Fullerenes: applications and generalizations

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I. General setting
A $d$-polytope: the convex hull of a finite subset of $\mathbb{R}^d$.

A face of $P$ is the set $\{x \in P : f(x) = 0\}$ where $f$ is linear non-negative function on $P$.

A face of dimension $i$ is called $i$-face; for $i=0, 1, 2, d-2, d-1$ it is called, respectively, vertex, edge, face, ridge and facet.
The skeleton of polytope $P$ is the graph $G(P)$ formed by vertices, with two vertices adjacent if they form an edge. $d$-polytopes $P$ and $P'$ are of the same combinatorial type if $G(P) \cong G(P')$.

The dual skeleton is the graph $G^*(P)$ formed by facets with two facets adjacent if their intersection is a ridge. (Poincaré) dual polytopes $P$ and $P^*$ on sphere $S^{d-1}$: $G^*(P) = G(P^*)$.

Steinitz’s theorem: a graph is the skeleton of a 3-polytope if and only if it is planar and 3-connected, i.e., removing any two edges keep it connected.
Regular $d$-polytopes:
self-dual $d$-simplex $G(\alpha_d) = K_{d+1}$,
$d$-cube $G(\gamma_d) = H_d = (K_2)^d$ and
its dual $d$-cross-polytope $G(\beta_d) = K_{2d} - dK_2$. 
Euler formula

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

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

For a polyhedron (3-polytope on $S^2$), it is $f_0 - f_1 + f_2 = 2$.

$p$-vector: $(p_3, \ldots)$ where $p_i$ is number of $i$-gonal faces.

$v$-vector: $(v_3, \ldots)$ where $v_i$ is number of $i$-valent vertices.

So, $f_0 = \sum_{i\geq 3} v_i$, $f_2 = \sum_{i\geq 3} p_i$ and $2f_1 = \sum_{i\geq 3} iv_i = \sum_{i\geq 3} ip_i$.

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

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

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

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

buckminsterfullerene $C_{60}(I_h)$

truncated icosahedron, soccer ball

$F_{36}(D_{6h})$

elongated hexagonal barrel

$F_{24}(D_{6d})$
The range of fullerenes

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

Graphite lattice $(6^3)$ as $F_{\infty}$: the “largest fullerene"
Finite isometry groups

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

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

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

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

(point group) \( \text{Isom}(P) \subset \text{Aut}(G(P)) \) (combinatorial group)

Theorem (Mani, 1971)

Given a 3-connected planar graph \( G \), there exist a 3-polytope \( P \), whose group of isometries is isomorphic to \( \text{Aut}(G) \) and \( G(P) = G \).

All groups for fullerenes (Fowler et al) are:

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

24, $D_{6d}$

26, $D_{3h}$

28, $D_2$

28, $T_d$

30, $D_{5h}$

30, $C_{2v}$

30, $C_{2v}$
$A C_{540}$
What nature wants?

Fullerenes or their duals appear in Architecture and nanoworld:

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

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

**Conjecture**: FULLERENES
Almost all optimizers for Thomson and Tammes problems, in the range $25 \leq n \leq 125$ are fullerenes.

For $n > 125$, appear 7-gonal faces; for $n > 300$: almost always.

However, J. Graver, 2005: in all large optimizers, the 5- and 7-gonal faces occurs in 12 distinct clusters, corresponding to a unique underlying fullerene.
Skyrmions and fullerenes

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

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

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

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

Polyhedron of greatest volume $V$ with a given number of faces and a given surface $S$?

Polyhedron of least volume with a given number of faces circumscribed around the unit sphere?

Maximize Isoperimetric Quotient for solids. Schwarz, 1890:

$$IQ = 36 \pi \frac{V^2}{S^3} \leq 1 \text{ (with equality only for sphere)}$$

In Biology: the ratio $\frac{V}{S}$ ($= \frac{r}{3}$ for spherical animal of radius $r$) affects heat gain/loss, nutrient/gas transport into body cells and organism support on its legs.
Isoperimetric problem for polyhedra

<table>
<thead>
<tr>
<th>polyhedron</th>
<th>$IQ(P)$</th>
<th>upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tetrahedron</td>
<td>$\frac{\pi}{6\sqrt{3}} \simeq 0.302$</td>
<td>$\frac{\pi}{6\sqrt{3}}$</td>
</tr>
<tr>
<td>Cube</td>
<td>$\frac{\pi}{6} \simeq 0.524$</td>
<td>$\frac{\pi}{6}$</td>
</tr>
<tr>
<td>Octahedron</td>
<td>$\frac{\pi}{3\sqrt{3}} \simeq 0.605$</td>
<td>$\simeq 0.637$</td>
</tr>
<tr>
<td>Dodecahedron</td>
<td>$\frac{\pi\tau^{7/2}}{3.55^{4/2}} \simeq 0.755$</td>
<td>$\frac{\pi\tau^{7/2}}{3.55^{4/2}}$</td>
</tr>
<tr>
<td>Icosahedron</td>
<td>$\frac{\pi\tau^{4}}{15\sqrt{3}} \simeq 0.829$</td>
<td>$\simeq 0.851$</td>
</tr>
</tbody>
</table>

IQ of Platonic solids

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

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

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

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

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

\[
\Gamma\left(\frac{n}{2}\right) = \begin{cases} 
\frac{(n/2)!}{\sqrt{\pi}} & \text{for even } n \\
\frac{\sqrt{\pi} (n-2)!!}{2^{n/2}} & \text{for odd } n
\end{cases}
\]
Five Platonic solids

- OCTAHEDRON: Air
- CUBE: Earth
- TETRAHEDRON: Fire
- DODECAHEDRON: the Universe
- ICOSAHEDRON: Water
**Goldberg Conjecture**

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

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

<table>
<thead>
<tr>
<th>polyhedron</th>
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<th>upper bound</th>
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</thead>
<tbody>
<tr>
<td>Dodecahedron $F_{20}(I_h)$</td>
<td>$\frac{\pi \tau^{7/2}}{3.5^{5/4}} \simeq 0.755$</td>
<td>$\frac{\pi \tau^{7/2}}{3.5^{5/4}}$</td>
</tr>
<tr>
<td>Truncated icosahedron $C_{60}(I_h)$</td>
<td>$\simeq 0.9058$</td>
<td>$\simeq 0.9065$</td>
</tr>
<tr>
<td>Chamfered dodecahedron $C_{80}(I_h)$</td>
<td>$\simeq 0.928$</td>
<td>$\simeq 0.929$</td>
</tr>
<tr>
<td>Sphere</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>
II. Icosahedral fullerenes
Icosahedral fullerenes

Call icosahedral any fullerene with symmetry $I_h$ or $I$

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

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

$C_{80}(I_h) = (2, 0)$-dodecahedron
chamfered dodecahedron
$C_{60}(Ih)$: (1, 1)-dodecahedron

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

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

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

Call icosadeltahedron the dual of an icosahedral fullerene $C^*_20T(I_h)$ or $C^*_20T(I)$.

