Nets and Tiling

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Introduction to tiling theory
and its application to crystal nets

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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

Berkeley 37.9 N, 122.3 W

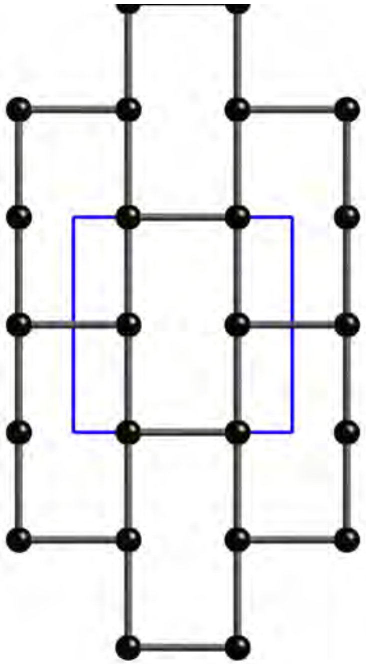
Tempe 33.4 N, 121.9 W

As far as we are concerned

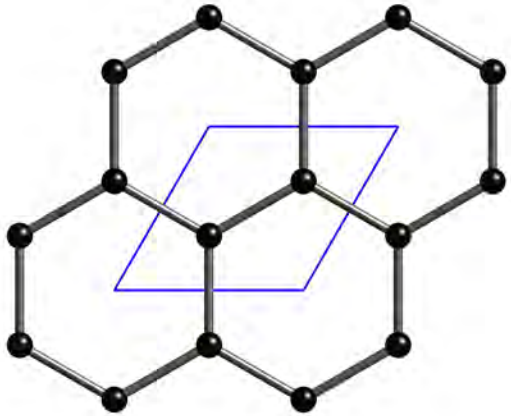
Tilings in two dimensions are edge-to-edge
(each edge is common to just two tiles)

In three dimensions face-to-face
(each face common to just two tiles)

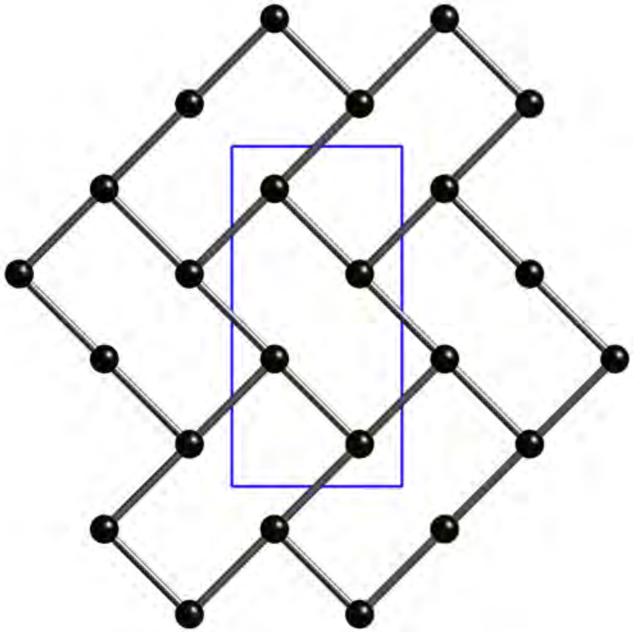
Three different embeddings of **the same abstract tiling**



brick wall
*c*2*mm*

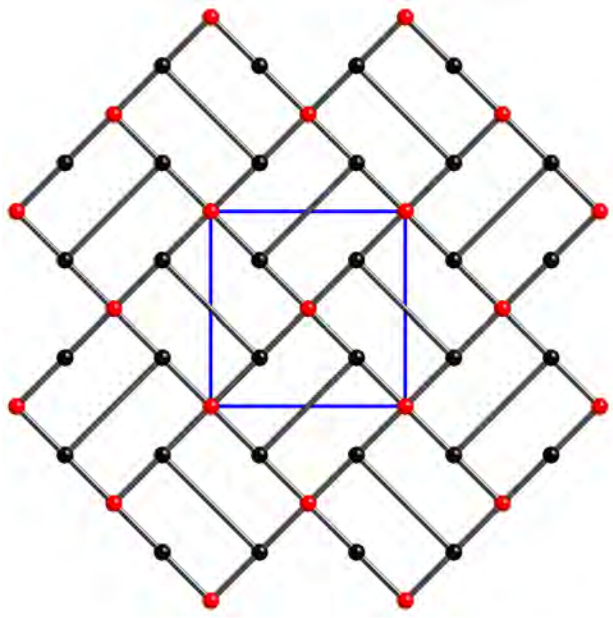


honeycomb
*p*6*mm*

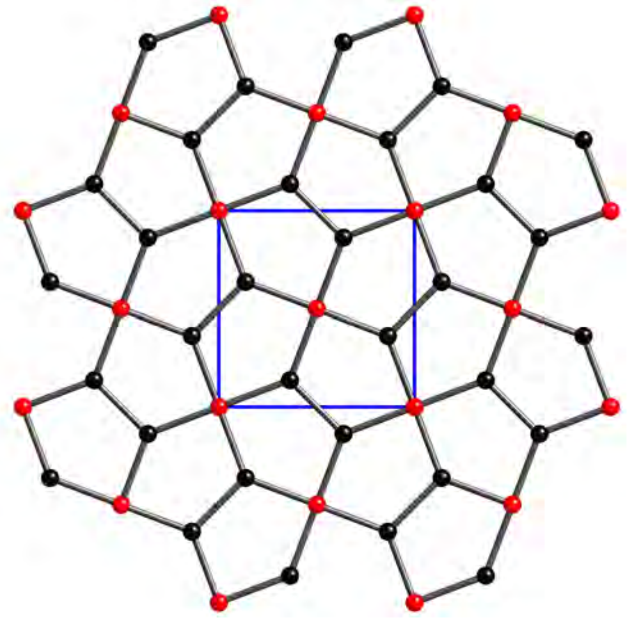


herringbone
*p*2*gg*

Again, two embeddings of the same abstract tiling



double brick

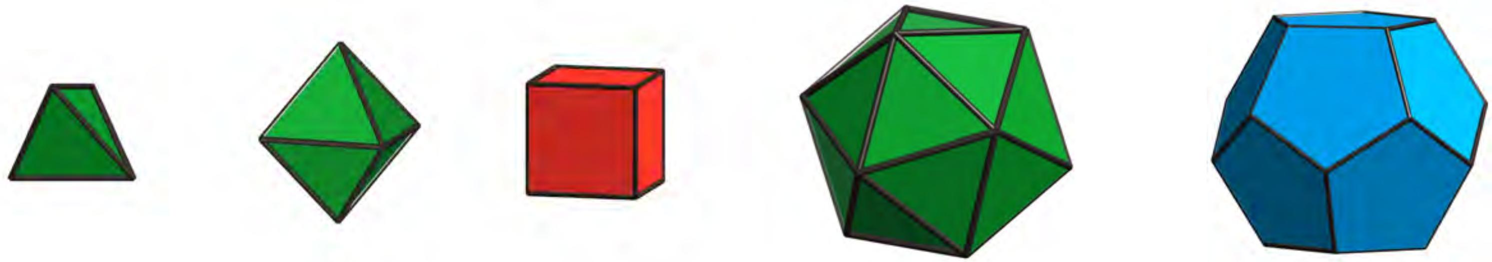


Cairo tiling

Both have same symmetry, *p*4*gm*. The Cairo conformation is the minimum density for equal edges.

Recall Steinitz theorem

Planar 3-connected graph is graph of a convex polyhedron

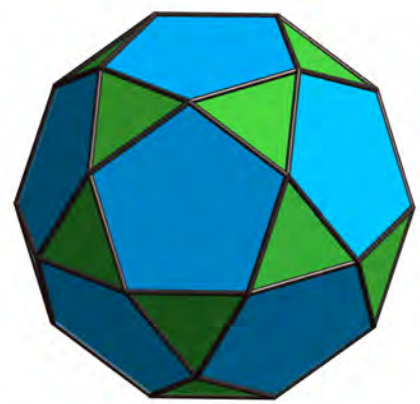


3^3 3^4 4^3 3^5 5^3

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

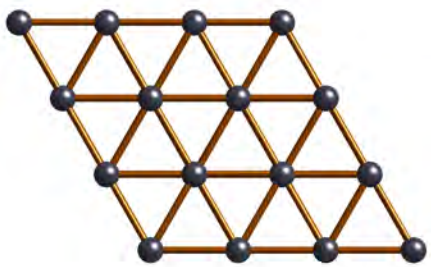
3.4.3.4

3.5.3.5

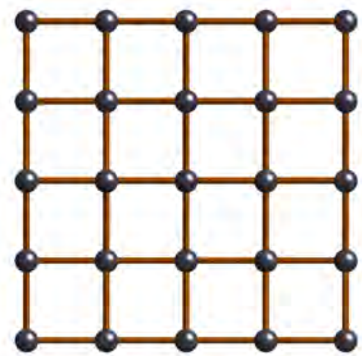


Quasiregular polyhedra: one kind of vertex, one kind of edge

Tiling of the plane - regular tilings
one kind of vertex, one kind of edge, one kind of face



