Extended Family of Fullerenes

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This is a joint work with Mathieu DUTOUR SIKIRIC and Mikhail SHTOGRIN, presented at Int. Conferenc "Computers in Scientific Discovery 7" (CSD 7), July 19–23, 2015, Richmond, USA

Overview

Definition of a fullerene

A (geometric) fullerene F_v is a simple (i.e., 3-valent) polyhedron (putative carbon molecule) whose v vertices (carbon atoms) are arranged in $p_5 = 12$ pentagons and $p_6 = (\frac{v}{2} - 10)$ hexagons.

- F_v exist for all even $v \geq 20$ except $v = 22$.
  $1, 0, 1, 1, 2, 3, 6 \dots, 1812, \dots 214127713, \dots$ isomers F_v for $v=$ $20, 22, 24, 26, 28, 30, 32 \dots, 60, \dots, 200, \dots$.
  Graphite lattice $\{6^3\}$ can be seen as *"largest fullerene"* F_∞.
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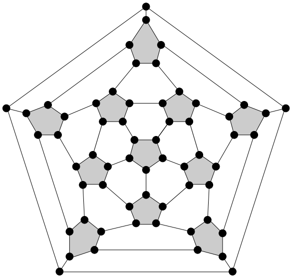
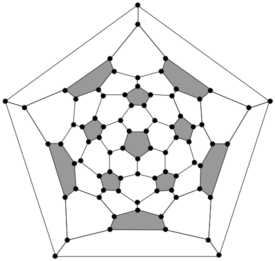
- Thurston, 1998, implies: the number of F_v grows as v^9.
- Only 4 Frank–Kasper fullerenes (having isolated hexagons): unique ones F_{20}, F_{24}, F_{26} and $F_{28}(T_d)$, one of two F_{28}.
  ∞ of IP fullerenes (isolated pentagons; denote such by C_v); the smallest is the truncated Icosahedron $C_{60}(I_h)$.
- Curl–Kroto–Smalley, 1985, synthesised it as carbon allotrope backminsterfullerene (Nobel Prize, 1996, in Chemistry). But Goldberg (1935, 1937) and rev. Kirkman, 1882: 80 of 89 F_{44}.

Original Goldberg–Coxeter construction

Any icosahedral fullerene (i.e., of symmetry I_h or I), has $v{=}20(p^2{+}pq{+}q^2)$ with $0{\le}q{\le}\, p$; I_h for $p = q \neq 0$ and for $q = 0$. Below are cases of $C_{60}(I_h)$; $(p, q){=}(1, 1)$, truncated Icosahedron, and $C_{80}(I_h)$; $(p, q){=}(2, 0)$, chamfered Dodecahedron. Besides Dodecahedron, they are only icosahedral fullerenes with $v \le 80$.





This construction: parameterization by a Gaussian integer $pi{+}q$.

Extended family of fullerenes; of interest are:

- $(\{a, b\}, k)$ on $\mathbb{S}^2$, $\mathbb{P}^2$, $\mathbb{T}^2$ or $\mathbb{K}^2$, i.e., k-valent maps with only a- and b-gonal faces, of curvature $1 + \frac{i}{k} - \frac{i}{2} \geq 0$ for $i = a, b$.
- b-icosahedrites, i.e., $(\{3, b\}, 5)$-$\mathbb{S}^2$ with $b{\geq}4$.
- G-fulleroids, i.e., $(\{5, b\}, 3)$-$\mathbb{S}^2$ with $b{>}6$ and symmetry G.
- c-superfullerenes $(\{5, 6, c\}, 3)$-$\mathbb{S}^2$, in which all 5- and c-gons belong to 12 isomorphic disjoint clusters of faces.
- c-disk-fullerenes, i.e., $(\{5, 6, c\}, 3)$-$\mathbb{S}^2$ with $p_c = 1$.

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- Azulenoids, i.e., $(\{5,6,7\},3)$-$\mathbb{T}^2$; such tori have $p_5=p_7$.
- Schwartzits, i.e., $(\{5,6,7\},3)$- and $(\{5,6,8\},3)$-maps of genus $g\geq 2$ on minimal surfaces of constant negative curvature.
- Plane fullerenes, i.e., $(\{5,6\},3)$-$\mathbb{E}^2$; such planes have $p_5\leq 6$.
- Also, space fullerenes ($\mathbb{E}^3$-tilings by fullerenes) and fullerene manifolds (manifolds whose 2-faces are only 5- or 6-gonal).

Main considered properties of those maps

- Usual ones: symmetries, computer enumeration (wnen feasible), generation, connectivity and so on.
- Parameterization by complex numbers, esp. Goldberg–Coxeter construction (1-parameter case) using rings $\mathbb{Z}[\omega]$ and $\mathbb{Z}[i]$.
- By analogy with v-, p-vectors enumerating map's vertices and faces, edges are represented by z-vector enumerating zigzags (left-right circuits doubly covering edge-set). Main interesting cases: knot (unique zigzag), pure (no zigzag self-intersects) and tight (no railroad, i.e. pair of "parallel" zigzags) maps. Similar theory is build for central circuits of even-valent maps.

Besides relevant papers, this material is presented in our book: M.Deza, M.Dutour Sikiric and M.Shtogrin, *Geometric Structure of Chemistry-relevant Graphs*, Springer, 2015, to appear, which complemented previous book: M.Deza and M.Dutour Sikiric, *Geometry of Chemical Graphs*, Cambridge University Press, 2008.

Fullerenes and other 7 families of parabolic $(\{a, b\}, k)$-spheres

(R,k)-spheres: curvature $\kappa_i = 1 + \frac{i}{k} - \frac{i}{2}$ of i-gons

- Fix $R \subset \mathbb{N}$. An (R,k)-sphere is a k-regular, $k \geq 3$, map on $\mathbb{S}^2$ whose faces are i-gons, $i \in R$. Let m=min and M=$\max_{i \in R} i$.
- Let v, e and $f = \sum_i p_i$ be the map's numbers of vertices, edges and faces, where p_i is the number of i-gonal faces. So, $kv = 2e = \sum_i ip_i$ and *Euler formula* $v - e + f = 2$ become $2 = \sum_i p_i \kappa_i$, where $\kappa_i = 1 + \frac{i}{k} - \frac{i}{2}$ is the curvature of i-gons.
- $\kappa_m \geq 0$ implies $m < \frac{2k}{k-2}$; so, $m \geq 3$, implies $3 \leq m, k \leq 5$, i.e. 5 Platonic parameters $(m,k) = (3,3), (4,3), (3,4), (5,3), (3,5)$.

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- (R,k)-sphere is elliptic if $M{<}\frac{2k}{k-2}$, i.e., $\min_{i \in R}\kappa_i > 0$; then either 1) $k = 3$, $M \leq 5$, or 2) $k \in \{4,5\}$, $M \leq 3$.
  So, for $m \geq 3$, such are only Octahedron, Icosahedron and 10 $(\{3,4,5\},3)$-spheres: 8 dual deltahedra and the Cube's truncations on 1 or 2 opposite vertices (Dürer octahedron).
  In other words, five Platonic and seven $(\{3,4,5\},3)$-spheres.

Parabolic (R, k)-spheres

- (R, k)-sphere is parabolic if $M = \frac{2k}{k-2}$, i.e. $\min_{i \in R} \kappa_i = 0$.
  So, $(M, k) = (6, 3), (4, 4), (3, 6)$ (Euclidean parameter pairs).
  Exclusion of i-faces with $\kappa_i < 0$ simplifies enumeration, while number p_M of *flat* ($\kappa_M = 0$) M-gonal faces not being restricted, there is an infinity of such (R, k)-spheres.
- The number of such v-vertex (R, k)-spheres with $|R| = 2$ increases polynomially with v.
  Such spheres admit parametrization and description in terms of rings of (*Gaussian* if $k=4$ and *Eisenstein* if $k=3, 6$) *integers*.
  All eight series of such spheres will be considered in detail.

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  All eight series of such spheres will be considered in detail.
- (R, k)-sphere is hyperbolic if $M > \frac{2k}{k-2}$, i.e. $\min_{i \in R} \kappa_i < 0$; it do not admit above, in general. We will consider only simplest cases, say: icosahedrites, i.e. $(\{3, 4\}, 5)$-spheres (number of such v-vertex spheres grows at least exponentially with v) and fulleroids, i.e. $(\{5, b\}, 3)$-spheres with $b \geq 7$.

8 families of parabolic $(\{a, b\}, k)$-spheres

- An $(\{a, b\}, k)$-sphere is an (R, k)-sphere with $R = \{a, b\}$, $1 \le a < b$. It has $v = \frac{1}{k}(ap_a + bp_b)$ vertices.
- Such parabolic sphere has $b = \frac{2k}{k-2}$; so, $(b, k) = (6, 3)$, $(4, 4)$, $(3, 6)$ and Euler formula become $2 = \kappa_a p_a = (1 + \frac{a}{k} - \frac{a}{2})p_a = (1 - \frac{a}{b})p_a$.
- So, $p_a = \frac{2b}{b-a}$ and all possible (a, p_a) are:
  $(5, 12)$, $(4, 6)$, $(3, 4)$, $(2, 3)$ for $(b, k) = (6, 3)$;
  $(3, 8)$, $(2, 4)$ for $(b, k) = (4, 4)$;
  $(2, 6)$, $(1, 3)$ for $(b, k) = (3, 6)$.
- Those 8 families can be seen as spheric analogs of the regular plane partitions $\{6^3\}$, $\{4^4\}$, $\{3^6\}$ with p_a *disclinations* ("defects") κ_a added to get the curvature 2 of the sphere.

8 parabolic families: existence criterions

Grűnbaum–Motzkin, 1963: criterion for $k{=}3 \le a$;
Grűnbaum, 1967: for $(\{3,4\},4)$-spheres;
Grűnbaum–Zaks, 1974: for $a = 1, 2$.

k	(a,b)	smallest one	it exists if and only if	p_a	v	Ord	Gr
3	$(5,6)$	Dodecahedron	$p_6 \neq 1$	12	$20{+}2p_6$	v^9	28
3	$(4,6)$	Cube	$p_6 \neq 1$	6	$8{+}2p_6$	v^3	16
4	$(3,4)$	Octahedron	$p_4 \neq 1$	8	$6{+}p_4$	v^5	18
6	$(2,3)$	$\text{Bundle}_6{=}6{\times}K_2$	p_3 is even	6	$2{+}\frac{p_3}{2}$	v^4	22
3	$(3,6)$	Tetrahedron	p_6 is even	4	$4{+}2p_6$	v	5
4	$(2,4)$	$\text{Bundle}_4{=}\ 4{\times}K_2$	p_4 is even	4	$2{+}p_4$	v	5
3	$(2,6)$	$\text{Bundle}_3{=}3{\times}K_2$	$p_6{=}(k^2{+}kl{+}l^2){-}1$	3	$2{+}2p_6$	v	2
6	$(1,3)$	Trifolium	$p_3{=}2(k^2{+}kl{+}l^2){-}1$	3	$\frac{1+p_3}{2}$	v	3
5	$(3,4)$	Icosahedron	$p_4 \neq 1$	$2p_4{+}20$	$2p_4{+}12$	exp	38

8 families of parabolic $(\{a, b\}, k)$-spheres

- Let us denote $(\{a, b\}, k)$-sphere with v vertices by $\{a, b\}_v$.
- $(\{5, 6\}, 3)$- and $(\{4, 6\}, 3)$-spheres are models of molecules of (chemical) fullerenes and boron nitrides., respectively.
- $(\{a, b\}, 4)$-spheres are minimal projections of alternating links, whose components are their *central circuits* (those going only ahead) and crossings are the vertices.
- Bundle$_m$ is $m \times K_2$. Trifolium $\{1, 3\}_1$ is the 3-*rose* $3 \times (vv)$.
- b-icosahedrites $((\{3, b\}, 5)$-spheres) are hypebolic if $b>3$, $p_b>0$, since $p_3=p_b(3b\text{-}10)+20$ and $\kappa_b = \frac{10-3b}{10b} < 0$.

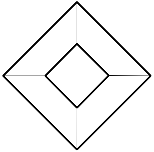
Generation of 4 simplest parabolic $(\{a, b\}, k)$-spheres

- $(\{3,6\},3)$- (Grűnbaum–Motzkin, 1963) and $(\{2,4\},4)$-spheres (Deza–Shtogrin, 2003) admit a 2-parametric description (by 2 Gaussian integers) and also a description by 3 integers.

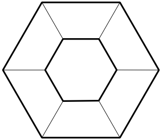
- 1-parametric description: $(\{2,6\},3)$-spheres are given by the *Goldberg–Coxeter construction* from Bundle$_3$ $\{2,6\}_2{=}3{\times}K_2$.
- $(\{1,3\},6)$-spheres come by this construction (extended on 6-regular spheres) from Trifolium $\{1,3\}_1{=}3{\times}(vv)$.

