Michel Marie Deza

Research Professor, School of Information Science, JAIST

Discrete Geometry, Combinatorics and Applications

Some recent research topics:

I. Fullerenes: IQ and virus structure

II. Space fullerenes and metallic alloys

III. Railroads and zigzags in fullerenes

IV. Ambiguous boundaries of polycycles

Recent books

- **Geometry of Cuts and Metrics** (with M.Laurent), Springer, 1997.
- **Scale-Isometric Polytopal Graphs in Hypercubes and Cubic Lattices** (with V.Grishukhin and M.Shtogrin), Imperial College Press and World Scientific, 2004.
- **Dictionary of Distances** (with E.Deza), Elsevier, 2006.
- **Geometry of Chemical Graphs** (with M.Dutour), Cambridge University Press, 2008.
- **Encyclopedia of Distances** (with E.Deza), Springer, 2009.

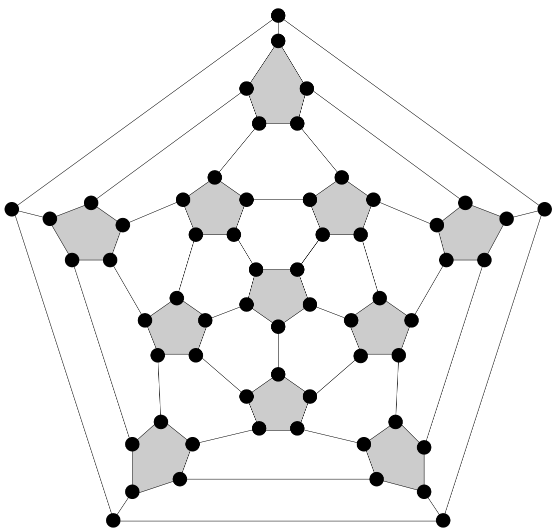
I. Fullerenes: IQ and virus structure

- A fullerene F_n is polyhedron with n 3-valent vertices and only pentagonal and hexagonal faces. Clearly, $p_5 = 12$ and $p_6 = \frac{n}{2} - 10$. F_n exist for all even $n \geq 20$ but $n = 22$.
- Fullerenes or their duals are ubiquitous in Organic Chemistry and Biology (virus capsids, clathrine coated vesicles). Also, energy minimizers in Thomson problem (n unit charged particles on sphere) and Skyrme problem (baryonic number n of nucleons), while maximizers, in Tammes problem, of minimum distance between n points on sphere.
- **Conjecture**: among 3-valent polyhedra with given number $m \geq 12$ of faces, the "best" approximation of sphere are are fullerenes; for instance, their Isoperimetric Quotient $IQ = 36\pi\frac{V^2}{S^3}$ is closest to the maximum (1 for sphere).

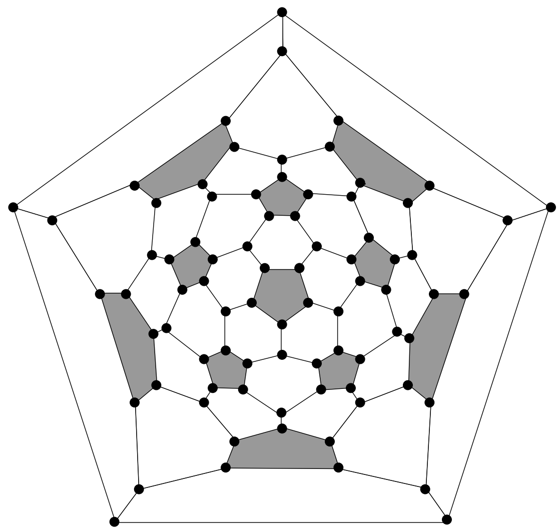
Icosahedral fullerenes

Call icosahedral a fullerene of maximal symmetry I_h or I.

- n=$20T$ for T=a^2+ab+b^2 (triangulation number), $0 \leq b \leq a$.
- I for $0 < b < a$ and I_h for $a = b \neq 0$ or $b = 0$.
- Dodecahedron $F_{20}(I_h)$: smallest ((a,b)=$(1,0)$, T=1).



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



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

$C_n(G)$: a fullerene F_n of symmetry G with isolated 5-gons.

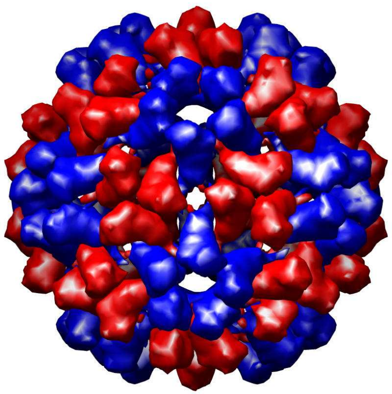
Icosadeltahedra

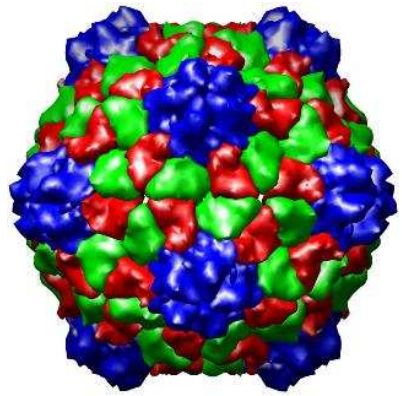
Icosadeltahedron C^*_{20T}: dual of an icosahedral fullerene.

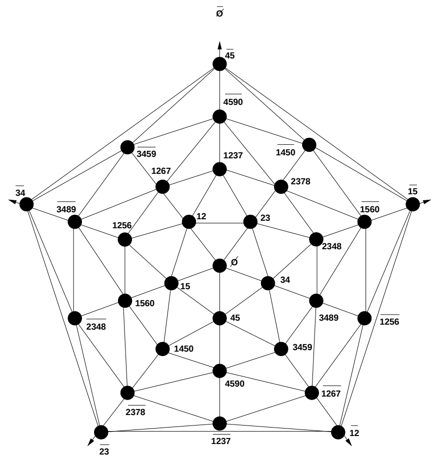
- Geodesic domes: Fuller, patent 1954
- Carbon $C_{60}(I_h)$: Kroto-Curl-Smalley, Nobel prize 1996
- Capsids of viruses: Caspar and Klug, Nobel prize 1982: virion capsomers are $10T+2$ vertices of C^*_{20T}, since capsomers organized quasi-equivalently: in minimal number T of locations with non-equivalent bonding. All virions, except some complex ones, are helical or ($\approx \frac{1}{2}$ of all and almost all human) icosahedral.

