Nets and Tiling

Michael O'Keeffe

Introduction to tiling theory
and its application to crystal nets

Arizona State University

Start with tiling in two dimensions.

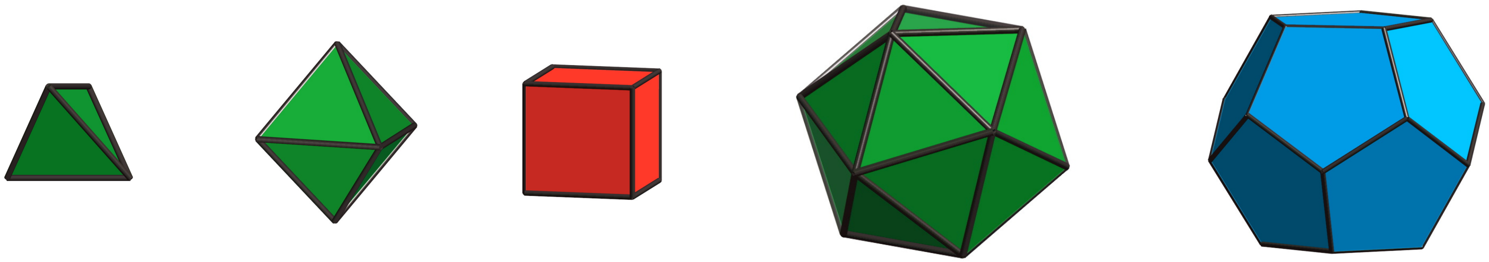
Surface of sphere and plane

Sphere is two-dimensional. We require only two coordinates to specify position on the surface of a sphere:

The coordinates of

Hong Kong 22.3 N, 114.2 E

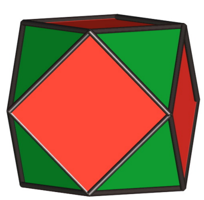
Tempe ` 33.4 N, 278.1 E



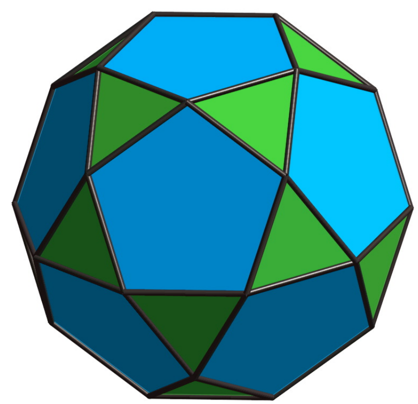
3^4 3^4 4^3 3^5 5^3

Tilings of the sphere (polyhedra) - regular polyhedra.
one kind of vertex, one kind of edge, one kind of face

3.4.3.4



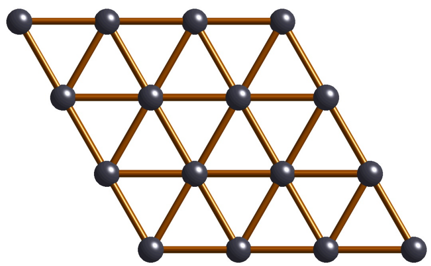
3.5.3.5



Quasiregular polyhedra: one kind of vertex, one kind of edge

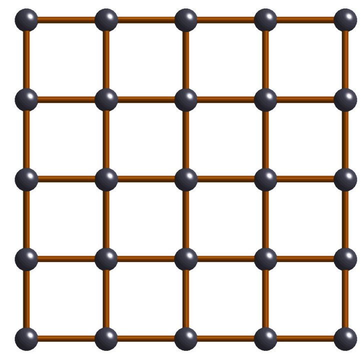
Tiling of the plane - regular tilings

one kind of vertex, one kind of edge, one kind of face



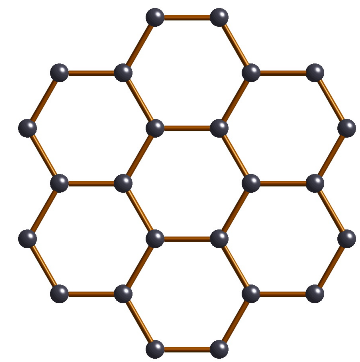
3^6

hexagonal lattice



4^4

square lattice



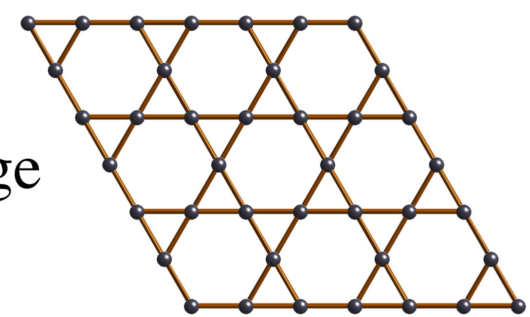
6^3

honeycomb net

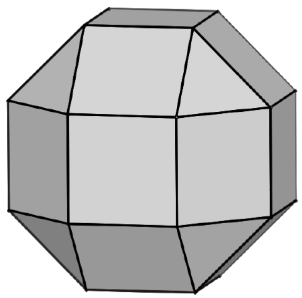
quasiregular

one kind of vertex, one kind if edge

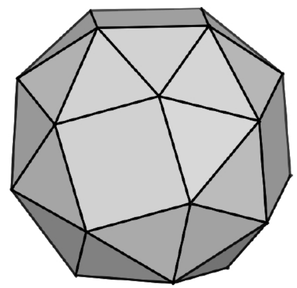
3.6.3.6 kagome net



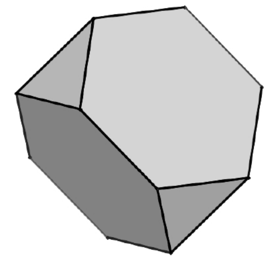
cubic archimedean polyhedra - one kind of vertex



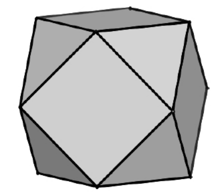
rhombi-
cuboctahedron
rco 3.4^3 $[3^8.4^{18}]$



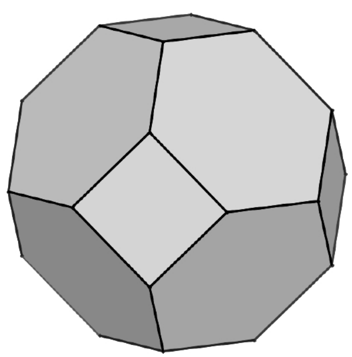
snub cube
snc $3^4.4$ $[3^{32}.4^6]$



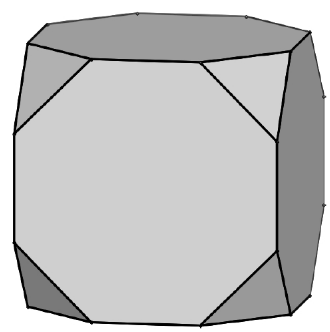
truncated
tetrahedron
tte 3.6^2 $[6^4.4^4]$



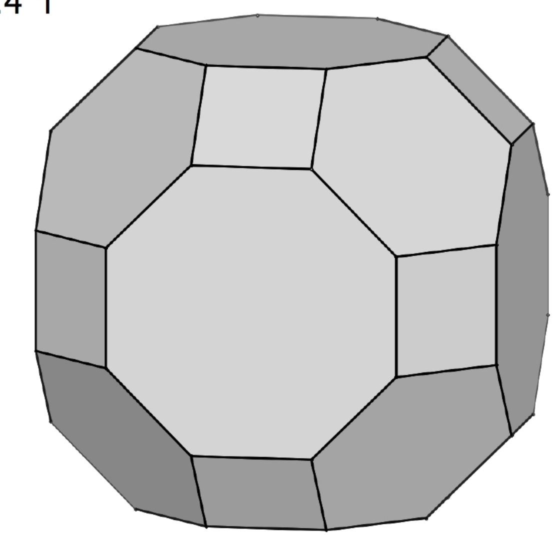
cuboctahedron
cuo 3.4.3.4 $[3^8.4^6]$



truncated octahedron
tro 4.6^2 $[4^6.6^8]$

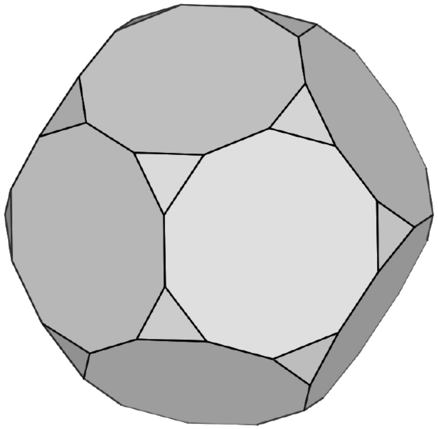


truncated cube
tcu 3.8^2 $[3^8.8^6]$

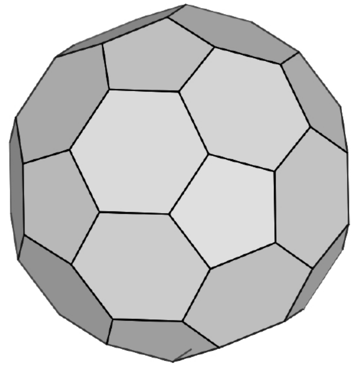


truncated cuboctahedron
tco 3.6.3.8 $[4^{12}.6^8.8^6]$

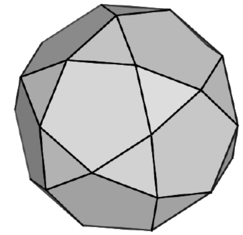
icosahedral Archimedean poyhedra - one kind of vertex



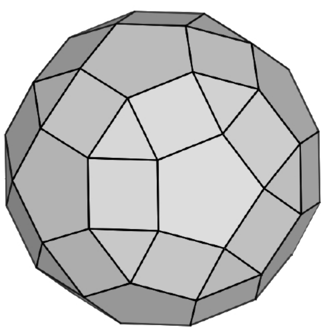
truncated
dodecahedron
tdo 3.10^2 [$3^{20}.10^{12}$]



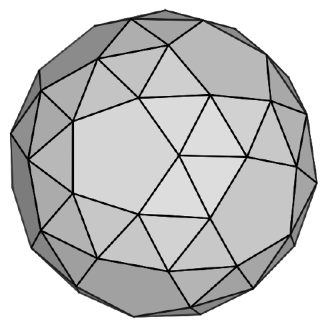
truncated
icosahedron
tic 5.6^2 [$5^{12}.6^{20}$]



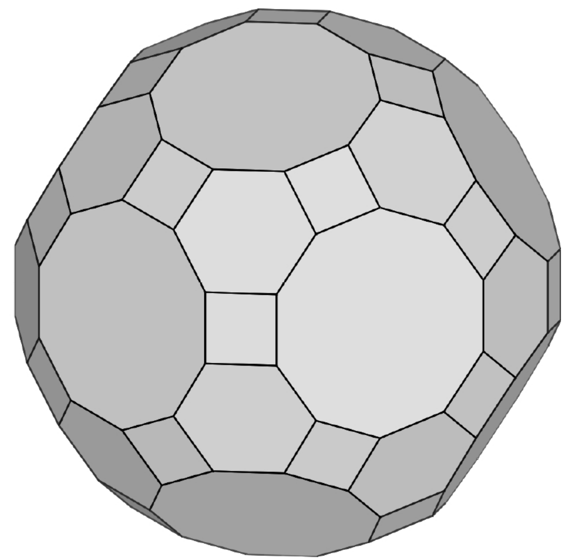
icosidodecahedron
ido 3.5.3.5 [$3^{20}.5^{12}$]



rhombi-
icosidodecahedron
ric 3.4.5.4 [$3^{20}.4^{30}.5^{12}$]



snub
dodecahedron
snd $3^4.5$ [$3^{80}.5^{12}$]



truncated-
icosidodecahedron
tid 4.6.10 [$4^{30}.6^{20}.10^{12}$]