- $(\{2,3\},6)$-spheres, except of $6 \times K_2$ and $3 \times K_3$, are the duals of $(\{3,4,5,6\},3)$-spheres with six new vertices put on edges. Example: $(\{5,6\},3)$-spheres with 5-gons organized in 6 pairs.
- $(\{1,2,3\},6)$-spheres with $v{>}3$, except of 5 infinite series, are the duals of $(\{3,4,5,6\},3)$-$\mathbb{S}^2$ with splitting (into a 2-gon or into a 2-gon, enclosing a 1-gon) of some edges.

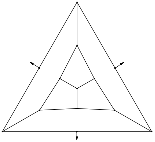
First four $(\{4,6\},3)$- and $(\{5,6\},3)$-spheres (fullerenes)



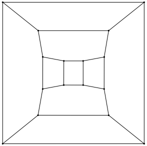
O_h (6^4)



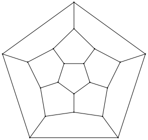
D_{6h} (18^2)



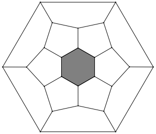
D_{3h} $(6^2; 30)$



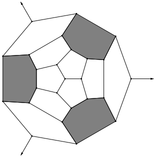
D_{2d} (24^2)



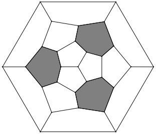
I_h (10^6)



D_{6d} $(12; 60)$



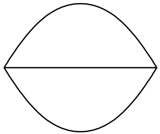
D_{3h} $(12^3; 42)$



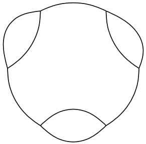
T_d (12^7)

First four $(\{2,6\},3)$- and $(\{3,6\},3)$-spheres

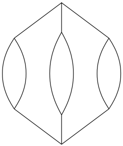
Number of $(\{2,6\}_v$'s is nr. of representations $v{=}2(k^2+kl+l^2)$, $0 \le l \le k$ $(GC_{k,l}(\{2,6\}_2))$. It become 2 for $v{=}7^2{=}5^2{+}15{+}3^2$.



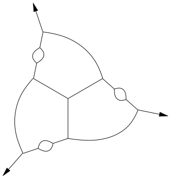
D_{3h} (6)



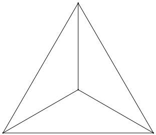
D_{3h} (6^3)



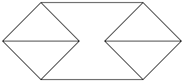
D_{3h} (12^2)



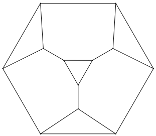
D_3 (42)



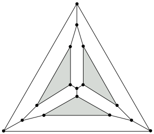
T_d (4^3)



D_{2h} $(8^2, 4^2)$

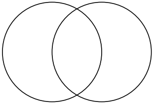


T_d (12^3)

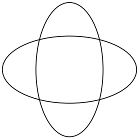


T_d (8^6)

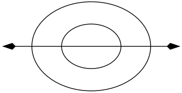
First four $(\{2,4\},4)$- and $(\{3,4\},4)$-spheres



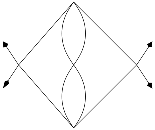
D_{4h} 2^2_1 (2^2)



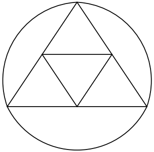
D_{4h} 4^2_1 (4^2)



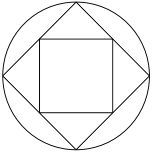
D_{2h} 2×2^2_1 $(2^2, 4)$



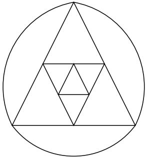
D_{2d} 6^2_2 (6^2)



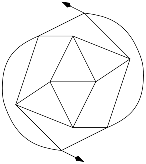
O_h 6^3_2 (4^3)
Borr. rings



D_{4d} 8_{18} (16)



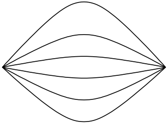
D_{3h} 9_{40} (18)
(Herschel)*



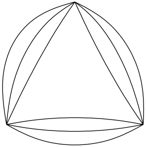
D_2 10^2_{56}
$(6; 14)$

Above links/knots are given in Rolfsen, 1976 and 1990, notation.
Herschel graph: smallest non-Hamiltonian polyhedral graph.

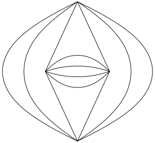
First four $(\{2,3\},6)$- and $(\{1,3\},6)$-spheres



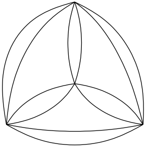
D_{6h} (2^3)



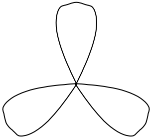
D_{3h} $(3;6)$



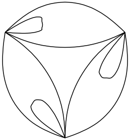
D_{2d} $(2^2;8)$



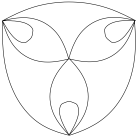
T_d (3^4)



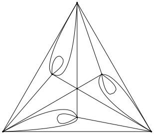
C_{3v} (3)



C_{3h} $(3;6)$



C_{3v} (6^2)



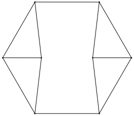
C_3 (21)

$(\{a, b\}, k)$-spheres with $p_b \leq 3$: listings

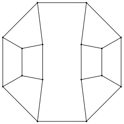
$(\{a, b\}, k)$-spheres with $p_b \leq 2 < a < b$

- Remind: $(a, k)=(3,3),(4,3),(3,4),(5,3),(3,5)$ if $k, a \geq 3$.
- The only $(\{a, b\}, k)$-spheres with $p_b \leq 1$ are 5 Platonic (a^k): Tetrahedron, Cube ($Prism_4$), Octahedron ($APrism_3$), Dodecahedron (snub $Prism_5$), Icosahedron (snub $APrism_3$).
- There exists unique trivial 3-connected $(\{a, b\}, k)$-sphere with $p_b=2$ for $(\{4, b\}, 3)$-, $(\{3, b\}, 4)$-, $(\{5, b\}, 3)$-, $(\{3, b\}, 5)$-: D_{bh} $Prism_b$ and D_{bd} $APrism_b$, snub $Prism_b$, snub $APrism_b$: two b-gons separated by b-ring of 4-gons, $2b$-ring of 3-gons, two b-rings of 5-gons, two $3b$-rings of 3-gons.
- Also, for $t \geq 2$, 10 non-trivial $(\{a, at\}, k)$-spheres with $p_{at}=2$: 5 $(\{a, ta\}, k)$-spheres are (D_{th}) necklaces of polycycles $\{a^k\}$-e; 3 are (D_{th}) necklaces of t v-split $\{3^4\}$ and e-split $\{5^3\}$, $\{3^5\}$; $(\{3, 3t\}, 5)$-spheres C_{th}, D_t are necklaces of t v-, f-split $\{3^5\}$.

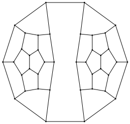
$(\{a, b{=}ta\}, k)$-spheres with $p_b = 2$, $k{=}3, 4, 5$; case $t{=}2$



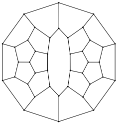
D_{2h}: $a{=}3$



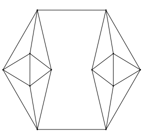
$a{=}4$



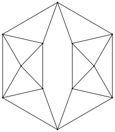
$a{=}5$



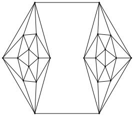
$a{=}5$



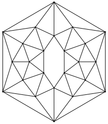
$a{=}3$ D_{2h}



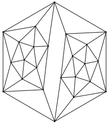
$a{=}3$ D_{2h}



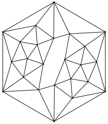
$a{=}3$ D_{2h}



$a{=}3$ D_{2h}



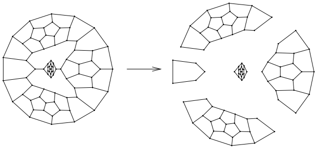
$a{=}3$ C_{2h}



$a{=}3$ D_2

Proof method: elementary (a, k)-polycycles

- A (a, k)-polycycle is a 2-connected plane graph with faces partitioned in a-gonal proper faces and holes, exterior face among them, so that vertex degrees are in $\{2, \dots, k\}$ and can be $< k$ only for a vertex lying on the boundary of a hole.
- Any (a, k)-polycycle decomposes uniquely along its bridges (non-boundary going hole-to-hole, possibly, same, edges) into elementary ones. Cf. integer factorisation into primes.
- We listed them for $\kappa_a = 1 + \frac{a}{k} - \frac{a}{2} \geq 0$. Othervise, continuum.



This $(\{5, 15\}, 3)$-sphere with $p_{15} = 3$ is a 3-holes $(\{5\}, 3)$-polycycle It decomposes into five 1-hole elementary $(\{5\}, k)$-polycycles.

$(\{a, b\}, 3)$-spheres with $p_b = 3$

- $(\{a, b\}, k)$-sphere with $p_b = 3$ exists if and only if $b \equiv 2, a, 2a - 2\,(mod\,2a)$ and $b \equiv 4, 6\,(mod\,10)$ if a=5.
- There are 7 such spheres with t=$\lfloor \frac{b}{6} \rfloor$=0 and 3+4+5+17 of them for any $t \geq 1$.
- Such sphere are unique if b is not $\equiv a\,(mod\,2a)$ and then their symmetry is D_{3h}, except $(a, k) = (3, 5)$.

Symmetry groups of $(\{a, b\}, k)$-spheres

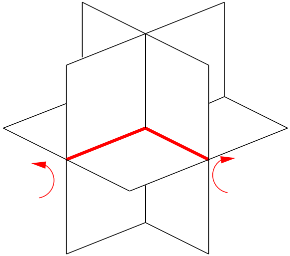
Finite isometry groups

All finite groups of isometries of 3-space $\mathbb{E}^3$ are classified.
In Schoenflies notations, they are:

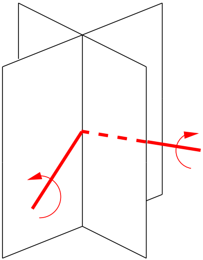
- C_1 is the trivial group
- C_s is the group generated by a plane reflexion
- $C_i = \{I_3, -I_3\}$ is the inversion group
- C_m is the group generated by a rotation of order m of axis Δ
- C_{mv} ($\simeq$ dihedral group) is the group generated by C_m and m reflexion containing Δ
- $C_{mh} = C_m \times C_s$ is the group generated by C_m and the symmetry by the plane orthogonal to Δ
- S_{2m} is the group of order $2m$ generated by an antirotation, i.e. commuting composition of a rotation and a plane symmetry

Finite isometry groups D_m, D_{mh}, D_{md}

- D_m ($\simeq$ dihedral group) is the group generated 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}

Remaining 7 finite isometry groups

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

While (point group) $Isom(P) \subset Aut(G(P))$ (combinatorial group), Mani, 1971: for any 3-polytope P, there is a map-isomorphic 3-polytope P' (so, with the same skeleton $G(P') = G(P)$), such that the group $Isom(P')$ of its isometries is isomorphic to $Aut(G)$.

8 parabolic families: symmetry groups

1. 28 for $\{5,6\}_v$: C_1, C_s, C_i; C_2, C_{2v}, C_{2h}, S_4; C_3, C_{3v}, C_{3h}, S_6; D_2, D_{2h}, D_{2d}; D_3, D_{3h}, D_{3d}; D_5, D_{5h}, D_{5d}; D_6, D_{6h}, D_{6d}; T, T_d, T_h; I, I_h (Fowler–Manolopoulos, 1995)
2. 16 for $\{4,6\}_v$: C_1, C_s, C_i; C_2, C_{2v}, C_{2h}; D_2, D_{2h}, D_{2d}; D_3, D_{3h}, D_{3d}; D_6, D_{6h}; O, O_h (Deza–Dutour, 2005)
3. 5 for $\{3,6\}_v$: D_2, D_{2h}, D_{2d}; T, T_d (Fowler–Cremona,1997)
4. 2 for $\{2,6\}_v$: D_3, D_{3h} (Grűnbaum–Zaks, 1974)
5. 18 for $\{3,4\}_v$: C_1, C_s, C_i; C_2, C_{2v}, C_{2h}, S_4; D_2, D_{2h}, D_{2d}; D_3, D_{3h}, D_{3d}; D_4, D_{4h}, D_{4d}; O, O_h (Deza-Dutour-Shtogrin, 2003)
6. 5 for $\{2,4\}_v$: D_2, D_{2h}, D_{2d}; D_4, D_{4h}, all in $[D_2, D_{4h}]$ (same)
7. 3 for $\{1,3\}_v$: C_3, C_{3v}, C_{3h} (Deza–Dutour, 2010)
8. 22 for $\{2,3\}_v$: C_1, C_s, C_i; C_2, C_{2v}, C_{2h}, S_4; C_3, C_{3v}, C_{3h}, S_6; D_2, D_{2h}, D_{2d}; D_3, D_{3h}, D_{3d}; D_6, D_{6h}; T, T_d, T_h (same)

38 for icosahedrites $(\{3,4\},5)$- (same, 2011).