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

Dual $C^*_60(I_h)$, $(a, b) = (1, 1)$

pentakis-dodecahedron

GRAVIATION (Esher 1952)

omnicapped dodecahedron
**Icosadeltahedra in Architecture**

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

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

US pavilion, World Expo 1967, Montreal

Spaceship Earth, Disney World’s Epcot, Florida
Icosadeltahedra $C^*_n$ with $a = 2$

$Icosadeltahedra \ C^*_n$ with $a = 2$

$Icosadeltahedra \ C^*_n$ with $a = 2$

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$Icosadeltahedra \ C^*_n$ with $a = 2$

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$Icosadeltahedra \ C^*_n$ with $a = 2$

$Icosadeltahedra \ C^*_n$ with $a = 2$
$C_{60}(I_h)$ in leather

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

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

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

$C_{180}^*(I_h)$ as omnicapped buckminsterfullerene $C_{60}$
Triangulations, spherical wavelets

Dual 4-chamfered cube
$(a, b) = (2^4 = 16, 0), O_h$

Dual 4-cham. dodecahedron
$C_{5120}^*, (a, b) = (2^4 = 16, 0), I_h$

Used in Computer Graphics and Topography of Earth
III. Fullerenes in Chemistry and Biology
Fullerenes in Chemistry

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

- **Graphite sheet**: bi-lattice $(6^3)$, Voronoi partition of the hexagonal lattice $(A_2)$, “infinite fullerene”

- **Diamond packing**: bi-lattice $D$-complex, $\alpha_3$-centering of the lattice f.c.c. = $A_3$

- **Fullerenes**: 1985 (Kroto, Curl, Smalley): Cayley $A_5$, $C_{60}(I_h)$, tr. icosahedron, football; Nobel prize 1996 but Ozawa (in japanese): 1984. “Cheap” $C_{60}$: 1990. 1991 (Iijima): nanotubes (coaxial cylinders). Also isolated chemically by now: $C_{70}$, $C_{76}$, $C_{78}$, $C_{82}$, $C_{84}$. If $> 100$ carbon atoms, they go in concentric layers; if $< 20$, cage opens for high temperature. Full. alloys, stereo org. chemistry, carbon: semi-metal.
Allotropes of carbon

- **Diamond**: cryst. tetrahedral, electro-isolating, hard, transparent. Rarely $> 50$ carats, unique $> 800ct$: Cullinan $3106ct = 621g$. Kuchner: diamond planets?

- **Hexagonal diamond** (lonsdaleite): cryst. hex., very rare; 1967, in shock-fused graphite from several meteorites

- **ANDR** (aggregated diamond nanorods): 2005, hardest

- **Graphite**: cryst. hexagonal, soft, opaque, el. conducting

- **Graphene**: 2004, $2D$-carbon 1-atom thick, very conduc. and strained into semiconducting is better than silicon

- **Amorphous carbon** (no long-range pattern): synthetic; coal and soot are almost such

- **Fullerenes**: 1985, spherical; only soluble carbon form

- **Nanotubes**: 1991, cylindric, few nm wide, upto few mm; **nanobudes**: 2007, nanotubes combined with fullerenes
Allotropes of carbon: pictures

a) Diamond  
b) Graphite  
c) Lonsdaleite  
d) $C_{60}$  
e) $C_{540}$  
f) $C_{70}$  
g) Amorphous carbon  
h) single-walled carbon nanotube
The (n,m) nanotube is defined by the vector $C_h = na_1 + ma_2$ in infinite graphene sheet $\{6^3\}$ describing how to roll it up; $T$ is the tube axis and $a_1, a_2$ are unit vectors of $\{6^3\}$ in 6-gon. It is called zigzag, chiral, armchair if $m=0$, $0<m<n$, $m=n$ resp.
Other allotropes of carbon

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

graphite:  

diamond:
Carbon and Anthropic Principle

- Nucleus of lightest elements H, He, Li, Be (and Boron?) were produced in seconds after Big Bang, in part, by scenario: Deuterium $H^2$, $H^3$, $He^3$, $He^4$, $H$, $Li^7$. If weak nuclear force was slightly stronger, 100% hydrogen Univers; if weaker, 100% helium Univers.

- Billion years later, by atom fusion under high $t^0$ in stars

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

(12 nucleons, i.e., protons/neutrons), then Ni, O, Fe etc.

"Happy coincidence": energy level of C $\simeq$ the energies of 3 He; so, reaction was possible/probable.

- Without carbon, no other heavy elements and life could not appear. $C$: 18.5% of human (0.03% Universe) weight.
La$_{C_{82}}$
first Endohedral Fullerene compound

$C_{10}Ph_9OH$
Exohedral Fullerene compound (first with a single hydroxy group attached)
First non-preferable fullerene compound

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

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

*In silico*: from $C_{60}$ and $F_{40}(T_d)$; cf. 2 atoms in quasicrystals
### Onion-like metallic clusters

#### Palladium icosahedral 5-cluster

\[ Pd_{561}L_{60}(O_2)_{180}(OAc)_{180} \]

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

### Icosahedral and cuboctahedral metallic clusters
Nanotubes and Nanotechnology

Helical graphite  Deformed graphite tube
Nested tubes (concentric cylinders) of rolled graphite; use(?): for composites and “nanowires”
Applications of nanotubes/fullerenes

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

- **El. conductivity** of alcali-doped $C_{60}$: insulator $K_2C_{60}$ but superconductors $K_3C_{60}$ at $18K$ and $Rb_3C_{60}$ at $30K$ (however, it is still too low transition $T_c$)

- **Catalists for hydrocarbon upgrading** (of heavy oils, methane into higher HC, thermal stability of fuels etc.)