9 Archimedean tilings

Picture is from O'Keeffe & Hyde Beeok

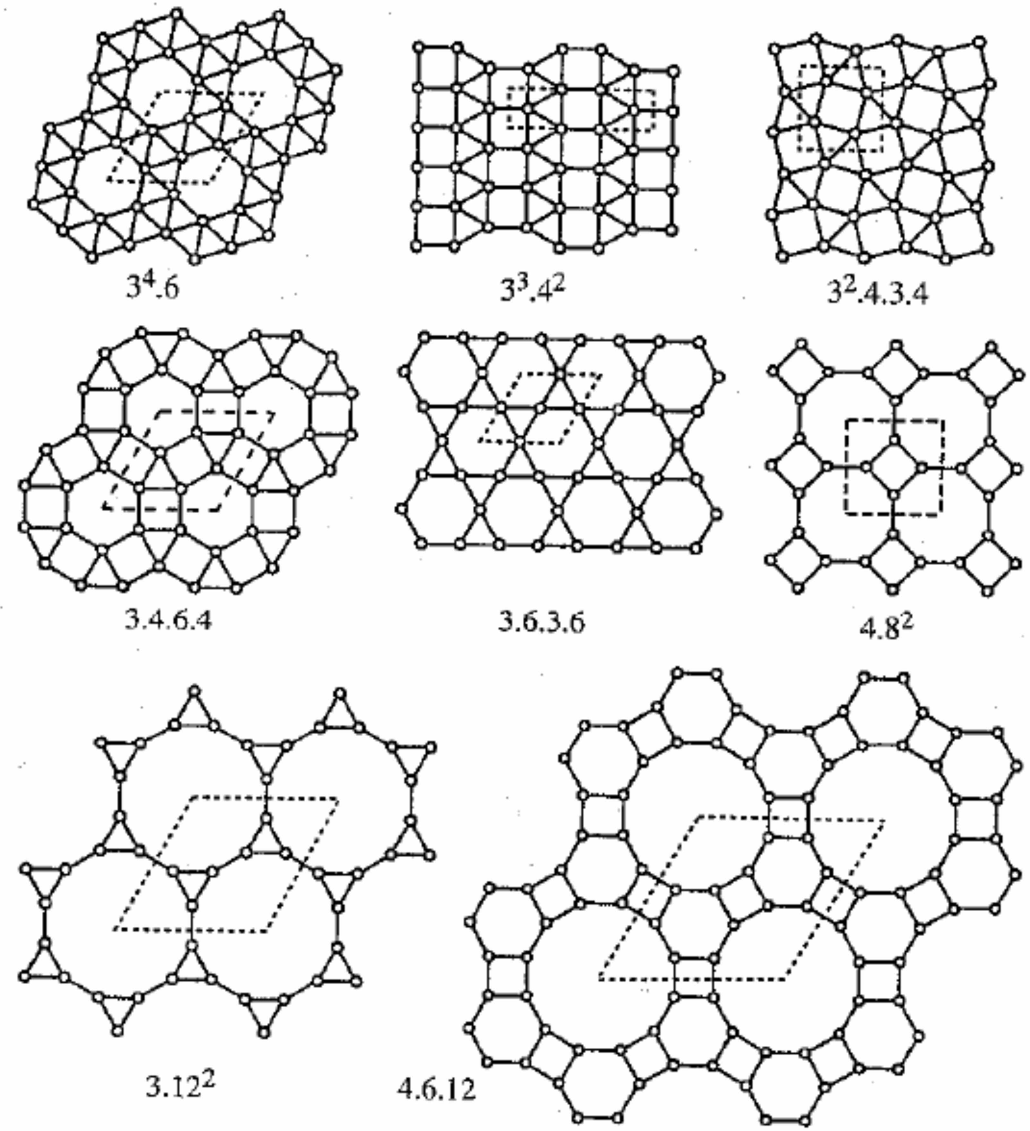
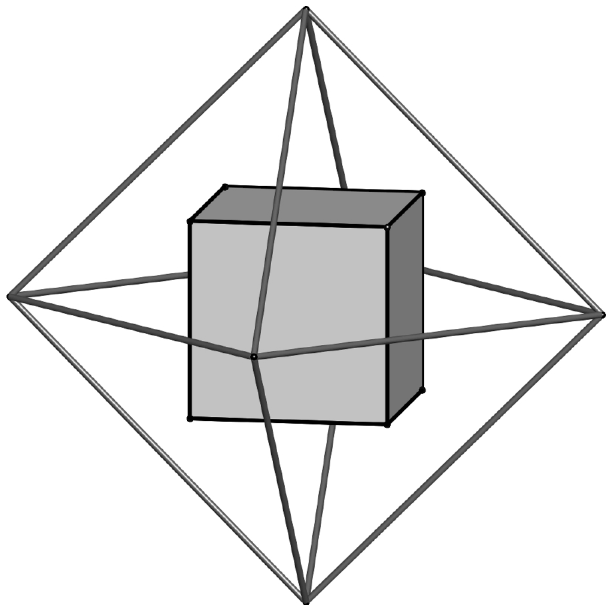
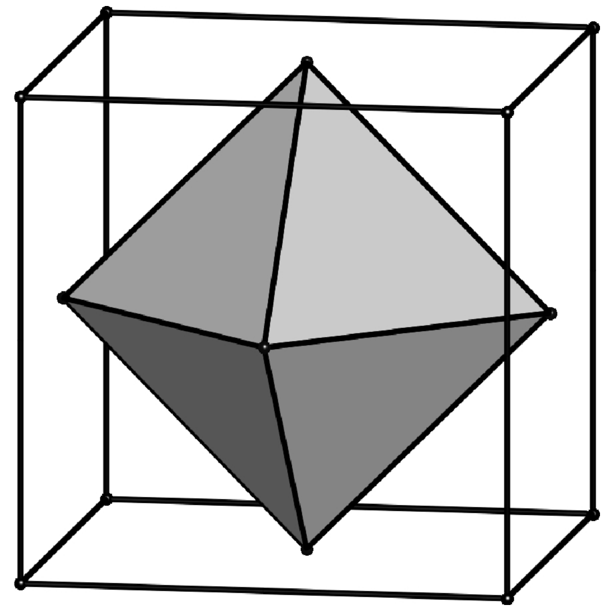


Fig. 5.39. The Archimedean tilings. Top row: $3^4.6$, $3^3.4^2$ and $3^2.4.3.4$. Middle row: 3.4.6.4, 3.6.3.6 and 4.8^2. Bottom row: 3.12^2 and 4.6.12. Unit cells are outlined with broken lines.

Duals of two-dimensional tilings vertices <—> faces

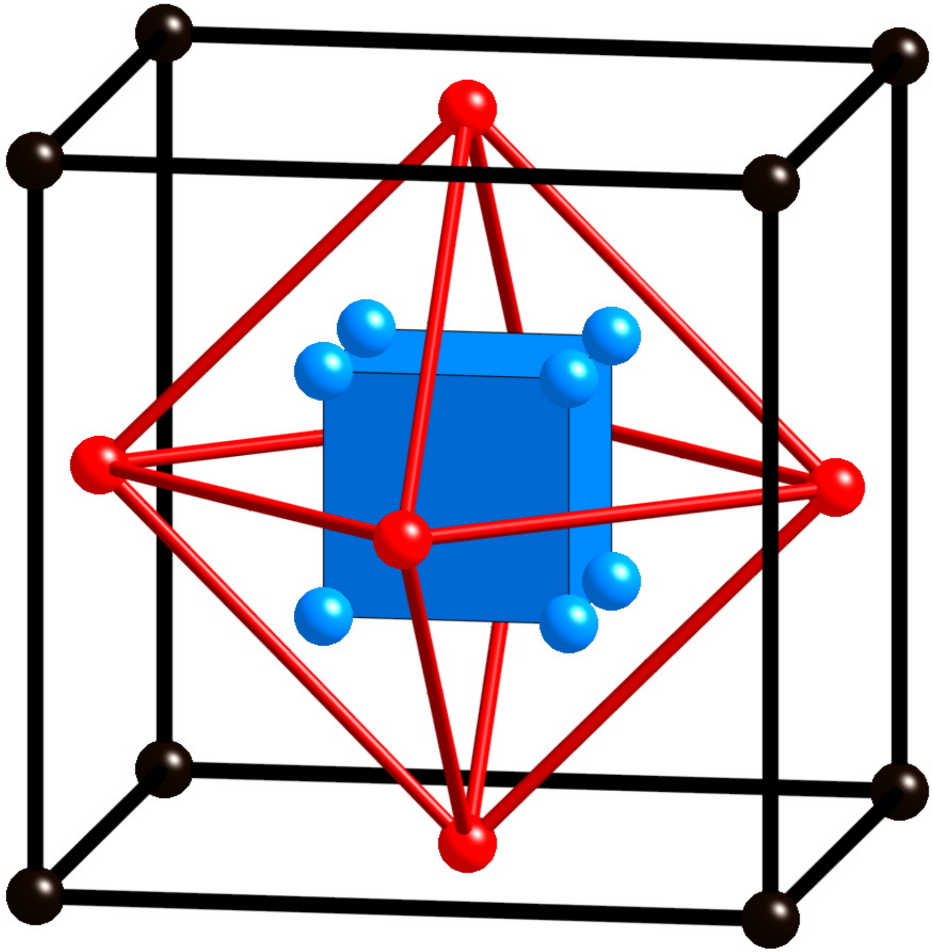


dual of octahedron 3^4
is cube 4^3



dual of cube 4^3
is octahedron 3^4

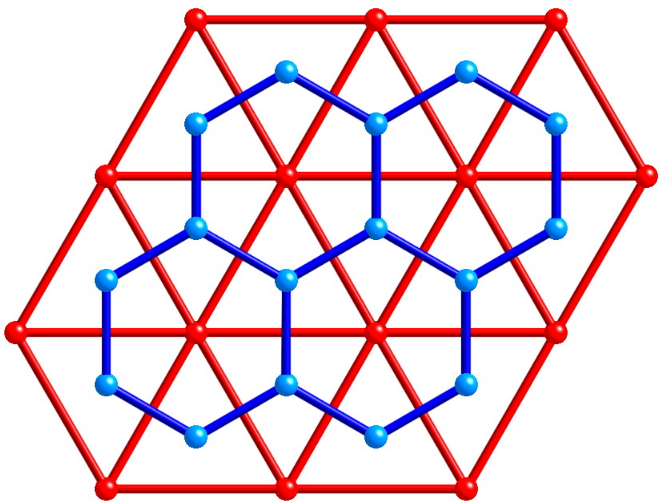
dual of dual is the original
tetrahedron is self-dual



Duals:
edges <-> faces

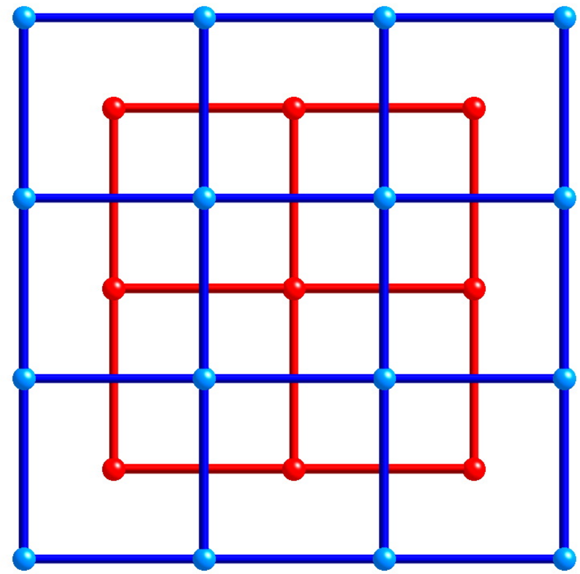
The dual of a dual
is the original

Duals of 2-D periodic nets



$3^6 <=> 6^3$

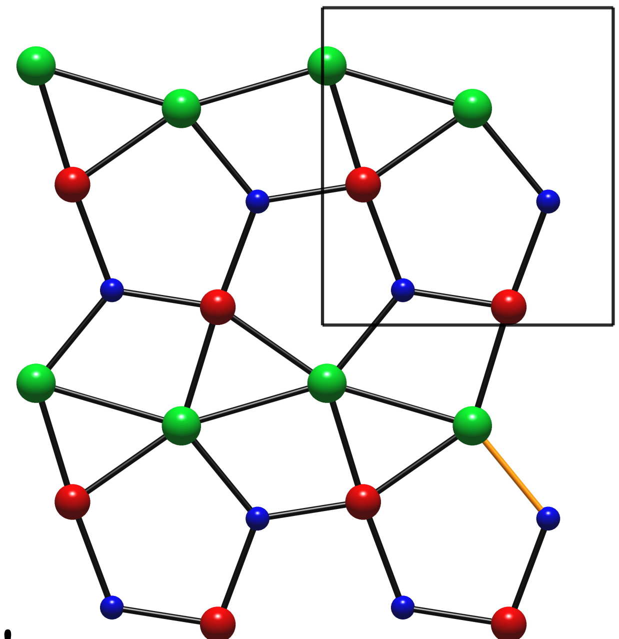
AlB$_2$

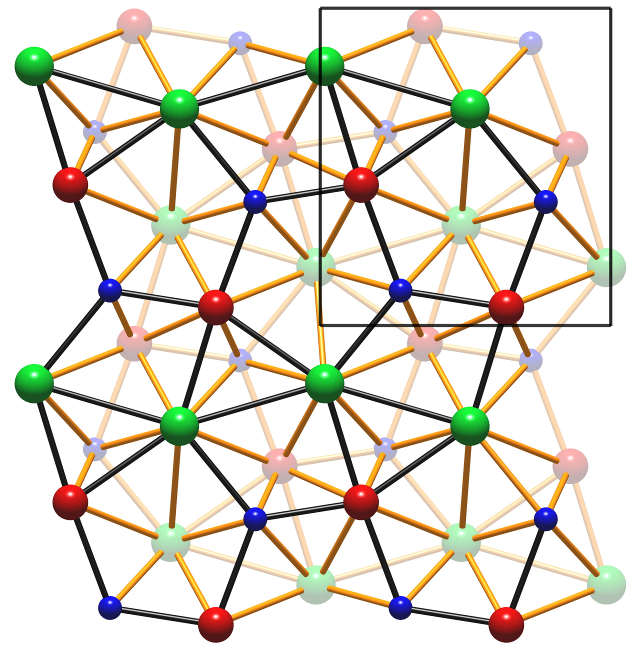


$4^4 <=> 4^4$

self-dual

self-dual nets in crystal structures see O'Keeffe & Hyde book for many more!