Cowpea mosaic virus CPCM: $T = 3$

Plant *comovirus* infecting cowpea leafs; high yields 1-2 g/kg



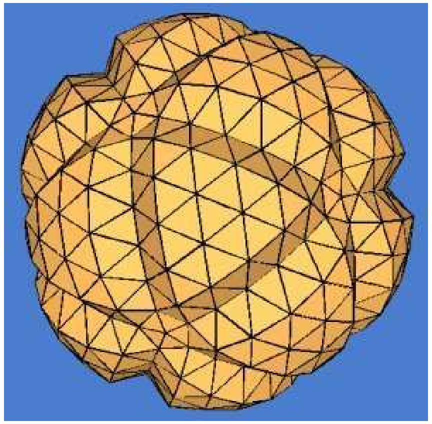




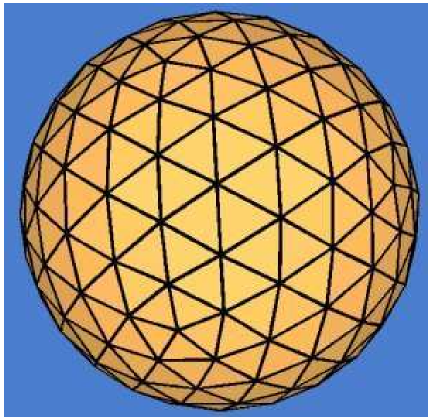
$C^*_{60}(I_h)$, $(a, b) = (1, 1), T = 3$

pentakis-dodecahedron

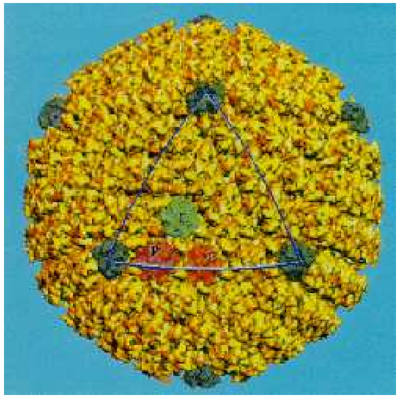
Icosadeltahedra with $T = a^2$



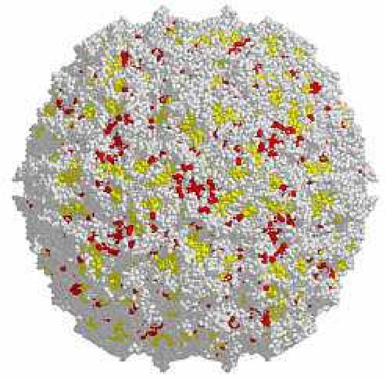
$a = 7, b = 0$



$a = 5, b = 0$



$(4, 0)$; HSV1 herpes



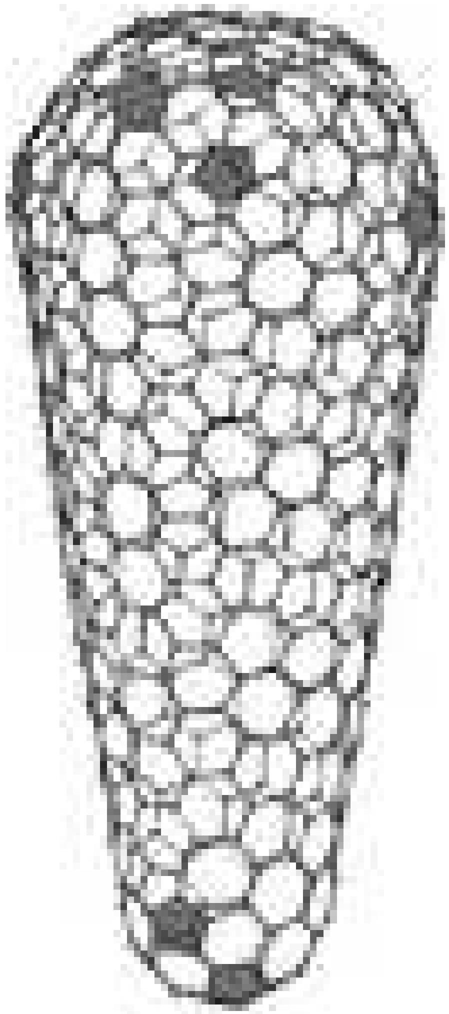
$(5, 0)$; PRD1 polyo

Largest viruses observed (directly by EM) have $T = 25$.

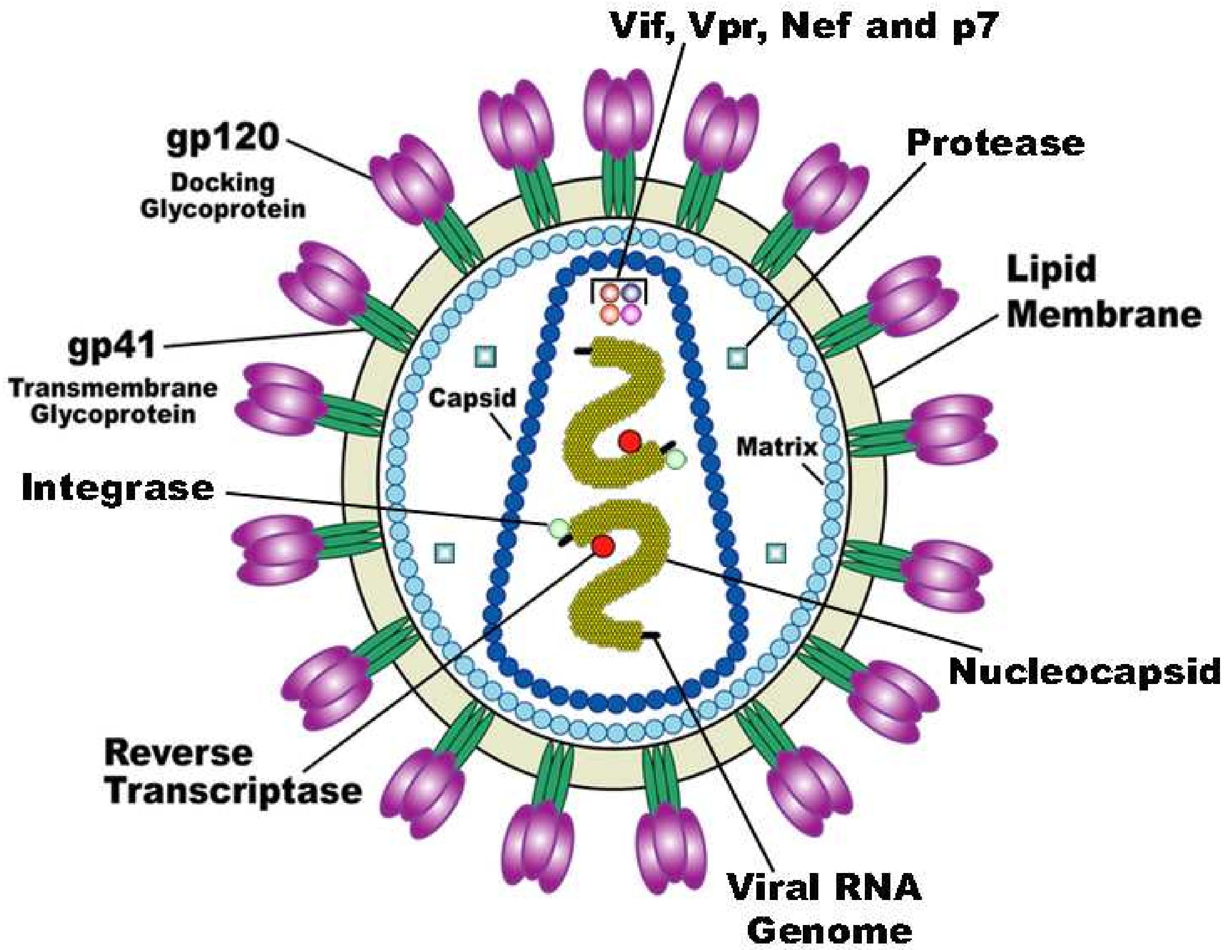
Capsids of icosahedral viruses

(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)
$(7,10)$	219	$C^*_{4380}(I)_{dextro?}$	*Algal virus PpV01*

HIV conic fullerene; which $F_n(G)$ it is?