- **Pharmaceceuticals**: protease inhibitor since derivatives of $C_{60}$ are highly hydrophobic and antioxidant (they soak cell-damaging free radicals)

- **Superstrong materials, nanowires?**

- **Now/soon**: buckyfilms, sharper scanning microscope
Nanotubes/fullerenes: hottest sci. topics

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

Chem. compounds ranking: \( C_{60} \) 5.2, gallium nitride 2.1, …

\( h \)-index of a topic, compound or a scholar is the highest number \( T \) of published articles on this topic, compound or by this scholar that have each received \( \geq T \) citations.

\( h \)-\( b \) index of a topic or compound is \( h \)-index divided by the number of years that papers on it have been published.
Chemical context

- **Crystals**: from basic units by symm. operations, incl. translations, excl. order 5 rotations (“cryst. restriction”). Units: from few (inorganic) to thousands (proteins).

- Other very symmetric mineral structures: **quasicrystals**, **fullerenes** and like, icosahedral packings (no translations but rotations of order 5).

- Fullerene-type polyhedral structures (polyhedra, nanotubes, cones, saddles, …) were first observed with carbon. But also inorganic ones were considered: boron nitrides, tungsten, disulphide, allumosilicates and, possibly, fluorides and chlorides. May 2006, Wang-Zeng-al.: first **metal hollow cages** $Au_n = F_{2n-4}^*$ $(16 \leq n \leq 18)$. $F_{28}^*$ is the smallest; the gold clusters are flat if $n < 16$ and compact (solid) if $n > 18$. 

- p. 48
Stability of fullerenes

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

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

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

The best $I$-structure: same number of positive and negative eigenvalues.
Fullerene Kekule structure

- **Perfect matching** (or 1-factor) of a graph is a set of disjoint edges covering all vertices. A Kekule structure of an organic compound is a perfect matching of its carbon skeleton, showing the locations of double bonds.

- A set $H$ of disjoint 6-gons of a fullerene $F$ is a **resonant pattern** if, for a perfect matching $M$ of $F$, any 6-gon in $H$ is $M$-alternating (its edges are alternatively in and off $M$).

- **Fries number** of $F$ is maximal number of $M$-alternating hexagons over all perfect matchings $M$; **Clar number** is maximal size of its resonant pattern.

- A fullerene is $k$-resonant if any $i \leq k$ disjoint hexagons form a resonant pattern. Any fullerene is 1-resonant; **conjecture**: any preferable fullerene is 2-resonant. Zhang et al, 2007: all 3-resonant fullerenes: $C_{60}(I_h)$ and a $F_{4m}$ for $m = 5, 6, 7, 8, 9, 9, 10, 12$. All 9 are $k$-resonant for $k \geq 3$. 
Life fractions

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

<table>
<thead>
<tr>
<th></th>
<th>Atom</th>
<th>DNA</th>
<th>Cryo-EM</th>
<th>Prion</th>
<th>Virus capsides</th>
</tr>
</thead>
<tbody>
<tr>
<td>size nm</td>
<td>≃ 0.25</td>
<td>≃ 2</td>
<td>≃ 5</td>
<td>11</td>
<td>20 – 50 – 100 – 400</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>SV40, HIV, Mimi</td>
</tr>
</tbody>
</table>

- **Viruses**: 4th domain (Acytota)?
  But crystals also self-assembly spontaneously.

- **Viral eukaryogenesis** hypothesis (Bell, 2001).
Icosahedral viruses

- Virus: *virion*, then (rarely) cell parasite.
- Watson and Crick, 1956: "viruses are either spheres or rods". In fact, all, except most complex (as brick-like pox virus) and enveloped (as conic HIV) are helical or ($\approx \frac{1}{2}$ of all) icosahedral.
- Virion: protein shell (*capsid*) enclosing genome (RNA or DNA) with $3 - 911$ protein-coding genes.
- Shere-like capsid has $60T$ protein subunits, but EM resolves only clusters (*capsomers*), incl. 12 *pentamers* (5 bonds) and 6-mers; plus, sometimes, 2- and 3-mers.
- Bonds are flexible: $\sim 5^0$ deviation from mean direction. Self-assembly: slight but regular changes in bonding.
Caspar- Klug (quasi-equivalence) principle: virion minimizes by organizing capsomers in min. number $T$ of locations with non-eqv. bonding. Also, icosah. group generates max. enclosed volume for given subunit size. But origin, thermodynamics and kinetics of this self-assembly is unclear. Modern computers cannot evaluate capsid free energy by all-atom simulations.)

So, capsomers are $10T + 2$ vertices of icosadeltahedron $C^*_{20T}$, $T = a^2 + ab + b^2$ (triangulation number). It is symmetry of capsid, not general shape (with spikes).

Lower pseudo-equivalence when 2-, 3-mers appear and/or different protein type in different locations.

Hippocrates: disease = icosahedra (water) body excess
# Capsids of icosahedral viruses

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

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

Foot-and-Mouth virus, $T = 3$
Viruses with (pseudo) $T = 3$

Poliovirus (polyomyelitis)

Human Rhinovirus (cold)
Viruses with $T = 4$

Human hepatitis B

Semliki Forest virus
More $T = a^2$ viruses

Sindbis virus,
$T = 4$

Herpes virus,
$T = 16$
Human and simian papilloma viruses

Polyoma virus,  
\[ T = 7d \]

Simian virus 40,  
\[ T = 7d \]
Viruses with $T = 13$

Rice dwarf virus

Bluetongue virus
Viruses with $T = 25$

PRD1 virus

Adenovirus (with its spikes)
More $I_h$-viruses

Pseudomonas phage phiKZ,  
$T = 27$

HTLV1 virus,  
$T = 36$
Special viruses

Archeal virus STIV, $T = 31$

Algal chlorella virus PBCV1 (4th: $\approx 331,000$ bp), $T = 169$

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

Capsid core

Shape (spikes): $T \simeq 71$?
Mimivirus and other giants

Largest (400nm), >150 (bacteria *Micoplasma genitalium*), \(\frac{1}{30}\) of its host *Acanthamoeba Polyphaga* (record: \(\frac{1}{10}\)).