8 families: Goldberg–Coxeter construction $GC_{k,l}(.)$

With $\mathbf{T}$=$\{T, T_d, T_h\}$, $\mathbf{O}$=$\{O, O_h\}$, $\mathbf{I}$=$\{I, I_h\}$, $\mathbf{C_1}$=$\{C_1, C_s, C_i\}$, $\mathbf{C_m}$=$\{C_m, C_{mv}, C_{mh}, S_{2m}\}$, $\mathbf{D_m}$=$\{D_m, D_{mh}, D_{md}\}$, we get

1. for $(\{5,6\},3)$-: $\mathbf{C_1}$, $\mathbf{C_2}$, $\mathbf{C_3}$, $\mathbf{D_2}$, $\mathbf{D_3}$, $\mathbf{D_5}$, $\mathbf{D_6}$, $\mathbf{T}$, $\mathbf{I}$
2. for $(\{2,3\},6)$-: $\mathbf{C_1}$, $\mathbf{C_2}$, $\mathbf{C_3}$, $\mathbf{D_2}$, $\mathbf{D_3}$, $\{D_6, D_{6h}\}$, $\mathbf{T}$
3. for $(\{4,6\},3)$-: $\mathbf{C_1}$, $\mathbf{C_2}\setminus S_4$, $\mathbf{D_2}$, $\mathbf{D_3}$, $\{D_6, D_{6h}\}$, $\mathbf{O}$
4. for $(\{3,4\},4)$-: $\mathbf{C_1}$, $\mathbf{C_2}$, $\mathbf{D_2}$, $\mathbf{D_3}$, $\mathbf{D_4}$, $\mathbf{O}$
5. for $(\{3,6\},3$-: $\mathbf{D_2}$, $\{T, T_d\}$ $\{D_3, D_{3h}\}$
6. for $(\{2,4\},4)$-: $\mathbf{D_2}$, $\{D_4, D_{4h}\}$
7. for $(\{2,6\},3)$-: $\mathbf{D_3}\setminus D_{3d}$= $\{D_3, D_{3h}\}$
8. for $(\{1,3\},6)$-: $\mathbf{C_3}\setminus S_6$=$\{C_3, C_{3v}, C_{3h}\}$

if $(\{3,4\},5)$-: $\mathbf{C_1}$, $\mathbf{C_2}$, $\mathbf{C_3}$, $\mathbf{C_4}$, $\mathbf{C_5}$, $\mathbf{D_2}$, $\mathbf{D_3}$, $\mathbf{D_4}$, $\mathbf{D_5}$, $\mathbf{T}$, $\mathbf{O}$, $\mathbf{I}$.

8 families: Goldberg–Coxeter construction $GC_{k,l}(.)$

With $\mathbf{T}=\{T, T_d, T_h\}$, $\mathbf{O}=\{O, O_h\}$, $\mathbf{I}=\{I, I_h\}$, $\mathbf{C_1}=\{C_1, C_s, C_i\}$, $\mathbf{C_m}=\{C_m, C_{mv}, C_{mh}, S_{2m}\}$, $\mathbf{D_m}=\{D_m, D_{mh}, D_{md}\}$, we get

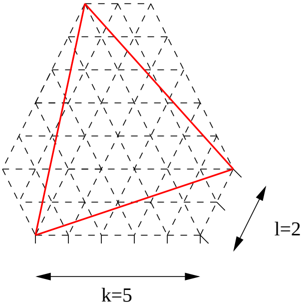
1. for $(\{5,6\},3)$-: $\mathbf{C_1}$, $\mathbf{C_2}$, $\mathbf{C_3}$, $\mathbf{D_2}$, $\mathbf{D_3}$, $\mathbf{D_5}$, $\mathbf{D_6}$, $\mathbf{T}$, $\mathbf{I}$
2. for $(\{2,3\},6)$-: $\mathbf{C_1}$, $\mathbf{C_2}$, $\mathbf{C_3}$, $\mathbf{D_2}$, $\mathbf{D_3}$, $\{D_6, D_{6h}\}$, $\mathbf{T}$
3. for $(\{4,6\},3)$-: $\mathbf{C_1}$, $\mathbf{C_2}\backslash S_4$, $\mathbf{D_2}$, $\mathbf{D_3}$, $\{D_6, D_{6h}\}$, $\mathbf{O}$
4. for $(\{3,4\},4)$-: $\mathbf{C_1}$, $\mathbf{C_2}$, $\mathbf{D_2}$, $\mathbf{D_3}$, $\mathbf{D_4}$, $\mathbf{O}$
5. for $(\{3,6\},3$-: $\mathbf{D_2}$, $\{T, T_d\}$ $\{D_3, D_{3h}\}$
6. for $(\{2,4\},4)$-: $\mathbf{D_2}$, $\{D_4, D_{4h}\}$
7. for $(\{2,6\},3)$-: $\mathbf{D_3}\backslash D_{3d}= \{D_3, D_{3h}\}$
8. for $(\{1,3\},6)$-: $\mathbf{C_3}\backslash S_6=\{C_3, C_{3v}, C_{3h}\}$

if $(\{3,4\},5)$-: $\mathbf{C_1}$, $\mathbf{C_2}$, $\mathbf{C_3}$, $\mathbf{C_4}$, $\mathbf{C_5}$, $\mathbf{D_2}$, $\mathbf{D_3}$, $\mathbf{D_4}$, $\mathbf{D_5}$, $\mathbf{T}$, $\mathbf{O}$, $\mathbf{I}$.
Spheres of blue symmetry are $GC_{k,l}$ from 1st such; so, given by one complex (Gaussian for $k=4$, Eisenstein for $k=3,6$) parameter.
Goldberg, 1937 and Coxeter, 1971: $\{5,6\}_v(I, I_h)$, $\{4,6\}_v(O, O_h)$, $\{3,6\}_v(T, T_d)$. Dutour-Deza, 2004 and 2010: for other cases.

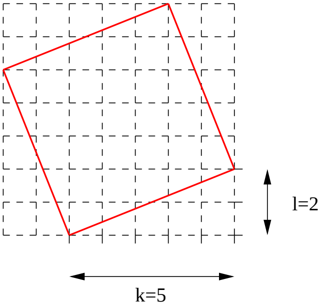
Goldberg–Coxeter construction and parameterizing

Goldberg–Coxeter (1 parameter) construction $GC_{k,l}(.)$

- Take a 3- or 4-regular plane graph G. The faces of dual graph G^* are triangles or squares, respectively.
- Break each face into pieces according to parameter (k, l). *Master polygons* below have area $\mathcal{A}(k^2+kl+l^2)$ or $\mathcal{A}(k^2+l^2)$, where $\mathcal{A}$ is the area of a small polygon.



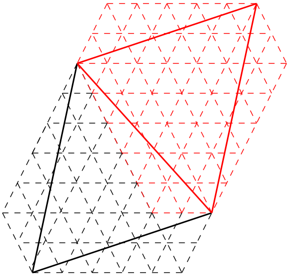
3−valent case



4−valent case

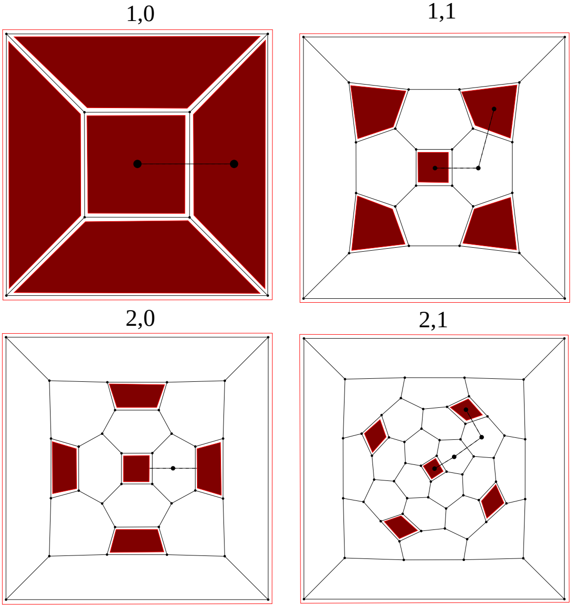
Gluing the pieces together in a coherent way

- Gluing the pieces so that, say, 2 non-triangles, coming from subdivision of neighboring triangles, form a small triangle, we obtain another triangulation or quadrangulation of the plane.

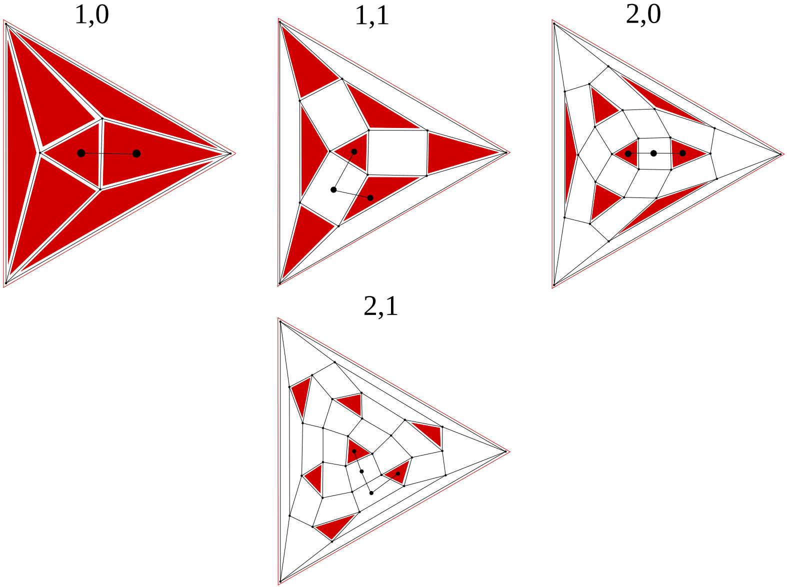


- The dual is a 3- or 4-regular plane graph, denoted $GC_{k,l}(G)$; we call it Goldberg–Coxeter construction.
- It works for any 3- or 4-regular map on oriented surface.

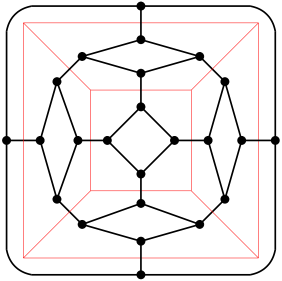
$GC_{k,l}(Cube)$ for $(k, l) = (1, 0), (1, 1), (2, 0), (2, 1)$



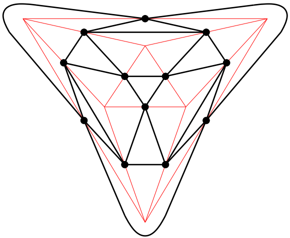
Goldberg–Coxeter construction from Octahedron



The case $(k, l)=(1, 1)$ of $GC_{k,l}(G)$



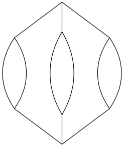
For 3-regular $G=(V, E)$,
$GC_{1,1}$ is called leapfrog
($\frac{1}{3}$-truncation of the dual),
$3|V|$ vertices.
Truncated Octahedron



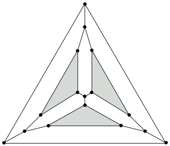
For 4-regular $G=(V, E)$,
$GC_{1,1}$ is called medial
($\frac{1}{2}$-truncation),
$|E|$ vertices
Cuboctahedron

The case $(k, l)=(k, 0)$ of $GC_{k,l}(G)$: k-inflation

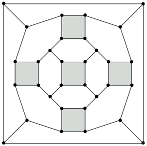
Chamfering (*quadrupling*) $GC_{2,0}(G)$ of smallest $(\{a, b\}, k)$-spheres, $(a, b)=(2, 6), (3, 6), (4, 6), (5, 6)$ and $(2, 4), (3, 4), (1, 3), (2, 3)$, are:



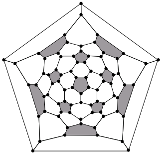
D_{3h} (12^2)



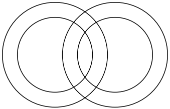
T_d (8^6)



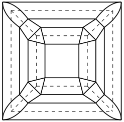
O_h (12^8)



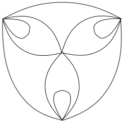
I_h (20^{12})



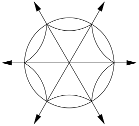
D_{4h} (4^4)



O_h (8^6)

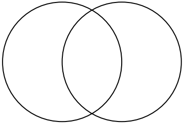


C_{3v} (6^2)

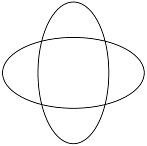


D_{6h} $(4^3, 6^2)$

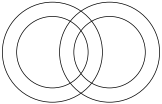
First four $GC_{k,l}(4\times K_2)$ and $GC_{k,l}(6\times K_2)$



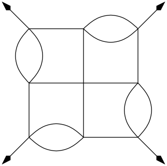
D_{4h} $4\times K_2$



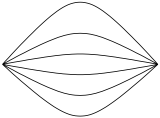
D_{4h} medial



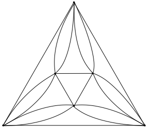
D_{4h} $G_{2,0}$



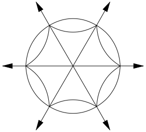
D_4 $G_{2,1}$



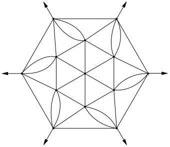
D_{6h} $6\times K_2$



D_{3d} $G_{1,1}$



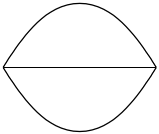
D_{6h} $G_{2,0}$



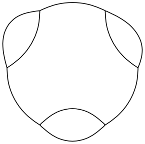
D_6 $G_{2,1}$

First four $GC_{k,l}(3\times K_2)$ and $GC_{k,l}(Trifolium = 3\times(vv))$

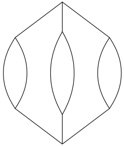
All $(\{2,6\},3)$-spheres are $G_{k,l}(3\times K_2)$: D_{3h}, D_{3h}, D_3 if $l{=}0$, k, else.