Capsid core
7+5 pentagons

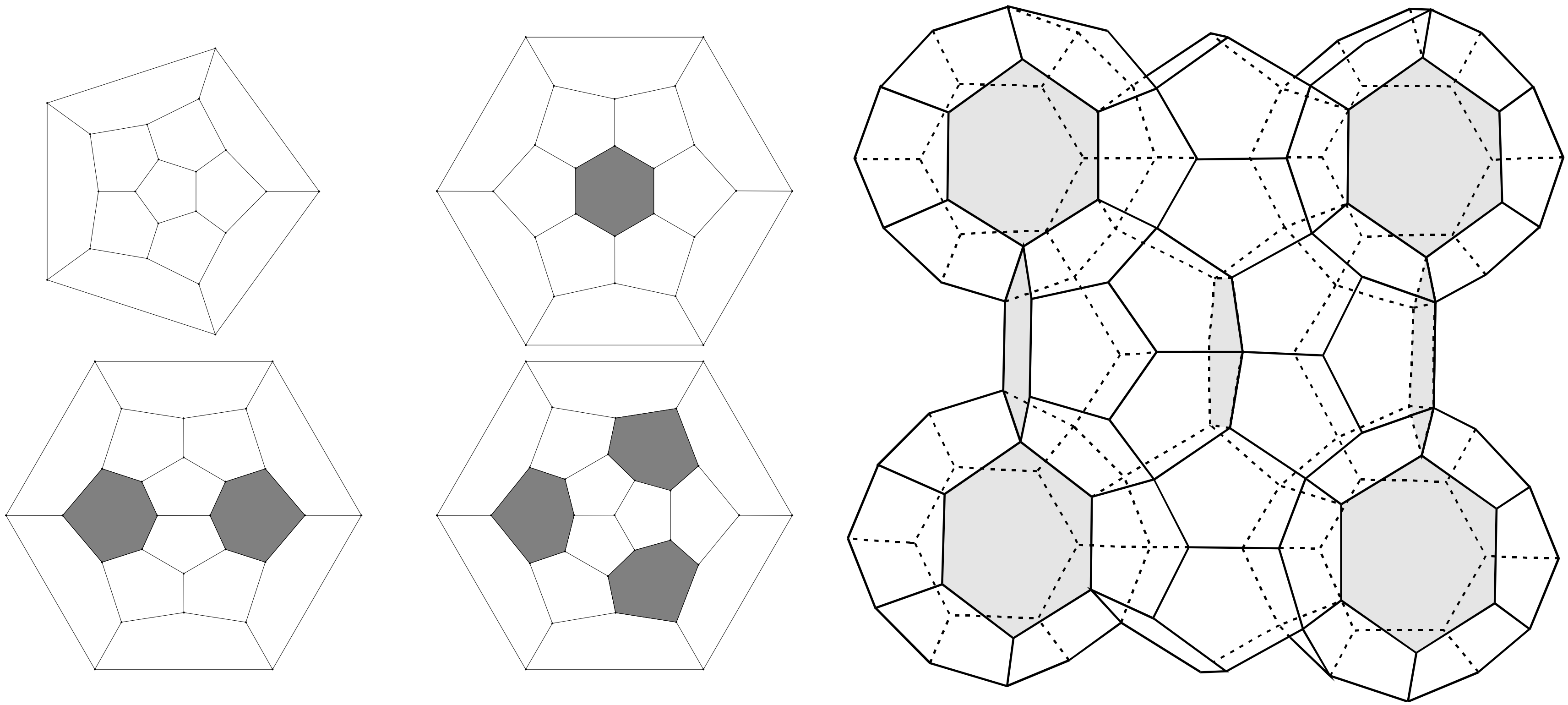


Icosahedral shape (spikes): $T \simeq 71$?

II. Space fullerenes and metallic alloys

Frank-Kasper polyhedra are all four fullerenes with isolated hexagons: $F_{20}(I_h)$, $F_{24}(D_{6d})$, $F_{26}(D_{3h})$, $F_{28}(T_d)$.

FK space fullerene: a 4-valent 3-periodic comb. $\mathbb{E}^3$-tiling by them; space fullerene: such tiling by any fullerenes.
They occur in clathrate hydrates, zeolites, soap froths and tetrahedrally close-packed phases of metallic alloys.

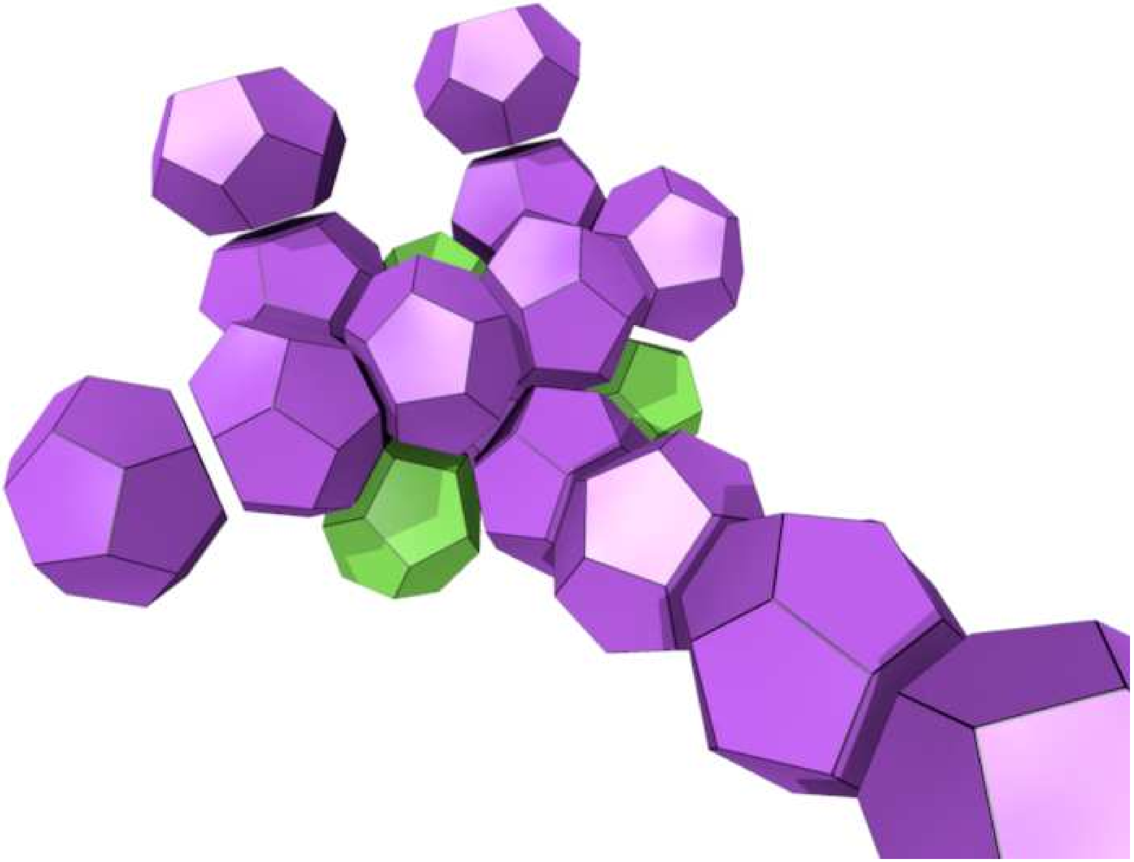


12 (of 24 known) FK space fullerenes

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 III, Zr_4Al_3	$P6/mmm$	13.43	3, 2, 2, 0	7
σ	ype IV, $Cr_{46}Fe_{54}$	$P4_2/mnm$	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	$Mg_{32}(Zn,Al)_{49}$	$Immm$	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