Largest genome: 1,181,404 bp; 911 protein-coding genes >182 (bacterium *Carsonella ruddii*). Icosahedral: \(T = 1179\)

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

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

Mathematical Chemistry use following fullerene-like maps:

- **Polyhedra** $(p_5, p_6, p_n)$ for $n = 4, 7$ or $8$ ($v_{\min} = 14, 30, 34$)
- Aulonia hexagona (E. Haeckel 1887): plankton skeleton

- **Azulenoids** $(p_5, p_7)$ on torus $g = 1$; so, $p_5 = p_7$

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

$(p_5, p_6, p_7) = (12, 142, 12)$,
$v = 432, D_{6d}$
Schwarzits \((p_6, p_7, p_8)\) on minimal surfaces of constant negative curvature \((g \geq 3)\). We consider case \(g = 3\):

![Schwarz P-surface](image1)

![Schwarz D-surface](image2)

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

\( D_{168} \): putative carbon, 1992, (Vanderbilt-Tersoff)

\[ (p_6, p_7 = 24), \quad v = 2p_6 + 56 = 56(p^2 + pq + q^2) \]

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

\( D_{56}, D_{168} \) and \((6, 7)\)-surfaces are analogs of \(F_{20}(I_h), F_{60}(I_h)\)
and icosahedral fullerenes.
(6, 8)-surfaces

Starting with (1, 0):

\[ P48 \text{ with } p_6 = 8 \]

while unit cell with \( p_6 = 0 \) is \( P32 \)-Dyck regular map \((8^3)\)
More \((6, 8)\)-surfaces

\[ v = 120, \ p_6 = 44 \]

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

Unit cell of \(p_6 = 0\): \(P32\) - Dyck regular map \((8^3)\)
A finite \((p, q)\)-polycycle is a plane 2-connected finite graph, such that:

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

![A (5, 3)-polycycle](image)
Examples of \((p, 3)\)-polycycles

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

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

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

<table>
<thead>
<tr>
<th>face orbit size</th>
<th>60</th>
<th>30</th>
<th>20</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>number of orbits</td>
<td>any</td>
<td>≤ 1</td>
<td>≤ 1</td>
<td>1</td>
</tr>
<tr>
<td>face degrees</td>
<td>5, $n$</td>
<td>any</td>
<td>$3t$</td>
<td>$2t$</td>
</tr>
</tbody>
</table>

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

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

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

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

Triacon $T_1$

Triacon $T_2$

Triacon $T_3$

Pentacon $P$
### $I$-fulleroids

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

Above $(5, n)$-spheres: unique for their $p$-vector $(p_5, p_n)$, $n > 7$
1st smallest icosahedral \((5, 7)\)-spheres

\[ F_{5,7}(I)a = P(C_{140}(I)); \quad v = 260 \]

Dress-Brinkmann (1996) 1st Phantasmagorical Fulleroid
2nd smallest icosahedral \((5, 7)\)-spheres

\[
F_{5,7}(I)b = T_1(C_{180}(I_h)); \quad v = 260
\]

Dress-Brinkmann (1996) 2nd Phantasmagorical Fulleroid
The smallest icosahedral \((5, 8)\)-sphere

\[ F_{5,8}(I_h) = P(C_{80}(I_h)); \quad v = 200 \]
The smallest icosahedral \((5, 9)\)-sphere

\[ F_{5,9}(I_h) = P(C_{60}(I_h)); \, v = 180 \]
The smallest icosahedral \((5, 10)\)-sphere

\[ F_{5,10}(I_h) = T_1(C_{60}(I_h)); \quad v = 140 \]
The smallest icosahedral \((5, 12)\)-sphere

\[ F_{5,12}(I_h) = T_3(C_{80}(I_h)); \quad v = 440 \]
The smallest icosahedral \((5, 14)\)-sphere

\[ F_{5,14}(I_h) = P(F_{5,12}(I_h)); \quad v = 560 \]
The smallest icosahedral \((5, 15)\)-sphere

\[ F_{5,15}(I_h) = T_2(C_{60}(I_h)); v = 260 \]
\textbf{\(G\)-fulleroids}

- \textbf{\(G\)-fulleroid}: cubic polyhedron with \(p = (p_5, p_n)\) and symmetry group \(G\); so, \(p_n = \frac{p_5 - 12}{n - 6}\).

- 
\textbf{Fowler et al., 1993}: \(G\)-fulleroids with \(n = 6\) (fullerenes) exist for 28 groups \(G\).

- 
\textbf{Kardos, 2007}: \(G\)-fulleroids with \(n = 7\) exists for 36 groups \(G\); smallest for \(G = I_h\) has 500 vertices. There are infinity of \(G\)-fulleroids for all \(n \geq 7\) if and only if \(G\) is a subgroup of \(I_h\); there are 22 types of such groups.

- 
\textbf{Dress-Brinkmann, 1986}: there are 2 smallest \(I\)-fulleroids with \(n = 7\); they have 260 vertices.

- 
\textbf{D-Delgado, 2000}: 2 infinite series of \(I\)-fulleroids and smallest ones for \(n = 8, 10, 12, 14, 15\).