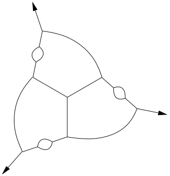
D_{3h} $3\times K_2$



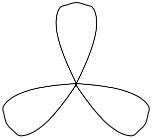
D_{3h} leapfrog



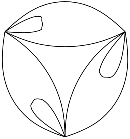
D_{3h} $G_{2,0}$



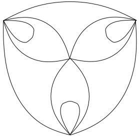
D_3 $G_{2,1}$



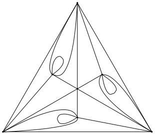
C_{3v} $3\times K_1$



C_{3h} $G_{1,1}$



C_{3v} $G_{2,0}$



C_3 $G_{2,1}$

All $(\{1,3\},6)$-spheres are $G_{k,l}(3\times K_1)$: C_{3v}, C_{3h}, C_3 if $l{=}0$, k, else.

Plane tilings $\{4^4\}$, $\{3^6\}$ and complex rings $\mathbb{Z}[i]$, $\mathbb{Z}[\omega]$

- The vertices of regular plane tilings $\{4^4\}$ and $\{3^6\}$ form each, convenient algebraic structures: lattice and ring. Path-metrics of those graphs are l_1- 4-*metric* and *hexagonal* 6-*metric*, resp.
- $\{4^4\}$: square lattice $\mathbb{Z}_2$ and ring $\mathbb{Z}[i]=\{z=k+li : k,l \in \mathbb{Z}\}$ of Gaussian integers with norm $N(z)=z\overline{z}=k^2+l^2=||(k,l)||^2$.
- $\{3^6\}$: hexagonal lattice $A_2=\{x \in \mathbb{Z}_3 : x_0+x_1+x_2=0\}$ and ring $\mathbb{Z}[\omega]=\{z=k+lw : k,l \in \mathbb{Z}\}$, where $\omega=e^{i\frac{\pi}{3}}=\frac{1}{2}(1+i\sqrt{3})$, of Eisenstein integers with norm $N(z)=z\overline{z}=k^2+kl+l^2=||(k,l)||^2$. We identify points $x=(x_0,x_1,x_2) \in A_2$ with $x_0+x_1\omega \in \mathbb{Z}[\omega]$.
- Both, $\mathbb{Z}[i]$ and $\mathbb{Z}[\omega]$ are unique factorization rings.
- A natural number $n=\prod_i p_i^{\alpha_i}$ is of form $n=k^2+l^2$ if and only if any α_i is even, whenever $p_i \equiv 3(mod\,4)$ (Fermat Theorem). It is of form $n=k^2+kl+l^2$ if and only if $p_i \equiv 2 \pmod 3$.
- The first cases of non-unicity with $gcd(k,l)=gcd(k_1,l_1)=1$ are $91=9^2+9+1^2=6^2+30+5^2$ and $65=8^2+1^2=7^2+4^2$. The first cases with $l=0$ are $7^2=5^2+15+3^2$ and $5^2=4^2+3^2$.

The bilattice of vertices of hexagonal plane tiling $\{6^3\}$

- We identify again the *hexagonal lattice* A_2 of the vertices of the plane tiling $\{3^6\}$ with *Eisenstein ring* $\mathbb{Z}[\omega]$.
- The hexagon centers of $\{6^3\}$ form $\{3^6\}$. Also, with vertices of $\{6^3\}$, they form $\{3^6\}$, rotated by 90° and scaled by $\frac{1}{3}\sqrt{3}$.
- The complex coordinates of vertices of $\{6^3\}$ are given by vectors $v_1{=}1$ and $v_2{=}\omega$. The lattice $L{=}\mathbb{Z}v_1{+}\mathbb{Z}v_2$ is $\mathbb{Z}[\omega]$.
- The vertices of $\{6^3\}$ form bilattice $L_1 \cup L_2$, where the bipartite complements, $L_1{=}(1{+}\omega)L$ and $L_2{=}1{+}(1{+}\omega)L$, are stable under multiplication. Using this,

$GC_{k,l}(G)$ for 6-regular graph G can be defined similarly to 3- and 4-regular case, but only for $z{=}k{+}l\omega{\in}L_2$, i.e. $k \equiv l \pm 1\,(mod\, 3)$. If $z \in L_1$, then $z{=}(1+\omega)s(k'{+}l'\omega)\omega$, where $k' \equiv l \pm 1'\,(mod\, 3)$ and $s{\geq}0$. Then $GC_{k,l}(G){:=}G_{k',l'}(Or^s(G))$ via oriented tripling $Or(G){:=}GC_{1,1}$, defined using vertex 2-coloring of bipartition of G^*.

Goldberg–Coxeter operation in ring terms

	3-regular G	4-regular G	6-regular G
the tiling	$\{3^6\}$	$\{4^4\}$	$\{6^3\}$
the lattice?	A_2	Z_2	bilattice $L_1 \cup L_2$
the ring	Eisenstein $\mathbb{Z}[\omega]$	Gaussian $\mathbb{Z}[i]$	Eisenstein $\mathbb{Z}[\omega]$
Euler formula	$\sum_i (6-i)p_i{=}12$	$\sum_i (4-i)p_i{=}8$	$\sum_i (3-i)p_i{=}6$
curvature 0	hexagons	quadrangles	triangles
ZC-circuits	zigzags	central circuits	both
$GC_{11}(G)$	leapfrog graph	medial graph	oriented tripling

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curvature 0	hexagons	quadrangles	triangles
ZC-circuits	zigzags	central circuits	both
$GC_{11}(G)$	leapfrog graph	medial graph	oriented tripling

- If $GC_z(G):=GC_{k,l}(G)$, then $GC_z(GC_{z'}(G))=GC_{zz'}(G)$, i.e. in ring terms, $GC_z(G)$ corresponds to scalar multiplication by z. Example: $GC_{2k^2,0}(G)=GC_{k,k}(GC_{k,k}(G))$ by $(k+ki)^2=2k^2i$.
- G has v vertices, then $GC_{k,l}(G)$ has $vN(z)$ vertices.
- $GC_z(G)$ has all rotational symmetries of G in 3- and 4-regular case, and all symmetries if $l=0, k$ in general case.
- $GC_z(G)=GC_{\overline{z}}(\overline{G})$, where $\overline{G}$ differs by a plane symmetry only.

Parameterizing parabolic $(\kappa_b = 0)$ $(\{a,b\},k)$-spheres

Thurston, 1993, implies: $(\{a,b\},k)$-spheres have p_a-2 parameters and the number of v-vertex ones is $O(v^{m-1})$ if $m{=}p_a-2\geq 2$.
Idea: since b-gons are of zero curvature, it suffices to give relative positions of a-gons having curvature $\kappa_i{=}1{+}\frac{a}{k}-\frac{a}{2}$.
At most p_a-1 vectors will do, since one position can be taken 0.
But once p_a-1 a-gons are specified, the last one is constrained.
The number of m-parametrized spheres with at most v vertices is $O(v^m)$ by direct integration. The number of such v-vertex spheres is $O(v^{m-1})$ if $m>1$, by a Tauberian theorem.

Parameterizing parabolic $(\kappa_b = 0)$ $(\{a,b\},k)$-spheres

Thurston, 1993, implies: $(\{a,b\},k)$-spheres have p_a-2 parameters and the number of v-vertex ones is $O(v^{m-1})$ if $m{=}p_a - 2 \geq 2$.
Idea: since b-gons are of zero curvature, it suffices to give relative positions of a-gons having curvature $\kappa_i{=}1{+}\frac{a}{k} - \frac{a}{2}$.
At most $p_a - 1$ vectors will do, since one position can be taken 0.
But once $p_a - 1$ a-gons are specified, the last one is constrained.
The number of m-parametrized spheres with at most v vertices is $O(v^m)$ by direct integration. The number of such v-vertex spheres is $O(v^{m-1})$ if $m > 1$, by a Tauberian theorem.

- Goldberg, 1937: $\{a,6\}_v$ (highest 2 symmetries): 1 parameter
  Fowler and al., 1988: $\{5,6\}_v$ (D_5, D_6 or T): 2 parameters.
- Grűnbaum–Motzkin, 1963: $\{3,6\}_v$: 2 parameters.
  Deza–Shtogrin, 2003: $\{2,4\}_v$; 2 (Gaussian int.) parameters.
- Thurston, 1993: $\{5,6\}_v$: 10 (Eisenstein integers) parameters
  Graver, 1999: $\{5,6\}_v$: 20 integer parameters.
- Rivin, 1994: $\{5,6\}_v$: parametrization by 18 dihedral angles.

Parameterizing (R,k)-spheres with $\min_{i\in R}\kappa_i \geq 0$

Thurston, 1998 (actually, 1993) parametrized (dually) all 19 series of $(\{3,4,5,6\},3)$-spheres. In general, such (R,k)-spheres are given by $m{=}\sum_{3\leq i<\frac{2k}{k-2}} p_i - 2$ complex parameters $z_1,\dots,z_m$.
The number of vertices is expressed as a non-degenerate Hermitian form $q{=}q(z_1,\dots,z_m)$ of signature $(1,m-1)$.
Let H^m be the cone of $z{=}(z_1,\dots,z_m)\in\mathbb{C}^m$ with $q(z)>0$.
Given (R,k)-sphere is described by different parameter sets; let $M{=}M(\{p_3,\dots,p_m\},k)$ be the discrete linear group preserving q.
For $k{=}3$, the quotient $H^m/(\mathbb{R}_{>0}\times M)$ is of finite covolume. Sah, 1994, deduced: the number of corresp. spheres grows as $O(v^{m-1})$
Dutour partially generalized above for other k and surface maps.

8 families: number of complex parameters by groups

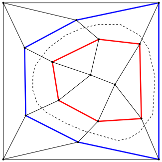
1. $\{5,6\}_v$ $\mathbf{C_1}(10)$, $\mathbf{C_2}(6)$, $\mathbf{C_3}(4)$, $\mathbf{D_2}(4)$, $\mathbf{D_3}(3)$, $\mathbf{D_5}(2)$, $\mathbf{D_6}(2)$, $\mathbf{T}(2)$, $\{I, I_h\}(1)$
2. $\{4,6\}_v$ $\mathbf{C_1}(4)$, $\mathbf{C_2}\backslash S_4(3)$, $\mathbf{D_2}(2)$, $\mathbf{D_3}(2)$, $\{D_6, D_{6h}\}(1)$, $\{O, O_h\}(1)$
3. $\{3,4\}_v$ $\mathbf{C_1}(6)$, $\mathbf{C_2}(4)$, $\mathbf{D_2}(3)$, $\mathbf{D_3}(2)$, $\mathbf{D_4}(2)$, $\{O, O_h\}(1)$
4. $\{2,3\}_v$ $\mathbf{C_1}(4)$, $\mathbf{C_2}(3)$, $\mathbf{C_3}(3)$, $\mathbf{D_2}(2)$, $\mathbf{D_3}(2)$, $\mathbf{T}(1)$, $\{D_6, D_{6h}\}(1)$
5. $\{3,6\}_v$ $\mathbf{D_2}$ (2) (also, 3 natural parameters), $\{T, T_d\}(1)$
6. $\{2,4\}_v$ $\mathbf{D_2}(2)$ (also, 3 natural parameters), $\{D_4, D_{4h}\}(1)$
7. $\{2,6\}_v$ $\{D_3, D_{3h}\}(1)$
8. $\{1,3\}_v$ $\{C_3, C_{3v}, C_{3h}\}(1)$

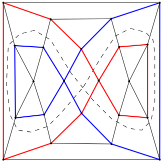
Thurston, 1998 implies: $(\{a,b\},k)$-$\mathbb{S}^2$ have $p_a - 2$ parameters and the number of v-vertex ones is $O(v^{m-1})$ if $m{=}p_a - 2 > 1$.

