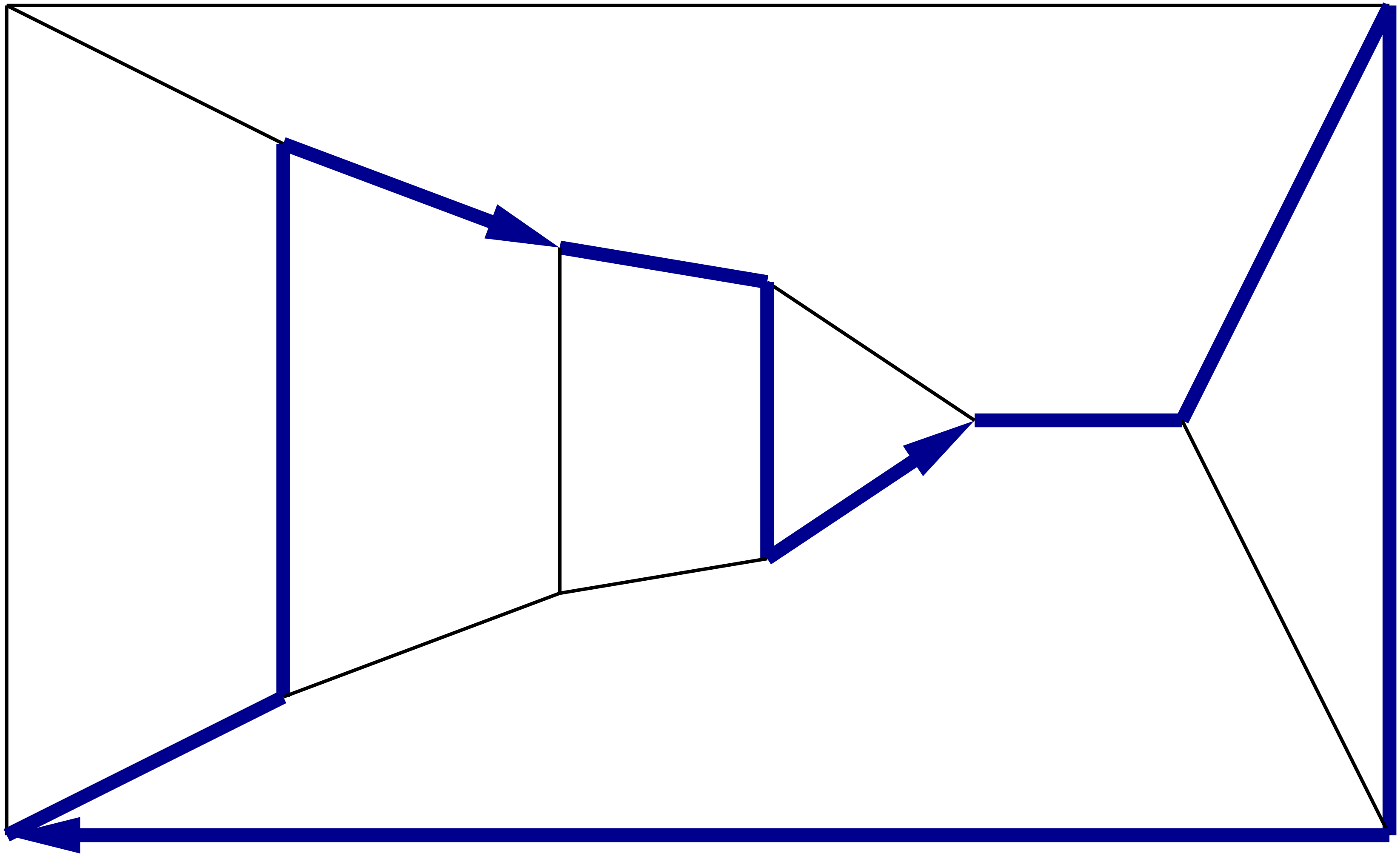
Zigzags

Continue it left−right alternatively ....



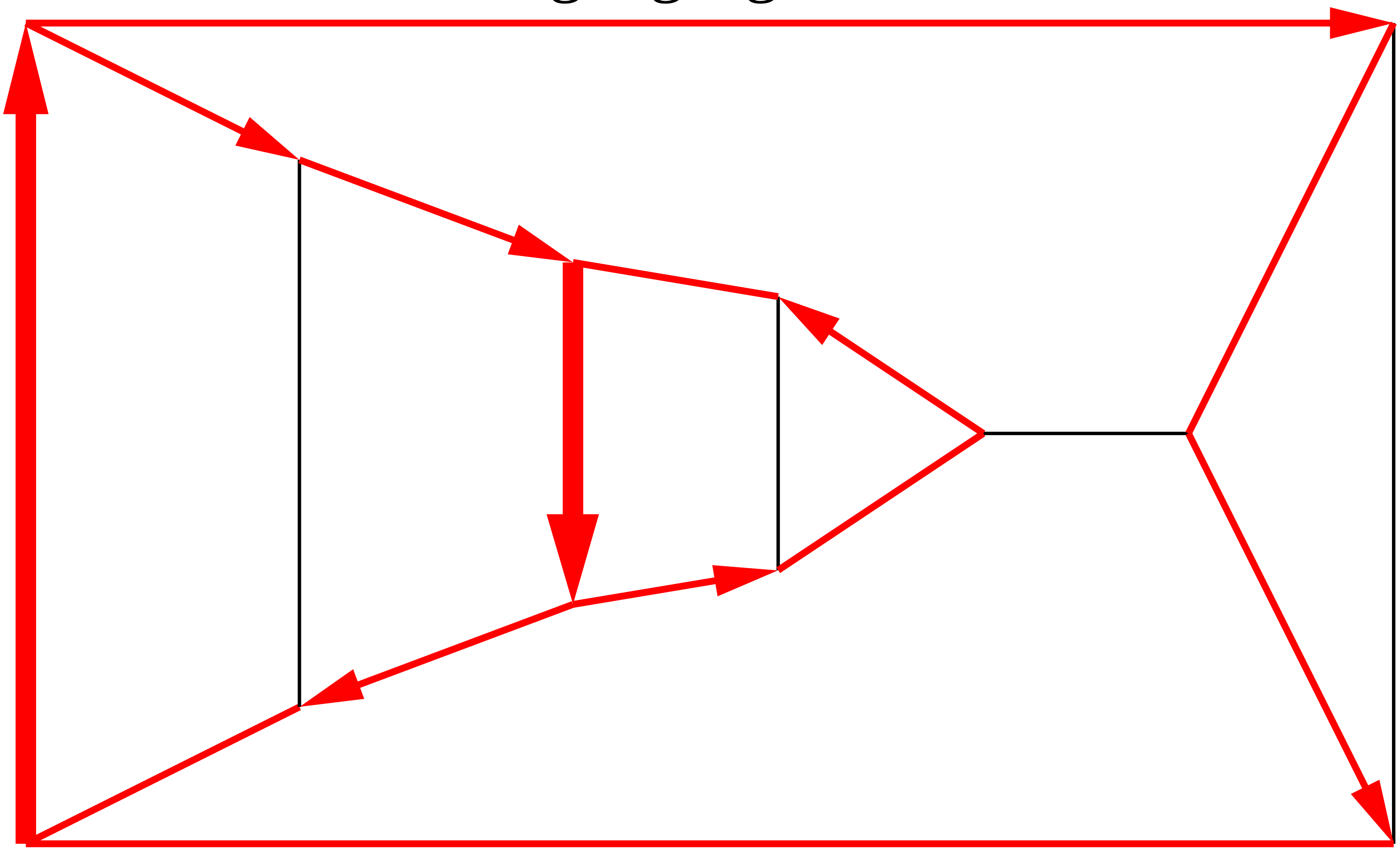
Zigzags

... until we come back.