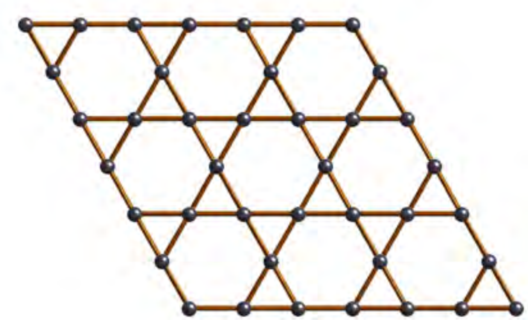
3^6
hexagonal lattice



4^4
square lattice

6^3
honeycomb net

quasiregular
one kind of vertex, one kind of edge
3.6.3.6 kagome net



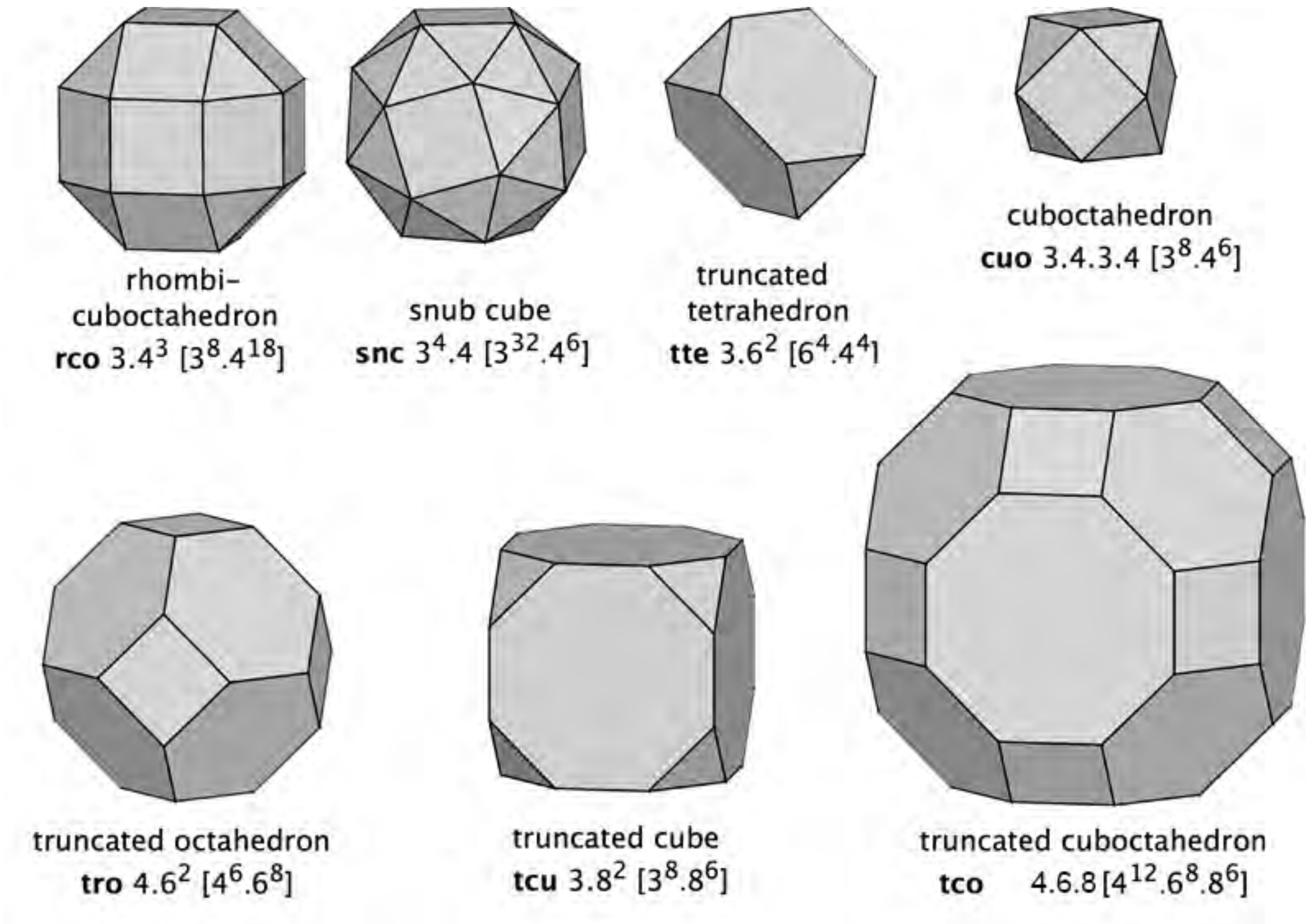
honey comb net is not a lattice

A lattice is a set of points related by translations

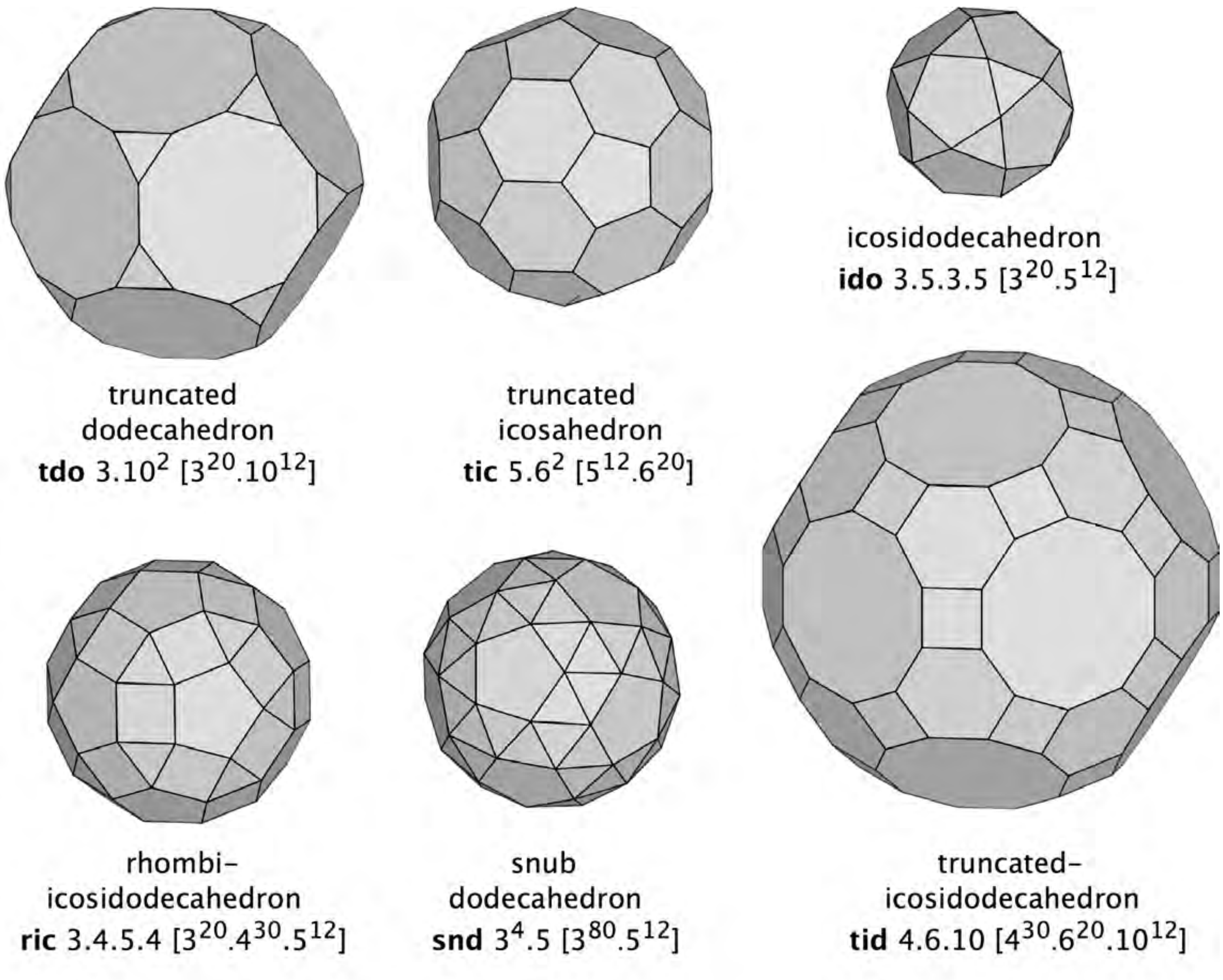
honeycombnet is actually a *lattice complex*