ZC-circuits and railroads of $(\{a, b\}, k)$-spheres

ZC-circuits

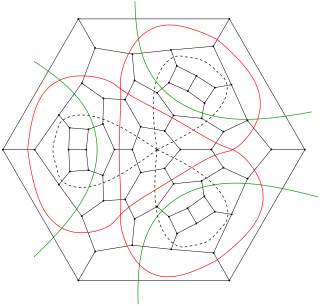
- The edges of any plane graph are doubly covered by zigzags (Petri or left-right paths), i.e., circuits such that any two but not three consecutive edges bound the same face.
- The edges of any *Eulerian* (i.e., even-valent) plane graph are partitioned by its central circuits (those going straight ahead).
- A ZC-circuit means *zigzag* or *central circuit* as needed. CC- or Z-vector ($\vec{cc}$ or $\vec{z}$) enumerate lengths of above circuits.
- A railroad in a 3-, 4- or 6-regular plane graph is a circuit of 6-, 4- or 3-gons, each adjacent to neighbors on opposite edges. Any railroad is bound by two "parallel" ZC-circuits. It (any if 4-, simple if 3- or 6-regular) can be collapsed into 1 ZC-circuit.



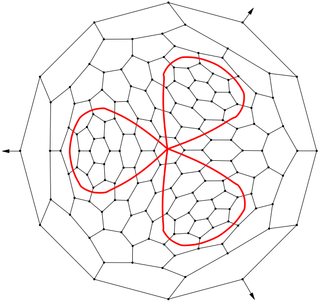


Trifolium $\{1, 3\}_1$ as a railroads flower

Railroads can be simple or self-intersect, including triply if $k = 3$. Smallest such $(\{4, 6\}, 3)$-$\mathbb{S}^2$ and fullerene $(\{5, 6\}, 3)$-$\mathbb{S}^2$ are below; they have a railroad of the form Trifolium (left one has 2 of them).



$\{4, 6\}_{66}(D_{3h})$ twice



$\{5, 6\}_{172}(C_{3v})$

Is any plane curve with at most triple self-intersections come so?

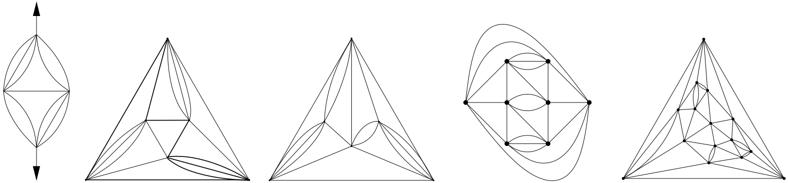
Number of ZC-circuits in tight $(\{a,b\},k)$-sphere

The number of ZC-circuits in a tight (no railroads) $(\{a,b\},k)$-$\mathbb{S}^2$:

- ≤ 15 for $\{5,6\}_v$ and ≤ 9 for $\{4,6\}_v$,
- ≤ 6 for $\{3,4\}_v$ and $\{2,3\}_v$,
- ≤ 3 for $\{3,6\}_v$ and $\{2,6\}_v$,
- ≤ 2 for $\{2,4\}_v$ and $= 0$ for $\{1,3\}_v$.
  All above bounds are sharp, except undecided $\{4,6\}_v$ (≤ 8?).
- Any $\{3,6\}_v$ has ≥ 3 zigzags with equality iff it is tight. All $\{3,6\}_v$ are tight iff $\frac{v}{4}$ is prime > 2 and none iff it is even.
- Any $\{2,4\}_v$ has ≥ 2 central circuits with equality iff it is tight. There is a tight one for any even v.

Small CC-knotted and/or z-knotted $(\{2,3\},6)$-$\mathbb{S}^2$

- The minimal number of central circuits or zigzags, 1, have CC-knotted and z-knotted $(\{2,3\},6)$-$\mathbb{S}^2$. They correspond to plane curves with only triple self-intersection points.
- Conjecture (holds if $v \leq 54$): any z-knotted $(\{2,3\},6)$-$\mathbb{S}^2$ has odd v and a CC-knotted one is also z-knotted iff v is odd.



4 D_2 **6** D_3 **6** C_2 **8** D_2 **15** C_1

Small CC-knotted $(\{2,3\},6)$-$\mathbb{S}^2$; only 5-th is also z-knotted.

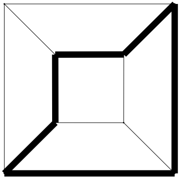
Tight pure $(\{a, b\}, k)$-spheres

Tight $(\{a, b\}, k)$-spheres with only simple ZC-circuits

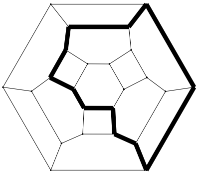
An $(\{a, b\}, k)$-sphere is pure if any of its ZC-circuits is simple.
The number of tight pure $(\{a, b\}, k)$-spheres is:

1. 9 for $\{5, 6\}_v$, 2 for $\{4, 6\}_v$, 8 for $\{3, 4\}_v$, 5 for $\{2, 3\}_v$;
2. all $\{2, 4\}_v$ are pure; ≥ 1 tight for any possible (i.e. even) v;
3. all $\{3, 6\}_v$ are pure; ≥ 1 tight for any odd $\frac{v}{4}$;
4. 0 for $\{2, 6\}_v$ and $\{1, 3\}_v$, since any ZC-circuit self-intersects.

Two such spheres $(\{4, 6\}, 3)$-$\mathbb{S}^2$: Cube and truncated Octahedron.

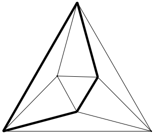


8 O_h (6^4)

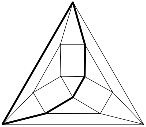


24 O_h (12^6)

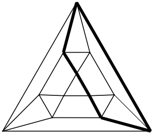
All tight $(\{3, 4\}, 4)$-spheres with only simple central circuits



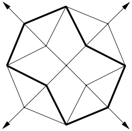
6 O_h (4^3) *Octahedron*



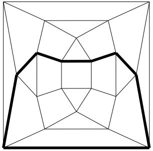
12 O_h (6^4) $GC_{11}(Oct.)$



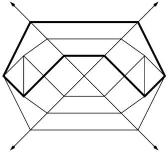
12 D_{3h} (6^4)



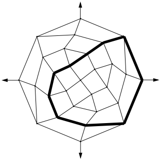
14 D_{4h} $(6^2, 8^2)$



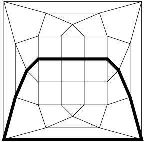
20 D_{2d} (8^5)



22 D_{2h} $(8^3, 10^2)$



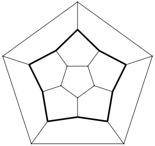
30 O (10^6) $GC_{21}(Oct.)$



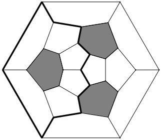
32 D_{4h} $(10^4, 12^2)$

A simple central circuit can be seen as a Jordan curve (closed simple plane curve). A (k, t)-AP (arrangements of pseudocircles) is a set of k Jordan curves where any two intersect in $= t$ points. For each, but $4, 6, 8$- above, the central circuits form a $(k, 2)$-AP.

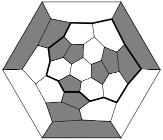
8 tight $(\{5,6\},3)$-spheres with only simple zigzags



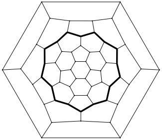
20 I_h (10^6)



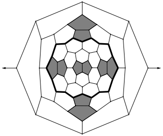
28 T_d (12^7)



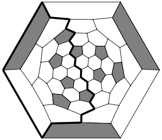
48 D_3 (16^9)



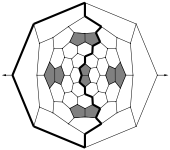
60 I_h (18^{10})



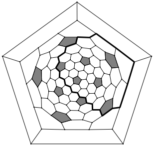
76 D_{2d} $(22^4, 20^7)$



88 T (22^{12})



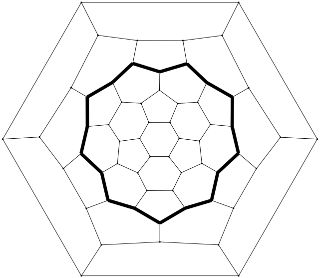
92 T_h $(24^6, 22^6)$



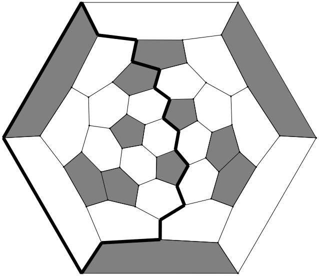
140 I, (28^{15})

The medial of a map G is the graph of edges of G with two being adjacent if they have a common vertex and face. It is a 4-regular plane graph; its central circuits correspond to the zizags of G.
The medials of all 9 fullerenes, but 5, 7-th above, form $(k,2)$-APs.

Remaining 9-th pure tight fullerene (2-nd 60-vertex one)



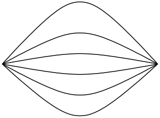
60 I_h (18^{10})



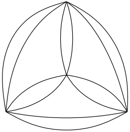
60 D_3 (18^{10})

This pair was first (affirmative) answer on a question in Grűnbaum, 1967, 2003 *Convex Polytopes* about existence of different *simple* polyhedra with the same v-, p- and z-vectors. Both above have $\vec{v}=(v_1,\dots,v_{60})=(3,\dots,3)$, $\vec{p}=(p_5,p_6)=(12,20)$ and $\vec{z}=(18^{10})$.

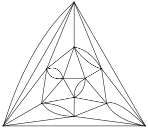
Tight $(\{2,3\},6)$-spheres with only simple ZC-circuits



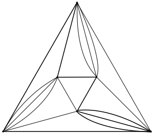
2 D_{6h} 2^3
6^2 ZC-tight



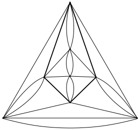
4 T_d 3^4
6^4



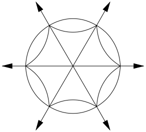
12 T_h 6^6
12^6



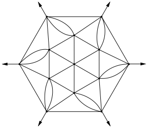
6 D_3 no
$12, 8^3$ z-tight



8 D_{2d} $5^4, 4$
no



D_{6h} $4^3, 6^2$
8^6 no



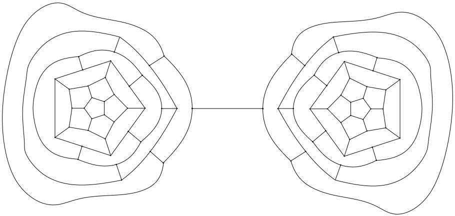
14 D_6 no
14^6 z-tight

All CC-pure w.tight: $1, 2, 3, 5, 6$th. All z-pure w.tight: $1, 2, 3, 4, 7$th
A $(\{2,3\},6)$-$\mathbb{S}^2$ is called ZC-tight if any ZC-circuit has a 2-gon on each side, and ZC-weakly tight if there are no parallel ZC-circuits.

c-disk fullerenes

c-disk and c-multidisk fullerenes

- Call a $(\{5,6,c\},3)$-$\mathbb{S}^2$, $p_c{=}1$, c-disk-fullerene c-DF, if c-gon not self-intersects and c-multidisk-fullerene c-MDF, else.
- Any c-DF or c-MDF has $p_5{=}c{+}6$, $v{=}2(p_6{+}c{+}\ 5)$ and there is an ∞ of c-DF's for any $c{\geq}1$ and of c-MDF's for any $c{\geq}8$
- Possible symmetry groups of a c-DF with $c{\neq}5, 6$ or c-MDF: C_k, $C_{k\nu}$ with $k \in \{1, 2, 3, 5, 6\}$ and k dividing c (symmetries stabilize c-gon and axis pass by a vertex, edge or face),



8-$MDF_{78}(C_{2\nu})$: min. 8-MDF and c-MDF with smallest c

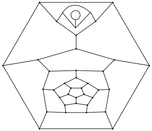
Fullerene c-disks: big picture

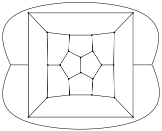
- Fullerene c-polycycle: an c-gon partitioned into 5- and 6-gons with vertices of degree 3 inside and 3 or 2 on the c-gon.
- c-disk fullerene: full. c-polycycle without degree 2 vertices; so, $p_5{=}p_6{+}6$. If $c \in \{5, 6\}$, it is a fullerene without a face.
- Fullerene c-patch: fullerene c-polycycle, which is a fullerene's part; so, $p_5{\leq}12$. It is a c-disk fullerene if f $c \in \{5, 6\}$.
- c-thimble fullerene: a 3-connected c-disk fullerene with only 5-gons adjacent to the c-gon. It exists if and only if $c \geq 5$. Smallest c-thimble has $c - 6{\leq}p_6{\leq}\lfloor\frac{3(c-5)}{2}\rfloor$; conj.: $=\lfloor\frac{3(c-5)}{2}\rfloor$.