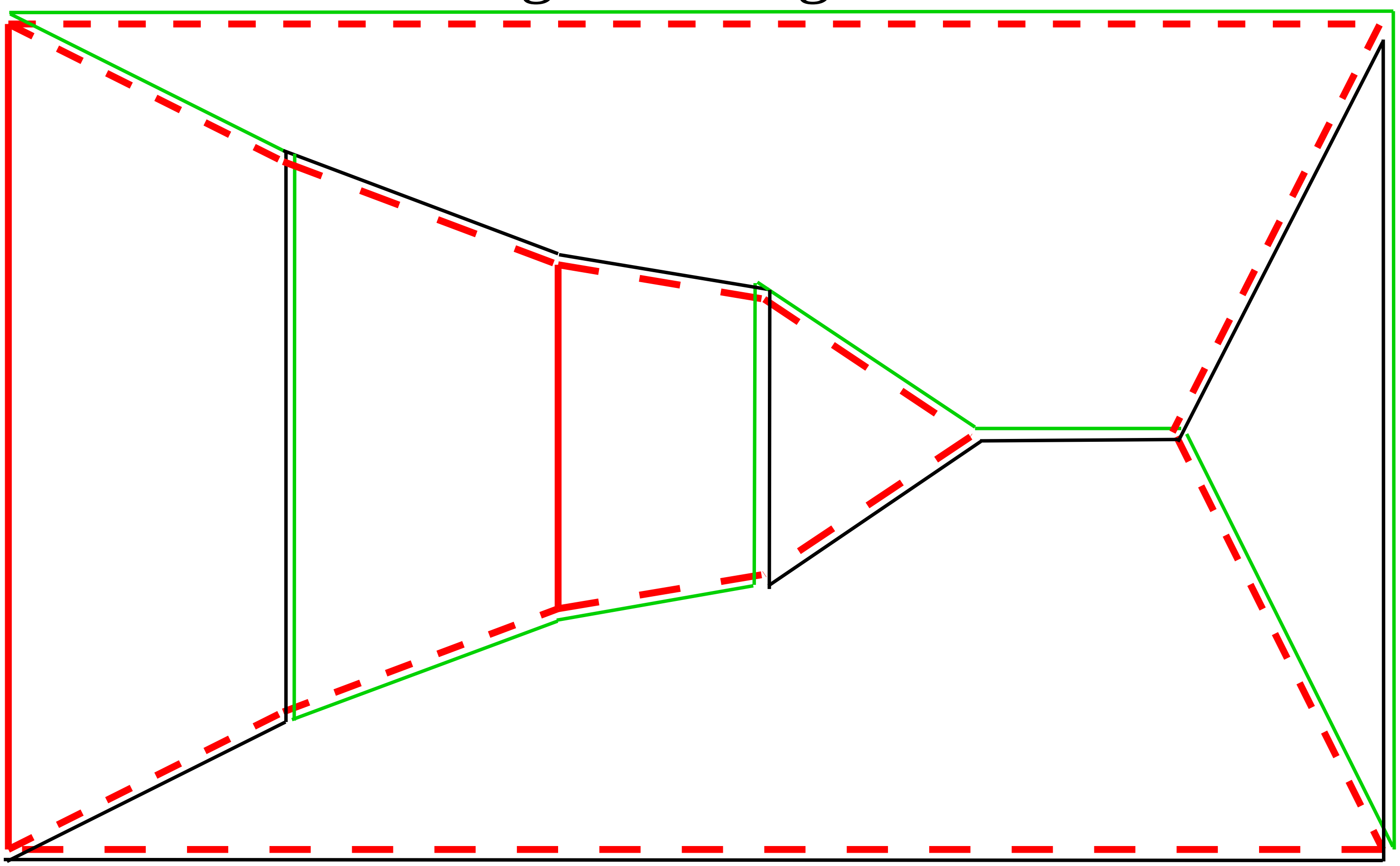
Zigzags

A self−intersecting zigzag



Zigzags

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



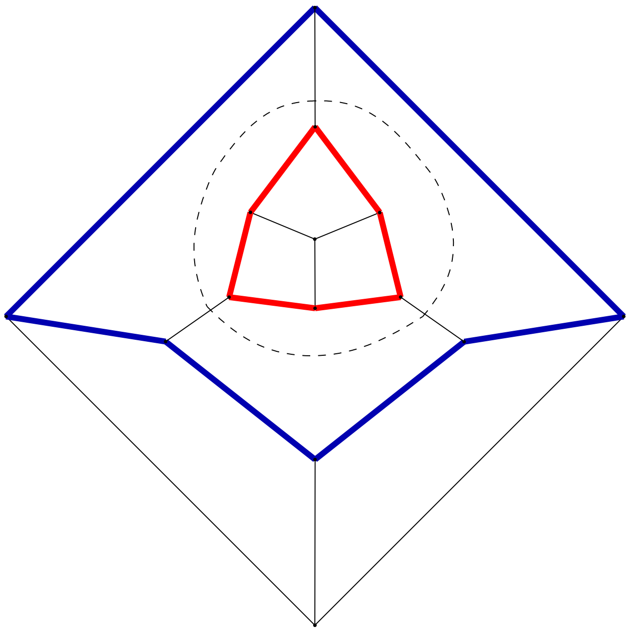
z−vector $\quad z=10^2,\ 16_{2,0}$

z-knotted fullerenes

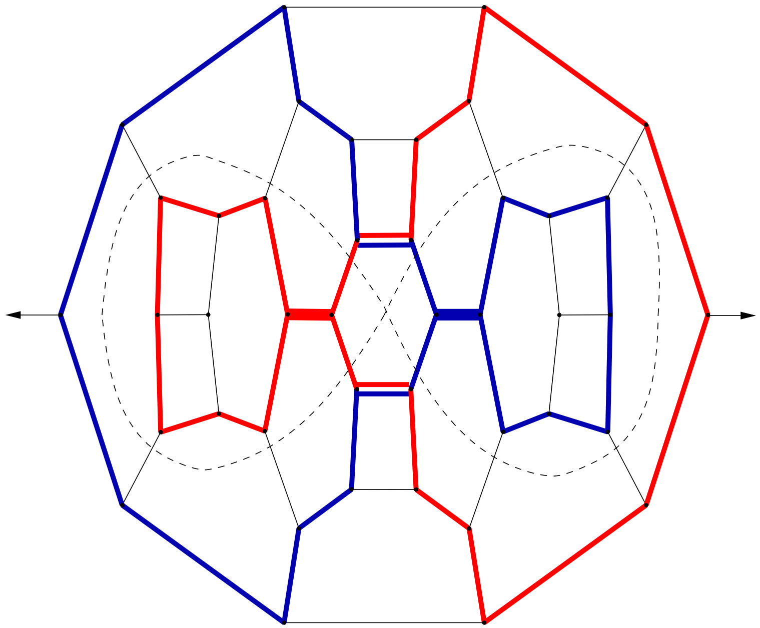
- A zigzag in a 3-valent plane graph G is a circuit such that any 2, but not 3 edges belong to the same face.
- Zigzags can self-intersect in the same or opposite direction.
- Zigzags doubly cover edge-set of G.
- A graph is z-knotted if there is unique zigzag.
- What is proportion of z-knotted fullerenes 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.



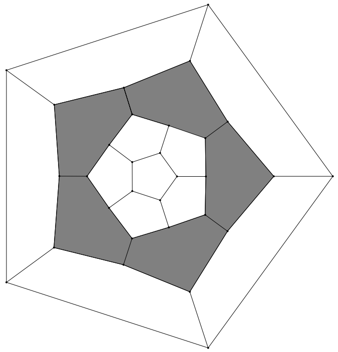
$4_{14}(D_{3h})$



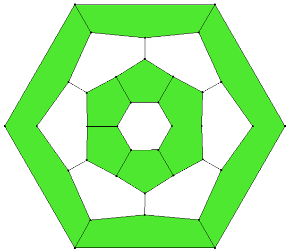
$4_{42}(C_{2v})$

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

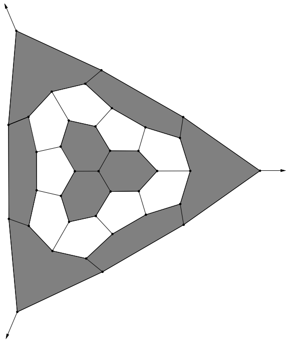
Some special fullerenes



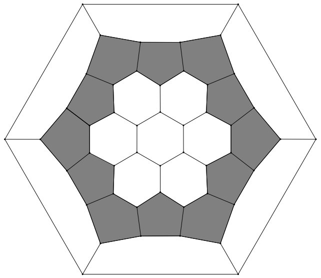
30, D_{5h}
all 6-gons
in railroad
(unique)