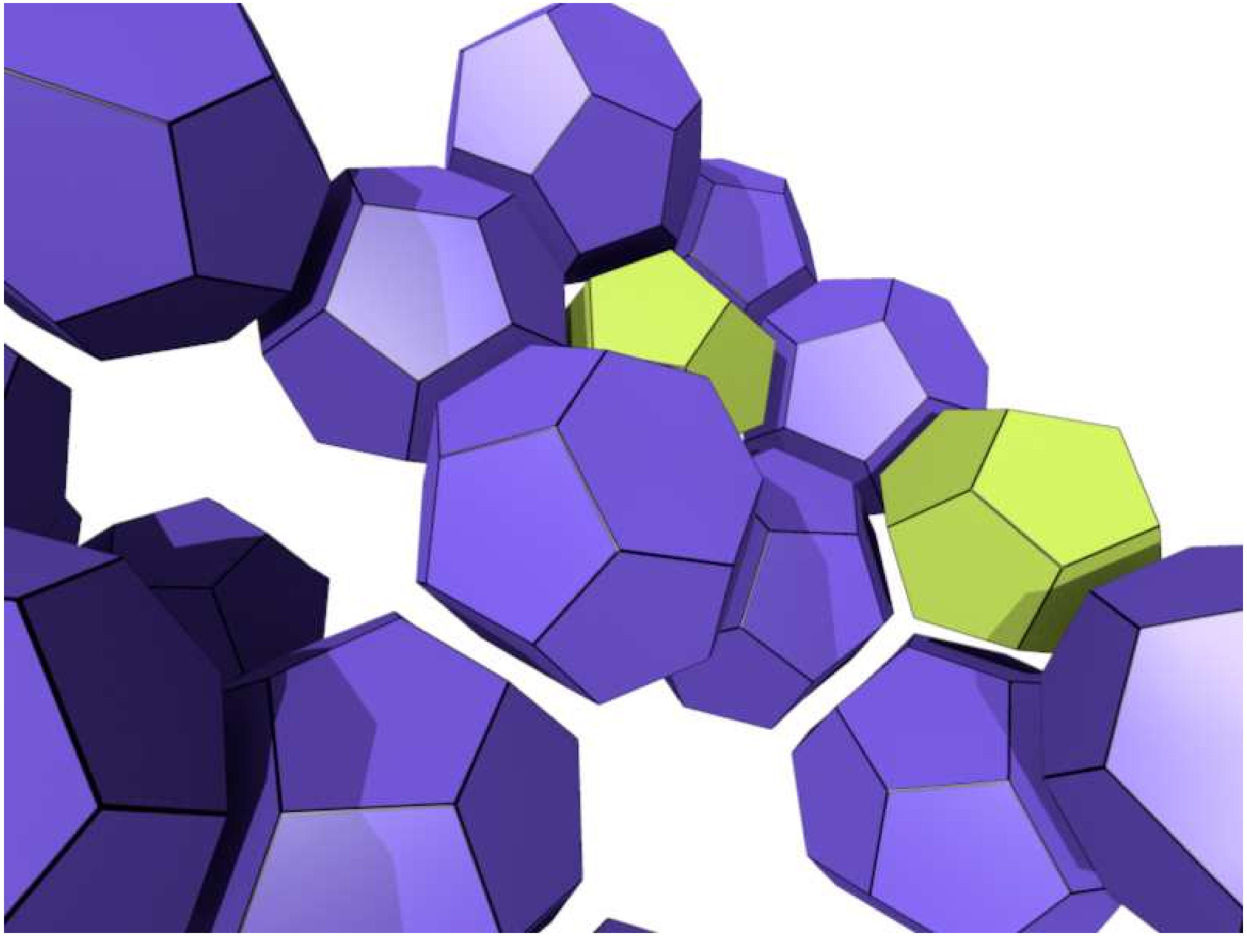
FK space fullerene A_{15}

Gravicenters of cells F_{20} (atoms Si in Cr_3Si) form the bcc network A_3^*. Unique with its fractional composition $(1,3,0,0)$.



FK space fullerenes C_{15} and C_{14}

C_{15}: atoms Mg in alloy $MgCu_2$ (gravicenters of cells F_{28}) form cubic diamond network.
C_{14}: $MgZn_2$, “ hexagonal diamond” (lonsdaleite) network.
C_{15}, C_{14} belong to a continuum of structures with $(2,0,0,1)$



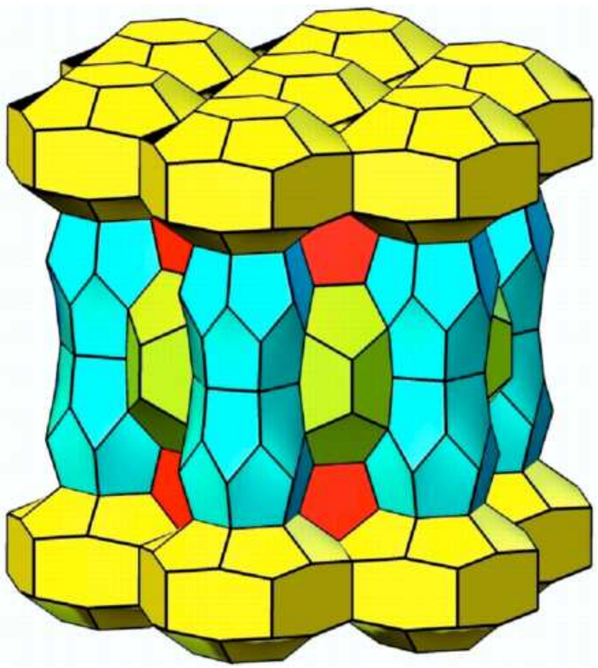
Computer enumeration

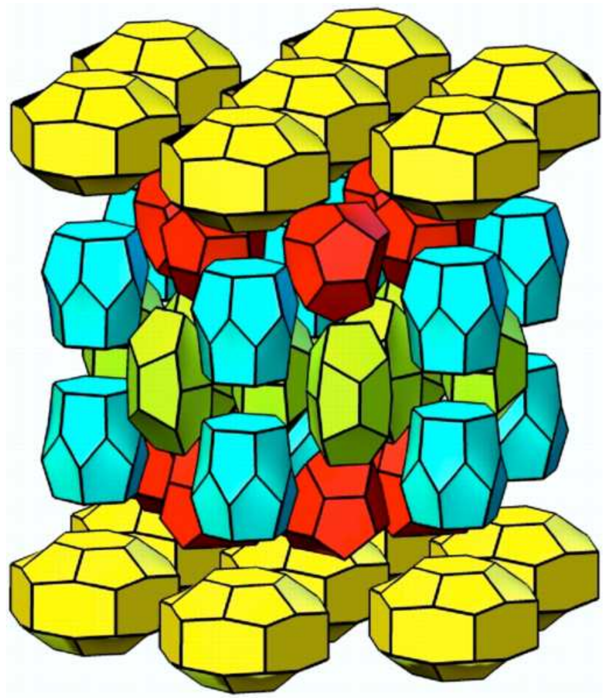
Dutour-Deza-Delgado, 2008: FK structures with ≤ 16 cells (not congruent, with curved faces) in reduced fund. domain.