- a set of symmetry-related points related by translations

cubic Archimedean polyhedra - one kind of vertex



icosahedral Archimedean poyhedra - one kind of vertex



8 Archimedean tilings

Picture is from O'Keeffe & Hyde Book

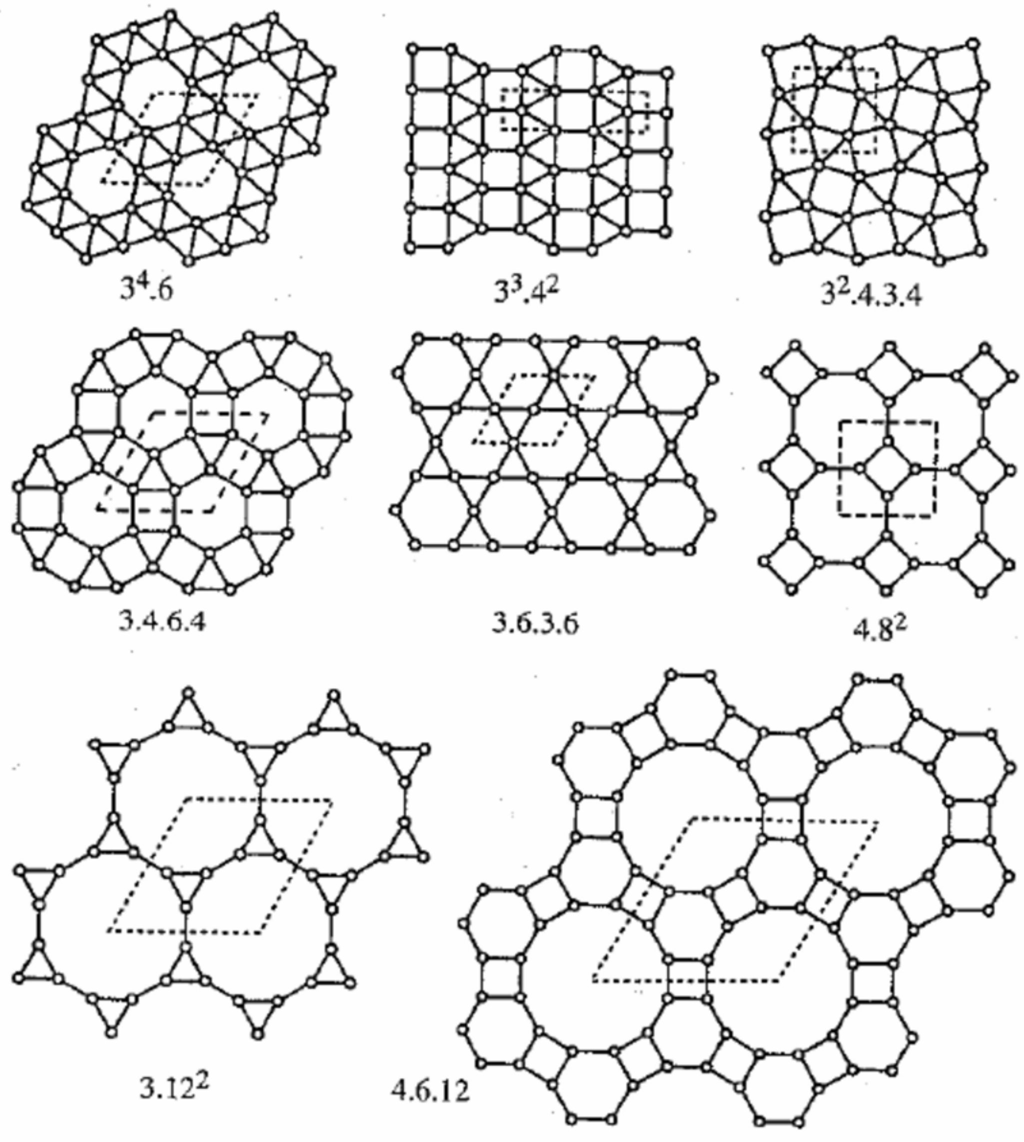
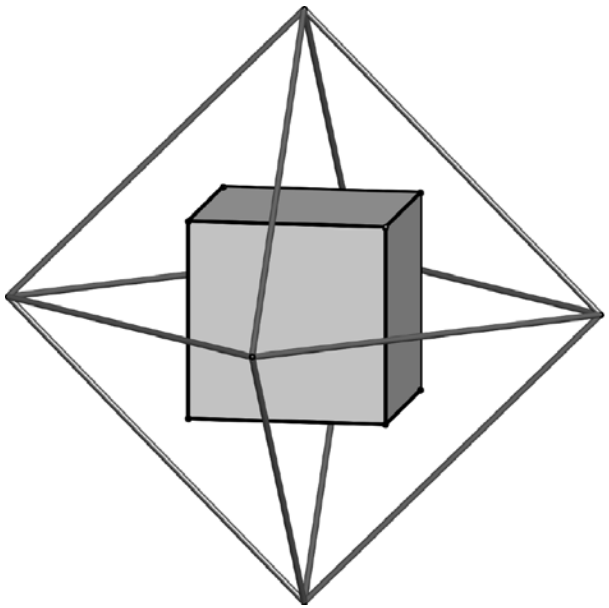
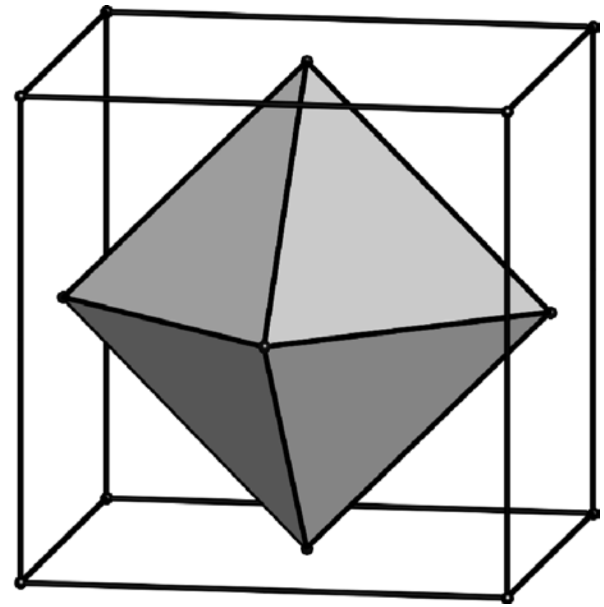


Fig. 5.39. The Archimedean tilings. Top row: $3^4.6$, $3^3.4^2$ and $3^2.4.3.4$. Middle row: 3.4.6.4, 3.6.3.6 and 4.8^2. Bottom row: 3.12^2 and 4.6.12. Unit cells are outlined with broken lines.