36, D_{6h}



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



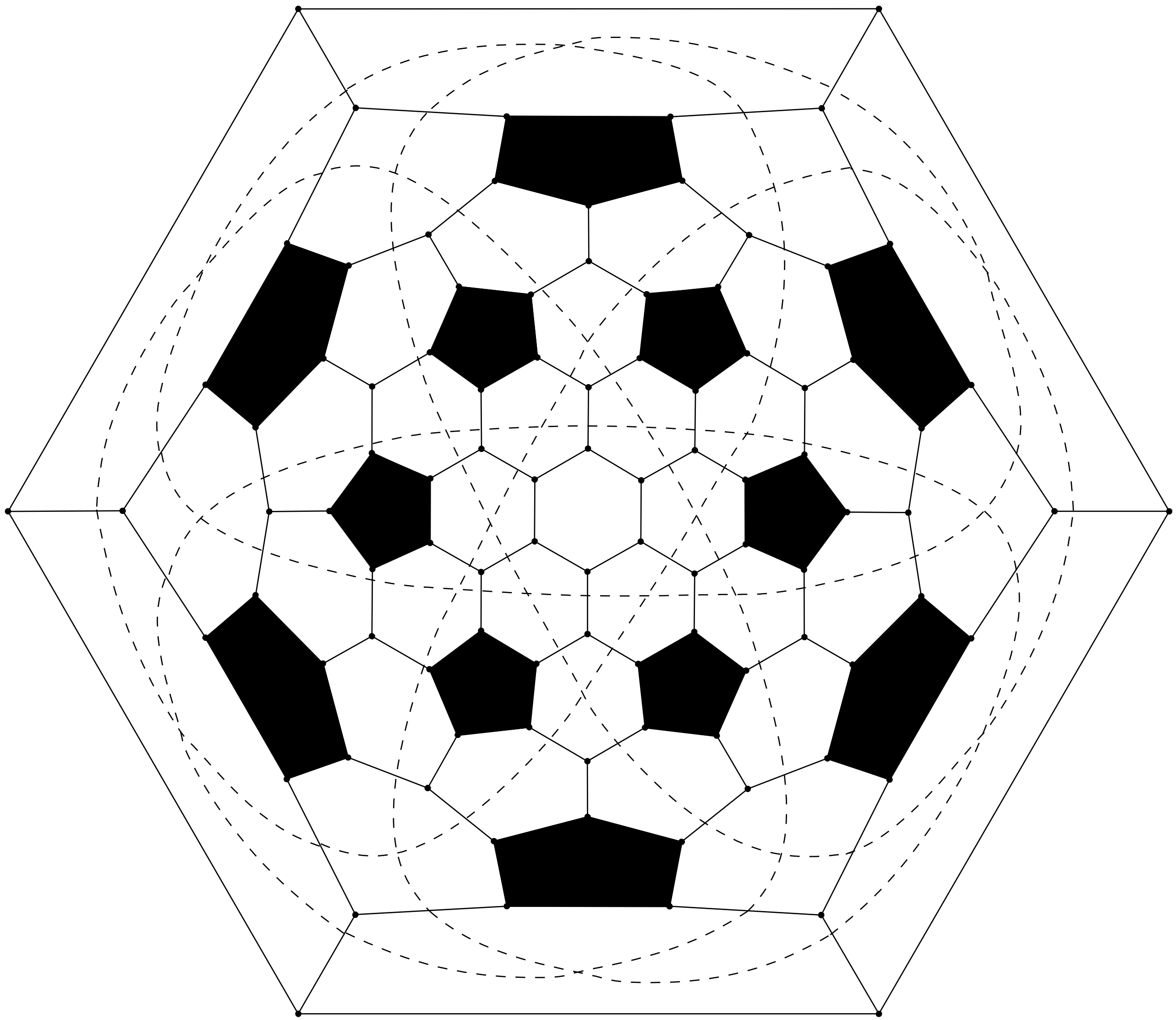
48, D_{6d}
all 5-gons
in alt. ring
(unique)

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.

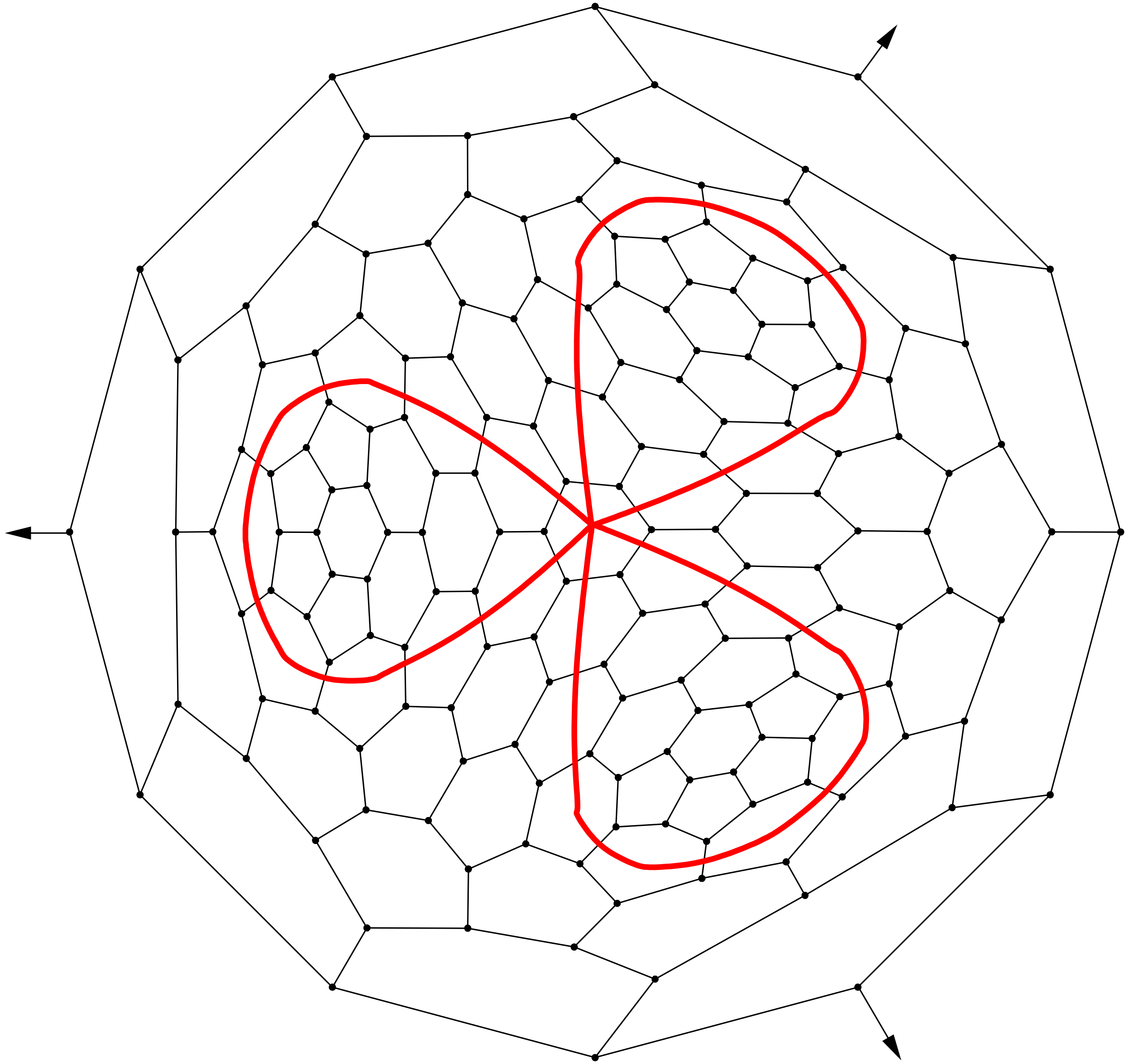
The skeleton of its dual is an isometric subgraph of $\frac{1}{2}H_8$.

First IPR fullerene with self-int. railroad



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

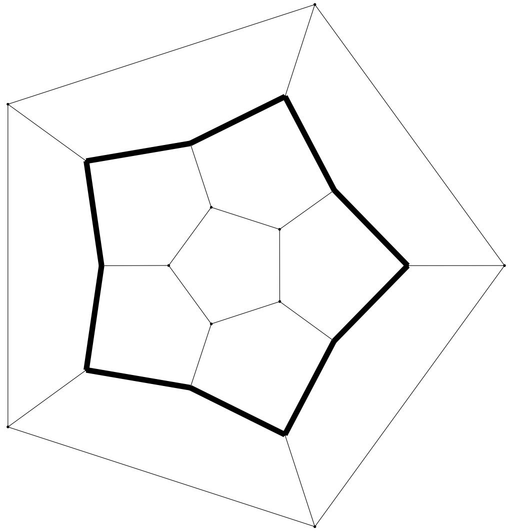
Triply intersecting railroad in $F_{172}(C_{3v})$



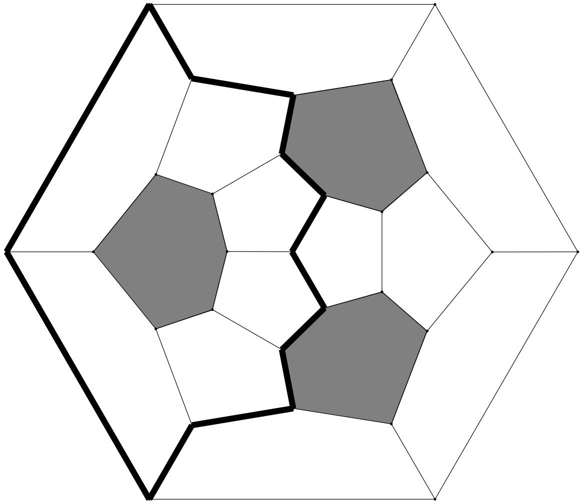
Tight fullerenes

- 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 $n \leq 200$).