$SrMgSi$ ($PbCl_2$) one of the most-common ternary structure types net and dual (same net displaced) alternate

Euler equation and genus.

For a (convex) polyhedron with

V vertices
E edges
F faces

$$V - E + F = 2$$

Euler equation and genus.

For a plane tiling with, per repeat unit

v vertices
e edges
f faces

$$v - e + f = 0$$

Euler equation and genus.

For a tiling on a surface of genus g, with, per repeat unit

v vertices
e edges
f faces

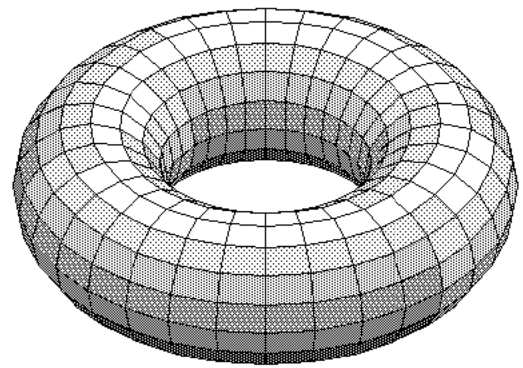
$$v - e + f = 2 - 2g$$

genus of a surface

sphere $g = 0$

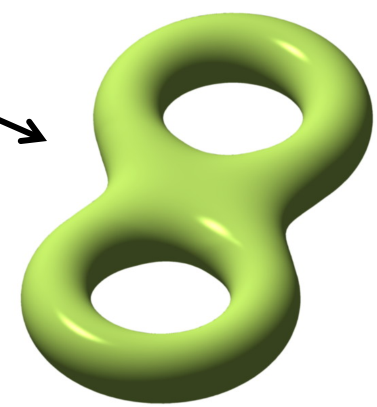
note all vertices
4^4 just like square
lattice

torus $g = 1$



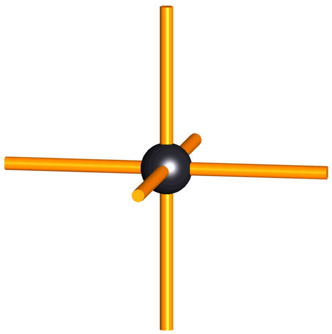
plane $g = 1$

double torus $g = 2$

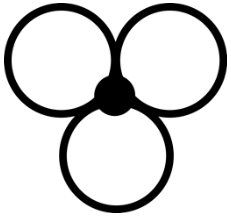


genus of a net = cyclomatic number of quotient graph

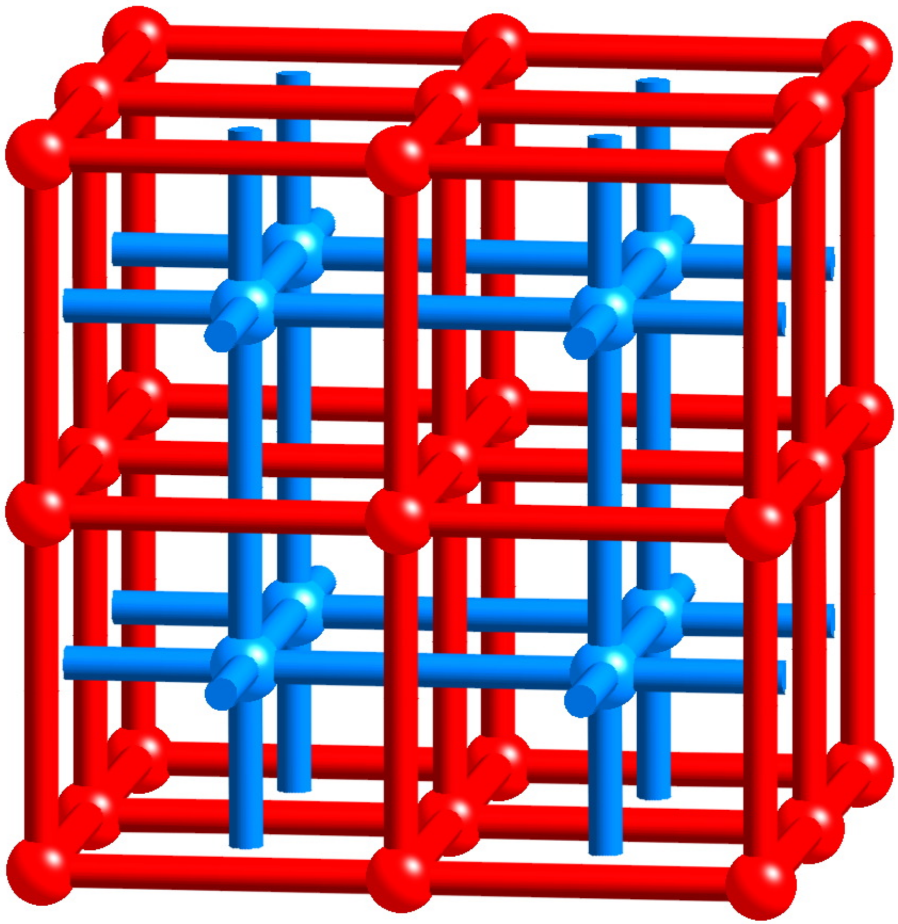
repeat unit
of **pcu**



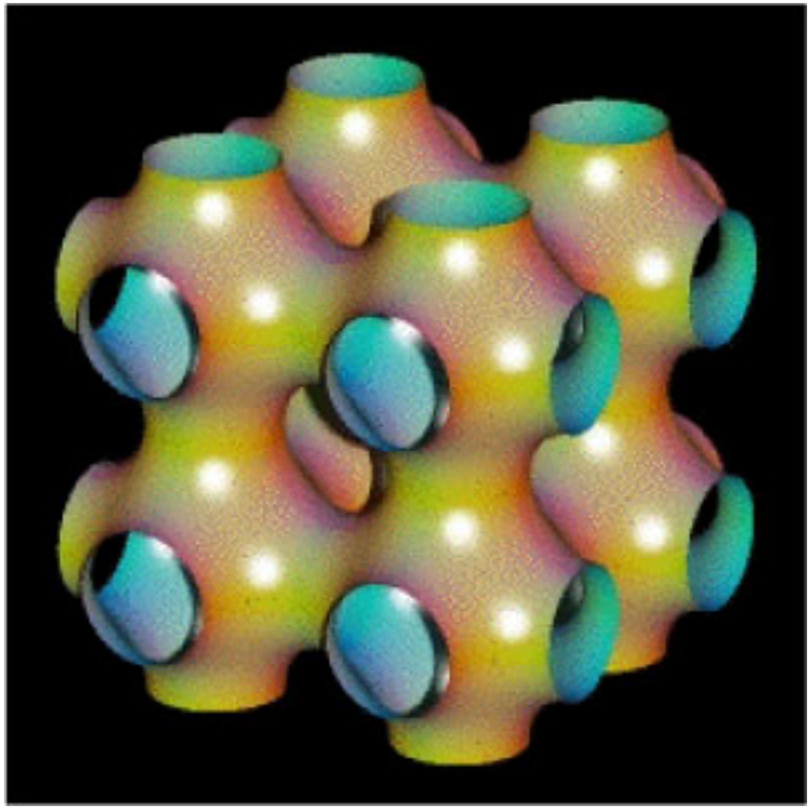
quotient
graph
cyclomatic
number = 3



genus of **pcu** net is 3



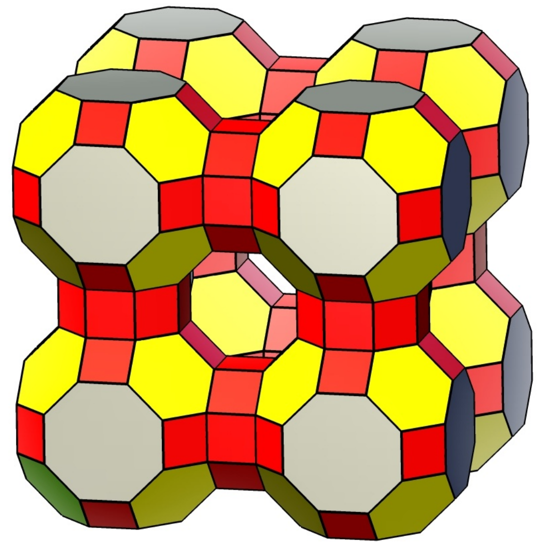
Two interpenetrating **pcu** nets



The *P* minimal surface separates the two nets.
Average curvature zero
Gaussian curvature neg.

infinite poyhedra – tilings of periodic surfaces

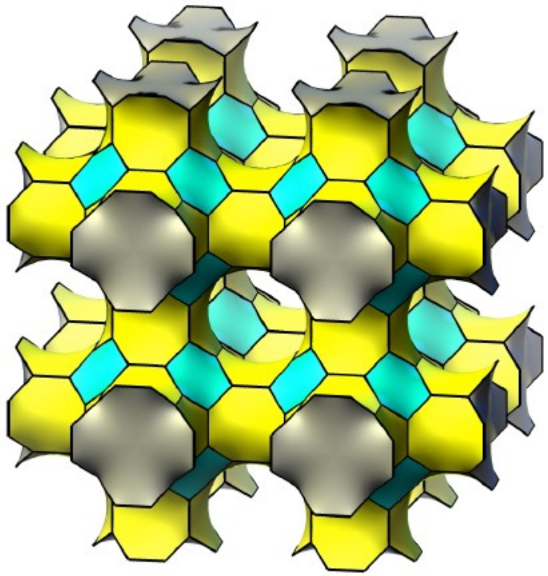
$4^3.6$ tiling of
the *P* surface (*g*= 3).