Duals of two-dimensional tilings vertices <—> faces

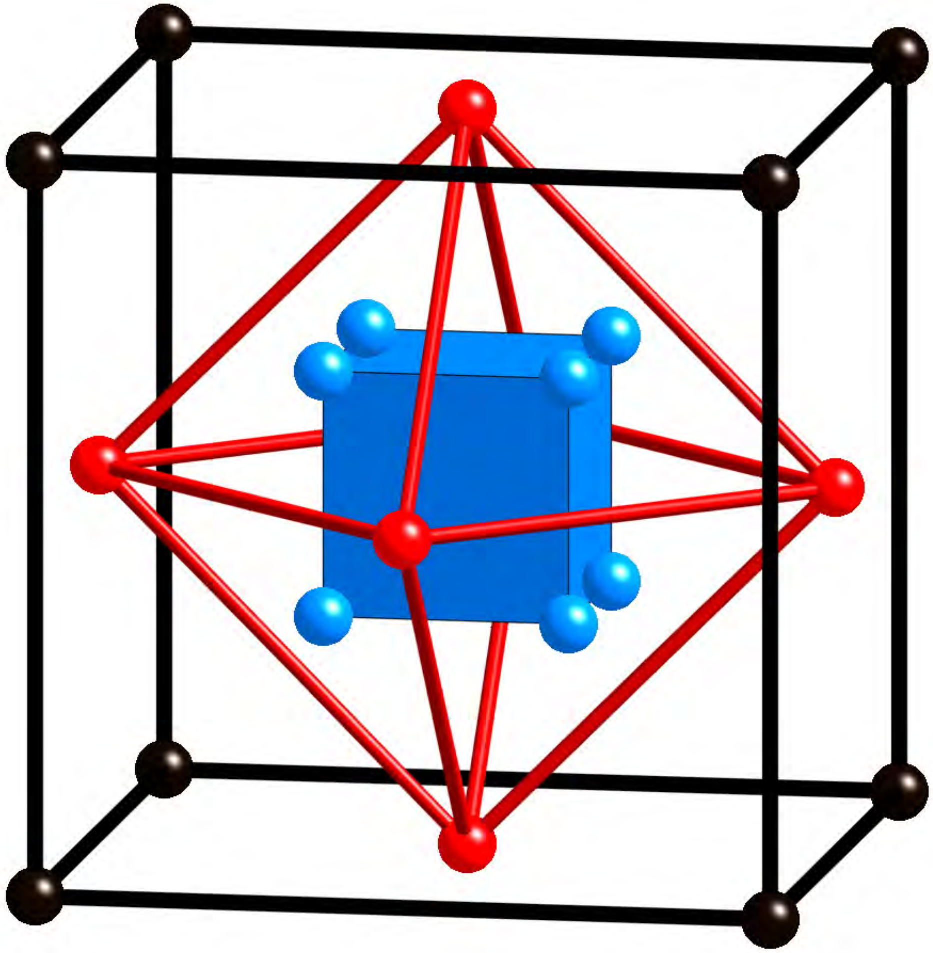


dual of octahedron 3^4
is cube 4^3



dual of cube 4^3
is octahedron 3^4

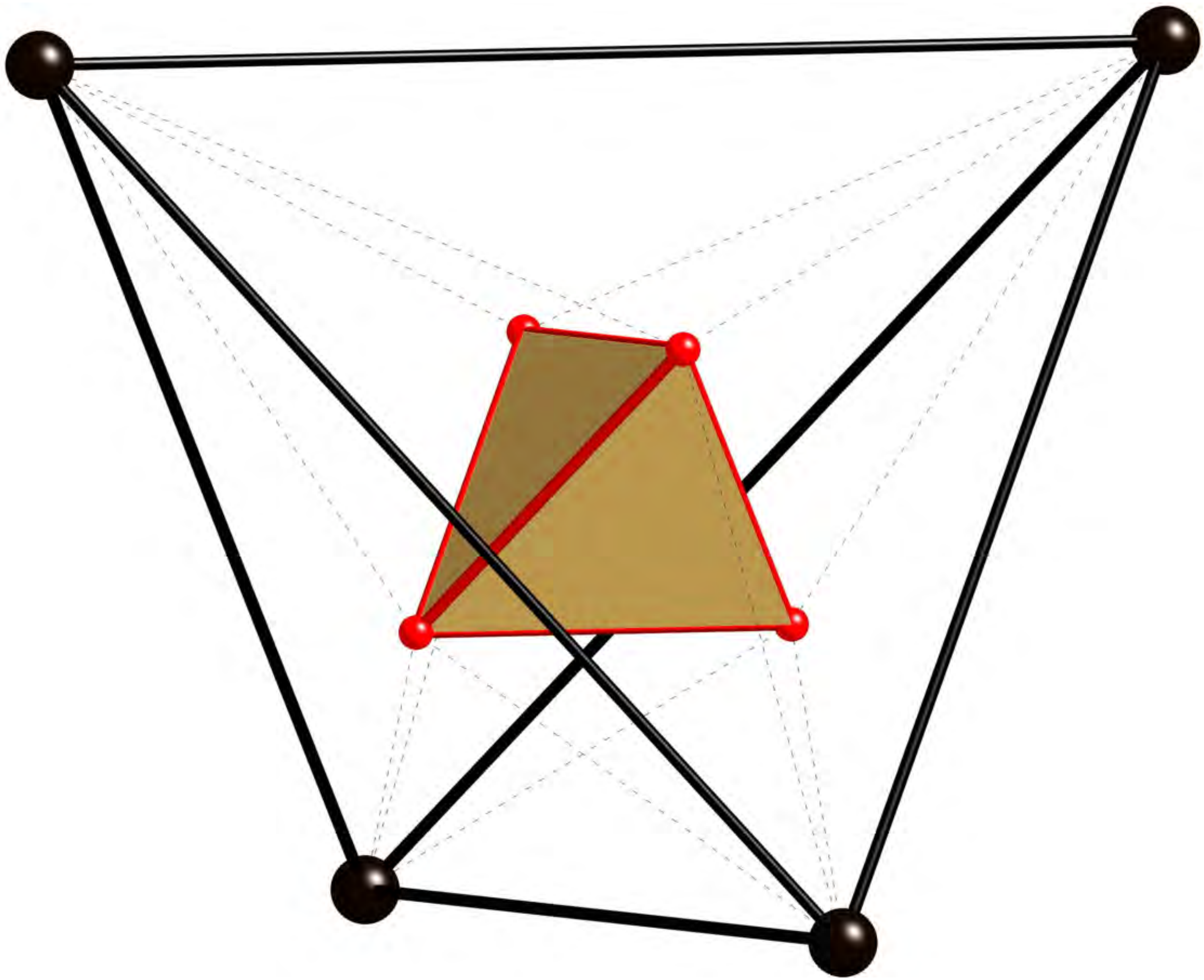
dual of dual is the original
tetrahedron is self-dual



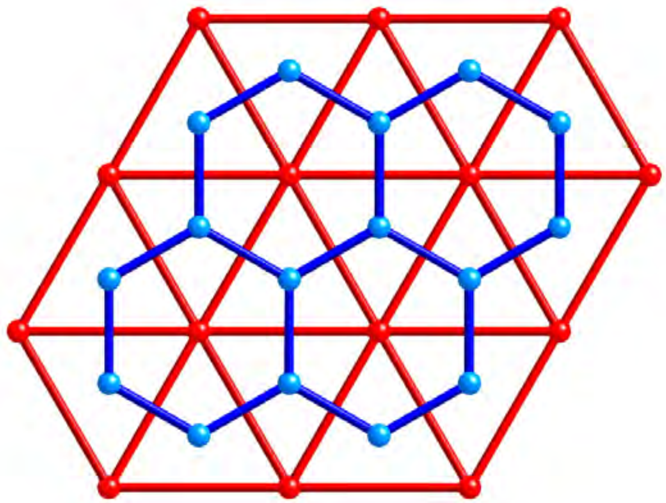
Duals:
edges <-> faces

The dual of a dual
is the original

tetrahedron is self-dual

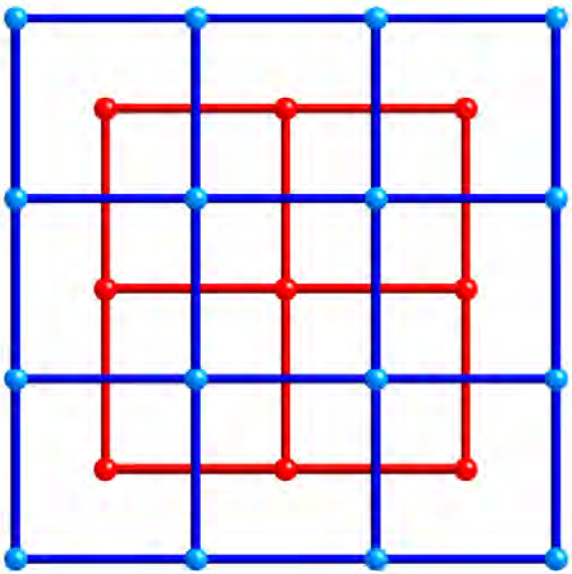


Duals of 2-D periodic nets



$3^6 <=> 6^3$

AlB_2



$4^4 <=> 4^4$

self-dual

Important terms:

Polyhedron convex solid with planar faces
has a planar three-connected graph.*

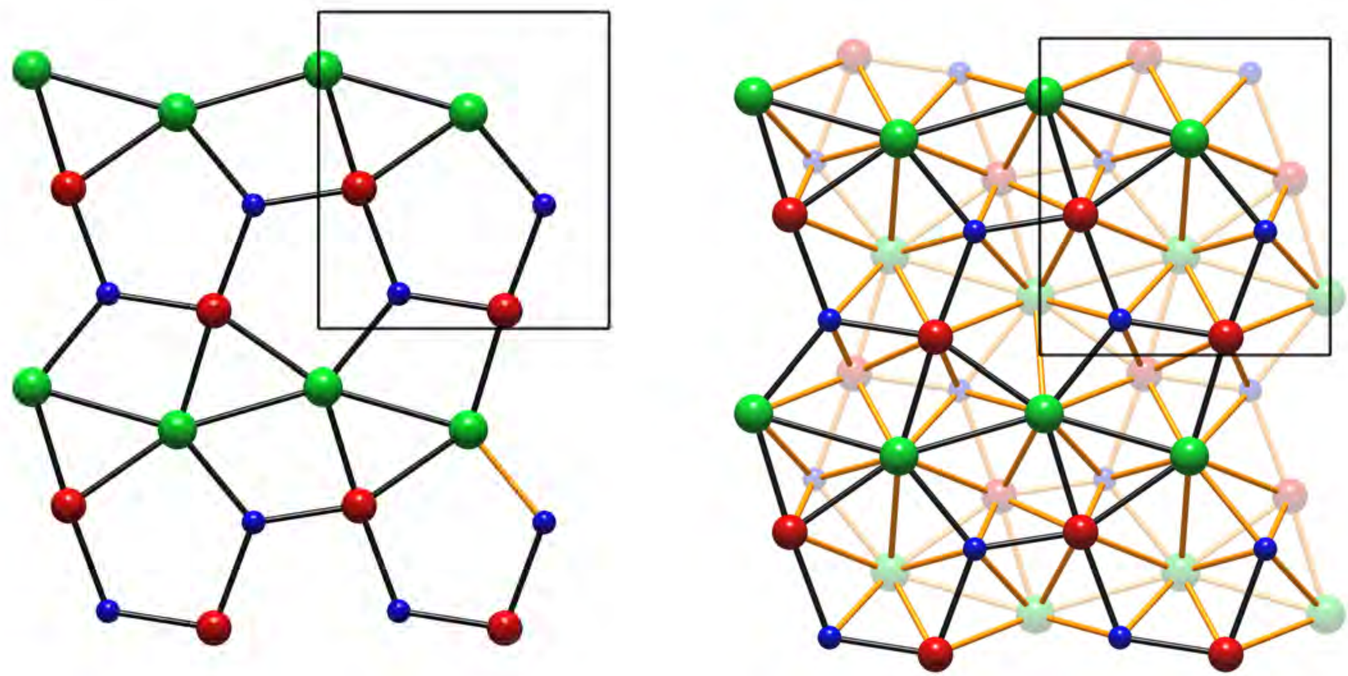
Simple polyhedron all vertices trivalent

Simplicial polyhedron all faces triangles

Simple and simplicial polyhedra are
duals of each other.