- 
\textbf{Jendrol-Trenkler, 2001}: \(I\)-fulleroids for all \(n \geq 8\).
All seven 2-isoohedral \((5, n)\)-planes

A \((5, n)\)-plane is a 3-valent plane tiling by 5- and \(n\)-gons. A plane tiling is 2-homohedral if its faces form 2 orbits under group of combinatorial automorphisms \(Aut\). It is 2-isoohedral if, moreover, its symmetry group is isomorphic to \(Aut\).
V. \(d\)-dimensional fullerenes (with Shtogrin)
\(d\)-fullerenes

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

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

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

<table>
<thead>
<tr>
<th>( g )</th>
<th>0</th>
<th>1 (or.)</th>
<th>2 (not or.)</th>
<th>1 (not or.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>surface</td>
<td>( S^2 )</td>
<td>( T^2 )</td>
<td>( K^2 )</td>
<td>( P^2 )</td>
</tr>
<tr>
<td>( p_5 )</td>
<td>12</td>
<td>0</td>
<td>0</td>
<td>6</td>
</tr>
<tr>
<td>( p_6 )</td>
<td>( \geq 0, \neq 1 )</td>
<td>( \geq 7 )</td>
<td>( \geq 9 )</td>
<td>( \geq 0, \neq 1, 2 )</td>
</tr>
<tr>
<td>3-fullerene</td>
<td>usual sph.</td>
<td>polyhex</td>
<td>polyhex</td>
<td>projective</td>
</tr>
</tbody>
</table>
Smallest non-spherical finite 3-fullerenes

Toric fullerene

Klein bottle fullerene

Projective fullerene
Non-spherical finite 3-fullerenes

- Projective fullerenes are antipodal quotients of centrally symmetric spherical fullerenes, i.e. with symmetry \( C_i, C_{2h}, D_{2h}, D_{6h}, D_{3d}, D_{5d}, T_h, I_h \). So, \( v \equiv 0 \pmod{4} \).

Smallest CS fullerenes \( F_{20}(I_h), F_{32}(D_{3d}), F_{36}(D_{6h}) \)

- Toroidal fullerenes have \( p_5 = 0 \). They are described by Negami in terms of 3 parameters.

- Klein bottle fullerenes have \( p_5 = 0 \). They are obtained as quotient of toroidal ones by a fixed-point free involution reversing the orientation.
Plane fullerenes (infinite 3-fullerenes)

- **Plane fullerene**: a 3-valent tiling of $E^2$ by (combinatorial) 5- and 6-gons.

- If $p_5 = 0$, then it is the graphite $\{6^3\} = F_\infty = 63$.

- **Theorem**: plane fullerenes have $p_5 \leq 6$ and $p_6 = \infty$.

- A.D. Alexandrov (1958): any metric on $E^2$ of non-negative curvature can be realized as a metric of convex surface on $E^3$.

  Consider plane metric such that all faces became regular in it. Its curvature is 0 on all interior points (faces, edges) and $\geq 0$ on vertices.

  A convex surface is at most half $S^2$. 
Space fullerenes (infinite 4-fullerene)

- 4 Frank-Kasper polyhedra (isolated-hexagon fullerenes): $F_{20}(I_h), F_{24}(D_{6d}), F_{26}(D_{3h}), F_{28}(T_d)$

- FK space fullerene: a 4-valent 3-periodic tiling of $E^3$ by them; space fullerene: such tiling by any fullerenes.

- FK space fullerenes occur in:
  - tetrahedrally close-packed phases of metallic alloys.
  - Clathrates (compounds with 1 component, atomic or molecular, enclosed in framework of another), incl. Clathrate hydrates, where cells are solutes cavities, vertices are $H_2O$, edes are hydrogen bonds; Zeolites (hydrated microporous aluminosilicate minerals), where vertices are tetrahedra $SiO_4$ or $SiAlO_4$, cells are $H_2O$, edges are oxygen bridges.
  - Soap froths (foams, liquid crystals).
## 24 known primary FK space fullerenes

<table>
<thead>
<tr>
<th>t.c.p.</th>
<th>clathrate, exp. alloy</th>
<th>sp. group</th>
<th>$\bar{f}$</th>
<th>$F_{20}:F_{24}:F_{26}:F_{28}$</th>
<th>N</th>
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<tbody>
<tr>
<td>$A_{15}$</td>
<td>type I, $Cr_3Si$</td>
<td>$Pm\bar{3}n$</td>
<td>13.50</td>
<td>1, 3, 0, 0</td>
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<tr>
<td>$C_{15}$</td>
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<td>$Fd\bar{3}m$</td>
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<td>$C_{14}$</td>
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<tr>
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<td>$MoNi$</td>
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<tr>
<td>$P$</td>
<td>$Mo_{42}Cr_{18}Ni_{40}$</td>
<td>$Pbnm$</td>
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## 24 known primary FK space fullerenes

<table>
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<tr>
<th>t.c.p.</th>
<th>exp. alloy</th>
<th>sp. group</th>
<th>( \bar{f} )</th>
<th>( F_{20} : F_{24} : F_{26} : F_{28} )</th>
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<tr>
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<td>Im3</td>
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<tr>
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FK space fullerene $A_{15}$ ($\beta$-$W$ phase)

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

Cubic $N=24$; gravicenters of cells $F_{28}$ (atoms $Mg$ in $MgCu_2$) form diamond network (centered $A_3$). Cf. $MgZn_2$ forming hexagonal $N=12$ variant $C_{14}$ of diamond: lonsdaleite found in meteorites, 2nd in a continuum of $(2, 0, 0, 1)$-structures.
It is also not determined by its fract. composition \((3, 2, 2, 0)\).
**Computer enumeration**

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

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<th># 24</th>
<th># 26</th>
<th># 28</th>
<th>fraction</th>
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<th>n(known structure)</th>
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<td>26(−), 26($p\sigma$), 39($\mu$), not $M$</td>
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<td>16(1)</td>
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<td>0</td>
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<td>16(1)</td>
<td>8($A_{15}$)</td>
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<td>0</td>
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<td>known</td>
<td>18(4)</td>
<td>12($C_{14}$), 24($C_{15}$), 36(6-layer), 54(9-layer)</td>
</tr>
</tbody>
</table>
Conterexamples to 2 old conjectures

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

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

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

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

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

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

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

Closer to impossible 5 or $\bar{f} = 12$ (120-cell, $S^3$-tiling by $F_{20}$) means lower energy. Minimal $\bar{f}$ for simple (3, 4 tiles at each edge, vertex) $E^3$-tiling by a simple polyhedron is 14 (tr.oct).
Non-$FK$ space fullerene: is it unique?