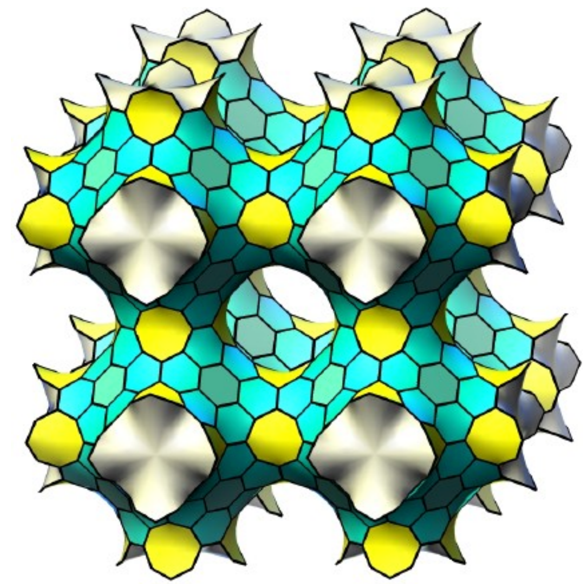
4-coordinated
net **rho** (net of
framework of
zeolite **RHO**)

for the polyhedron
$v = 48, e = 96, f = 44, v - e + f = -4 = 2 - 2g$

net has vertex symbol 4.4.4.6.8.8



6.8^2



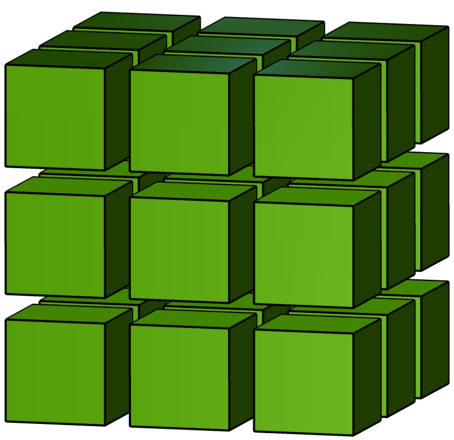
$(6^3)(6^2.8)_2$

tilings of *P* surface ("Schwarzites")

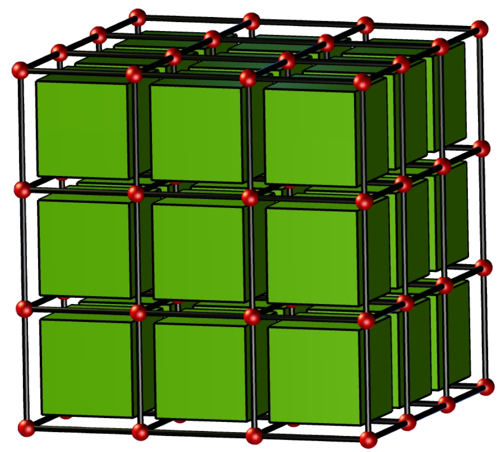
— suggested as possible low energy polymorphs of carbon

Tiling in 3 dimensions

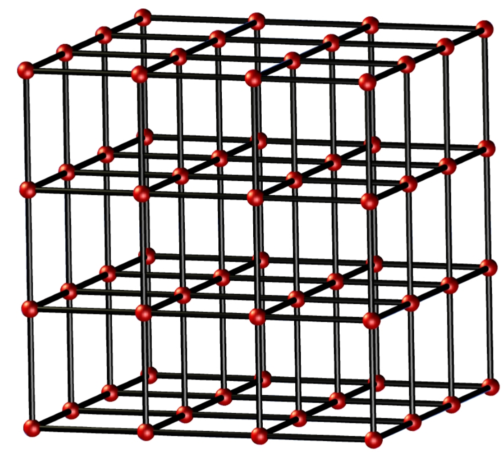
Filling space by generalized polyhedra (*cages*) in which at least two edges meet at each vertex and two faces meet at each edge. Tilings are "face-to-face"



exploded view of space filling by cube tiles

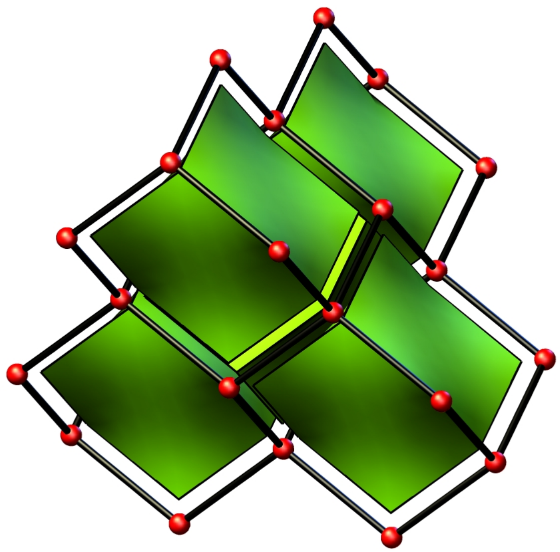


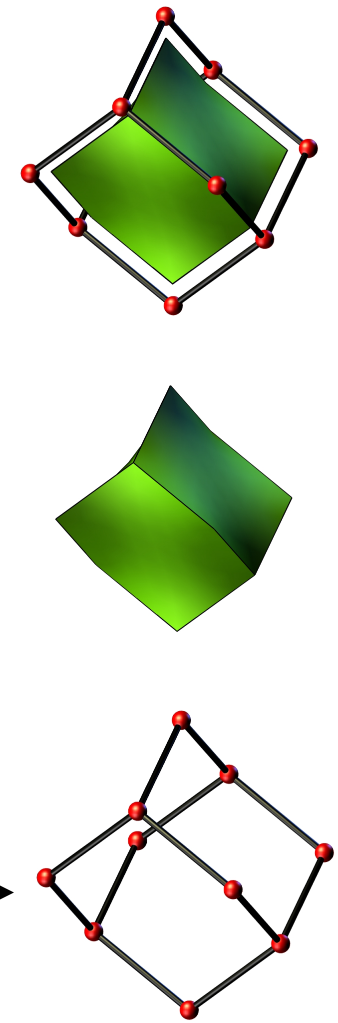
tiling plus net of vertices and edges



net "carried" by tiling **pcu**

Tiling that carries the diamond (**dia**) net
The tile (adamantane unit) is a *cage* with
four 3-coordinated and six 2-coordinated
there are four 6-sided faces i.e. [6^4]

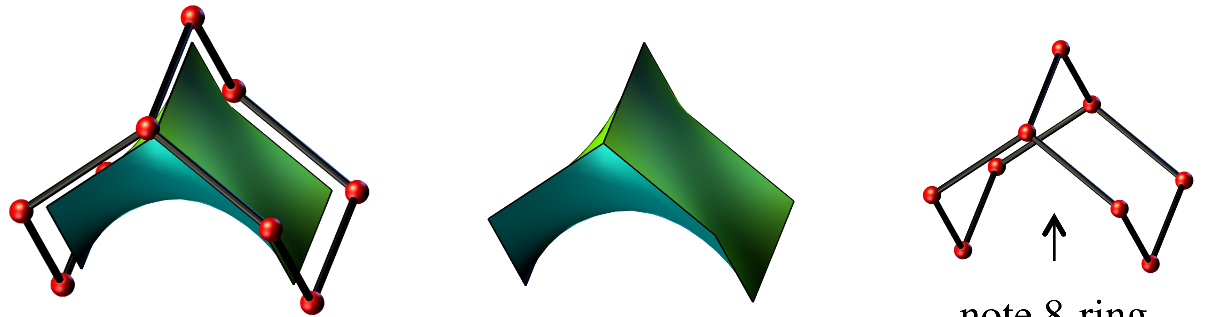




adamantane unit →

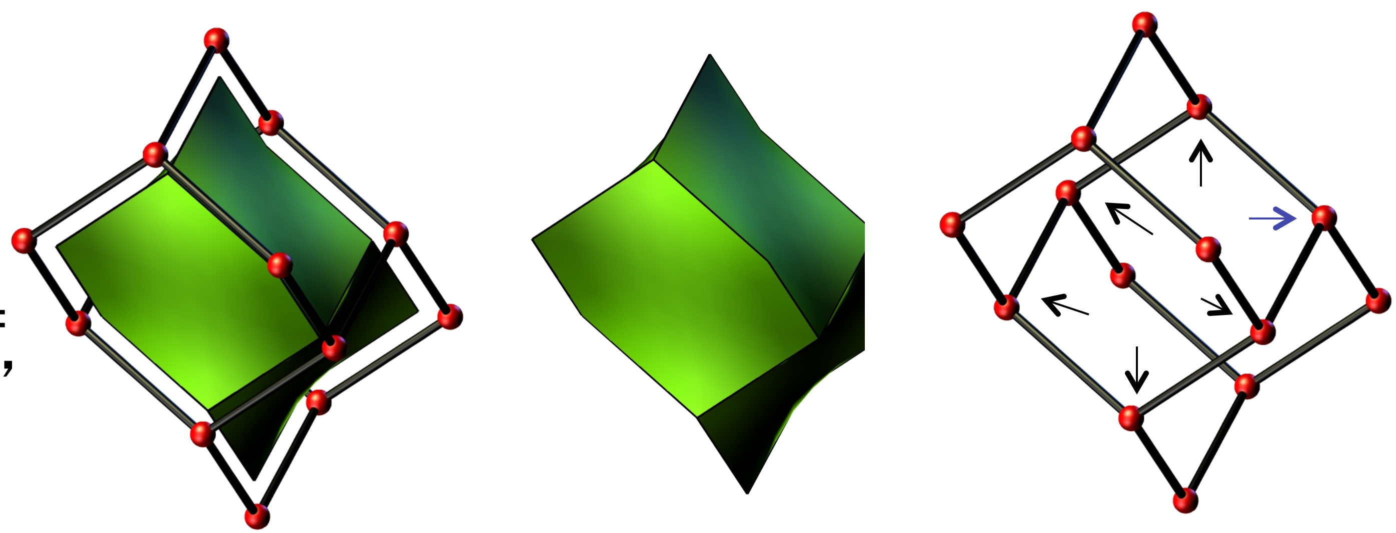
Tiles other than the adamantane unit for the diamond net

half adamantane



note 8-ring
(not a strong ring)

double adamantane = "congressane"



the arrows point to vertices on a 6-ring that is not a tile face

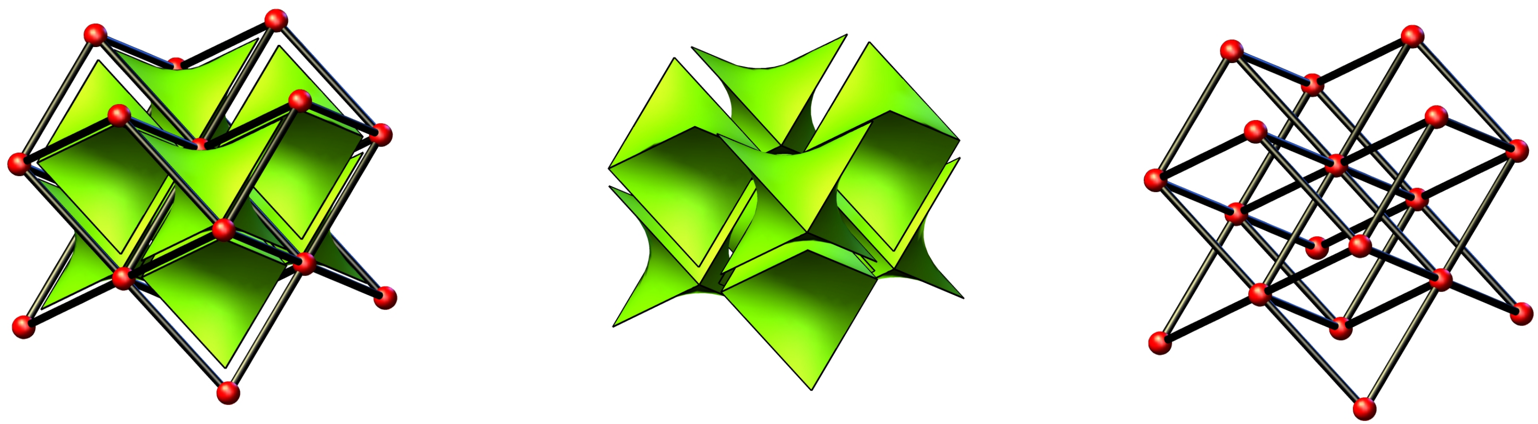
We have seen that if a net has a tiling at all, it has infinitely many made by joining or dividing tiles
The tiling by the adamantane unit appears to be the "natural" tiling for the diamond net. What is special about it? It fits the following definition:

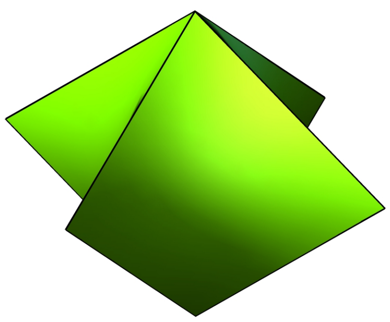
The **natural tiling** for a net is composed of the smallest tiles such that:

(a) the tiling conserves the maximum symmetry. (proper)
(b) all the faces of the tiles are strong rings.