*We will call non-conxex solids, maybe with
divalent vertices, ***cages***.

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

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

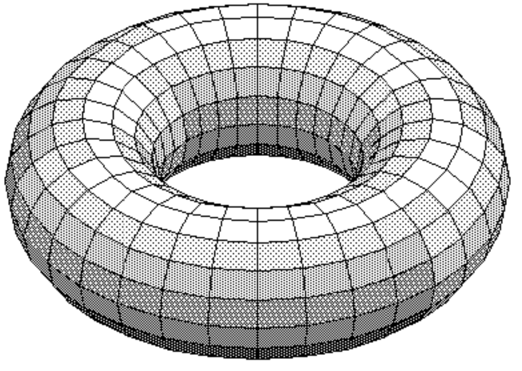
The surface of a body with g holes has genus g

genus of a surface

note all vertices 4^4 just like square lattice

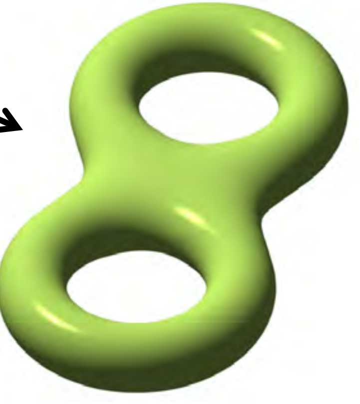
sphere $g = 0$

torus $g = 1$



plane $g = 1$

double torus $g = 2$

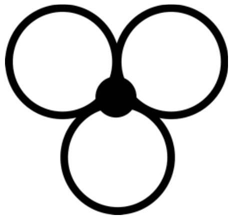


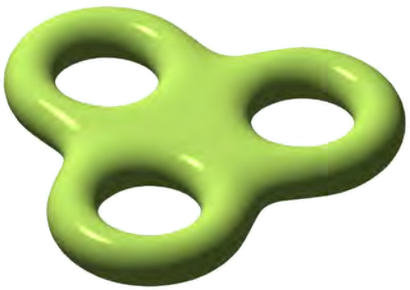
knotted torus still has $g = 1$

genus of a net = cyclomatic number of quotient graph

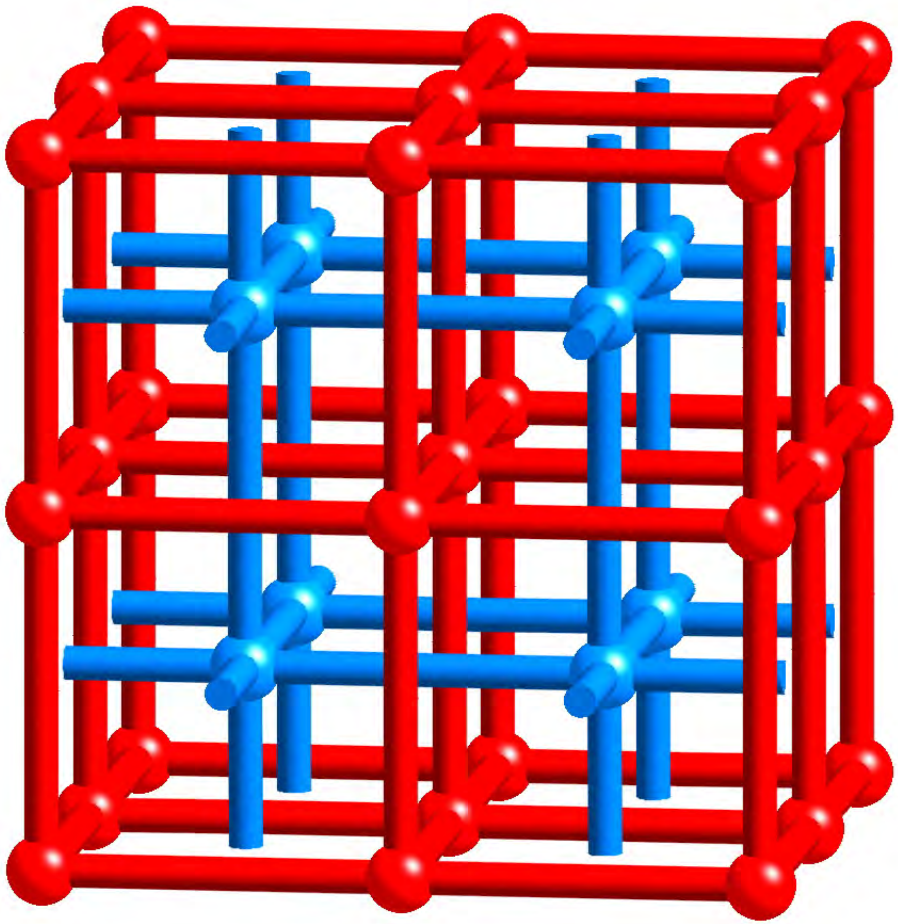
repeat unit
of **pcu**

quotient
graph
cyclomatic
number = 3

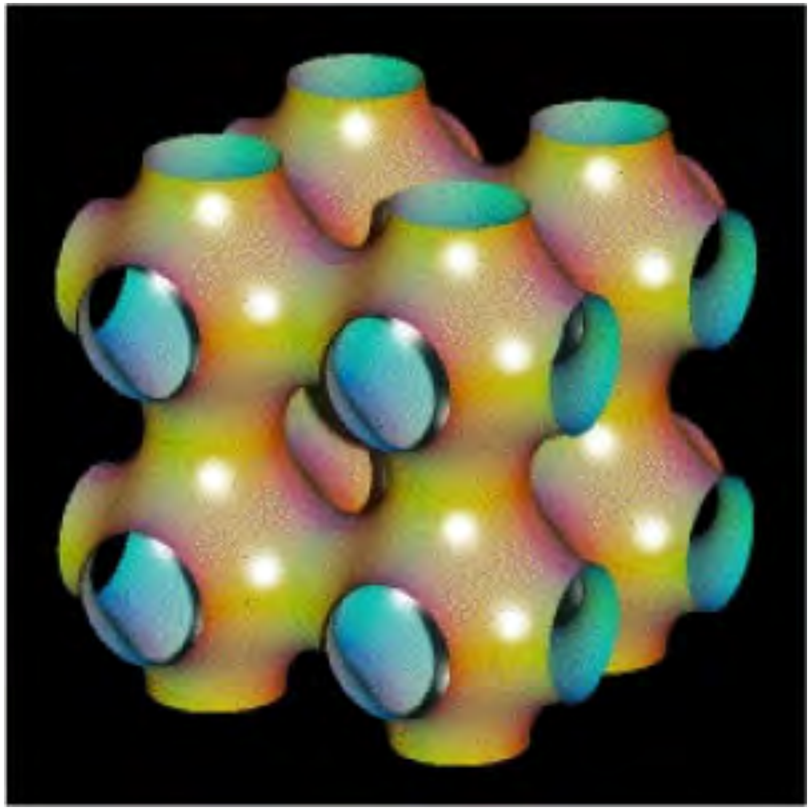




genus of **pcu** net is 3



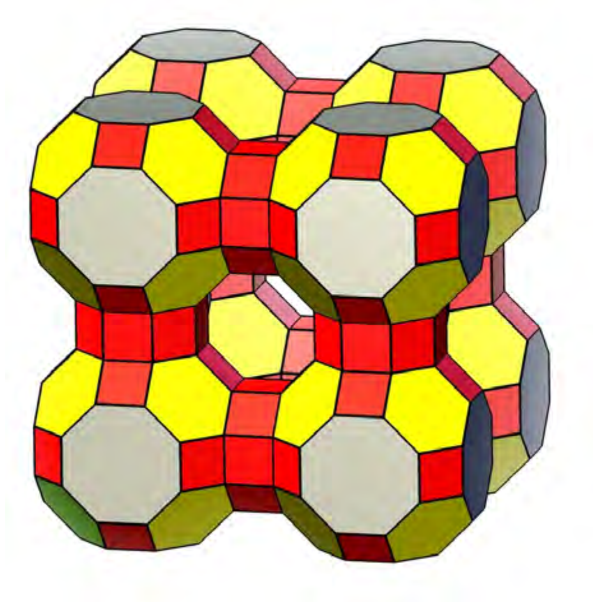
Two interpenetrating **pcu** nets



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

infinite poyhedra – tilings of periodic surfaces

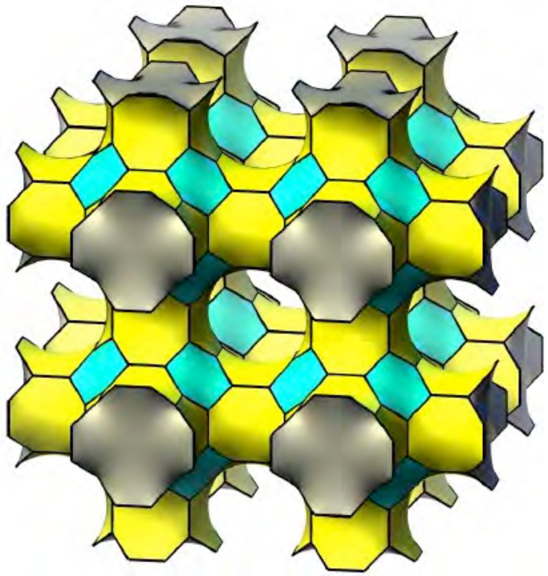
$4^3.6$ tiling of
the *P* surface *(*g = 3)



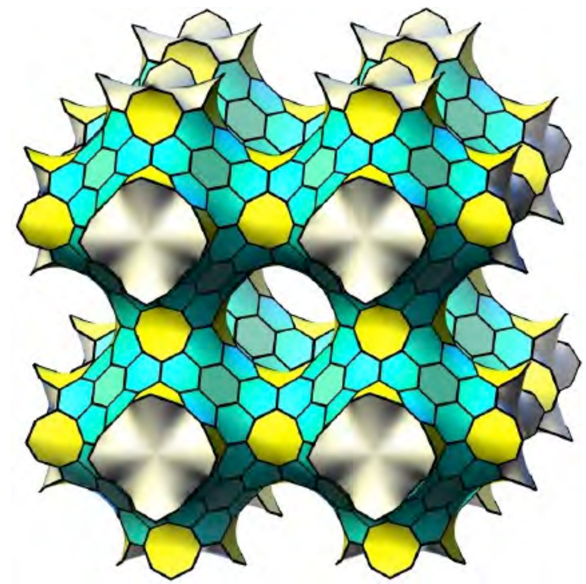
4-coordinated