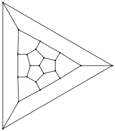
Connectivity of c-disk fullerenes

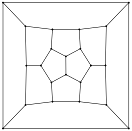
- Any c-MDF and 1-DF are 1-connected, but not 2-connected.
- Any c-DF is 2-connected; only 2-connected exist iff $c \geq 8$.
- Smallest such have $p_6 = 23, 17, 10, 8$ for $c = 8, 9, 10, 11$ and, for $c \geq 12$, $p_6 = 4, 5, 6$ if $c \equiv (\mod 10)$ to $4, 5, 6$ or $2, 3, 7, 8$ or $1, 9$
- Smallest 3-connected (i.e., polyhedral) ones have $m(c) :=$ $p_6 = 3, 2, 0, 1, 3, 4, 6, 7, 8$ for $3 \leq c \leq 11$ and (conj.) 6 for $c \geq 12$.
- Conjecture: 3-connected c-DF_v exists – except $(c, v) = (1, 42)$, $(3, 24)$, $(5, 22)$ – iff v is even and $v \geq 2(m(c) + c + 5)$.

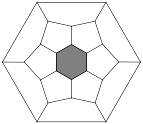
Minimal c-disk fullerenes

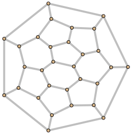

1 40, C_s

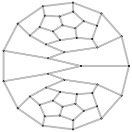

2 26, $C_{2\nu}$

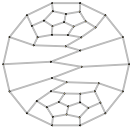

3 22, $C_{3\nu}$


4 22, $C_{2\nu}$


6 24 D_{6d}

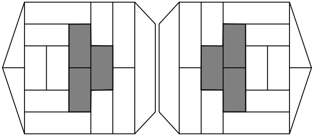

7 30, C_s


13 48, C_s

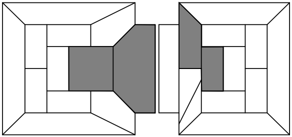

14 50, C_2

For $v \neq 13, 14$ above are minimal, but minimal 13- and 14-DF are 2-connected and have $p_6 = 5, 4$ respectively, i.e. less than 6 above.
Conjecture: for $c \geq 13$, minimal 3-connected c-disk is c-pentatube $B + Hex_3 + Pen_{c-12} + Hex_3 + B$ (symmetry C_s / C_2 for odd/even c).
All minimal c-DF, $5 \leq c \leq 9$, and a minimal 10-DF are c-thimbles.

Pure



20-$DF_{62}(C_{2\nu})$: not a 20-thimble, but all its 18 boundary faces are 5-gons; $\vec{z}=(10^2; 30^2_{0,3}, 40_{2,0}, 66_{4,5})$

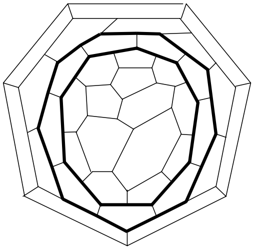


15-$DF_{48}(C_1)$ split in two parts with p_6=2 and two simple 10-zigzags; $\vec{z}=(10^4; 40_{0,4}, 64_{4,8})$

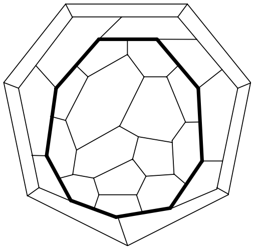
Reducibility of fullerene c-disks

- In a c-disk fullerene, a zigzag is an edge-circuit alternating left and right turns. The zigzags doubly cover the edges.
- A belt is simple circuit of 6-gons, adjacent to their neighbors on opposite faces. It is bounded by 2 disjoint simple zigzags. Call a c-DF tight if it has no a belt and reducible, otherwise.
- The belts of a full. c-thimble form a cylinder. So, c-thimbles are cuts of full. nanotubes: c-belt $\rightarrow$ two c-rings of 5-gons.
- Any simple zigzag in a tight c-disk fullerene has adjacent 5-gon on each side and intersects any other simple zigzag. So, the number of simple zigzags is at most $\frac{5(c+6)}{2}$.
- Each zigzag of a tight pure (all zigzags are simple) fullerene, is adjacent to at least two 5-gons on each side. So, their number is $\leq \frac{5(6+6)}{4}$=15. $F_{140}(I)$ has Z-vector 28^{15}.
- Besides 9 tight pure fullerenes, we have such 30-$DF_{336}(C_{6\nu})$.

Smallest pure c-disk fullerene with $15\geq c\neq 5,6$



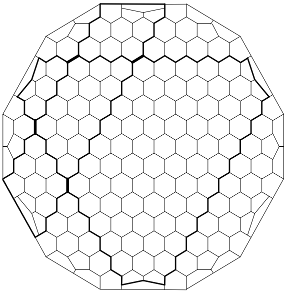
a reducible pure
7-$DF_{72}(C_1)$; $\vec{z}=(20^9,18^2)$

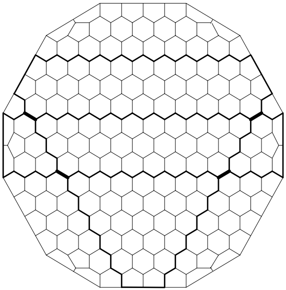


one of its reductions,
7-$DF_{54}(C_1)$; $\vec{z}=(18;144_{24,39})$

A 7-DF_{72} (unique pure c-DF with $p_6\leq 25$, $15\geq c\neq 5,6$) reduces to a tight 7-DF_{54}; any two zigzags of length $\neq 18$ intersect in two edges.

2-nd example: tight pure c-disk fullerene





tight pure 30-$DF_{336}(C_{6\nu})$
$\vec{z}$=$72, 66^2, 58^6, 56^3, 48^6$

tight 36-thimble $(C_{6\nu})$
simple zigzags: $2, 3$ bound.

Other known tight pure c-disk fullerenes are 9 fullerenes.

Fulleroids and icosahedrites

3 other interesting hyperbolic $(\{a,b,c\},k)$-spheres

Besides c-disk-fullerenes, are of interest

- lego-like fullerenes: $(\{5,6\},3)$-$\mathbb{S}^2$ in which all $12+p_6$ faces are partitioned into $p_a = 12$ or p_6 isomorphic clusters of faces

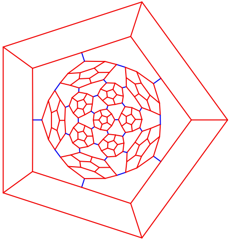
and the following fullerene relatives on $\mathbb{S}^2$ with largest faces having negative curvature:

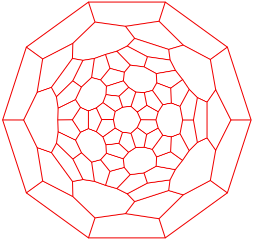
- c-superfullerenes: $(\{5,6,c\},3)$-$\mathbb{S}^2$ in which all 5- and c-gons belong to 12 isomorphic disjoint clusters of faces.
- G-fulleroids: $(\{5,b\},3)$-$\mathbb{S}^2$ with $b>6$ and given symmetry G.
- b-icosahedrites: $(\{3,b\},5)$-$\mathbb{S}^2$ with $b\geq 4$.

G-fulleroids: : $(\{5, b\}, 3)$-spheres with given symmetry G

- G-fulleroid: $(\{5, b\}, 3)$-$\mathbb{S}^2$ $(b>6)$ with group G; so, $p_b = \frac{p_5 - 12}{b-6}$.
- Fowler et al., 1993: fullerenes, seen as G-fulleroids with $b = 6$, exist for 28 groups G.
- Dress–Brinkmann, 1986: there are 2 smallest I-fulleroids with $b = 7$; they have 260 vertices
- Deza–Delgado, 2000: 2 infinite series of $\{I, I_h\}$-fulleroids and smallest ones for $b = 8, 10, 12, 14, 15$ (fullerene decorations). Jendrol–Trenkler, 2001: $\{I, I_h\}$-fulleroids for all $b \geq 8$.
- Kardos, 2007: G-fulleroids with $b = 7$ exists for 36 groups G. There are infinity of G-fulleroids for all $b \geq 7$ if and only if G is a subgroup of I_h; there are 22 types of such groups.
- There are 7 (with b=7, 7, 7, 7, 8, 8, 12) plane fulleroids, i.e. $(\{5, b\}, 3)$-$\mathbb{E}^2$, which are 2-isohedral (their symmetry group G is isomorphic to the group of combinatorial automorphisms Aut and their faces form two orbits under Aut).

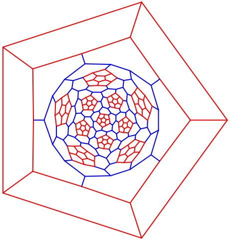
The smallest icosahedral $(5, 9)$- and $(5, 10)$-spheres

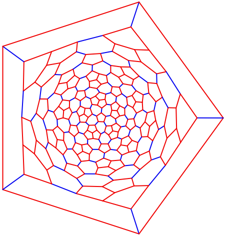




$(\{5, 9\}, 3)_{180}(I_h) = P(C_{60}(I_h))$ and $(\{5, 10\}, 3)_{140}(I_h) = T(C_{60}(I_h))$ are pentacon (subdivide each 5-gon into six 5-gons) and triacon (subdivide each 6-gon into three 5-gons) decorations of $C_{60}(I_h)$.

Dress–Brinkmann, 1996: smallest icosahedral $(\{5,7\},3)$-$\mathbb{S}^2$





$(\{5,7\},3)_{260a}(I) = P(C_{140}(I))$ and $(\{5,7\},3)_{260b}(I) = T(C_{180}(I_h))$
260*a*: a 7-superfullerene: 12 clusters of 5 7-gons around 6 6-gons

Ongoing: enumeration of lego-like fullerenes

Call a fullerene lego-like or b-lego-like if all its $p_a + p_b = 12 + p_6$ faces are partitioned into 12 or, resp., $p_6 < 12$ isomorphic clusters. So, the factor $f = \frac{p_b}{p_a} = \frac{p_6}{12}$ is an integer or, resp., inverse of integer.

- All $1, 1, 2, 6$ of, respectively, $24, 26, 28, 32$-vertex fullerenes are b-lego-like with factor $f = \frac{1}{6}, \frac{1}{4}, \frac{1}{3}, \frac{1}{2}$, respectively.
- Lego like-fullerene has $20 + 24f$ vertices; their enumeration for $f = 1, 2, 3, 4$ is ongoing (Dutour and Deza).
- Goldgerg-Coxeter fullerene $GC_{k,k-1}$ has $20(k^2+k(k\text{-}1)+1)$= $20+120\binom{k}{2}$ vertices. Its $12+60\binom{k}{2}$ faces are partitioned into 12 clusters: 5-gon surrounded by k coronas of 6-gons.
- Examples, besides above infinite series: tight pure $F_{92}(T_h)$ and many 44-vertex fullerenes, say, all of symmetry D_{3d} or D_{3h}.

New frontier: to enumerate c-superfullerenes

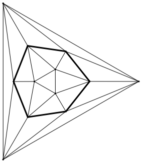
- c-superfullerenes exist iff $c \geq 5$; 5-superfullerenes are exactly fullerenes (their 12 clusters are exactly 12 pentagons). 6-superfullerenes are fullerenes with faces *partitioned* into 12 isomorphic clusters; exp. $C_{140}(I)$) (its faces occur in 12 clusters of 5 6-gons around each 5-gon) and all $GC_{k,l}$ from it.
- In Haeckel, 1887, skeletons of radiolarian zooplankton *Aulonia hexagona* are represented by $(\{5,6,7\},3)$- and $(\{5,6,8\},3)$-$\mathbb{S}^2$
- Many energy potential minimizers (in Thomson problem for n unit charged particles on sphere $\mathbb{S}^2$) and maximizers (in Tammes problem of minimum distance between n points on sphere) are dual fullerenes or dual 7-superfullerenes.
- Above $(\{5,7\},3)_{260a}(I) = P(C_{140}(I))$ with $(p_5,p_7) = (72,60)$ is the smallest icosahedral 7-superfullerene.
- In 2 IP C_{80}, I_h and D_{5h}, each 6-gon is adjacent to two 5-gons; their pentacons give two 8-superfullerenes with 200 vertices.