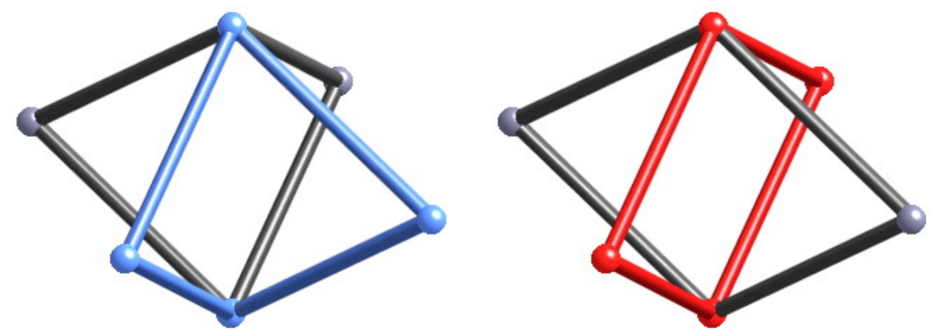
Notice that not all strong rings are necessarily faces
A net may have more than one tiling that fits these criteria. In that case we reject faces that do not appear in all tilings.

natural tiling for body-centered cubic (**bcu**)





one tile



blue is 4-ring face of tile = **essential ring**
red is 4-ring (strong) not essential ring

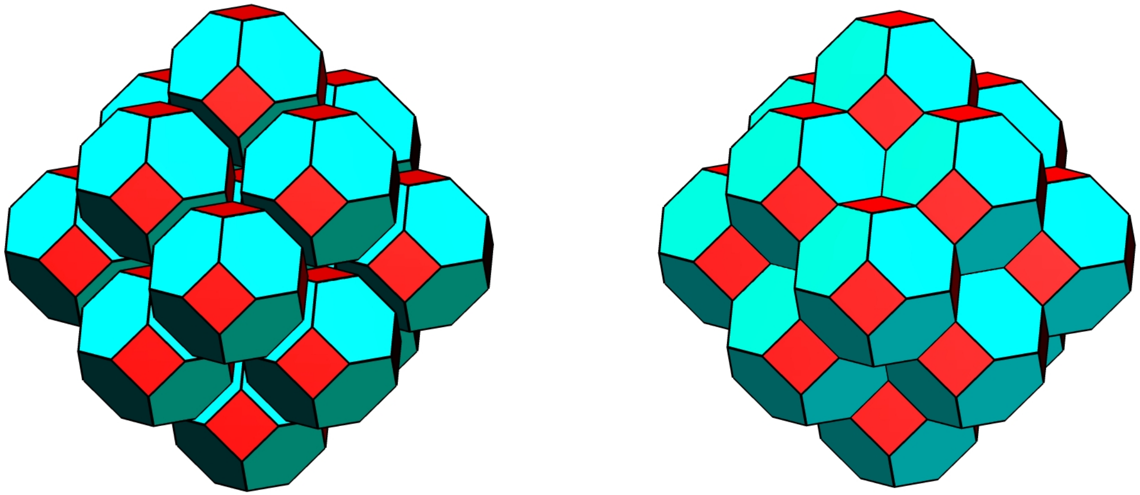
Simple tiling

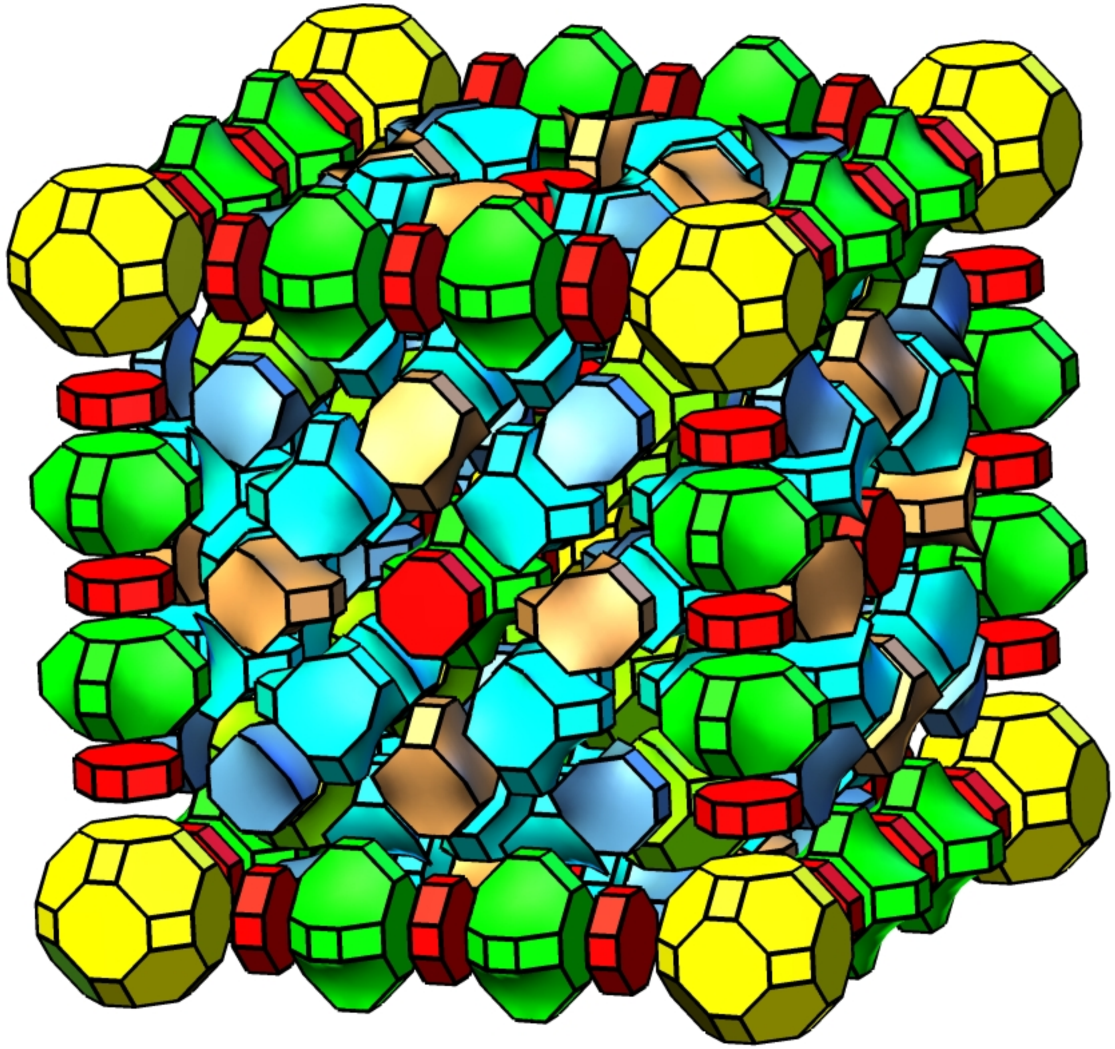
A **simple polyhedron** is one in which exactly two faces meet at each edge and three faces meet at each vertex.

A **simple tiling** is one in which exactly two tiles meet at each face, three tiles meet at each edge and four tiles meet at each vertex (and the tile is a simple polyhedron).

They are important as the structures of foams, zeolites etc.

The example here is a tiling by truncated octahedra which carries the sodalite net (**sod**).

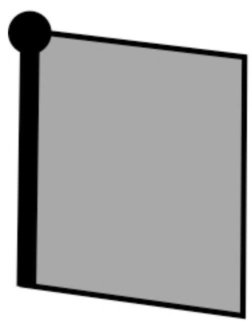




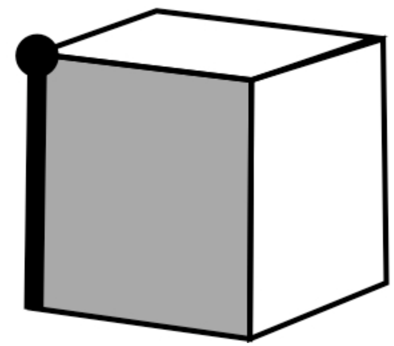
natural tiling of a complex net - that of the zeolite paulingite

Flags

regular tilings are flag transitive



2-D flag
vertex-edge-2D tile



3-D flag
vertex-edge-face-3D tile

Regular tilings and Schläfli symbols

(a) in spherical (constant positive curvature) space,
(b) euclidean (zero curvature) space
(c) hyperbolic (constant negative curvature) space

i.e. in S^d, E^d, and H^d (d is dimensionality)

H. S. M. Coxeter 1907-2003
Regular Polytopes, Dover 1973
The Beauty of Geometry, Dover 1996

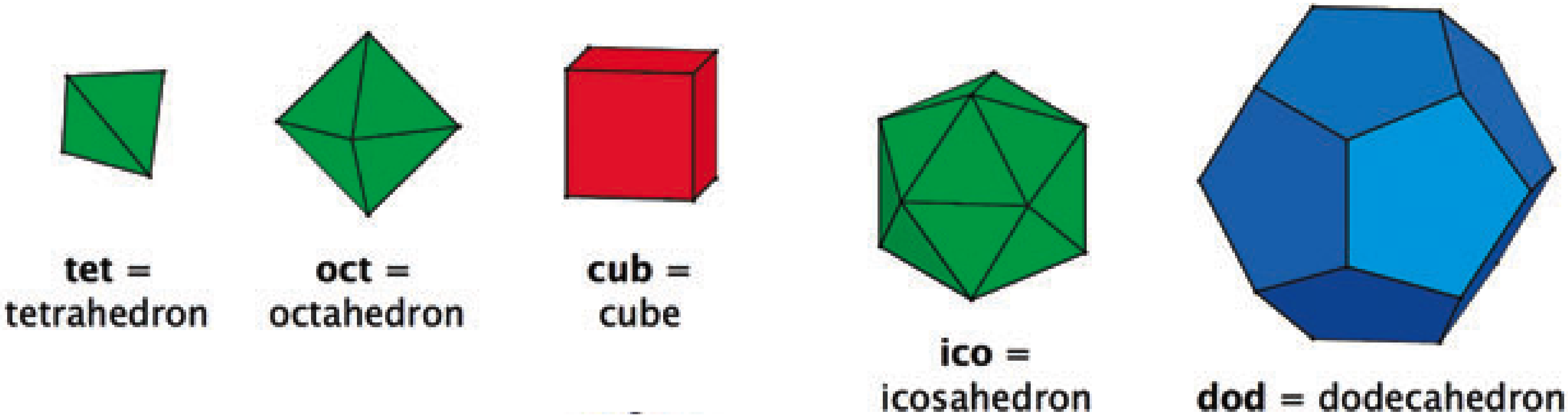
Start with one dimension.
Polygons are the regular polytopes in S^1
Schläfli symbol is {p} for p-sided

{∞} is degenerate case - an infinite linear group of line segments. Lives in E^1

Two dimensions. The symbol is {p,q} which means that q {p} meet at a point three cases:

case (a) $1/p + 1/q > 1/2 \rightarrow$ tiling of S^2

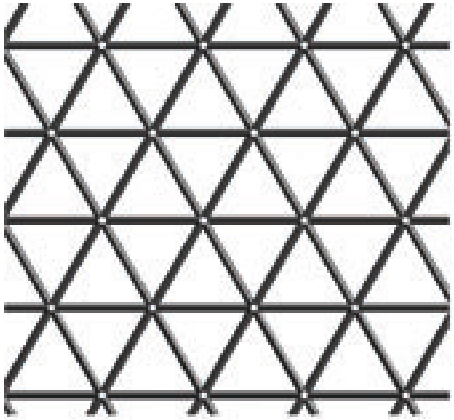
{3,3} tetrahedron
{3,4} octahedron
{3,5} icosahedron
{4,3} cube
{5,3} dodecahedron



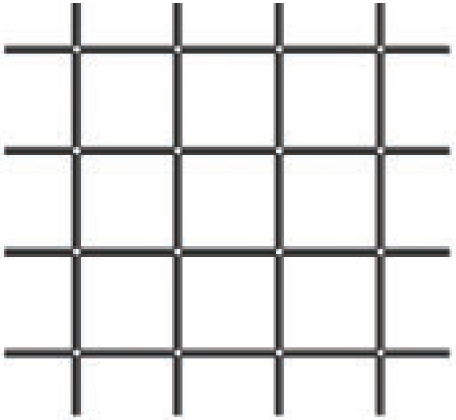
Two dimensions. The symbol is {p,q}
which means that q {p} meet at a point
three cases:

case (b) $1/p + 1/q = 1/2$ → tiling of E^2

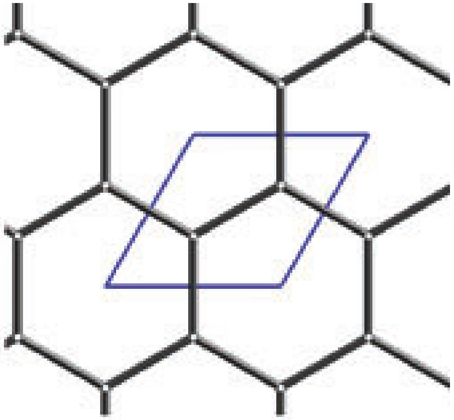
{3,6} hexagonal lattice
{4,4} square lattice
{6,3} honeycomb



hxl =
hexagonal lattice



sql =
square lattice

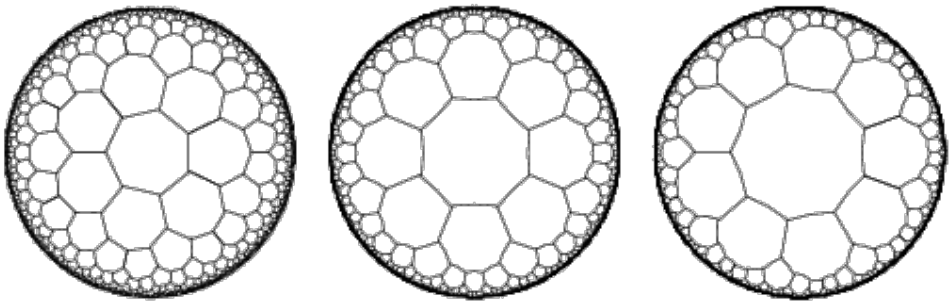


hcb =
honeycomb

Two dimensions. The symbol is {p,q} which means that q {p} meet at a point infinite number of cases:

case (c) $1/p + 1/q < 1/2 \rightarrow$ tiling of H^2

any combination of p and q (both >2) not already seen



{7,3} {8,3} {9,3}

space condensed to a Poincaré disc

Three dimensions. Schläfli symbol {p,q,r}
which means r {p,q} meet at an edge.