net **rho** (net of
framework of
zeolite **RHO**)

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

3-periodic net has vertex symbol 4.4.4.6.8.8



6.8^2

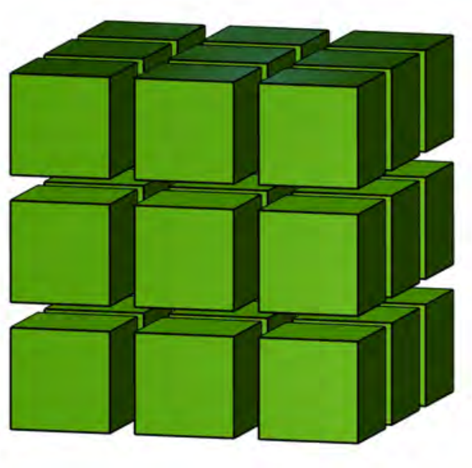


$(6^3)(6^2.8)_2$

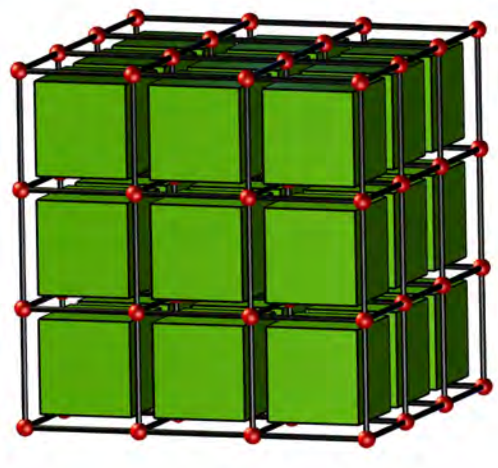
tilings of *P* surface ("Schwarzites")
— suggested as possible low energy polymorphs of carbon

Tiling in 3 dimensions

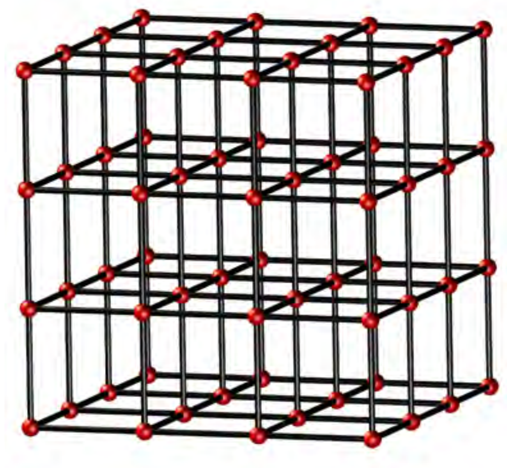
Filling space by generalized polyhedra (*cages*) in which at least two edges meet at each vertex and two faces meet at each edge. Tilings are "face-to-face"



exploded view of space filling by cube tiles

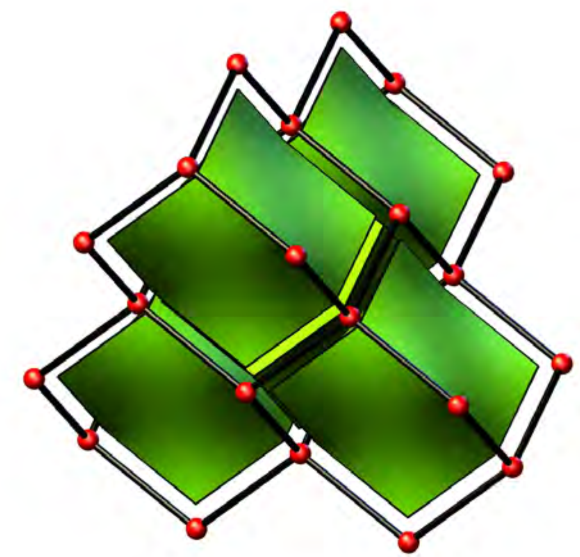


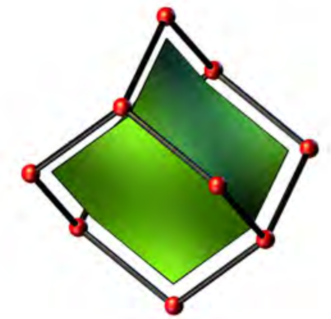
tiling plus net of vertices and edges

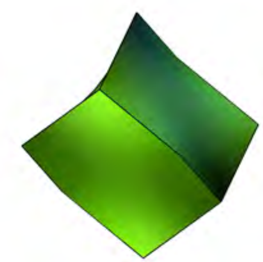


net "carried" by tiling **pcu**

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]



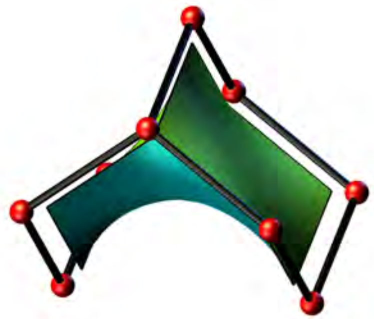


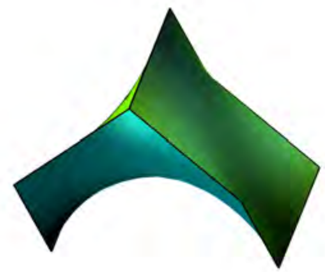


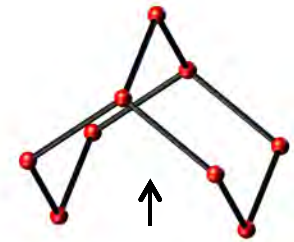
adamantane unit →

Tiles other than the adamantane unit for the diamond net (These are not *proper* – they have lower symmetry)