Icosahedrites, i.e., $(\{3,4\},5)$-spheres

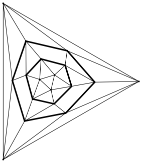
- They have $p_3 = 2p_b + 20$ and $v = 2p_b + 12$ vertices.
- Agregating $\mathbf{C_1}$=$\{C_1, C_s, C_i\}$, $\mathbf{C_m}$=$\{C_m, C_{mv}, C_{mh}, S_{2m}\}$, $\mathbf{D_m}$= =$\{D_m, D_{mh}, D_{md}\}$, $\mathbf{T}$=$\{T, T_d, T_h\}$, $\mathbf{O}$=$\{O, O_h\}$, $\mathbf{I}$=$\{I, I_h\}$, all 38 symmetries of $(\{3,4\},5)$-spheres are: $\mathbf{C_1}$, $\mathbf{C_m}$, $\mathbf{D_m}$ for $2 \le m \le 5$ and $\mathbf{T}$, $\mathbf{O}$, $\mathbf{I}$.
- p_a is fixed in for parabolic $(\{a,b\},k)$-spheres permitting Goldberg–Coxeter construction and parametrization of graphs which imply the polynomial growth of their number. It does not happen for icosahedrites; no parametrization for them.
- Their number is $1, 0, 1, 1, 5, 12, 63, 246, 1395, 7668, 45460$ for $v = 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 32$. It grows at least exponentially with v.

Proof for the number of icosahedrites

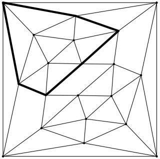
A weak zigzag ia a left/right, but never extreme, edge-circuit.
If a v-vertex icosahedrite has a simple weak zigzag of length 6, a (v+6)-vertex one come by inserting a corona (6-ring of three 4-gons alternated by three pairs of adjacent 3-gons) instead of it.
But such spheres exist for v=18, 20, 22; so, for $v \equiv 0, 2, 4 (mod\, 6)$.
There are two options of inserting corona; so, the number of v-vertex icosahedrites grows at least exponentially.



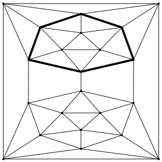
12 I_h
$wZ = 6^{10}$
$Z = 10^6$



18 D_3
$6^2, 8^3; 54_{0,9}$
$90_{27,18}$



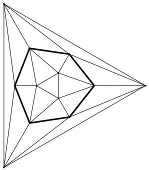
20 D_{2d}
$6^4, 20^2; 18^2_{0,3}$
$10^4; 30^2_{3,0}$



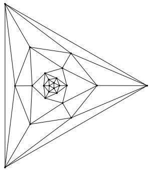
22 D_{5h}
$6^{10}; 50_{15,0}$
$10^2; 90_{15,20}$

An usual (strong) zigzag is a left/right, both extreme, edge-circuit.

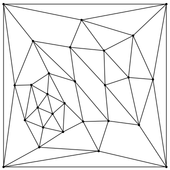
Pure (i.e. with simple $\vec{z}$ and/or $\vec{wz}$) icosahedrites are rare



12, I_h min.
$\vec{wz}$=6^{10}
$\vec{z}$= 10^6

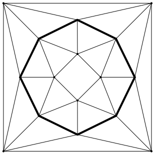


24, D_{3d} min.
$6^8, 36^2$
$6, 10^6, 18^3$

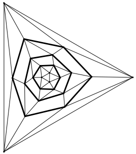


28, D_{2h} min.
$6^6, 12^4, 14^4$
$10^6, 20^4$

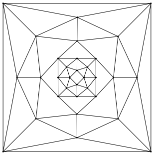
All known icosahedrites with only simple usual zigzags



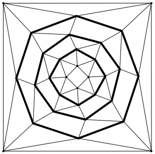
16, D_{4d} min
$\vec{wz}$= $8, 24^3$
$\vec{z}$=$40_{0,8}, 40_{8,0}$



24, S_6 min.
$6^3, 10^3, 36^2$
$60^2_{6,6}$



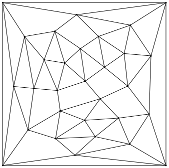
32, D_{4d}
$8^2, 24^2, 48^2$
$8; 40^2_{8,0}, 72_{0,8}$



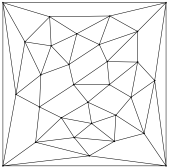
32, S_8 min.
$8^3, 40, 48^2$
$80^2_{8,8}$

Majority of icosahedrites are knotted

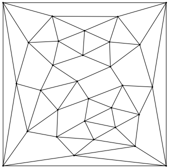
Silent majority of icosahedrites with $v \geq 28$: those of symmetry C_1 and consisting of 1 or 2 zigzags. They even include siblings (having the same $(\vec{z}, \vec{wz})$) of superknots (having $\vec{z} = \vec{wz} = 5v_{i,\frac{5v}{2}-i}$).



30, C_1
$\vec{wz}=\vec{z}=150_{41,34}$



30, C_1
$\vec{wz}=\vec{z}=150_{41,34}$

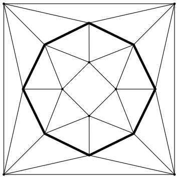


30, C_1
$\vec{wz}=\vec{z}=150_{41,34}$

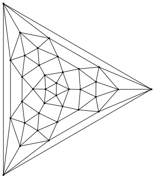
Smallest triple of superknots, which are siblings

Two problems on b-icosahedrites $(\{3, b\}, 5)$-$\mathbb{S}^2$

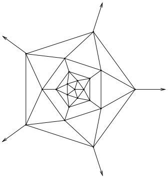
- With $(b, v; G) = (4, 24; O), (5, 60; I), (b, 4b; D_{bd})$, Snub Cube, Snub Dodecahedron and Snub $APrism_b$ with $b \geq 4$ are b-gon-transitive $(\{3, b\}, 5)$-spheres with 2 orbits of 3-gons. PROBLEM: to enumerate $(\{3, b\}, 5)$-spheres, which are b-gon-transitive and/or have at most 3 orbits of 3-gons.
- A 3-connected map is pR_i face-regular if any its p-gonal face is adjacent to exactly i of its other p-gonal faces. No $(\{3, b\}, 5)$-sphere, besides Icosahedron $3R_3$, is $3R_i$ but there is infinity of bR_i $(\{3, b\}, 5)$-spheres for $i = 0, 1, 2$. PROBLEM: to describe bR_i $(\{3, b\}, 5)$-spheres with $2 < i < b$.



$4R_0$: $G_4 = 2K_1$



$4R_1$: $G_4 = 6K_2$



$4R_2$: $G_4 = C_5$

Parabolic $(\{a, b\}, k)$-maps on surfaces

Parabolic (R,k)-maps

- Given $R \subset \mathbb{N}$ and a surface $\mathbb{F}^2$, an (R,k)-$\mathbb{F}^2$ is a k-regular map M on surface $\mathbb{F}^2$ whose faces have gonalities $i \in R$.
- Euler characteristic $\chi(M)$ is $v-e+f$, where v, e and $f=\sum_i p_i$ are the numbers of vertices, edges and faces of M.
- Since $kv{=}2e{=}\sum_i ip_i$, Euler formula $\chi = v - e + f$ becomes Gauss-Bonnet-like one $\chi(M) = \sum_i p_i\kappa_i$.
- Again, let our maps be parabolic, i.e., $\min_{i\in R}(1+\frac{i}{k}-\frac{i}{2})=0$. So, $M{=}max\{i \in R\}{=}\frac{2k}{k-2}$ and $(M,k){=}(6,3), (4,4), (3,6)$.
- There are infnity of parabolic maps (R,k)-$\mathbb{F}^2$, since the number p_M of *flat* ($\kappa_M{=}0$) faces is not restricted.
- So, $\chi(\mathbb{F}^2) \geq 0$. But all such connected *closed* (compact and without boundary) irreducible surfaces $\mathbb{F}^2$ are: sphere $\mathbb{S}^2$, torus $\mathbb{T}^2$ (two orientable), real projective plane $\mathbb{P}^2$ and Klein bottle $\mathbb{K}^2$ with $\chi=2,0,1,0$, respectively.
- Also, $\chi(\mathbb{F}^2)=0$, i.e. $\mathbb{F}^2$ is $\mathbb{T}^2$ or $\mathbb{K}^2$, if and only if $R=\{m\}$.

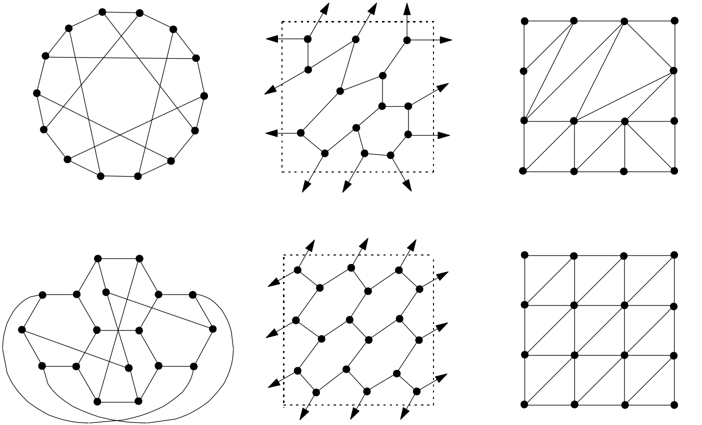
The $(\{a, b\}, k)$-maps on torus and Klein bottle

So, $\{a, b\}, k)$-$\mathbb{T}^2$ and $(\{a, b\}, k)$-$\mathbb{K}^2$ have $a = b = \frac{2k}{k-2}$ and $(a = b, k)$ should be $(6, 3), (3, 6)$ or $(4, 4)$.

We consider only polyhedral maps, i.e. no loops or multiple edges (1- or 2-gons), and any two faces intersect in edge, point or $\emptyset$ only.

Smallest such $\mathbb{T}^2$- and $\mathbb{K}^2$-maps for $(a{=}b, k){=}(4, 4), (6, 3), (3, 6)$:
as 4-regular quadrangulations: K_5 and $K_{2,2,2}$ $(p_4 = 5, 6)$;
as 6-regular triangulations: K_7 and $K_{3,3,3}$ $(p_3 = 14, 18)$;
as 3-regular polyhexes: Heawood graph (dual K_7) and dual $K_{3,3,3}$ $(p_6{=}7, 9)$. Two those graphs are the smallest $\mathbb{T}^2$- and $\mathbb{K}^2$-fullerenes

Smallest $\mathbb{T}^2$- and $\mathbb{K}^2$-fullerenes: dual K_7 and dual $K_{3,3,3}$



3-regular polyhexes on $\mathbb{T}^2$, cylinder, Möbius surface, $\mathbb{K}^2$ are $\{6^3\}$'s quotients by fixed-point-free group of isometries, generated by: two translations, a transl., a glide reflection, transl. *and* glide reflection.

8 parabolic families on the projective plane

(R, k)-maps on the projective plane are the antipodal quotients of centrally symmetric (R, k)-$\mathbb{S}^2$; so, halving their p-vector and v.

The point symmetry groups with inversion operation are: T_h, O_h, I_h, C_{mh}, D_{mh} with even m and D_{md}, S_{2m} with odd m. So, they are

1. 9 for $\{5, 6\}_v$: C_i, C_{2h}, D_{2h}, D_{3d}, D_{6h}, S_6, T_h, D_{5d}, I_h
2. 7 for $\{2, 3\}_v$: C_i, C_{2h}, D_{2h}, D_{3d}, D_{6h}, S_6, T_h
3. 6 for $\{4, 6\}_v$: C_i, C_{2h}, D_{2h}, D_{3d}, D_{6h}, O_h
4. 6 for $\{3, 4\}_v$: C_i, C_{2h}, D_{2h}, D_{3d}, D_{4h}, O_h
5. 2 for $\{2, 4\}_v$: D_{2h}, D_{4h}
6. 1 for $\{3, 6\}_v$: D_{2h}
7. 0 for $\{2, 6\}_v$ and $\{1, 3\}_v$
8. Cf. 12 for icosahedrites $((\{3, 4\}, 5)$-spheres$)$:
   C_i, C_{2h}, C_{4h}, D_{2h}, D_{4h}, D_{3d}, D_{5d}, S_6, S_{10}, T_h, O_h, I_h

6 parabolic families $(\{a,b\},k)$-$\mathbb{P}^2$: 1-parameterization

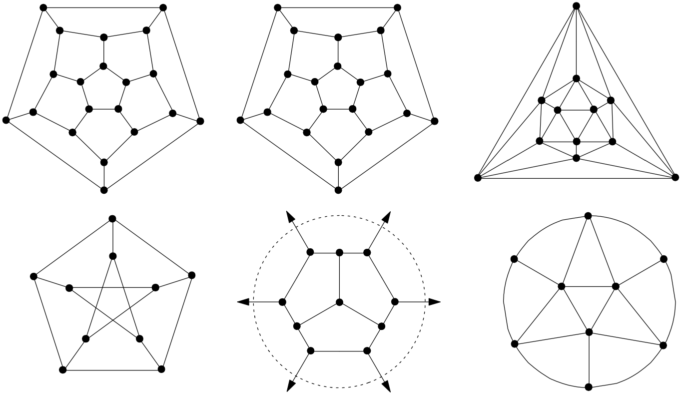
1. $\{5,6\}_v$: C_i, C_{2h}, D_{2h}, S_6, D_{3d}, D_{6h}, T_h, D_{5d}, I_h
2. $\{2,3\}_v$: C_i, C_{2h}, D_{2h}, S_6, D_{3d}, D_{6h}, T_h
3. $\{4,6\}_v$: C_i, C_{2h}, D_{2h}, D_{3d}, D_{6h}, O_h
4. $\{3,4\}_v$: C_i, C_{2h}, D_{2h}, D_{3d}, D_{4h}, O_h
5. $\{2,4\}_v$: D_{2h}, D_{4h}
6. $\{3,6\}_v$: D_{2h}

$(\{2,3\},6)$-spheres T_h and D_{6h} are $GC_{k,k}(2 \times \mathit{Tetrahedron})$ and, for $k \equiv 1,2 \pmod 3$, $GC_{k,0}(6 \times K_2)$, respectively. Other spheres of blue symmetry are $GC_{k,l}$ with $l = 0, k$ from the first such sphere.