Again 3 cases

case (a) Tilings of S^3 (finite 4-D polytopes)

{3,3,3} simplex
{4,3,3} hypercube or tesseract
{3,3,4} cross polytope (dual of above)
{3,4,3} 24-cell
{3,3,5} 600 cell (five regular tetrahedra meet at each edge)
{5,3,3} 120 cell (three regular dodecahedra meet at each edge)

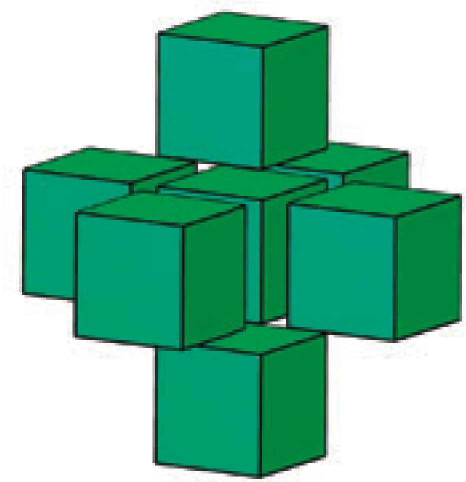
Three dimensions. Schläfli symbol {p,q,r} which means r {p,q} meet at an edge.

Again 3 cases

case (b) Tilings of E^3

{4,3,4} space filling by cubes self-dual

Only regular tiling of E^3

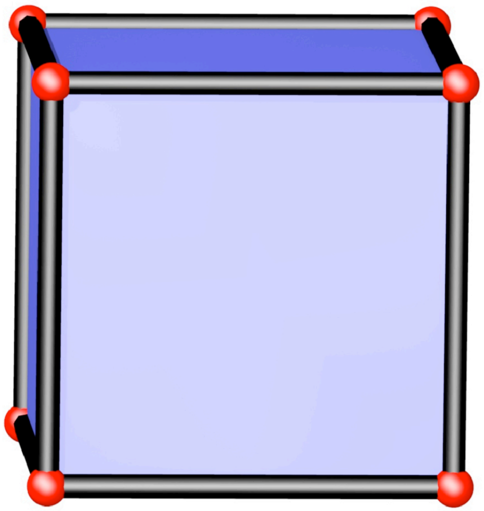


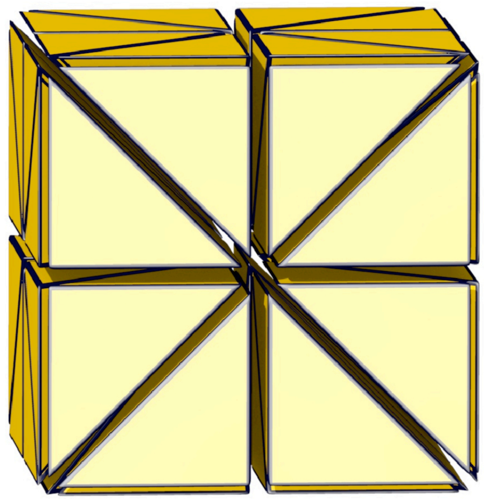
So what do we use for tilings that aren't regular?

Delaney-Dress symbol or D-symbol
(extended Schläfli symbol)

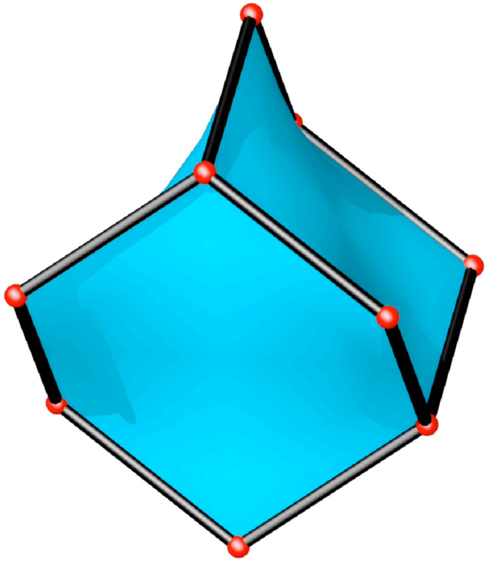
Introduced by Andreas Dress (Bielefeld) in
combinatorial tiling theory.

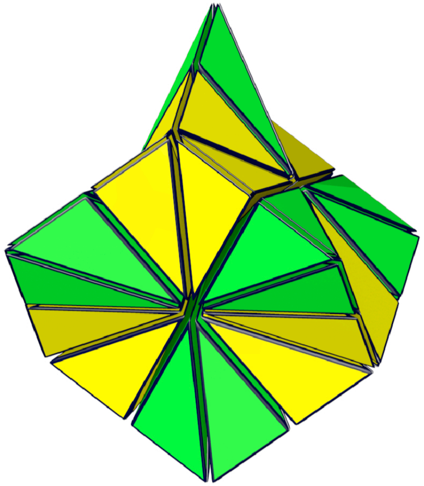
Developed by Daniel Huson
and Olaf Delgado-Friedrichs.





tile for **pcu**.
one kind of chamber
D-size = 1
D-symbol
<1.1:1 3:1,1,1,1:4,3,4>





tile for **dia**.
two kinds of chamber
D-size = 2
D-symbol
<1.1:2 3:2,1 2,1 2,2:6,2 3,6>

Q. How do you find the natural tiling for a net?

A. Use TOPOS

Q. How do you draw tilings?

A. Use 3dt

Transitivity

Let there be p kinds of vertex, q kinds of edge, r kinds of face and s kinds of tile. Then the transitivity is $pqrs$.

Unless specified otherwise, the transitivity refers to the natural tiling.

We shall see that there are five natural tilings with transitivity 1111; these are tilings of the **regular nets**. (There are at least two not-natural tilings with transitivity 1111 – these have natural tilings with transitivity 1121 and 1112 respectively)

Duals

A **dual tiling** tiling is derived from the original by centering the old tiles with new vertices, and connecting the new vertices with new edges that go through each old face.

The dual of a dual tiling is the original tiling

If a tiling and its dual are the same it is **self dual.**

The dual of a tiling with transitivity *pqrs* is *srqp*.

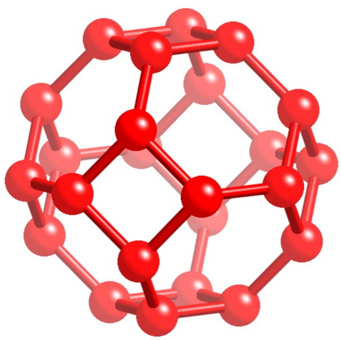
The dual of a natural tiling may not be a natural tiling.

If the natural tiling of a net is self-dual, the net is **naturally self dual**.

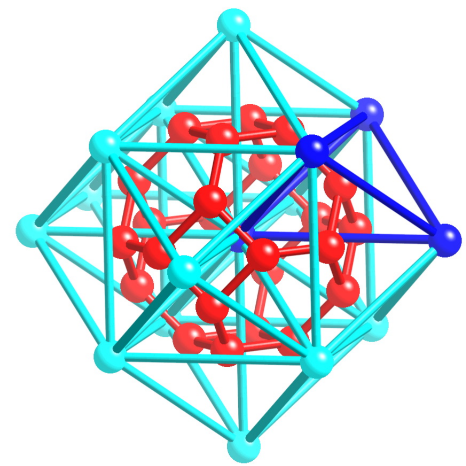
The faces (essential rings) of a natural tiling of a net are **catenated** with those of the dual.

Duals (cont)

The number of faces of a dual tile is the coordination number of the original vertex.
The number of vertices of a face of a dual tile is the number of tiles meeting at the corresponding edge of the original tiling.
The dual of a simple tiling is thus a tiling by tetrahedra (four 3-sided faces)



Sodalite (**sod**) tile part of a simple tiling



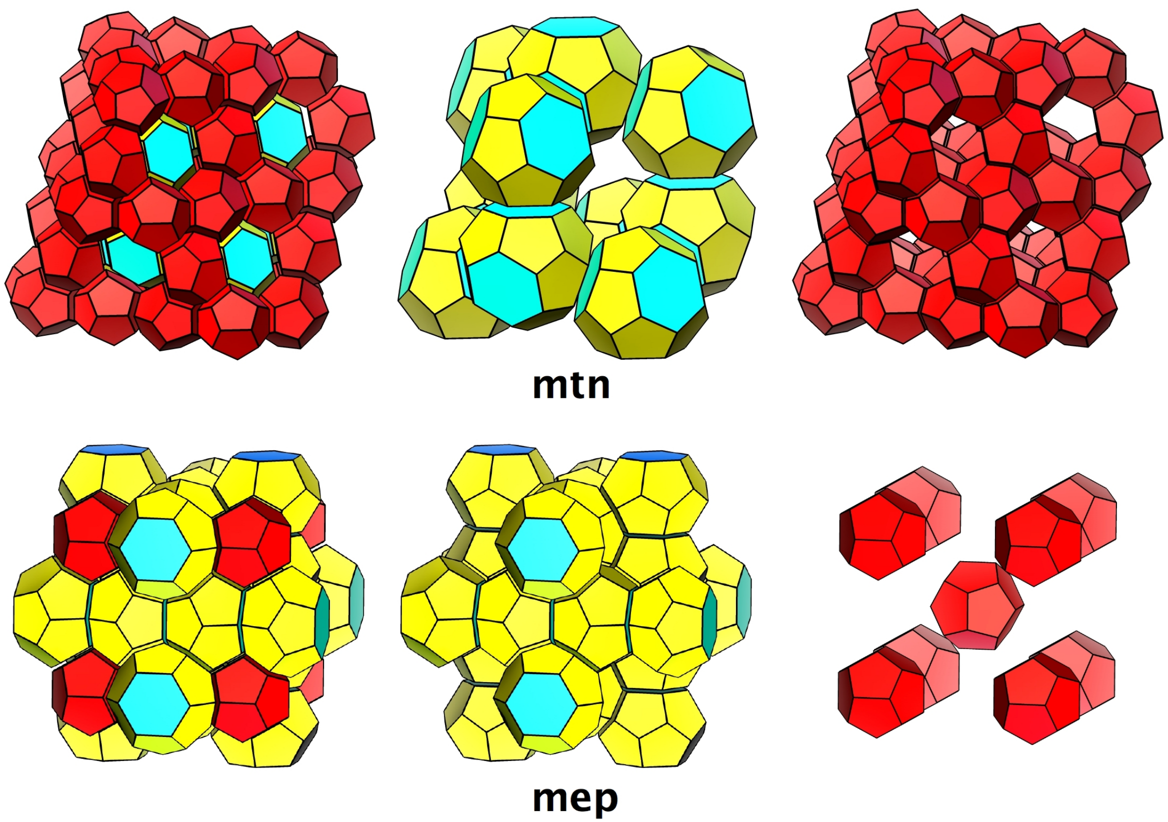
Dual tiling (blue) is **bcu-x** 14-coordinated body-centered cubic. A tiling by congruent tetrahedra

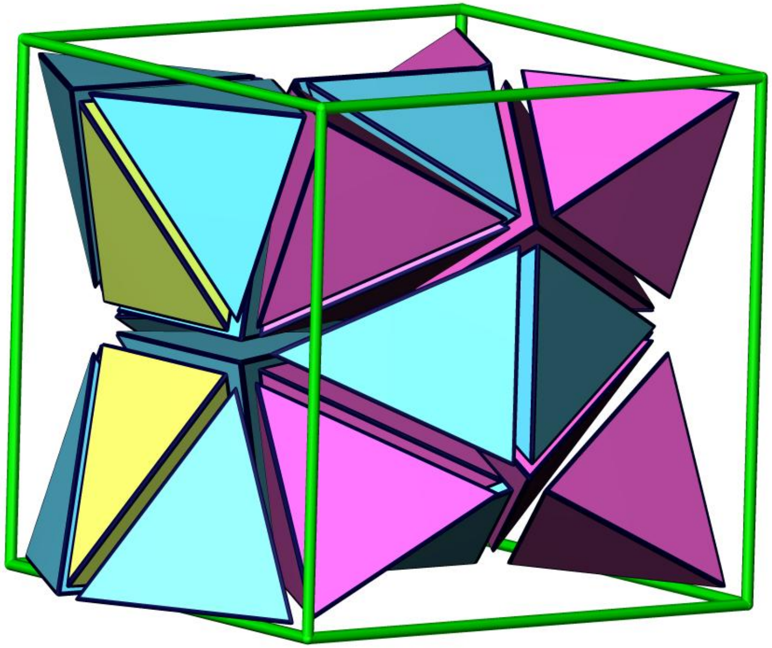
Some examples of dual structures

simple tiling
sodalite (**sod**)
type I clathrate (**mep**)
type II clathrate (**mtn**)