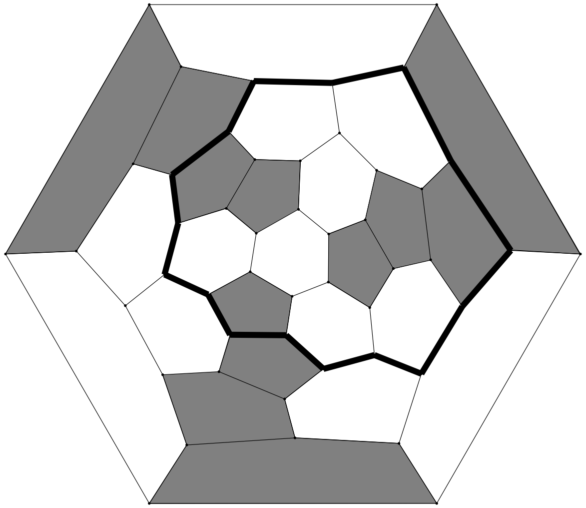
Tight F_n with simple zigzags



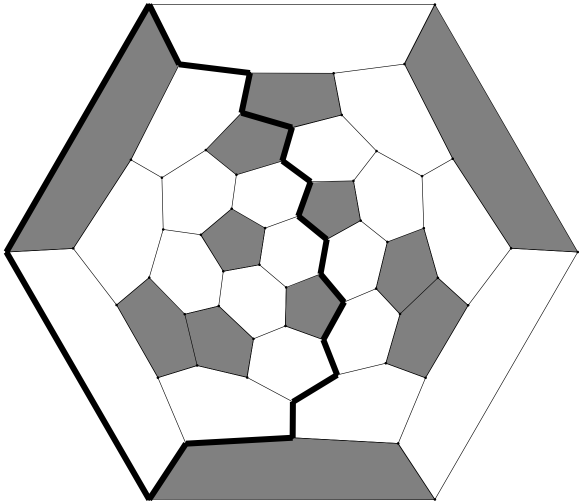
20 I_h, 20^6



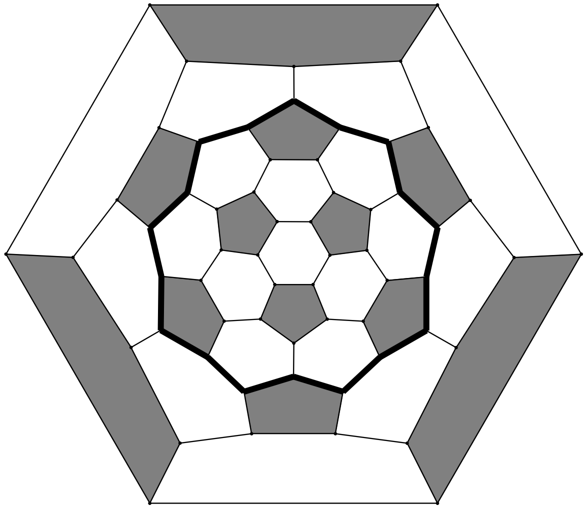
28 T_d, 12^7



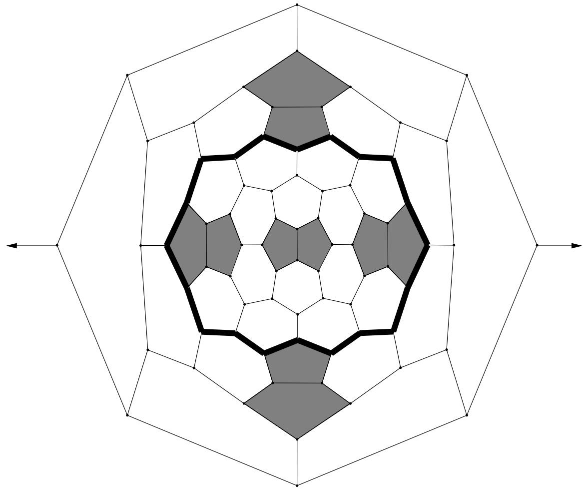
48 D_3, 16^9



60 D_3, 18^{10}

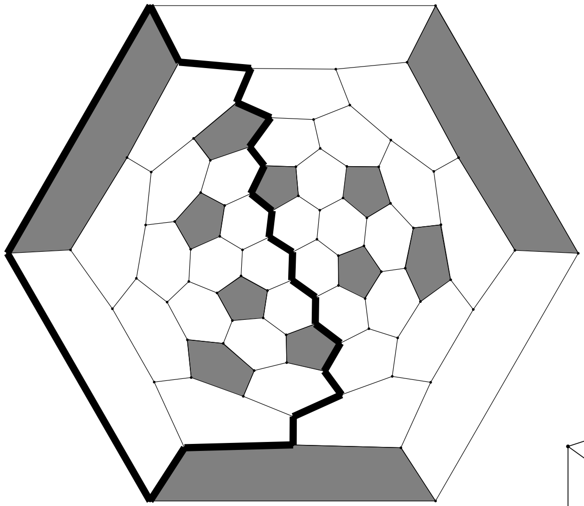


60 I_h, 18^{10}

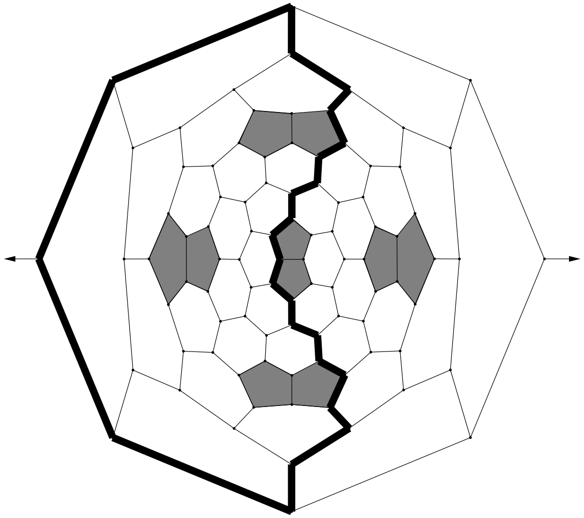


76 D_{2d}, $22^4, 20^7$

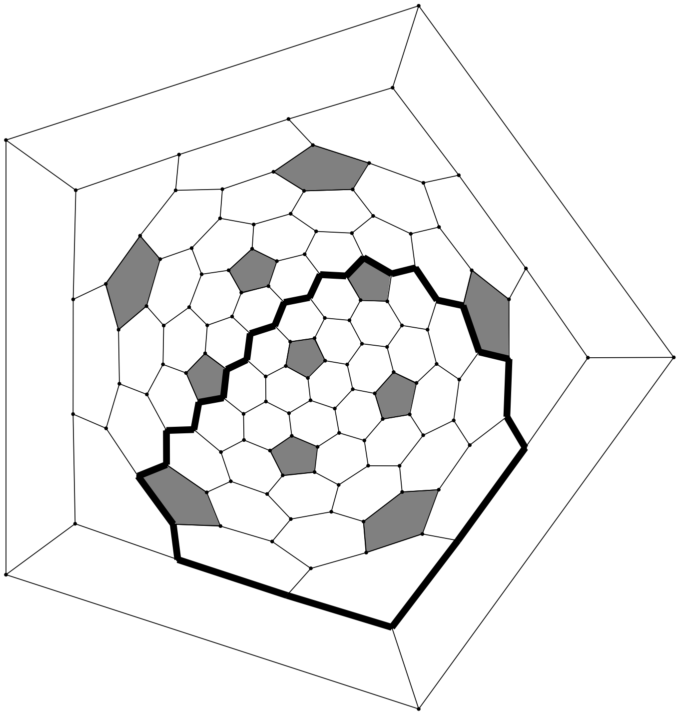
Tight F_n with simple zigzags



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



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



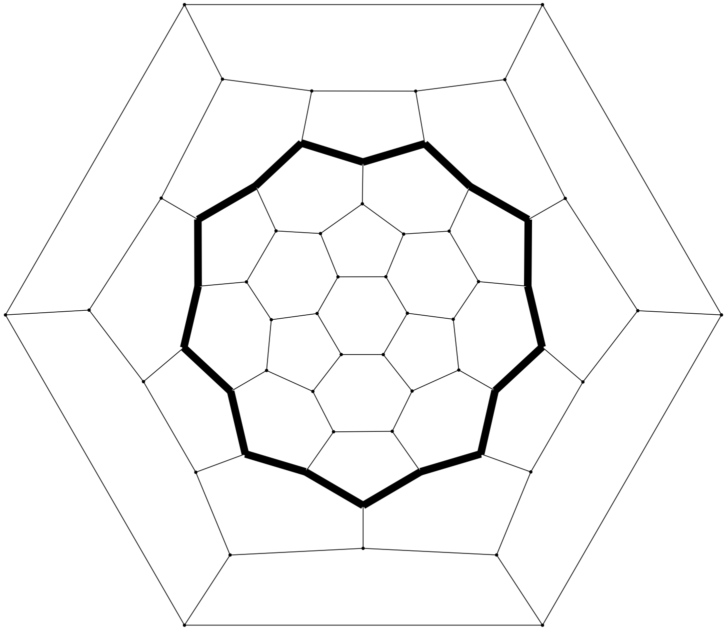
$140 \quad I,\ 28^{15}$

Tight F_n with only simple zigzags

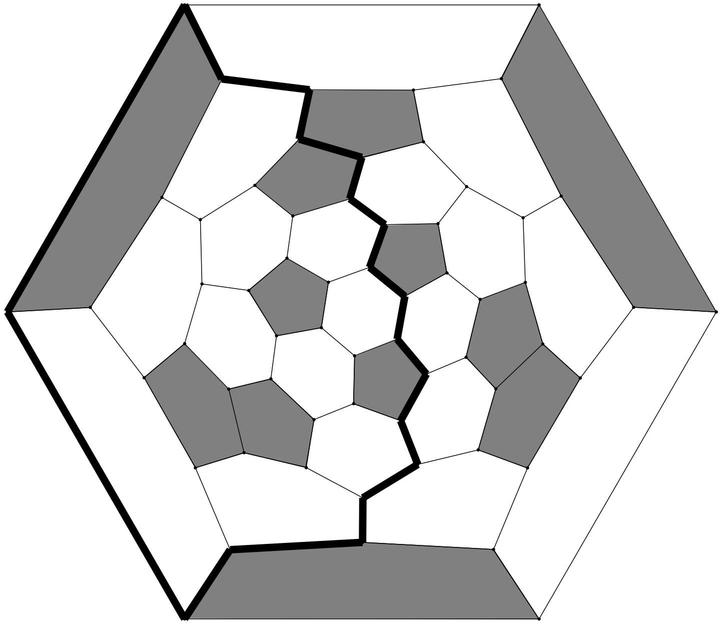
n	group	z-vector	orbit lengths	int. vector