So, each of 7 blue-symmetric families is described by one natural parameter k and contains $O(\sqrt{v})$ spheres with at most v vertices.

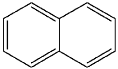
Petersen graph is the smallest projective plane's fullerene

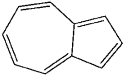
The smallest maps for $(\{a, b\}, k)$=$(\{5, 6\}, 3), (\{3, 4\}, 5), (\{4, 6\}, 3)$ are: Petersen graph (dual K_6), K_6 (half-Icosahedron; smallest $\mathbb{P}^2$-triangulation), K_4 (smallest $\mathbb{P}^2$-quadrangulation), i.e., the antipodal quotients of Dodecahedron, Icosahedron and Cube.

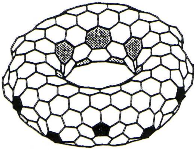


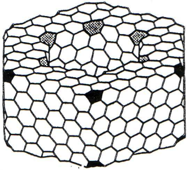
Two other $(\{5,6,c\},3)$-$\mathbb{F}^2$ used in Chemistry

- Azulenoids: $(\{5,6,7\},3)$-$\mathbb{T}^2$; so, $g{=}1$, $p_5{=}p_7$ (Kirby–Diudea, 2003, et al.), since *naftalen* and *azulen* are $C_{10}H_8$ isomers.









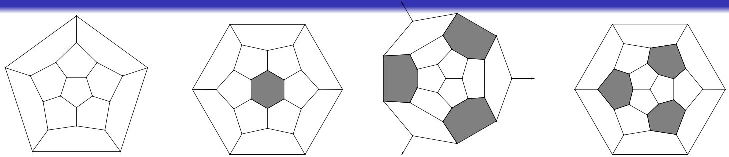
- Schwartzits: $(\{5,6,c\},3)$-$\mathbb{F}^2$ on minimal surfaces $\mathbb{F}^2$ of constant negative curvature ($g \geq 2$) with $c \geq 7$ (Terrones–MacKay, 1997, et al.)
  Knor et al., 2010: such $(\{6,c\},3)$-maps exist for any $g{\geq}2$, $p_6{\geq}0$ and $c{=}7,8,9,10,12$. For $c{=}7,8$ polyhedral maps exist.
  Analog of icos. fullerenes: $(\{6,7\},3)_v$ on D-surface, $g{=}3$, with $v{=}56(p^2{+}pq{+}q^2)$, starting with Klein regular map $\{7^3\}$.

Plane and space fullerenes

(Euclidean) plane fullerenes $(\{5,6\},3)$-$\mathbb{E}^2$

- An $(\{a,b\},k)$-$\mathbb{E}^2$ is a k-regular tiling of $\mathbb{E}^2$ by a- and b-gons.
- $(\{a,b\},k)$-$\mathbb{E}^2$ have $p_a \leq \frac{b}{b-a}$ and $p_b = \infty$. It follows from Alexandrov, 1958: any metric on $\mathbb{E}^2$ of non-negative curvature can be realized as a metric of convex surface on $\mathbb{E}^3$. In fact, 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-$\mathbb{S}^2$.
- There are ∞ of $(\{a,b\},k)$-$\mathbb{E}^2$ if $2 \leq p_a \leq \frac{b}{b-a}$ and 1 if $p_a = 0, 1$.
- For plane fullerenes (or *nanocones*) $(\{5,6\},3)$-$\mathbb{E}^2$, the number of *equivalence* (isomorphic up to a finite induced subgraph) classes is (Klein–Balaban, 2007) $2,2,2,1$ if $p_5 = 2,3,4,5$, resp.
- Nanotubes (case $p_5 = 6$) come by rolling up the graphite $\{6^3\}$.
- There are 7 (with $b = 7,7,7,7,8,8,12$) plane fulleroids, i.e. $(\{5,b\},3)$-$\mathbb{E}^2$, which are 2-isohedral (symmetry $G \approx Aut$ and faces form 2 orbits under comb. automorphisms group Aut).

General and FK space fullerenes



20, I_h 24 D_{6d} 26, D_{3h} 28, T_d

- Space fullerene is a 3-periodic 4-regular $\mathbb{E}^3$-tiling by fullerenes.
- FK space fullerene is such tiling by 4 Frank-Kasper fullerenes.
- They appear in crystallography of alloys (Frank–Kasper, 1958) clathrate hydrates, zeolites and bubble structures.
- Main cases A_{15}, C_{15}: clathrate hydrates of type I, II; zeolites MEP, MTN; metallic alloys, say, Cr_3Si, $MgCu_2$, respectively. Their *unit cells*: 2 F_{20}+6 F_{24} and 16 F_{20}+8 F_{28} cells, resp.
- Gravicenters of F_{20}'s in A_{15} form the bcc network A_3^*, while those of F_{28}'s in C_{15} form the diamond network, i.e., bi-lattice D-complex, or α_3-centered A_3/fcc network.
- Oceanic methane hydrate (of type I, i.e., A_{15}) contains 500-2500 Gt carbon; cf. $\sim$230 for other natural gas sources.

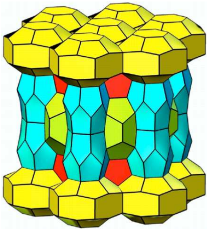
12 of 27 known before and 108 new FK space fullerenes

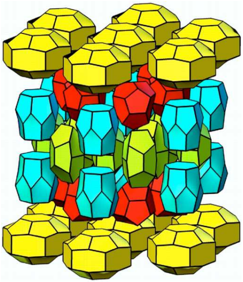
t.c.p.	clathrate exp.alloy	sp. group	$\overline{f}$	F_{20}:F_{24}:F_{26}:F_{28}	n	found
A_{15}	type I Cr_3Si	$Pm\overline{3}n$	13.50	1, 3, 0, 0	8	+
C_{15}	type II $MgCu_2$	$Fd\overline{3}m$	13.(3)	2, 0, 0, 1	24	+
C_{14}	type V $MgZn_2$	$P6_3/mmc$	13.(3)	2, 0, 0, 1	12	+
Z	type IV Zr_4Al_3	$P6/mmm$	13.43	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	

Dutour–Deza–Delgado, 2009, and Dutour–Deza, 2011, found 121 FK structures (including 13 among 27 known before) with $N \leq 21$ FK fullerenes in *reduced* (replacing automorphism group by its Biberbach, i.e. torsion-free, subgroup) fundamental domain.

First known non-FK space fullerene (Deza–Shtogrin, 1999)

Called now MDS, it is $\mathbb{E}^3$-tiling by F_{20}, F_{24} and its elongation $F_{36}(D_{6h})$ in ratio 7 : 2 : 1. Its mean face-size $\overline{s}\approx 5.091$ and mean number of faces in cell $\overline{f}=13.2$ are closest known to $\overline{s}=5$, $\overline{f}=12$ of impossible $\mathbb{E}^3$-tiling by F_{20} (cf. 120-*cell*), i.e. to lowest energy.





Delgado–O'Keeffe, 2006: all space fullerenes with $t \leq 7$ vertex orbits are 4 FK ($A_{15}, C_{15}, Z, C_{14}$) and MDS. O'Keeffe et al., 2010, on RCSR database: 7 new non-FK space fullerenes with $9 \leq t \leq 11$.

New frontier: to enumerate generalized perovskites

- 4-regular fullerene analogs: octahedites, i.e. 4-regular polyhedra with only 3- and 4-gonal faces; so, $p_3 = 8$.
- All octahedites without adjacent 4-gons: Octahedron $APrism_3$, $APrism_4$, $APrism_3^2$ and Cuboctahedron.
- Space octahedrite: 6-regular (octahedral, instead of tetrahedral, star) 3-periodic $\mathbb{E}^3$-tiling by them.
- Example: such tiling by Octahedron and Cuboctahedron, in proportion 1:1, is one of 28 uniform (vertex-transitive ones and by Platonic or semi-regular polyhedra) $\mathbb{E}^3$-tilings. Also, it is the mineral perovskite structure ABX_3, where anion X bonds to cations A, B. $MgSiO_3$ is the most abundant solid phase in the Earth, making $\approx 80\%$ of the lower mantle.
- To find other space octahedrites, it will require new tools.

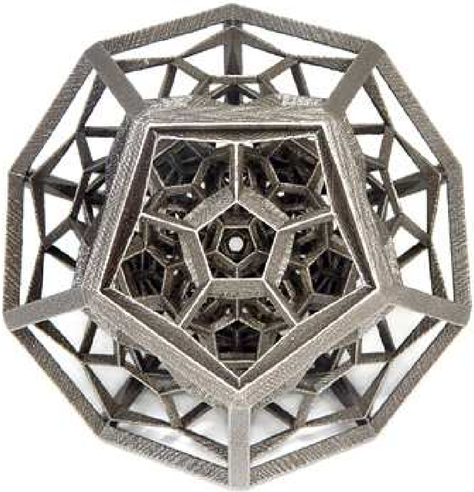
Fullerene manifolds

Fullerene manifolds

d-fullerene: (d-1)-dimensional d-valent compact connected manifold (loc. homeomorphic to $\mathbb{R}^{d-1}$) with 5- or 6-gonal 2-faces. Any its face is polytopal i-fullerene, $i \leq d$; so, $d \in \{2,3,4,5\}$, since (Kalai, 1990) any 5-polytope has a 3- or 4-gonal 2-face. Space fullerenes are 4-fullerenes in $\mathbb{E}^3$. Non-euclidean analogs are:

- Regular tilings of $\mathbb{S}^3$ by F_{20} (120-cell $\{533\}$) and of $\mathbb{H}^3$ by right-angled F_{24} (the *Löbell space* is its quotient).
- The *"greatest polyhex"*: convex hull, on the orosphere, of vertices of plane tiling $\{6^3\}$ (regular honeycomb $\{633\}$ in $\mathbb{H}^3$)
- The *"greatest polypent"*: tiling $\{5333\}$ of $\mathbb{H}^4$ by 120-cell and (a finite 5-fullerene) its quotient by the symmetry group; (a compact 4-manifold tiled by a finite number of 120-cell's).

Projection of 120-cell in 3-space



$\{533\}$: 600 vertices, 120 dodecahedral facets, $|Aut| = 14,400$

4- and 5-fullerenes

- All known finite 4-fullerenes are "mutations" of 120-cell by interfering in one of ways to construct it: tubes of 120-cells, coronas, inflation-decoration method, etc.
  Some putative facets: $F_n(G)$ with (n, G)=(20,I_h), (24,D_{6h}), (26,D_3), (28,T_d), (30,D_{5h}), (32,D_{3h}), (36,D_{6h}).
- All known 5-fullerenes come from $\{5333\}$'s by following ways.
  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 $\mathbb{R} \times \mathbb{S}^3$ (so, simply-connected).
  Finite compact ones: the quotients of $\{5333\}$ by its symmetry group (partitioned into 120-cells) and some gluings of them.

Quotient d-fullerenes

- Selberg, 1960, Borel, 1963: if a discrete group of motions of a symmetric space has a compact fundamental domain, then it has a torsion-free normal subgroup of finite index.
- So, the *quotient* of a d-fullerene by such symmetry group (its points are group orbits) is a finite d-fullerene.
- Exp. 1: Polyhexes on $\mathbb{T}^2$, cylinder, Möbius surface and $\mathbb{K}^2$ are the quotients of $\{6^3\}$ by discontinuous fixed-point-free group of isometries, generated by: 2 translations, a translation, a glide reflection, translation *and* glide reflection, respectively.
- Exp 2: Poincaré dodecahedral space: the quotient of 120-cell by I_h ; so, its f-vector is $(5, 10, 6, 1) = \frac{1}{120}\mathrm{f}(120\text{-cell})$.