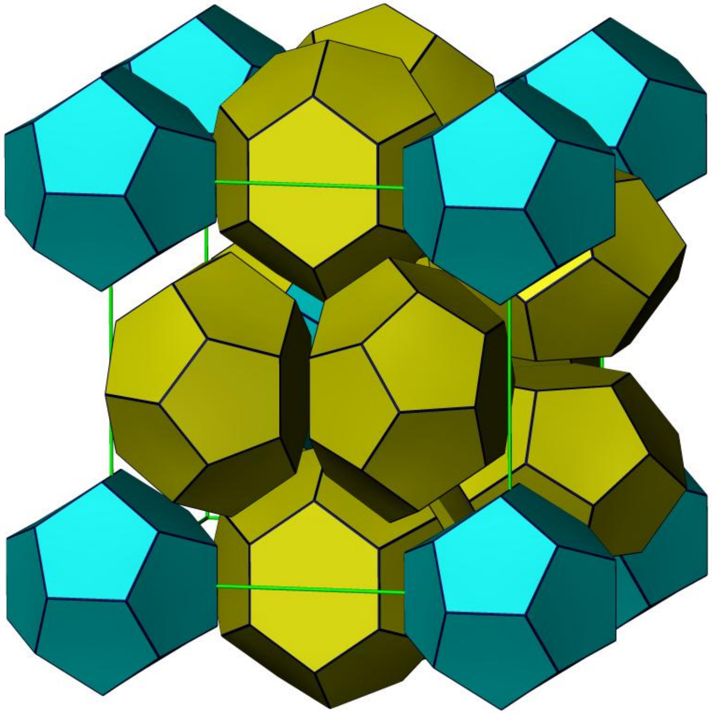
tiling by tetrahedra
body-centered cubic
A15 (Cr_3Si)
$MgCu_2$

Frank-Kasper



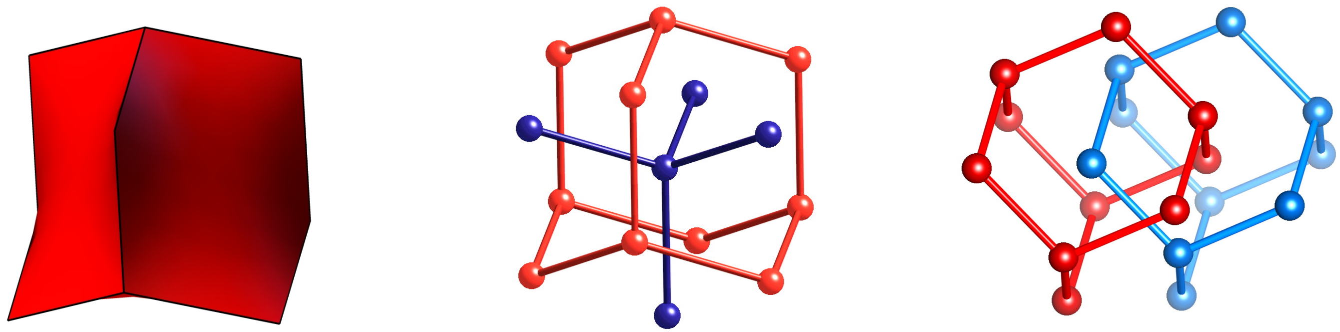


Cr_3Si (A15)

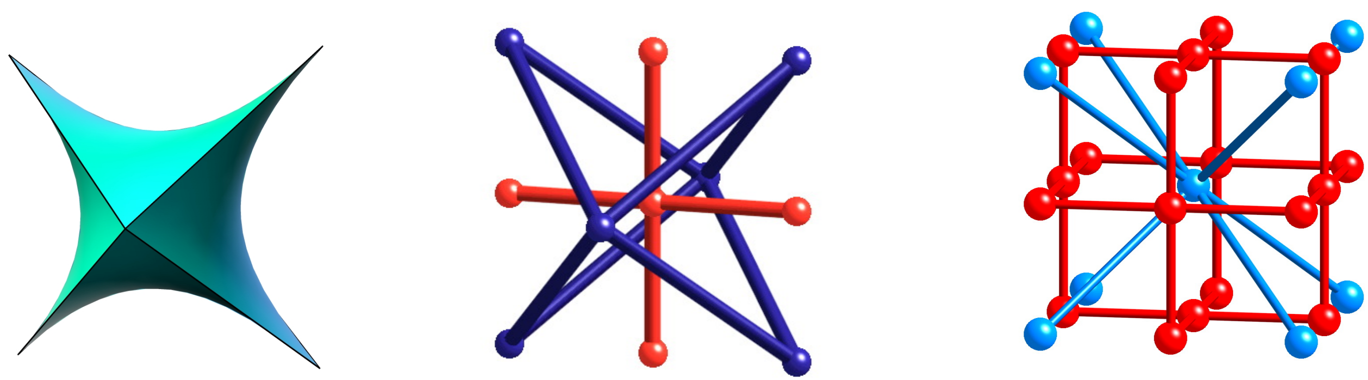


Type I clathrate
melanophlogite (MEP)
Weaire-Phelan foam

examples of duals

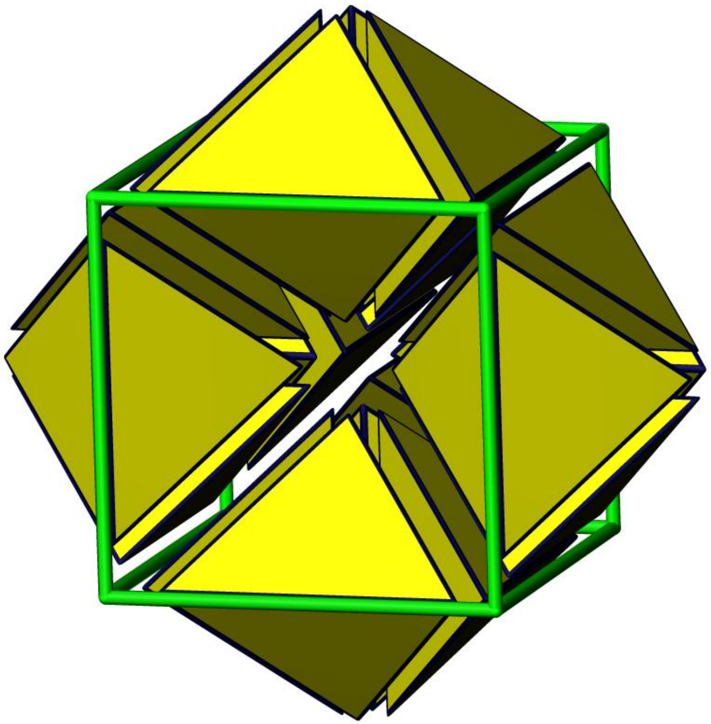


diamond (**dia**) is naturally self dual

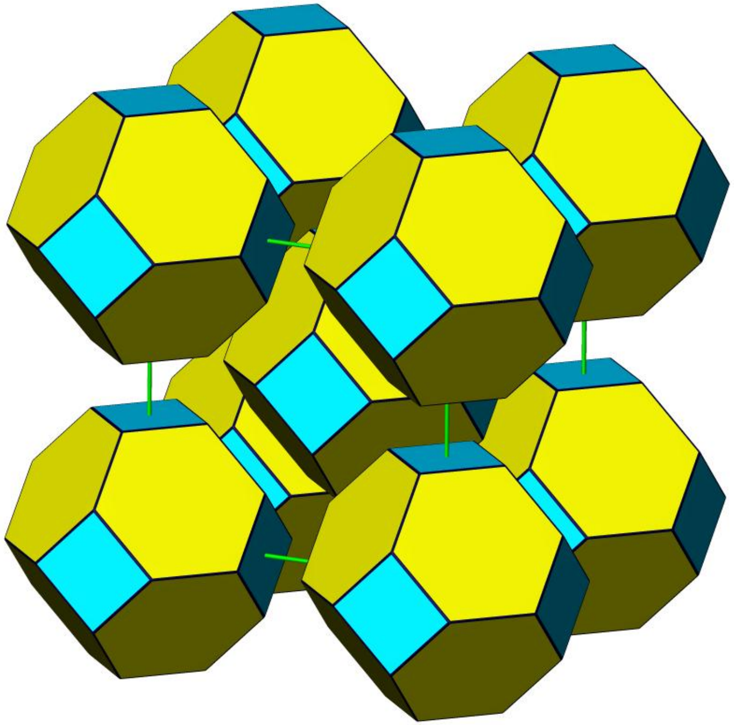


the dual of body-centered cubic (**bcu**) is the 4-coordinated NbO net (**nbo**)

Example of isohedral tiling by tetrahedra (Somerville tetrahedra). Only one that is also vertex transitive