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

Delgado, O’Keeffe: all space fullerenes with $\leq 7$ orbits of vertices are 4 FK ($A_{15}$, $C_{15}$, $Z$, $C_{14}$) and this one (3,3,5,7,7).
Weak Kelvin problem

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

Lord Kelvin, 1887: bcc$=A_3^*$

$IQ(\text{curved tr.Oct.}) \approx 0.757$

$IQ(\text{tr.Oct.}) \approx 0.753$

Weaire-Phelan, 1994: $A_{15}$

$IQ(\text{unit cell}) \approx 0.764$

2 curved $F_{20}$ and 6 $F_{24}$

In $\mathbb{R}^2$, the best is (Ferguson-Hales) graphite $F_\infty = (6^3)$. 
Projection of 120-cell in 3-space (G. Hart)

(533): 600 vertices, 120 dodecahedral facets, $|\text{Aut}| = 14400$
Regular (convex) polytopes

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

<table>
<thead>
<tr>
<th>regular polytope</th>
<th>group</th>
</tr>
</thead>
<tbody>
<tr>
<td>regular polygon (P_n)</td>
<td>(I_2(n))</td>
</tr>
<tr>
<td>Icosahedron and Dodecahedron</td>
<td>(H_3)</td>
</tr>
<tr>
<td>120-cell and 600-cell</td>
<td>(H_4)</td>
</tr>
<tr>
<td>24-cell</td>
<td>(F_4)</td>
</tr>
<tr>
<td>(\gamma_n)(hypercube) and (\beta_n)(cross-polytope)</td>
<td>(B_n)</td>
</tr>
<tr>
<td>(\alpha_n)(simplex)</td>
<td>(A_n=\text{Sym}(n+1))</td>
</tr>
</tbody>
</table>

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

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

<table>
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<th>5</th>
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### 3-dim. regular tilings and honeycombs

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<td></td>
<td></td>
<td></td>
<td></td>
<td>5335</td>
</tr>
<tr>
<td>$\delta_3$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4343*</td>
</tr>
</tbody>
</table>
**Finite 4-fullerenes**

- \( \chi = f_0 - f_1 + f_2 - f_3 = 0 \) for any finite closed 3-manifold, no useful equivalent of Euler formula.

- Prominent 4-fullerene: 120-cell.
  - **Conjecture**: it is unique equifacetted 4-fullerene \((\simeq Do = F_{20})\)

- Pasini: there is no 4-fullerene facetted with \( C_{60}(I_h) \) (4-football)

- Few types of putative facets: \( \simeq F_{20}, F_{24} \) (hexagonal barrel), \( F_{26}, F_{28}(T_d), F_{30}(D_{5h}) \) (elongated Dodecahedron), \( F_{32}(D_{3h}), F_{36}(D_{6h}) \) (elongated \( F_{24} \))

- \( \infty \): “greatest” polyhex is 633 (convex hull of vertices of 63, realized on a horosphere); its fundamental domain is not compact but of finite volume
4 constructions of finite 4-fullerenes

<table>
<thead>
<tr>
<th>120-cell*</th>
<th>600</th>
<th>$F_{20} = D_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_i^*$</td>
<td>560i + 40</td>
<td>$F_{20}, F_{30}(D_{5h})$</td>
</tr>
<tr>
<td>$B(F)$</td>
<td>30v(F)</td>
<td>$F_{20}, F_{24}, F(two)$</td>
</tr>
<tr>
<td>C(120-cell)</td>
<td>20600</td>
<td>$F_{20}, F_{24}, F_{28}(T_d)$</td>
</tr>
<tr>
<td>D(120-cell)</td>
<td>61600</td>
<td>$F_{20}, F_{26}, F_{32}(D_{3h})$</td>
</tr>
</tbody>
</table>

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

$A_i$: tube of 120-cells

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

$C, D$: any 4-fullerene decorations
Construction $A$ of polytopal 4-fullerenes

Similarly, tubes of 120-cell’s are obtained in $4D$
Inflation method

- Roughly: find out in simplicial $d$-polytope (a dual $d$-fullerene $F^*$) a suitable “large” $(d - 1)$-simplex, containing an integer number $t$ of “small” (fundamental) simplices.

- Constructions $C, D$: $F^* = 600$-cell; $t = 20, 60$, respectively.

- The decoration of $F^*$ comes by “barycentric homothety” (suitable projection of the “large” simplex on the new “small” one) as the orbit of new points under the symmetry group.
All known 5-fullerenes

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

No polytopal 5-fullerene exist.
Quotient $d$-fullerenes

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

Exp 1: Poincaré dodecahedral space

- quotient of 120-cell (on $S^3$) by the binary icosahedral group $I_h$ of order 120; so, $f$-vector
  $$(5, 10, 6, 1) = \frac{1}{120} f(120 - \text{cell})$$

- It comes also from $F_{20} = Do$ by gluing of its opposite faces with $\frac{1}{10}$ right-handed rotation

Quot. of $H^3$ tiling: by $F_{20}$: $(1, 6, 6, p_5, 1)$ Seifert-Weber space and by $F_{24}$: $(24, 72, 48 + 8 = p_5 + p_6, 8)$ Löbell space
Polyhexes on $T^2$, cylinder, its twist (Möbius surface) and $K^2$ are quotients of graphite 63 by discontinuous and fixed-point free group of isometries, generated by resp.:

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

The smallest polyhex has $p_6 = 1$: $\bullet \overrightarrow{\bullet} \overrightarrow{\bullet}$ on $T^2$.

The “greatest” polyhex is 633 (the convex hull of vertices of 63, realized on a horosphere); it is not compact (its fundamental domain is not compact), but cofinite (i.e., of finite volume) infinite 4-fullerene.
VI. Zigzags, railroads and knots in fullerenes
(with Dutour and Fowler)
Zigzags

A plane graph $G$
Zigzags

take two edges
Zigzags

Continue it left–right alternatively ....
Zigzags

... until we come back.
Zigzags

A self-intersecting zigzag
A double covering of 18 edges: 10+10+16

z-vector $z=10^2, 16_{2,0}$
**$z$-knotted fullerenes**

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

![Diagram of railroads and 3-valent plane graphs](image)

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

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

36, $D_{6h}$

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

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

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

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

The skeleton of its dual is an isometric subgraph of $\frac{1}{2}H_8$. 
First IPR fullerene with self-int. railroad

\[ F_{96}(D_{6d}) \text{; realizes projection of Conway knot } (4 \times 6)^* \]
Triply intersecting railroad in $F_{172}(C_{3v})$
Tight fullerene is one without railroads, i.e., pairs of "parallel" zigzags.