20	I_h	10^6	6	2^5
28	T_d	12^7	3,4	2^6
48	D_3	16^9	3,3,3	2^8
60, IPR	I_h	18^{10}	10	2^9
60	D_3	18^{10}	1,3,6	2^9
76	D_{2d}	$22^4, 20^7$	1,2,4,4	$4, 2^9$ and 2^{10}
88, IPR	T	22^{12}	12	2^{11}
92	T_h	$22^6, 24^6$	6,6	2^{11} and $2^{10}, 4$
140, IPR	I	28^{15}	15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

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 perfect matching of the fullerene skeleton, i.e., edges of self-intersection of type I cover exactly once its vertex-set. All, except $F_{100}(C_3)$ above, have symmetry C_1, C_2.

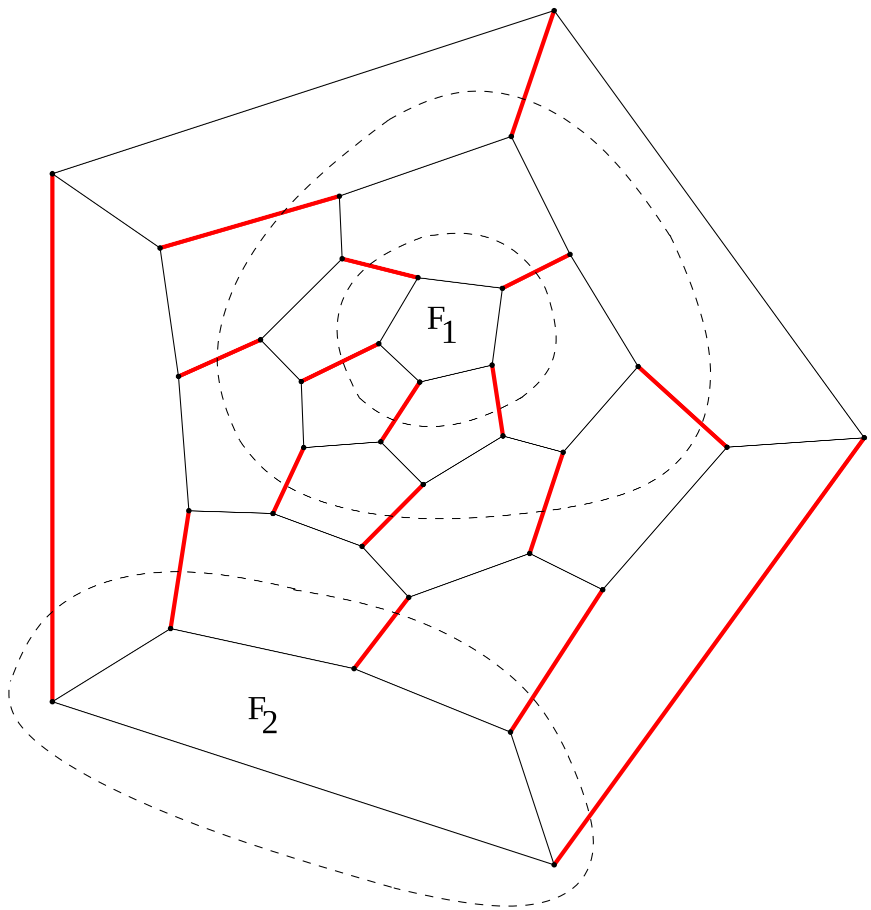
Perfect matching on fullerenes

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.



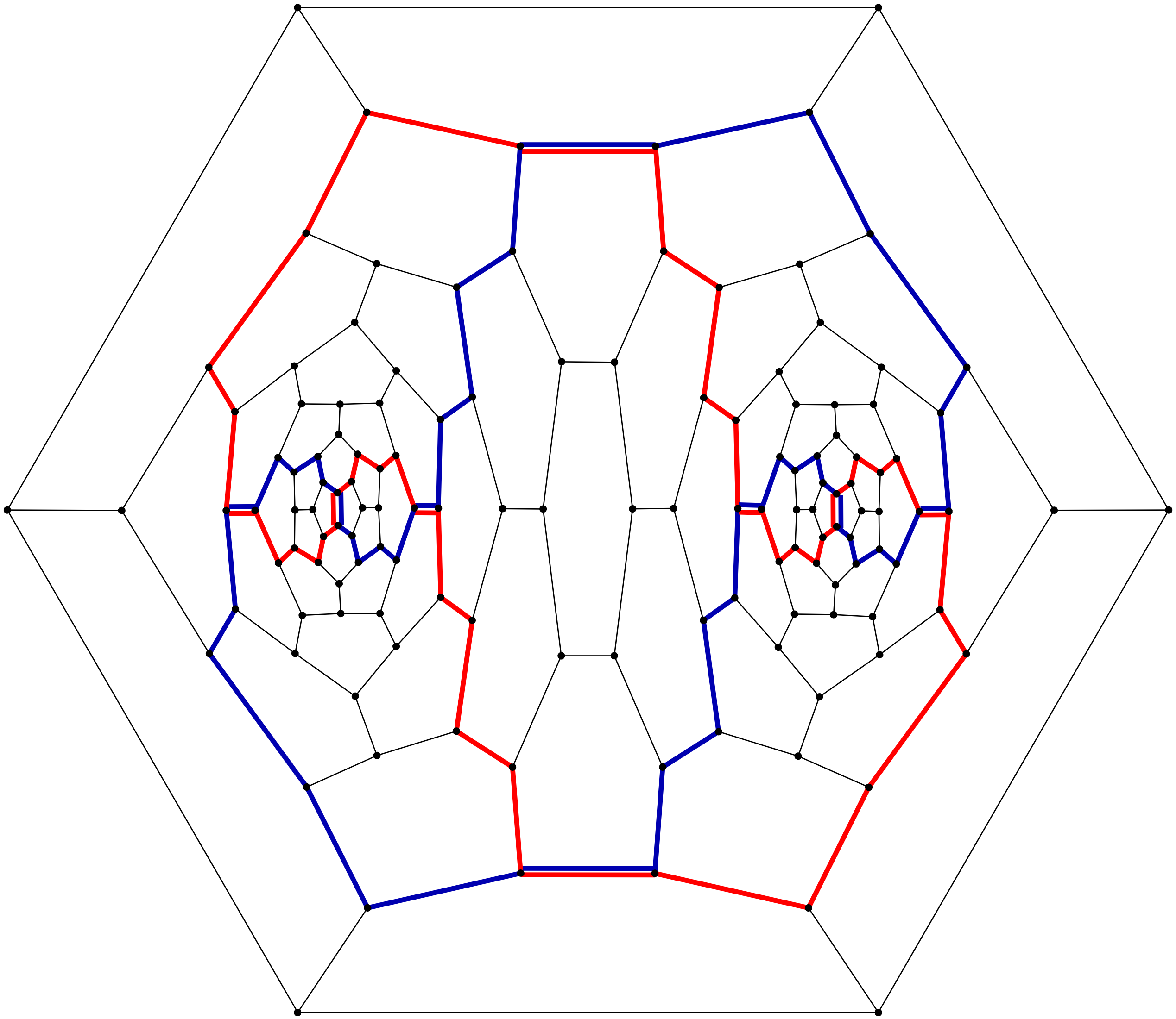
z-knotted fullerenes: statistics for $n \le 74$