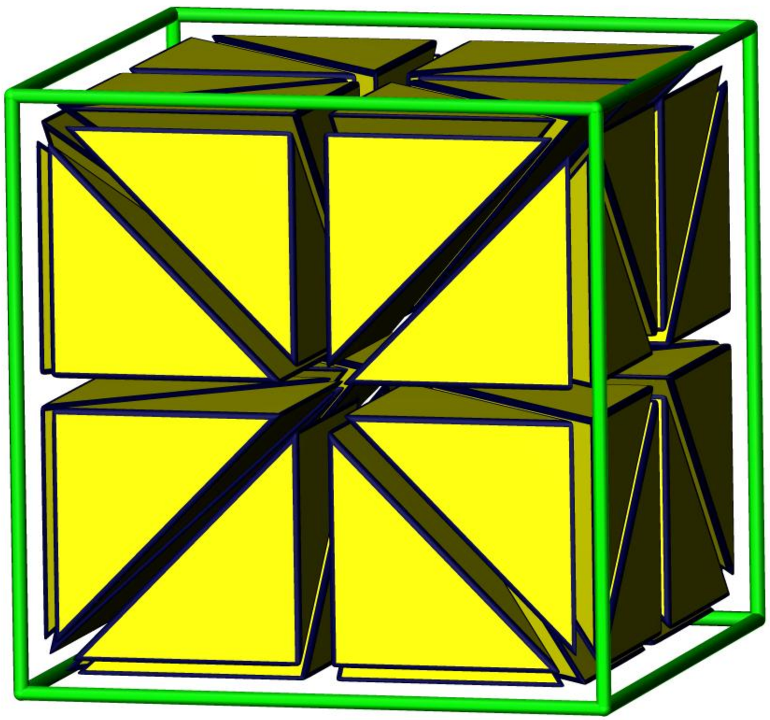


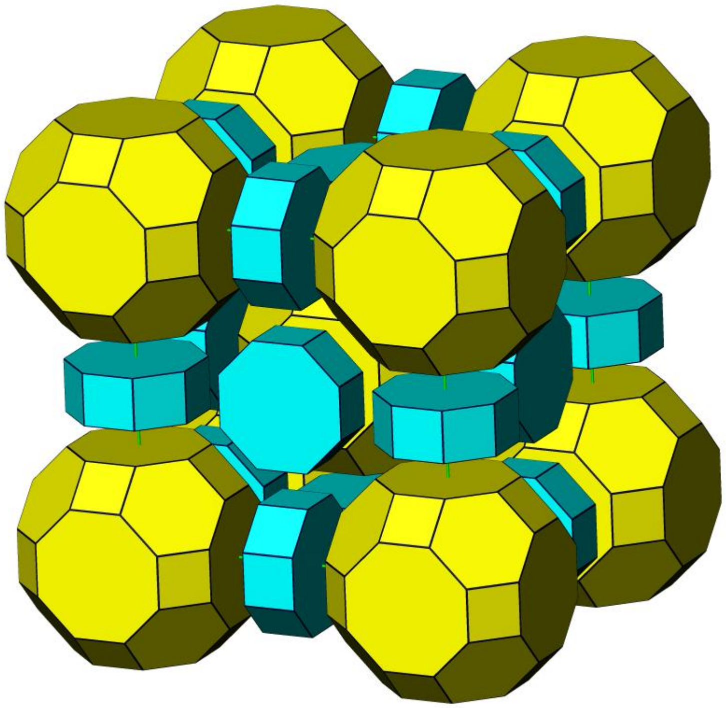
vertices are body-centered cubic



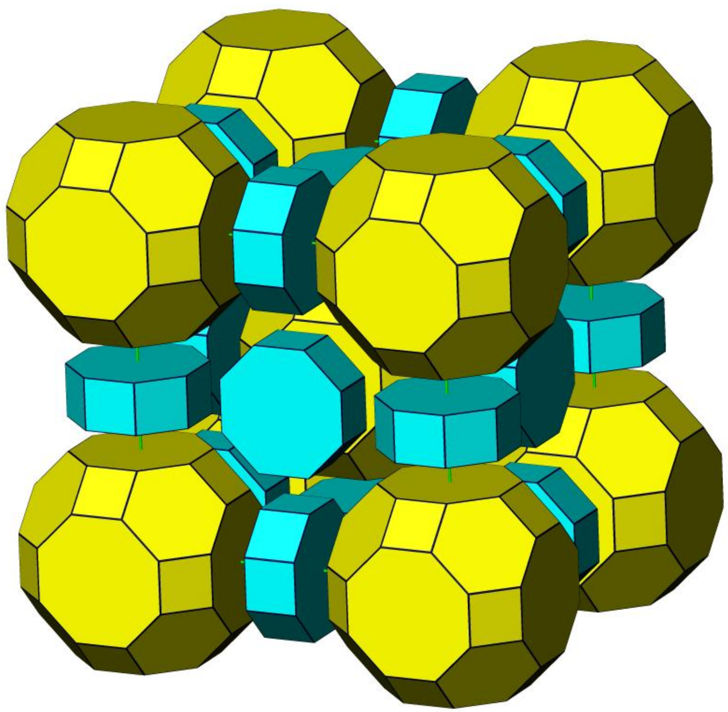
Dual structure (sodalite). "Kelvin structure"

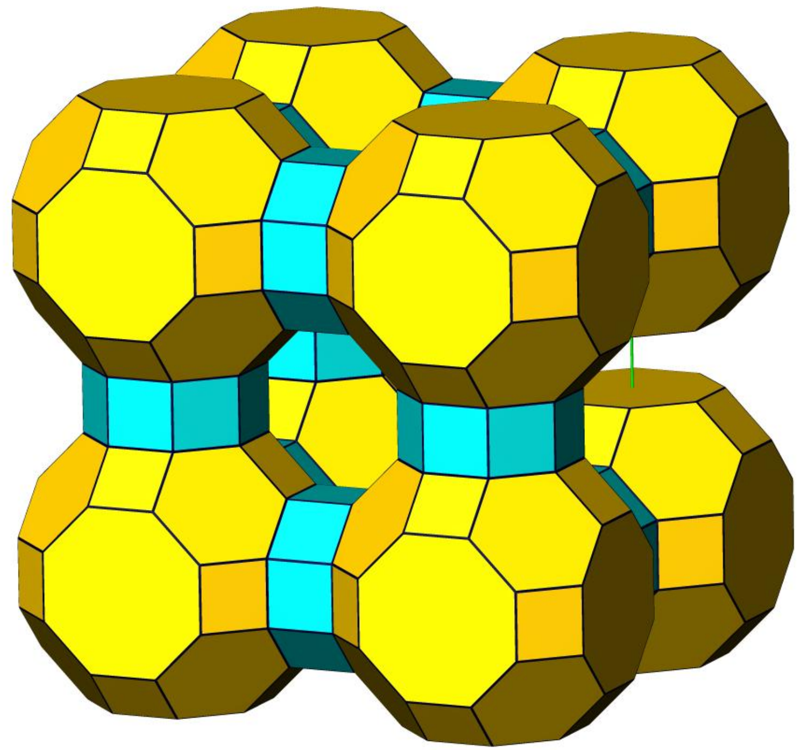
Another example: isohedral tiling by hlf-Somerville tetrahedra

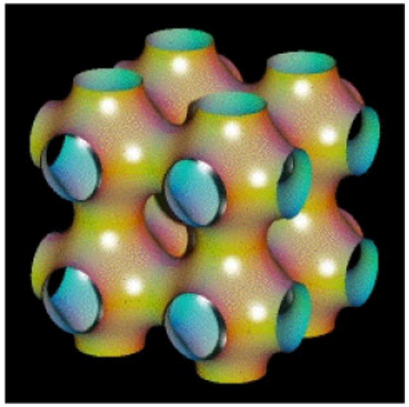




Dual structure -zeolite RHO

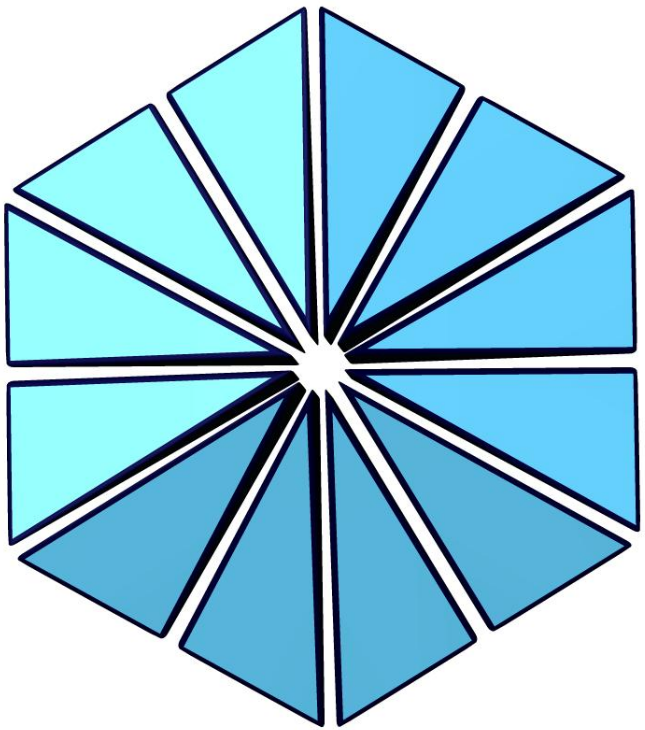




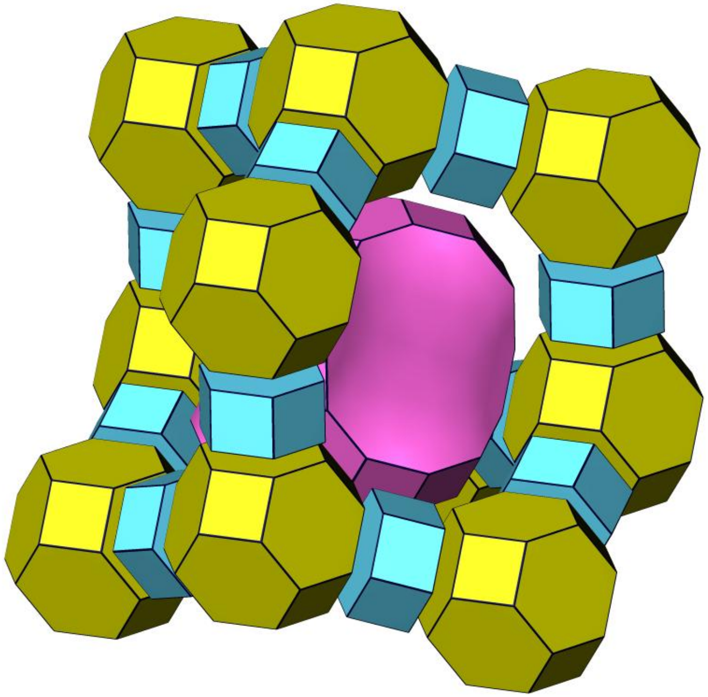


The 1-skeleton (net) of RHO
is also the 1-skeleton of a
3^3.6 tiling of a 3-periodic surface.
(Hyde and Andersson)

Yet another isohedral tiling by tetrahedra



12 tetrahedra forming a rhombohedron



Fragment of dual structure
Zeolite structure code FAU (faujasite) - billion dollar material!
Also a $3^4.6$ tiling of a surface

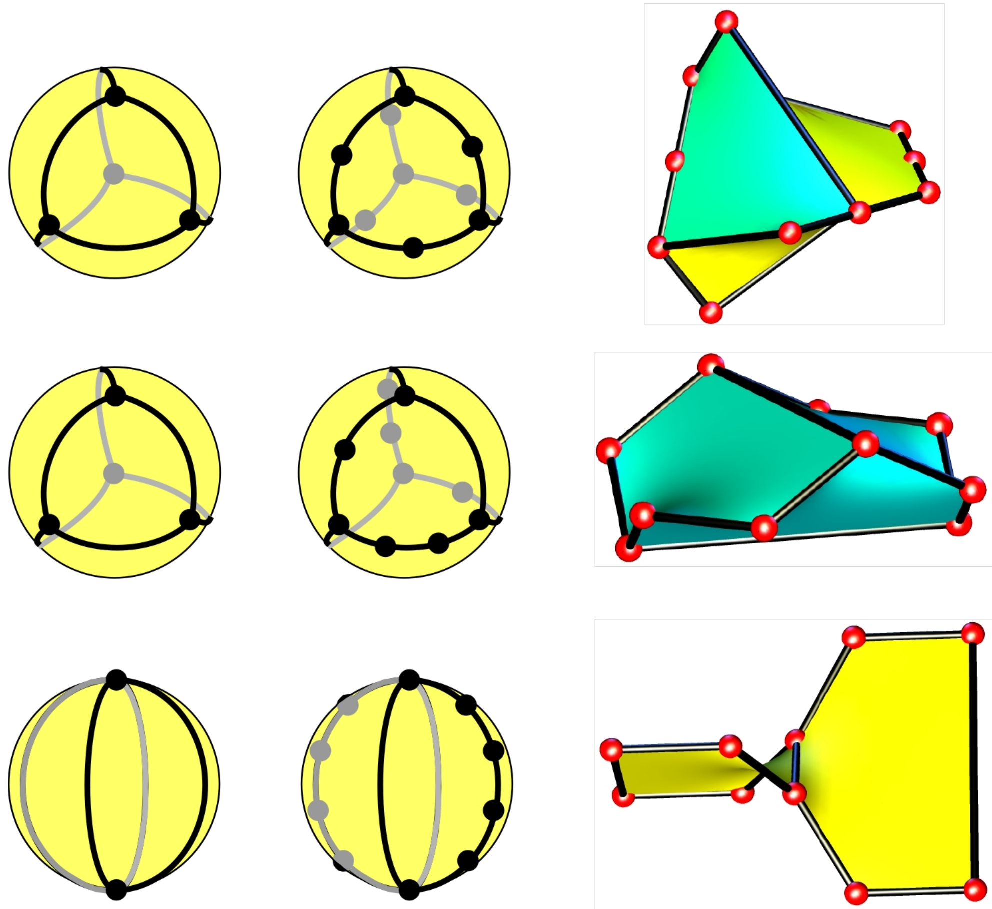
How to find edge-transitive nets?

A net with ine kind of edge has a tiling that is dual to a tiling with one kind of face.

So let's systematically enumerate all tilings with one kind of face. (faces can be two sided like a coin)

1. list all polyhedra with one kind of face
2. extend the faces with divalent vertices
3. see if the cages form proper tilings

O. Delgado-Friedrichs & M. O'Keeffe, *Acta Cryst. A*, **63**, 244 (2007)



Examples of $[6^4]$ face-transitive tiles

Table 1. Edge-transitive nets retrieved in this study listed by size of the Delaney-Dress symbol (D-symbol) of the proper tiling with smallest size. The 3-letter symbols are the RCSR (http://rcsr.anu.edu.au/) symbols.

D-symbol size	uninodal	binodal
1	**pcu**	
2	**bcu, dia, fcu, nbo**	**flu**
3	**reo, sod**	
4	**crs, hxg**	**ftw**
6	**acs**	
8	**rhr**	**bor, mgc, nia, ocu, rht, she, soc, spn, tbo, the, toc, ttt, twf,**
10	**lcs, lvt, lcy, srs**	**ith, scu, shp, stp**
12	**lcv**	**alb, pto**
14	**qtz**	**pts**
16	**bcs**	**sqc**
20	**thp**	**csq, ssa, ssb**
24	**ana**	**gar, iac, ibd, pyr, ssc**
28		**ifi**
32		**ctn, pth**

← **pcu** only regular tiling!

end