Clearly, any \( z \)-knotted fullerene (unique zigzag) is tight.

\[ F_{140}(I) \text{ is tight with } z = 28^{15} \text{ (15 simple zigzags)}. \]

Conjecture: any tight fullerene has \( \leq 15 \) zigzags.

Conjecture: All tight with simple zigzags are 9 known ones (holds for all \( F_n \) with \( n \leq 200 \)).
Tight $F_n$ with simple zigzags

- $20 \quad I_h, 20^6$
- $28 \quad T_d, 12^7$
- $48 \quad D_3, 16^9$
- $60 \quad D_3, 18^{10}$
- $60 \quad I_h, 18^{10}$
- $76 \quad D_{2d}, 22^4, 20^7$
Tight $F_n$ with simple zigzags

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

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

92 $T_h$, $24^6$, $22^6$
Tight $F_n$ with only simple zigzags

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

Conjecture: this list is complete (checked for $n \leq 200$). It gives 7 Grünbaum arrangements of plane curves.
Two $F_{60}$ with $z$-vector $18^{10}$

This pair was first answer on a question in B. Grunbaum "Convex Polytopes" (Wiley, New York, 1967) about non-existance of simple polyhedra with the same $p$-vector but different zigzags.
$z$-uniform $F_n$ with $n \leq 60$

<table>
<thead>
<tr>
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<th>orbit lengths</th>
<th>$z$-vector</th>
<th>int. vector</th>
</tr>
</thead>
<tbody>
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<td>$10^6$</td>
<td>$2^5$</td>
</tr>
<tr>
<td>28</td>
<td>$T_d:2$</td>
<td>4,3</td>
<td>$12^7$</td>
<td>$2^6$</td>
</tr>
<tr>
<td>40</td>
<td>$T_d:40$</td>
<td>4</td>
<td>$30^4_{0,3}$</td>
<td>$8^3$</td>
</tr>
<tr>
<td>44</td>
<td>$T:73$</td>
<td>3</td>
<td>$44^3_{0,4}$</td>
<td>$18^2$</td>
</tr>
<tr>
<td>44</td>
<td>$D_2:83$</td>
<td>2</td>
<td>$66^2_{5,10}$</td>
<td>36</td>
</tr>
<tr>
<td>48</td>
<td>$C_2:84$</td>
<td>2</td>
<td>$72^2_{7,9}$</td>
<td>40</td>
</tr>
<tr>
<td>48</td>
<td>$D_3:188$</td>
<td>3,3,3</td>
<td>$16^9$</td>
<td>$2^8$</td>
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<tr>
<td>52</td>
<td>$C_3:237$</td>
<td>3</td>
<td>$52^3_{2,4}$</td>
<td>$20^2$</td>
</tr>
<tr>
<td>52</td>
<td>$T:437$</td>
<td>3</td>
<td>$52^3_{0,8}$</td>
<td>$18^2$</td>
</tr>
<tr>
<td>56</td>
<td>$C_2:293$</td>
<td>2</td>
<td>$84^2_{7,13}$</td>
<td>44</td>
</tr>
<tr>
<td>56</td>
<td>$C_2:349$</td>
<td>2</td>
<td>$84^2_{5,13}$</td>
<td>48</td>
</tr>
<tr>
<td>56</td>
<td>$C_3:393$</td>
<td>3</td>
<td>$56^3_{3,5}$</td>
<td>$20^2$</td>
</tr>
<tr>
<td>60</td>
<td>$C_2:1193$</td>
<td>2</td>
<td>$90^2_{7,13}$</td>
<td>50</td>
</tr>
<tr>
<td>60</td>
<td>$D_2:1197$</td>
<td>2</td>
<td>$90^2_{13,8}$</td>
<td>48</td>
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<tr>
<td>60</td>
<td>$D_3:1803$</td>
<td>6,3,1</td>
<td>$18^{10}$</td>
<td>$2^9$</td>
</tr>
<tr>
<td>60</td>
<td>$I_h:1812$</td>
<td>10</td>
<td>$18^{10}$</td>
<td>$2^9$</td>
</tr>
</tbody>
</table>
$z$-uniform IPR $C_n$ with $n \leq 100$

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

IPR means the absence of adjacent pentagonal faces; IPR enhanced stability of putative fullerene molecule.
**IPR \( z \)-knotted \( F_n \) with \( n \leq 100 \)**

<table>
<thead>
<tr>
<th>( n )</th>
<th>signature</th>
<th>isomers</th>
</tr>
</thead>
<tbody>
<tr>
<td>86</td>
<td>43, 86*</td>
<td>( C_2:2 )</td>
</tr>
<tr>
<td>90</td>
<td>47, 88</td>
<td>( C_1:7 )</td>
</tr>
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<td></td>
<td>53, 82</td>
<td>( C_2:19 )</td>
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<td>71, 64</td>
<td>( C_2:6 )</td>
</tr>
<tr>
<td>94</td>
<td>47, 94*</td>
<td>( C_1:60; C_2:26, 126 )</td>
</tr>
<tr>
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<td>65, 76</td>
<td>( C_2:121 )</td>
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<td>69, 72</td>
<td>( C_2:7 )</td>
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<td>96</td>
<td>49, 95</td>
<td>( C_1:65 )</td>
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<td>53, 91</td>
<td>( C_1:7, 37, 63 )</td>
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<td>98</td>
<td>49, 98*</td>
<td>( C_2:191, 194, 196 )</td>
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<td>63, 84</td>
<td>( C_1:49 )</td>
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<td>75, 72</td>
<td>( C_1:29 )</td>
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<td>77, 70</td>
<td>( C_1:5; C_2:221 )</td>
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<td>100</td>
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<td>( C_1:371, 377; C_3:221 )</td>
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<td>53, 97</td>
<td>( C_1:29, 113, 236 )</td>
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<td>55, 95</td>
<td>( C_1:165 )</td>
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<td>65, 85</td>
<td>( C_1:31, 234 )</td>
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</table>