$\# 20$	$\# 24$	$\# 26$	$\# 28$	fraction	N(structure)
1	3	0	0	known	8(A_{15})
2	0	0	1	known	6,12(C_{14}),24(C_{15})
3	2	2	0	known	7(Z),14,28,28
3	3	2	0	conterexample	32
3	3	0	1	new	14,28,28
3	4	2	0	conterexample	18
4	5	2	0	known	22(cf. J complex)
5	2	2	1	new	20
5	8	2	0	known	15(cf. H complex),30(σ)
6	5	2	1	known	14,28,28,28,56,56(δ)
7	2	2	2	known	13,13,26,26(K_7Cs_6),26 ($p\sigma$)
7	4	2	2	conterexample	60
9	2	2	4	new	32

Non-FK space fullerene: is it unique?

Deza-Shtogrin, 1999: unique known non-FK space fullerene, 4-valent 3-periodic tiling of $\mathbb{E}^3$ by F_{20}, F_{24} and its elongation $F_{36}(D_{6h})$ in ratio $7:2:1$. So, new records: mean face-size ≈ 5.091<5.1 (C_{15}). Closer to impossible 5 (120-cell on 3-sphere) means energetically competitive with diamond.

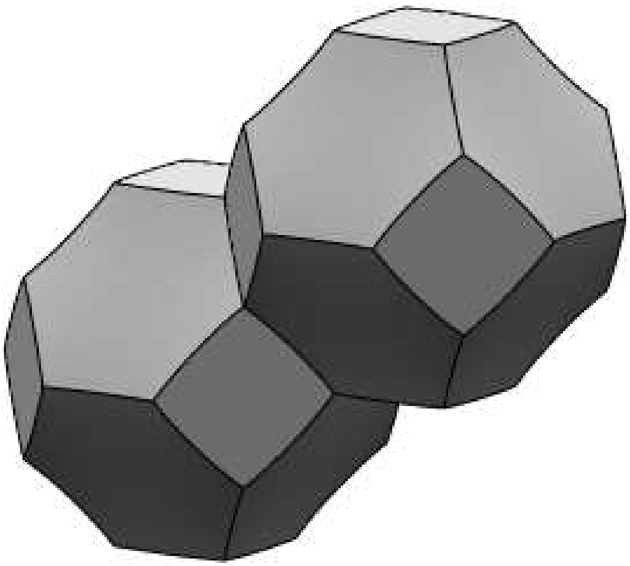


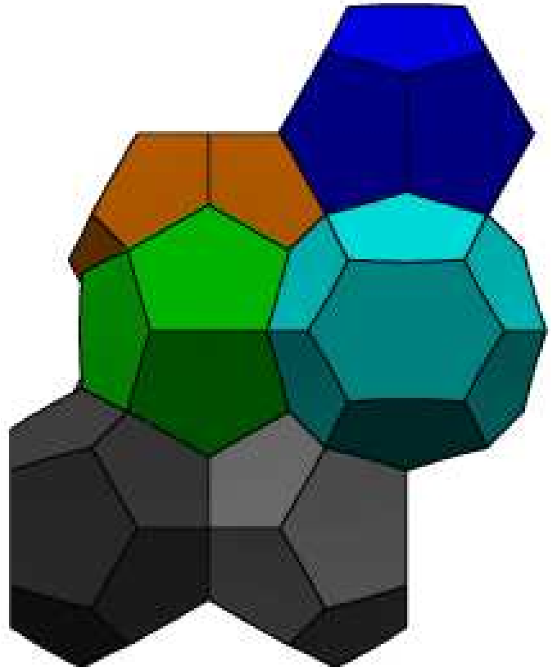


Delgado, O'Keeffe, 2007: all space fullerenes with ≤ 7 vertex-orbits are A_{15}, C_{15}, Z, C_{14} and this one (3,3,5,7,7).

Kelvin problem

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





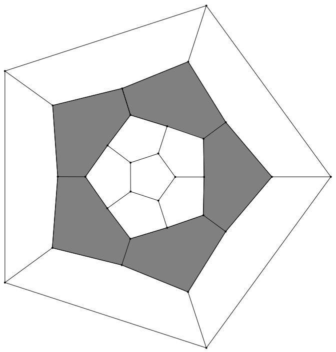
Lord Kelvin, 1887: bcc=A_3^*
IQ(curved tr.Oct.) ≈ 0.757
IQ(tr.Oct.) ≈ 0.753

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

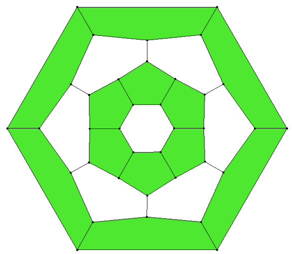
In $\mathbb{E}^2$, the best is (Ferguson, Hales) graphite $F_\infty = (6^3)$.

III. Railroads and zigzags in fullerenes

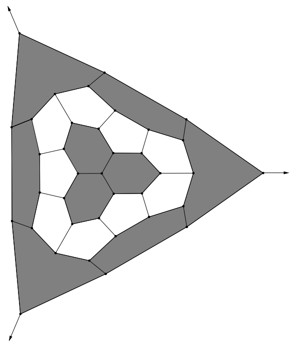
A railroad in a fullerene is a circuit of hexagons which are adjacent to two their neighbors on opposite faces.
Any railroad is bordered by two zigzags (left-right circuits).



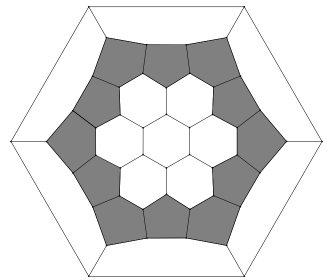
30, D_{5h}
all 6-gons
in railroad
(unique)