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 $\le n$-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



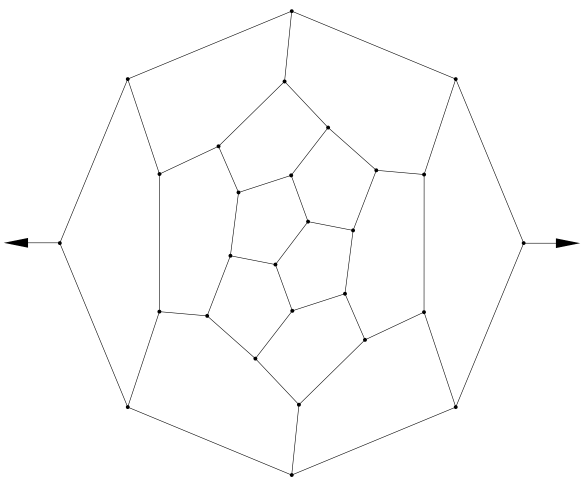
For any n, there is a fullerene F_{36n-8} with two simple zigzags having intersection $2n$; above $n = 4$.

Face-regular fullerenes

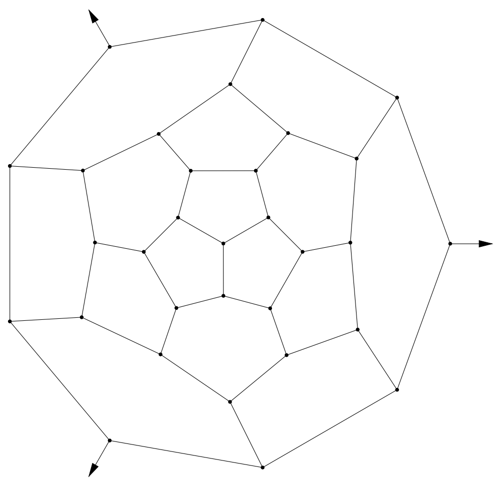
Face-regular fullerenes

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



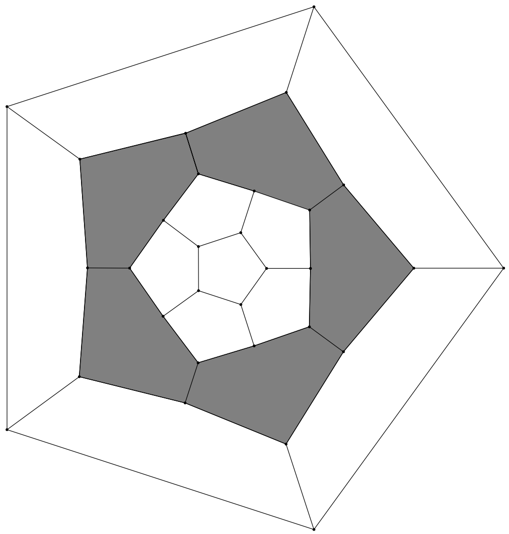
28, D_2



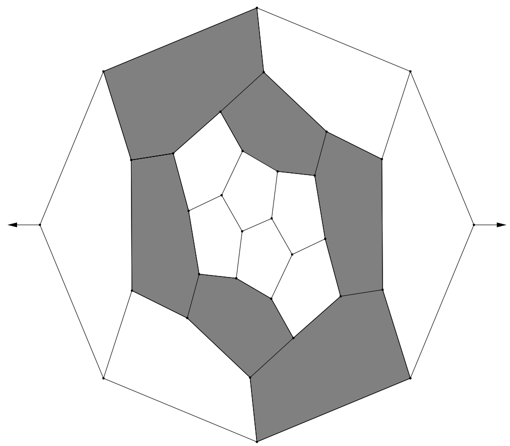
32, D_3

All fullerenes, which are $6R_1$

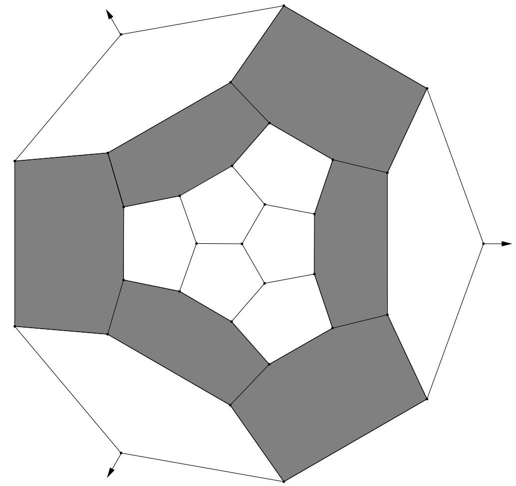
Fullerenes $6R_2$ with hexagons in 1 ring



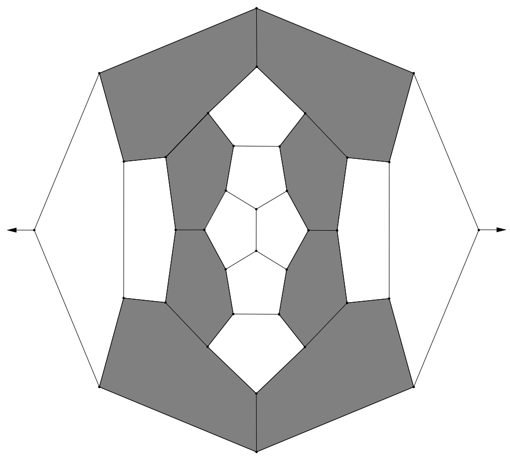
D_{5h}; 30



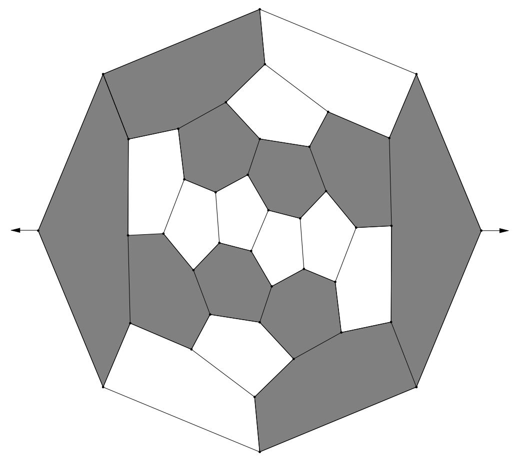
D_2; 32



D_{3d}; 32

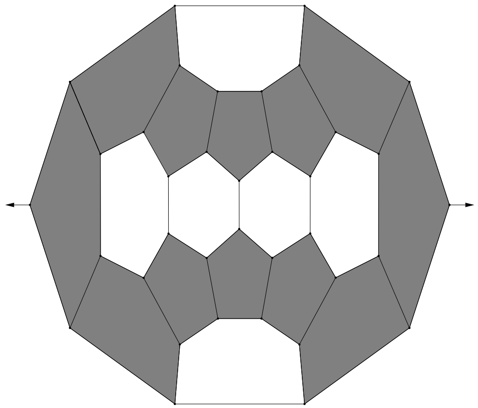


D_{2d}; 36

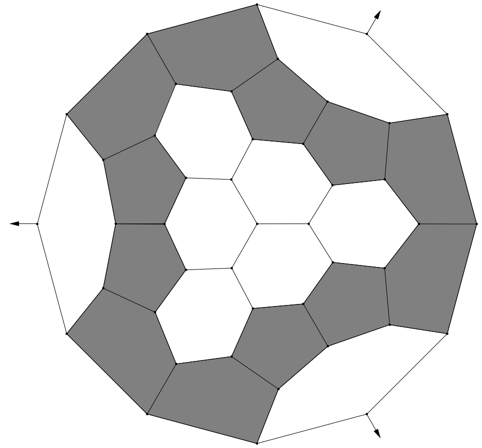


D_2; 40

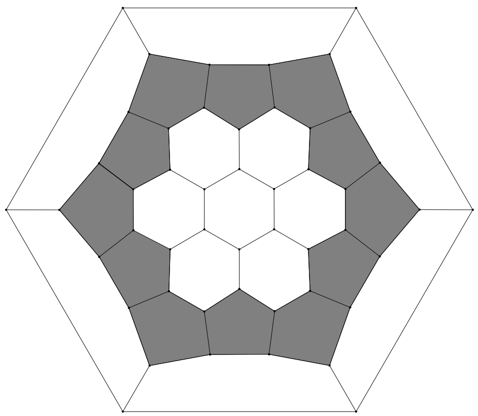
Fullerenes $5R_2$ with pentagons in 1 ring