half adamantane

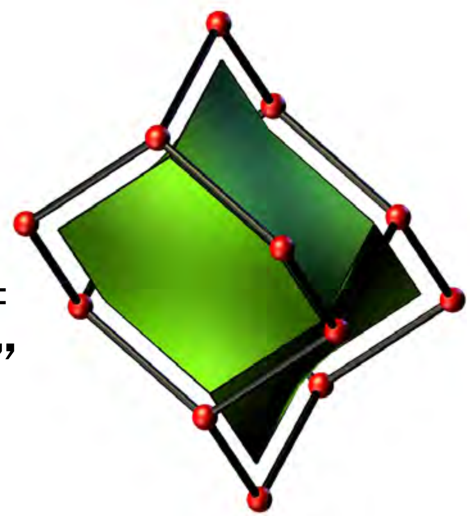


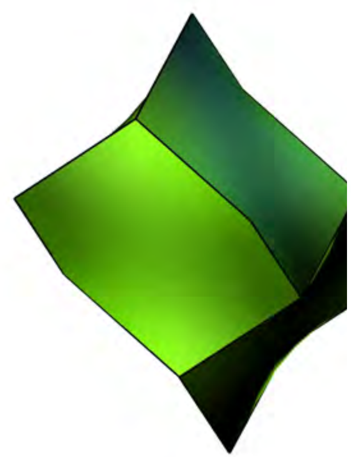


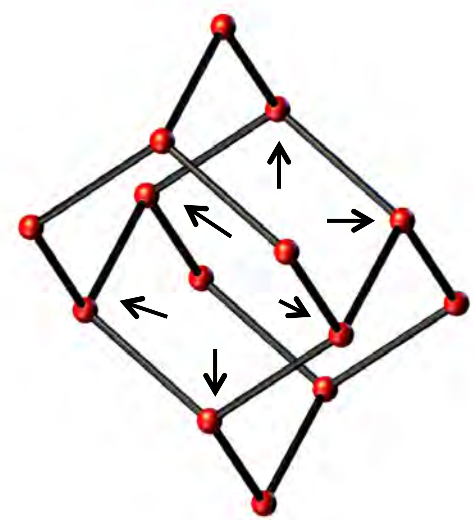


note 8-ring
(not a strong ring)

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:

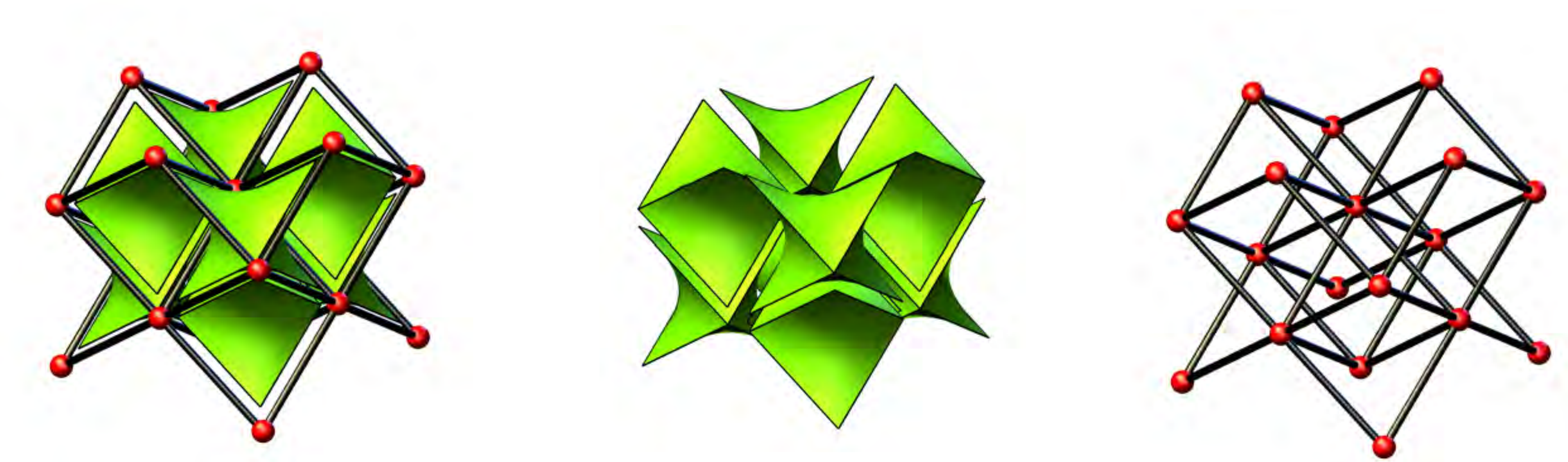
The **natural tiling** for a net is composed of the smallest tiles such that:

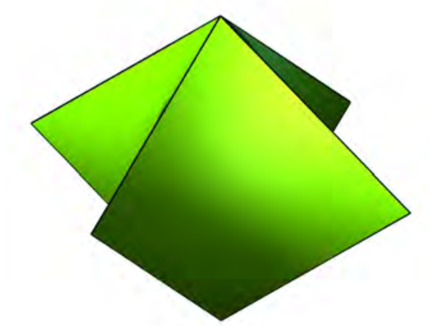
(a) the tiling conserves the maximum symmetry. (proper)
(b) all the faces of the tiles are strong rings.

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.

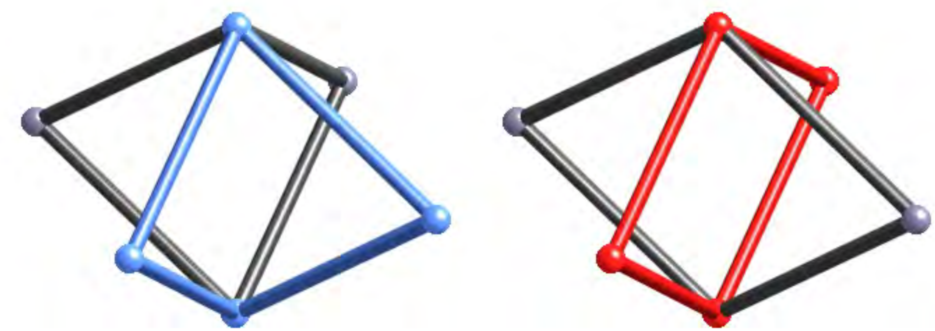
V. A. Blatov, O. Delgado-Friedrichs, M. O'Keeffe, D. M. Proserpio *Acta Cryst A* **2007**, *63*, 418.

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

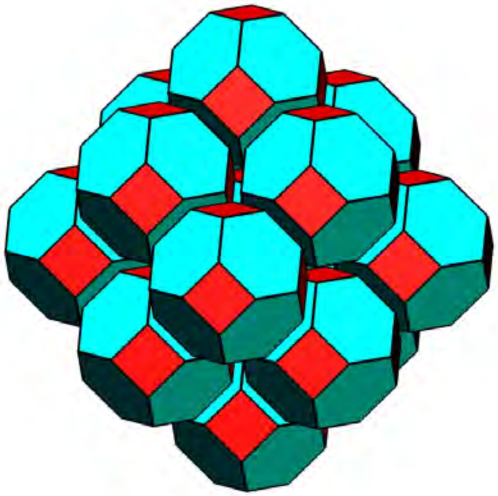
Simple tiling

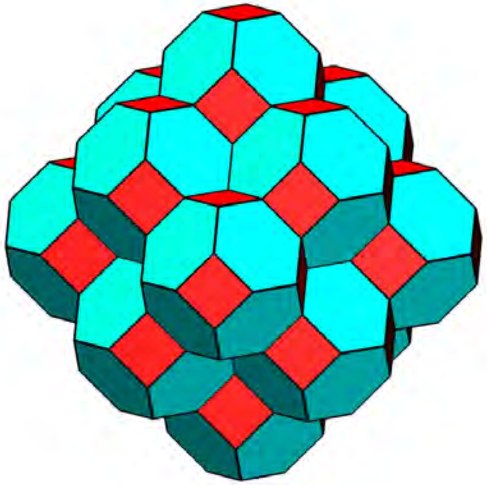
A **simple polyhedron** is one in which exactly two faces meet at each edge and three faces meet at each vertex.

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).