36, D_{6h} all
5-gons
in 2 rings

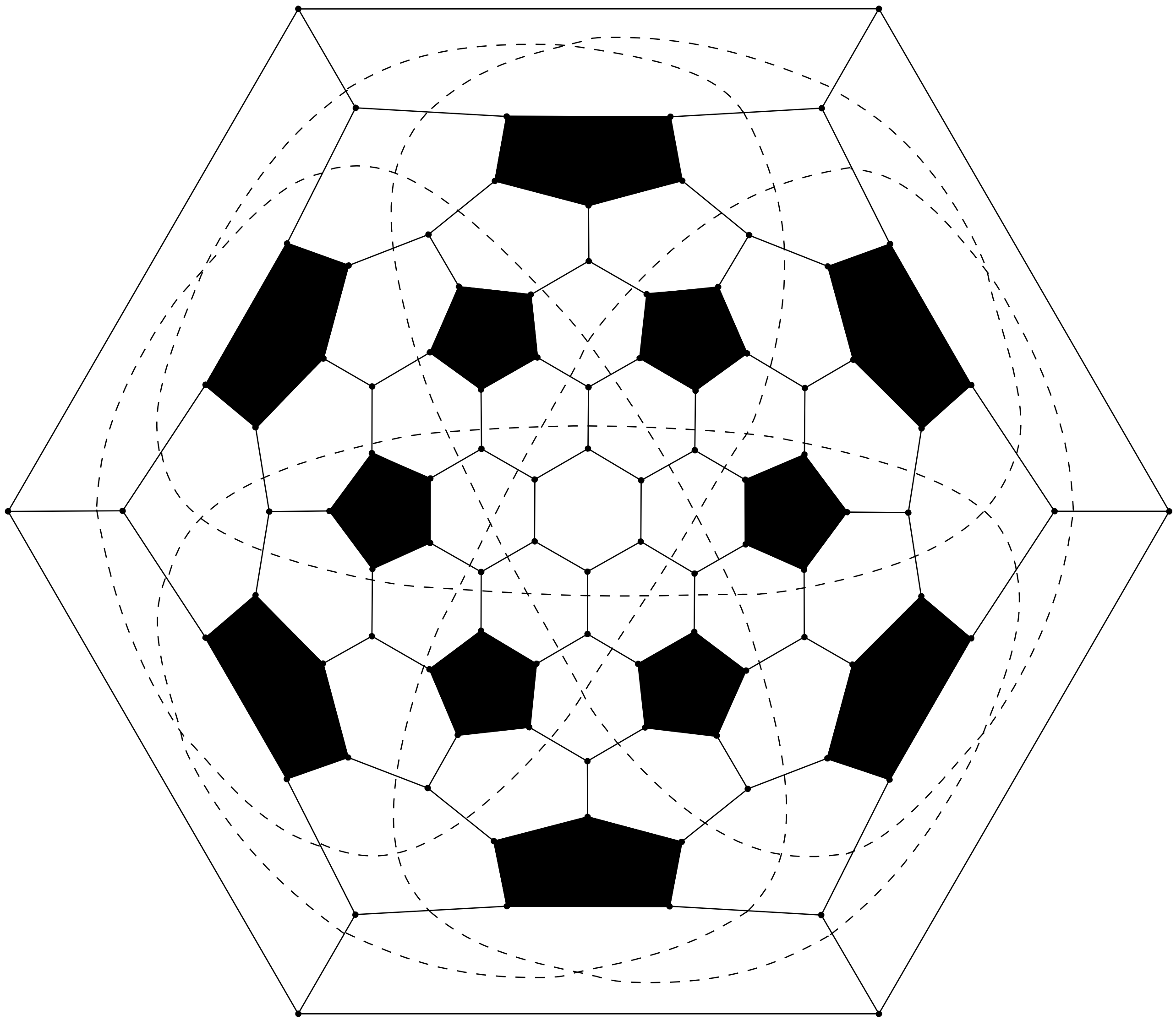


38, C_{3v}
all 5-, 6-
in rings
(unique)



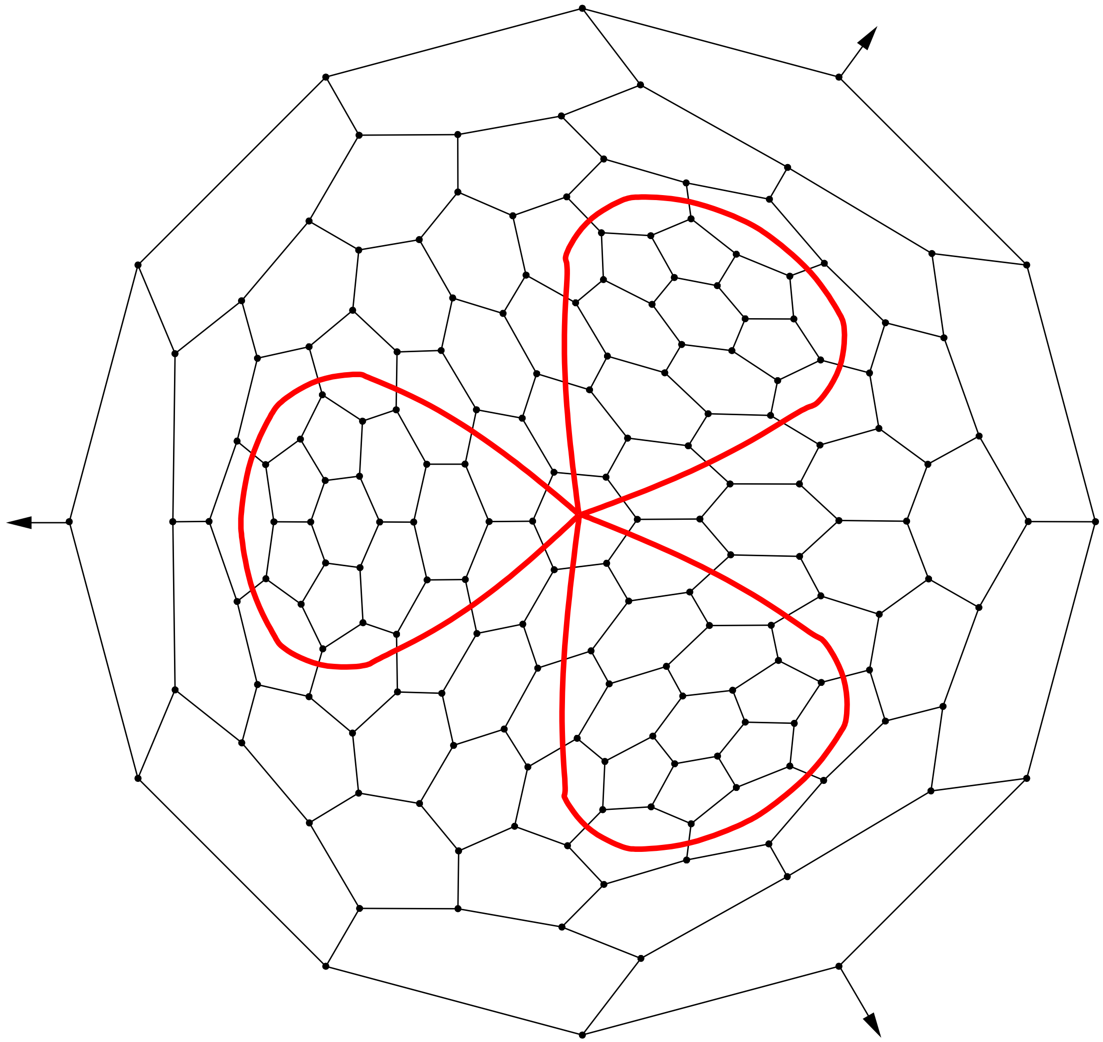
48, D_{6d}
all 5-gons
in alt. ring
(unique)

First IPR fullerene with self-int. railroad



Above $F_{96}(D_{6d})$ is IPR (its pentagons are isolated);
it realizes projection of Conway knot $(4 \times 6)^*$

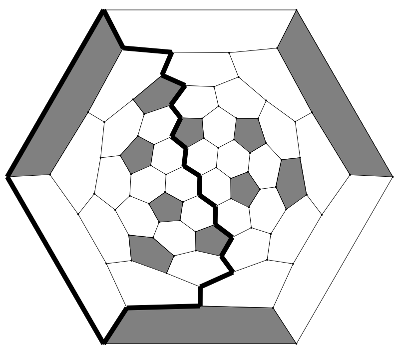
Fullerene with triply intersecting railroad