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

Let $G$ be a fullerene with one zigzag with self-intersection numbers $(\alpha_1, \alpha_2)$. Here is the smallest one, $F_{34}(C_2)$. →→

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

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

(iii) two faces, $F_1$ and $F_2$ are free of $PM$, $PM$ is organized around them in **concentric circles**.
**$z$-knotted fullerenes: statistics for $n \leq 74$**

<table>
<thead>
<tr>
<th>$n$</th>
<th>$#$ of $F_n$</th>
<th>$#$ of $z$-knotted</th>
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</thead>
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</tr>
<tr>
<td>36</td>
<td>15</td>
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<tr>
<td>74</td>
<td>14246</td>
<td>1970</td>
</tr>
</tbody>
</table>

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

- p. 134
For any $n$, there is a fullerene $F_{36n-8}$ with two simple zigzags having intersection $2n$; above $n = 4$. 
VII. Ringed fullerenes (with Grishukhin)
All fullerenes with hexagons in 1 ring

\[30, D_{5h}\]

\[32, D_{2}\]

\[32, D_{3d}\]

\[36, D_{2d}\]

\[40, D_{2}\]
All fullerenes with pentagons in 1 ring

36, $D_{2d}$

44, $D_{3d}$

48, $D_{6d}$

44, $D_2$
All fullerenes with hexagons in > 1 ring

32, $D_{3h}$

38, $C_{3v}$

40, $D_{5h}$
All fullerenes with pentagons in $> 1$ ring

$38, \ C_{3v}$

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

Infinite family:
$F_{24+12t}(D_{6d})$,
$t \geq 1$,
$D_{6h}$ if $t$ odd

Elongations of hexagonal barrel
VIII. Face-regular fullerenes
Face-regular fullerenes

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

<table>
<thead>
<tr>
<th>$i$</th>
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<th>3</th>
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<th>5</th>
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<tbody>
<tr>
<td># of $5R_i$</td>
<td>$\infty$</td>
<td>$\infty$</td>
<td>$\infty$</td>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td># of $6R_i$</td>
<td>4</td>
<td>2</td>
<td>8</td>
<td>5</td>
<td>7</td>
<td>1</td>
</tr>
</tbody>
</table>

28, $D_2$

All fullerenes, which are $6R_1$

32, $D_3$
All fullerenes, which are $6R_3$

- $R_3$ 36, $D_2$
- $R_2$ 44, $T$ (also $5R_2$)
- $R_1$ 48, $D_3$
- $R_0$ 52, $T$ (also $5R_1$)
- $I_h$ 60, $I_h$ (also $5R_0$)
All fullerenes, which are $6R_4$

$40, D_{5d}$

$56, T_d$ (also $5R_2$)

$68, D_{3d}$

$68, T_d$ (also $5R_1$)

$72, D_{2d}$

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

$80, I_h$ (also $5R_0$)
IX. Embedding of fullerenes
Fullerenes as isom. subgraphs of $\frac{1}{2}$-cubes

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

$F_{20}(I_h)(5, 0) \rightarrow \frac{1}{2}H_{10}$  $F_{20}^*(I_h)(5, 0) \rightarrow \frac{1}{2}H_{6}$
$F_{60}^*(I_h)(0, 3) \rightarrow \frac{1}{2}H_{10}$  $F_{80}(I_h)(0, 4) \rightarrow \frac{1}{2}H_{22}$

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

$F_{26}(D_{3h})(-, 0) \rightarrow \frac{1}{2}H_{12}$
$F_{40}(T_d)(2, -) \rightarrow \frac{1}{2}H_{15}$  $F_{44}(T)(2, 3) \rightarrow \frac{1}{2}H_{16}$
$F_{28}^*(T_d)(3, 0) \rightarrow \frac{1}{2}H_{7}$  $F_{36}^*(D_{6h})(2, -) \rightarrow \frac{1}{2}H_{8}$

Also, for graphite lattice (infinite fullerene), it holds:

$(6^3) = F_\infty(0, 6) \rightarrow H_\infty, Z_3$  and  $(3^6) = F_\infty^*(0, 6) \rightarrow \frac{1}{2}H_\infty, \frac{1}{2}Z_3$.  

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Embeddable dual fullerenes in cells

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

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

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

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

- Goldberg, 1937: all $F_n$ of symmetry $(I, I_h)$ are given by Goldberg-Coxeter construction $GC_{k,l}$.

- Fowler and al., 1988: all $F_n$ of symmetry $D_5$, $D_6$ or $T$ are described in terms of 4 integer parameters.

- Graver, 1999: all $F_n$ can be encoded by 20 integer parameters.

- Thurston, 1998: all $F_n$ are parametrized by 10 complex parameters.

- Sah (1994) Thurston’s result implies that the number of fullerenes $F_n$ is $\sim n^9$. 

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

Every such graph is obtained this way.

4 triangles in $\mathbb{Z}[\omega]$

The corresponding triangulation
Consider a fixed symmetry group and fullerenes having this group. In terms of complex parameters, we have:

<table>
<thead>
<tr>
<th>Group</th>
<th>#param.</th>
<th>Group</th>
<th>#</th>
<th>Group</th>
<th>#</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>10</td>
<td>$D_2$</td>
<td>4</td>
<td>$D_6$</td>
<td>2</td>
</tr>
<tr>
<td>$C_2$</td>
<td>6</td>
<td>$D_3$</td>
<td>3</td>
<td>$T$</td>
<td>2</td>
</tr>
<tr>
<td>$C_3$</td>
<td>4</td>
<td>$D_5$</td>
<td>2</td>
<td>$I$</td>
<td>1</td>
</tr>
</tbody>
</table>

For general fullerene ($C_1$) the best is to use `fullgen` (up to 180 vertices).

For 1 parameter this is actually the Goldberg-Coxeter construction (up to 100000 vertices).

For intermediate symmetry group, one can go farther by using the system of parameters (up to 1000 vertices).