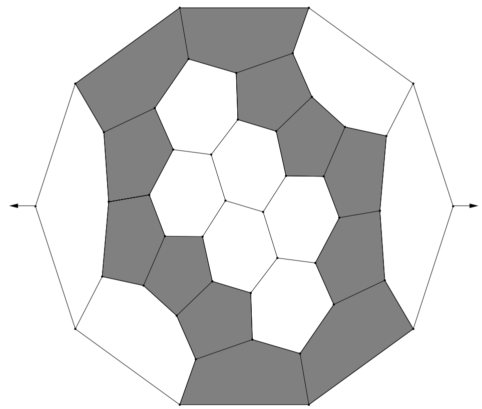
D_{2d}; 36



D_{3d}; 44

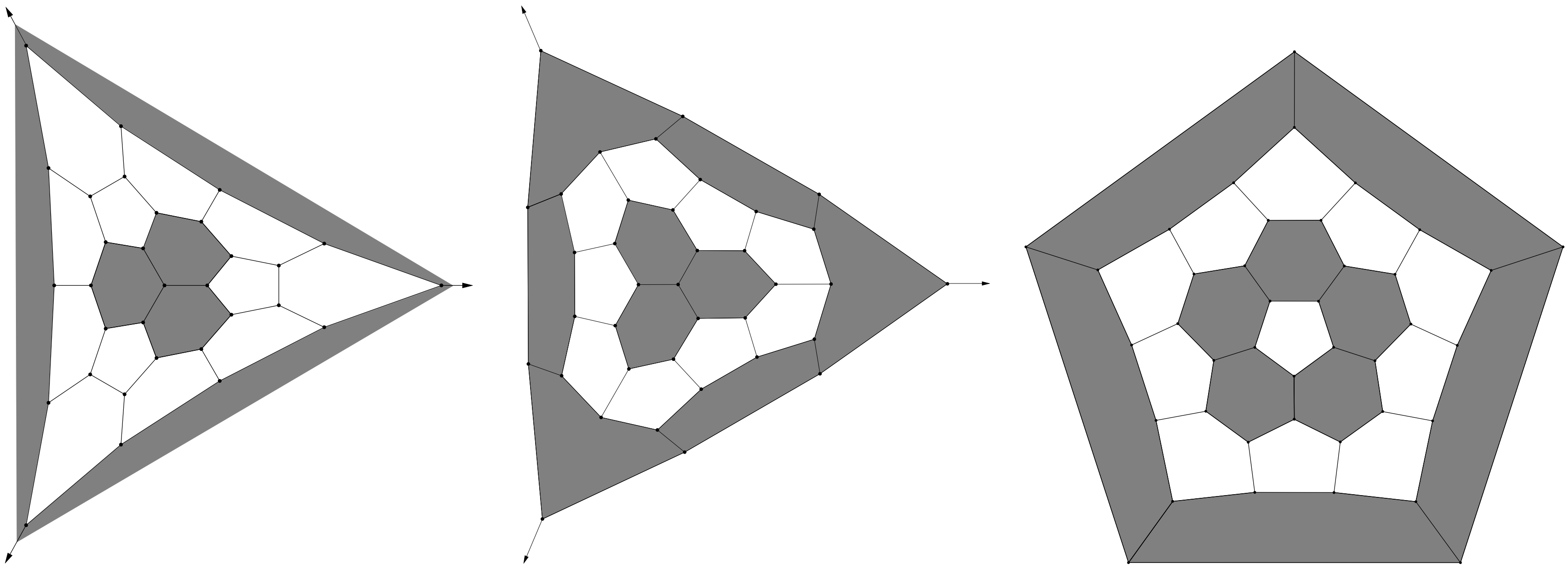


D_{6d}; 48



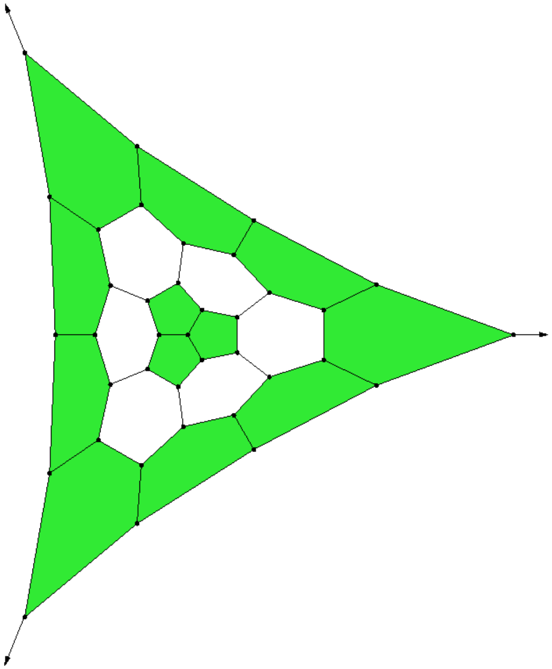
D_2; 44

Fullerenes $6R_2$ with hexagons in > 1 ring

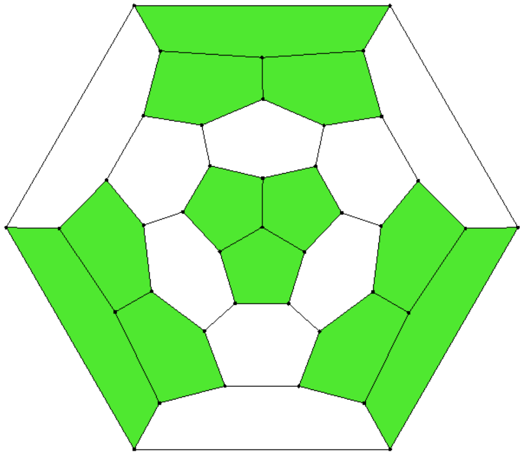


D_{3h}; 32 C_{3v}; 38 D_{5h}; 40

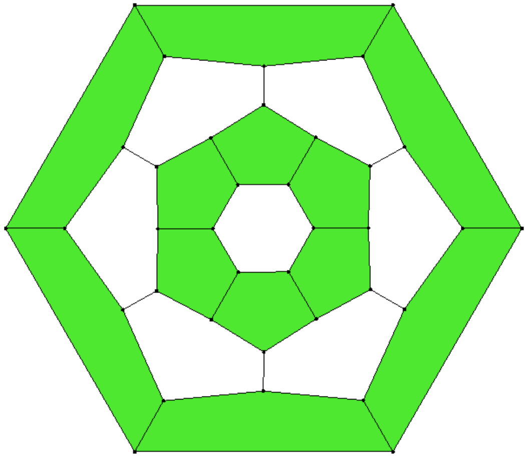
Fullerenes $5R_2$ with pentagons in > 1 ring