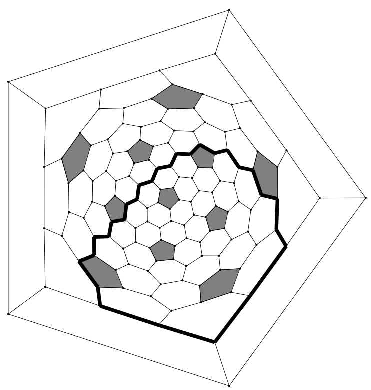
Conjecture: above $F_{176}(C_{3v})$ is smallest such fullerene

Tight fullerenes

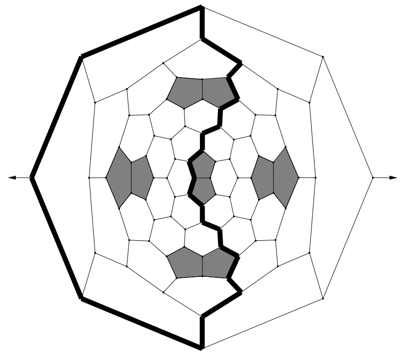
- Tight fullerene is one without railroads.
- $F_{140}(I)$ (below) is tight and has 15 zigzags, all simple.
  Conjecture: any tight fullerene has ≤ 15 zigzags.
- **Conjecture**: all tight fullerenes with simple (i.e., not self-intersecting) zigzags are 9 given below.