C_{3v}; 38

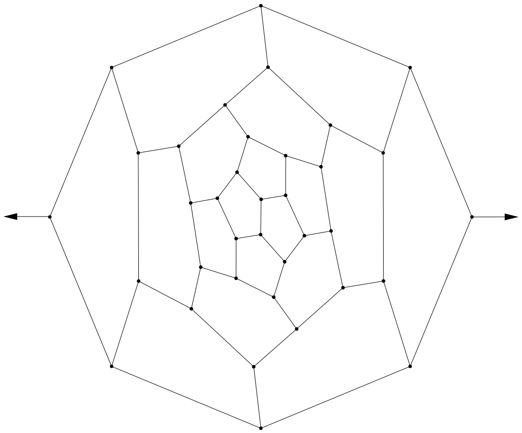


infinite family:
4 triples in F_{4t},
$t \geq 10$, from
collapsed 3_{4t+8}

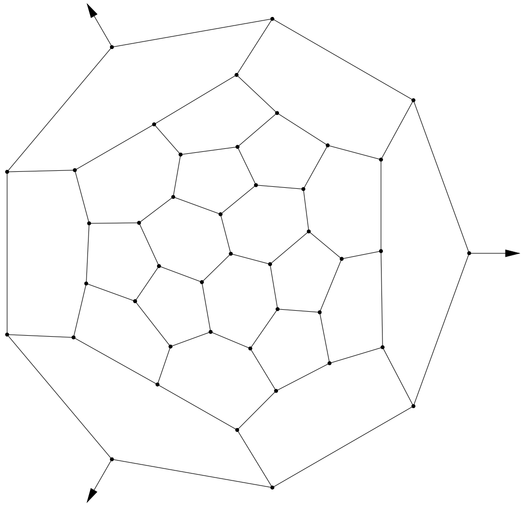


infinite family:
$F_{24+12t}(D_{6d})$,
$t \geq 1$,
D_{6h} if t odd
elongations of
hexagonal barrel

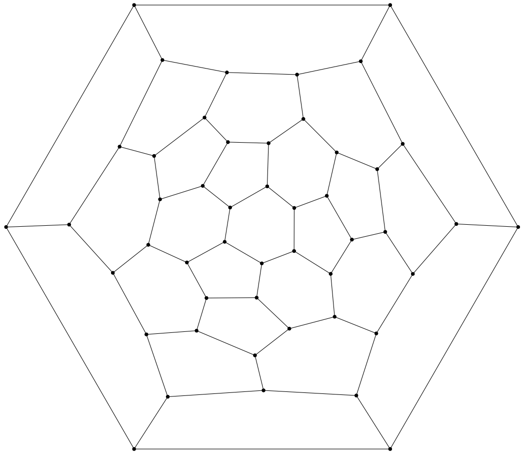
All fullerenes, which are $6R_3$



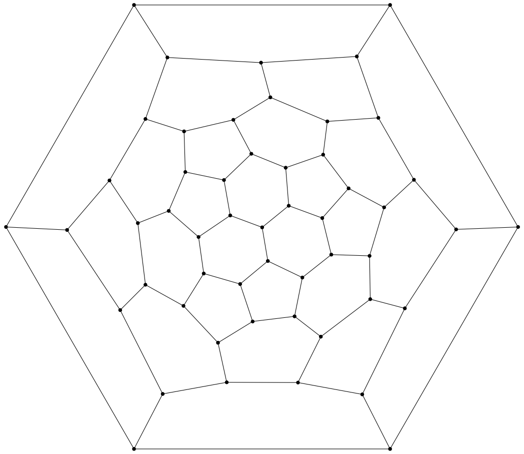
36, D_2



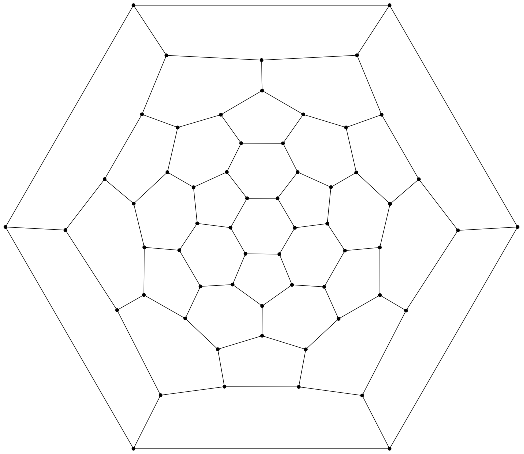
44, T (also $5R_2$)



48, D_3

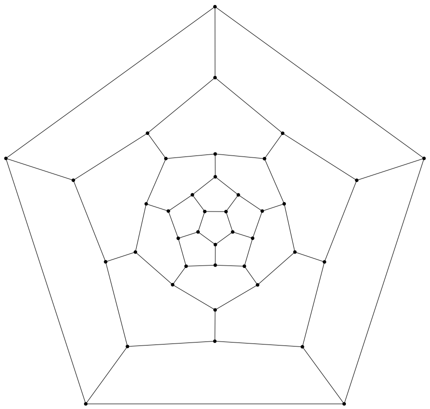


52, T (also $5R_1$)

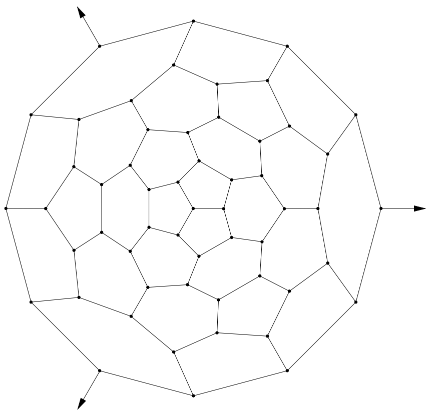


60, I_h (also $5R_0$)

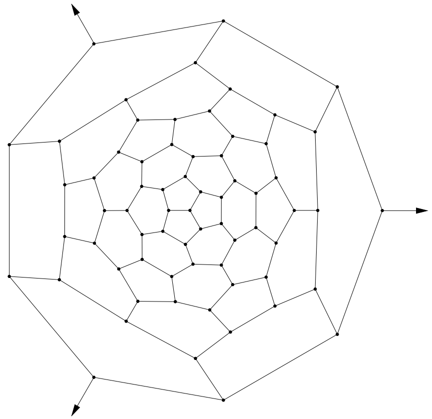
All fullerenes, which are $6R_4$



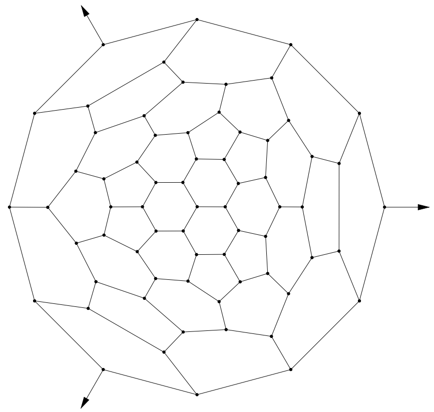
40, D_{5d}



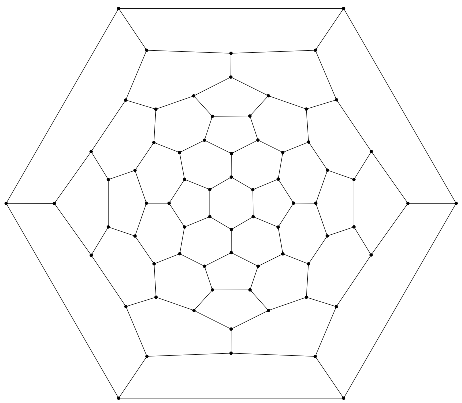
56, T_d
(also $5R_2$)



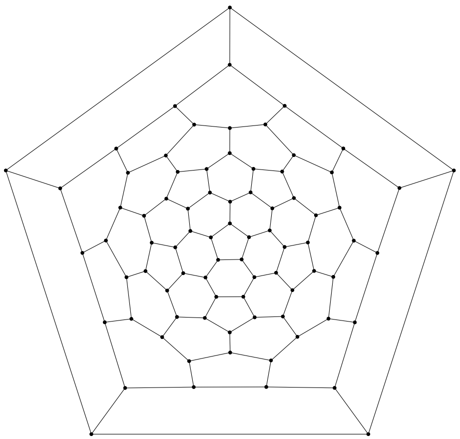
68, D_{3d}



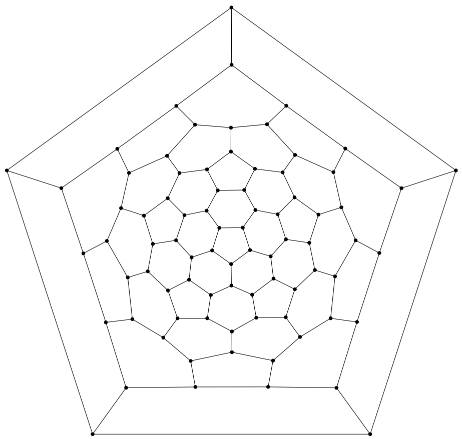
68, T_d
(also $5R_1$)



72, D_{2d}



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



80, I_h (also $5R_0$)

Embedding of fullerenes

Fullerenes as isom. subgraphs of half-cubes

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

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

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

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

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

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.

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