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

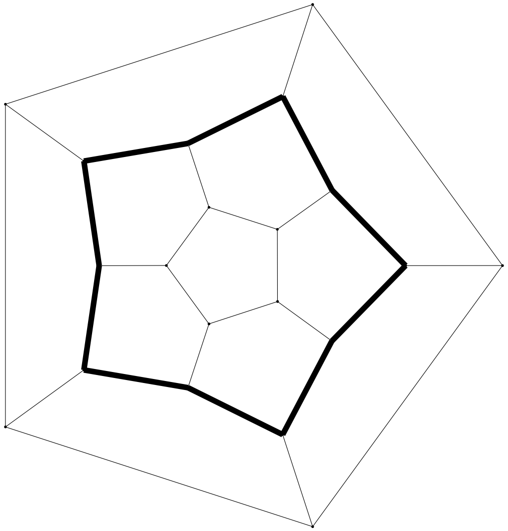


$140 \quad I,\ 28^{15}$

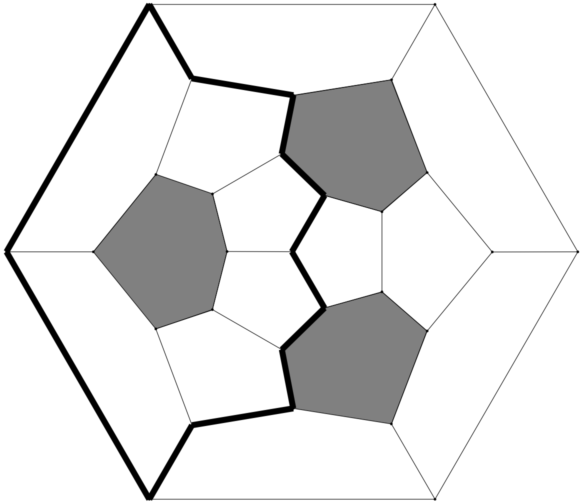


$92 \quad T_h,\ 24^6, 22^6$

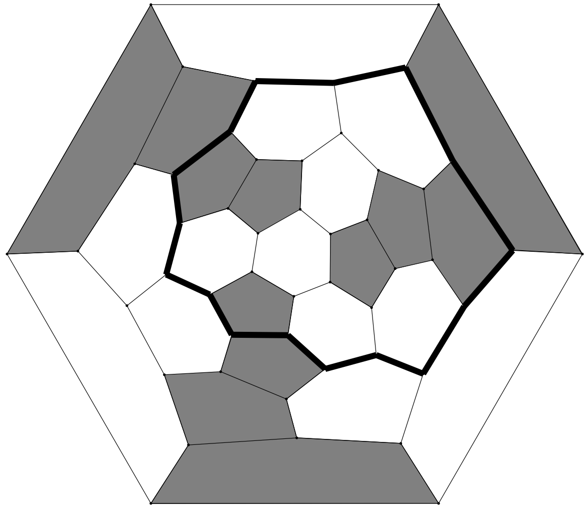
Other 6 tight F_n with simple zigzags



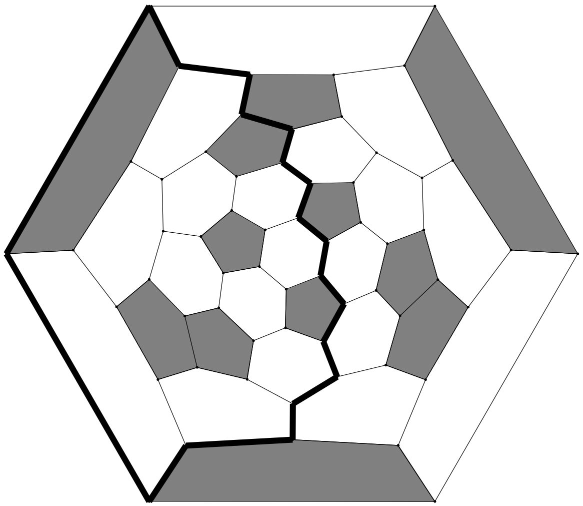
20 $I_h,\ 20^6$



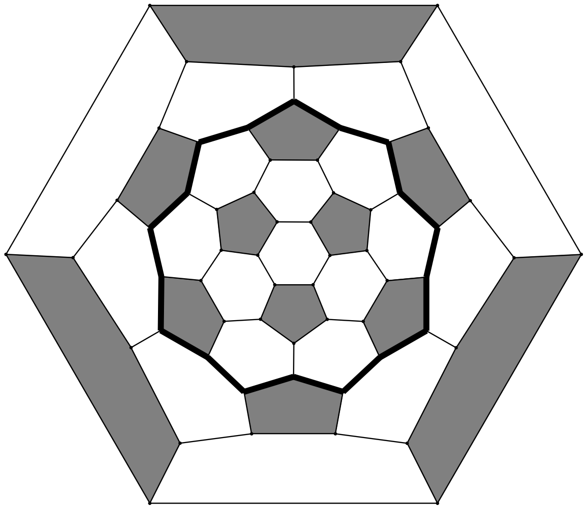
28 $T_d,\ 12^7$



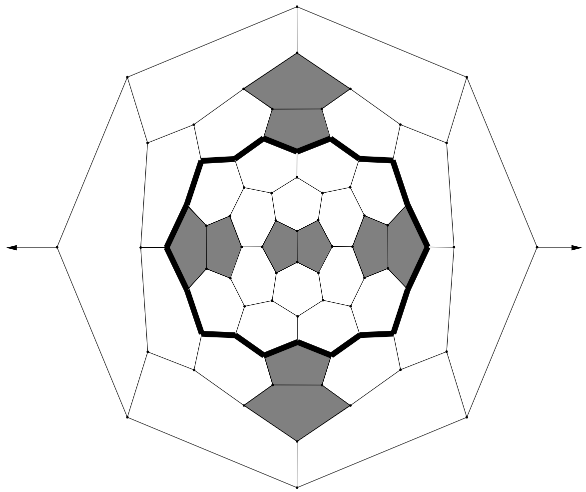
48 $D_3,\ 16^9$



60 $D_3,\ 18^{10}$



60 $I_h,\ 18^{10}$



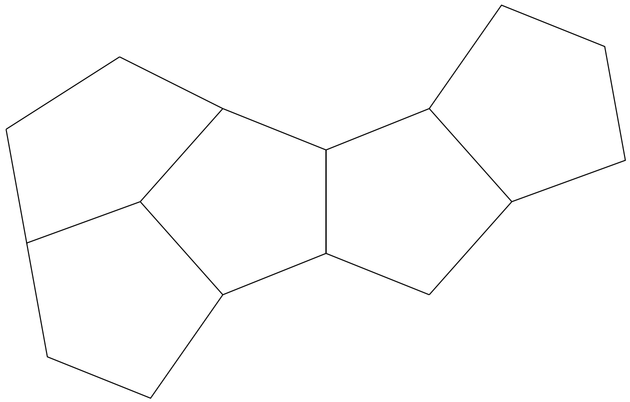
76 $D_{2d},\ 22^4, 20^7$

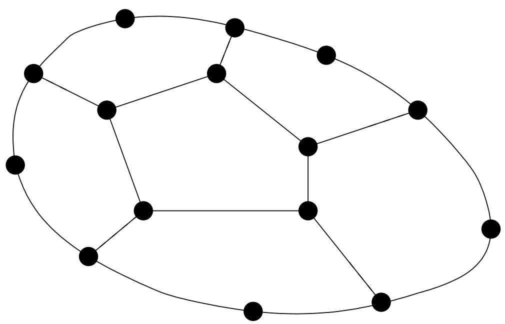
IV. Ambiguous polycycle boundaries

A n-polycycle is a plane 2-connected finite graph with:

- all interior faces are (combinatorial) n-gons,
- all interior vertices are of degree 3,
- all boundary vertices are of degree 2 or 3.

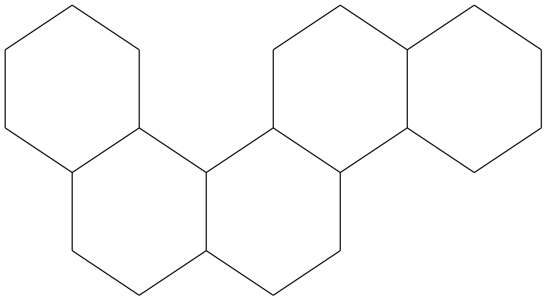
For example, 5-polycycles below have $1, 5$ interior vertices and $5, 10$ interior faces (pentagons, not necessarily regular).





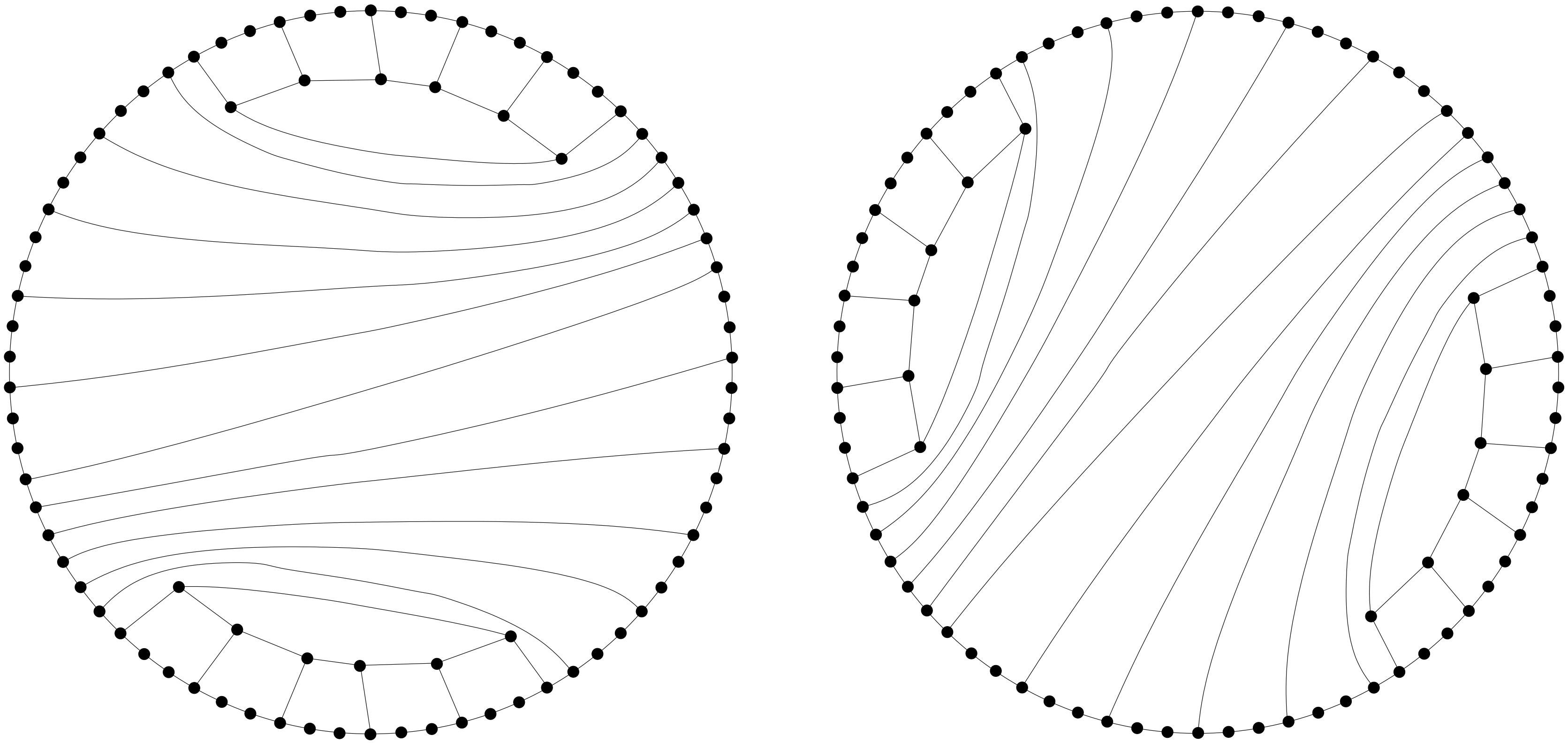
What boundary says about its filling(s?)

- The boundary of a n-polycycle defines it if $n = 3, 4$.
- Also, the boundary of a 6-polycycle defines it if it is of lattice type, i.e., its skeleton is a partial subgraph of the skeleton of the partition $\{6^3\}$ of the plane into hexagons.



- **Conjecture**: any n-polycycle with at most $4n$ n-gons is uniquely defined by its boundary. It holds for $n \leq 6$.

2 equi-boundary 6-polycycles



Boundary sequence: 40, 34 vertices of degree 2, 3, resp.

Symmetry groups: of boundary: C_{2v}, of polycycles: C_2.

Fillings: 24 hexagons, 12 interior vertices.

It is unique ambiguous boundary of a 5-polycycle filled by at most $24 = 4 \times 6$ hexagons.