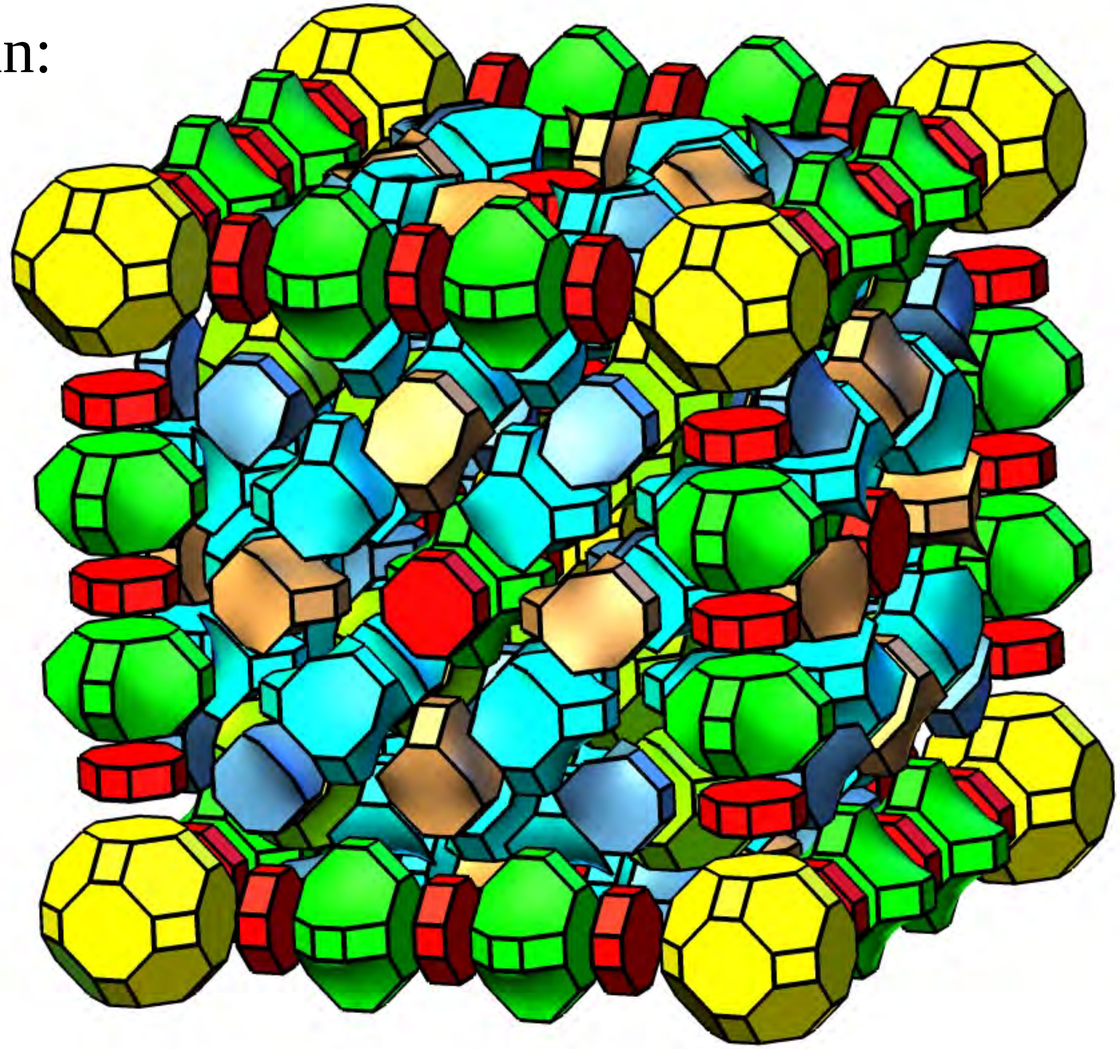
They are important as the structures of foams, zeolites etc.

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





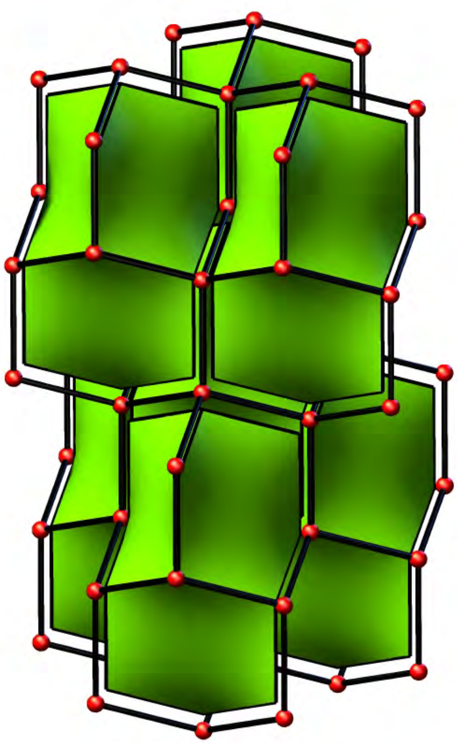
just for fun:



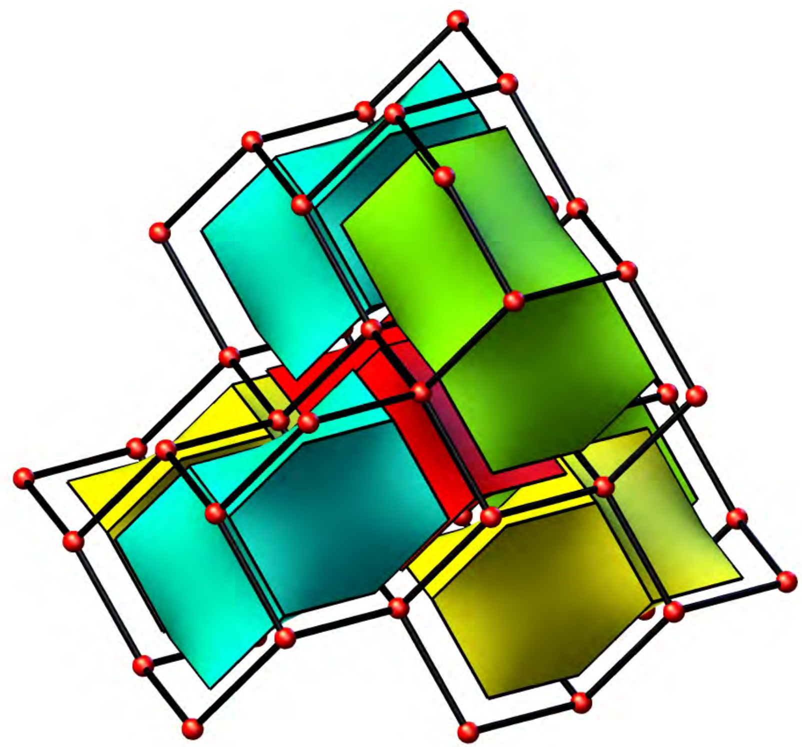
natural tiling of a complex net - that of the zeolite paulingite

PAU

The same tile can produce more than one tiling. Here the congressane (double adamantane) tile is used to form two different tilings that carry the diamond net. (But notice the symmetry of the tilings is lower than that of the net so they are not *proper* tilings).



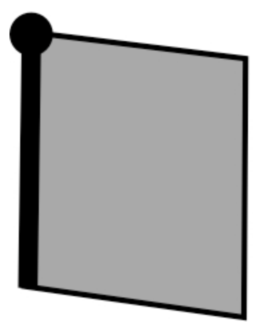
R-3m



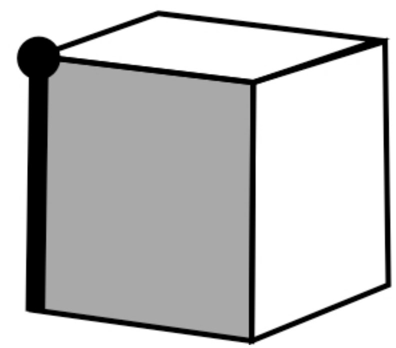
$P4_332$

Flags

regular tilings are flag transitive



2-D flag
vertex-edge-2D tile



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

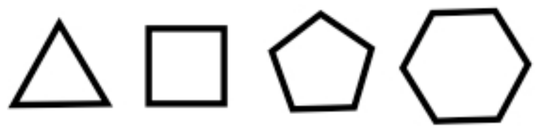
Regular tilings and Schläfli symbols

(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

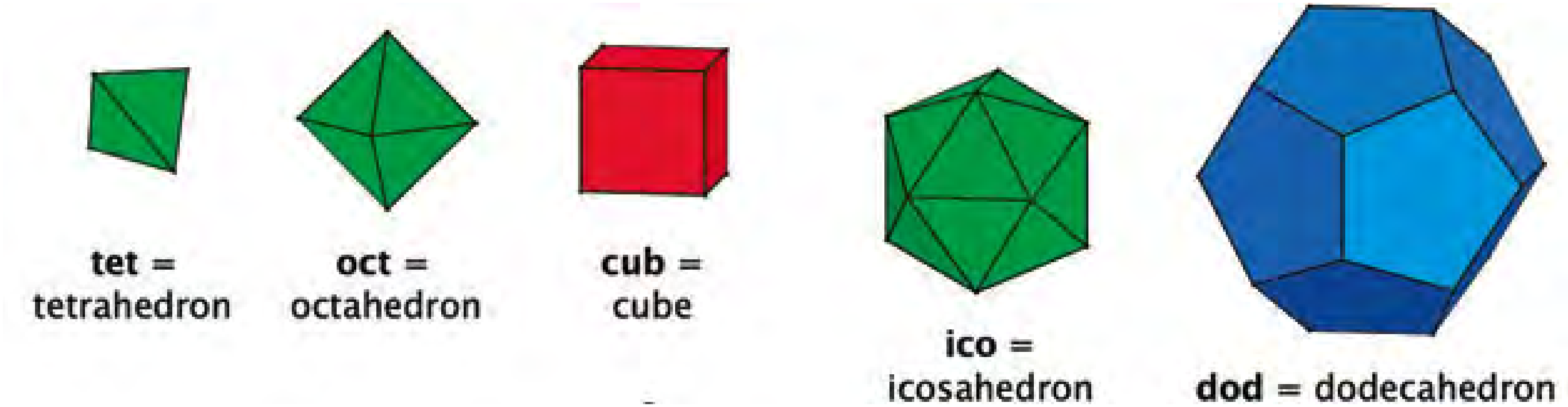


{∞} is degenerate case - an infinite linear group of line segments. Lives in E^1

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

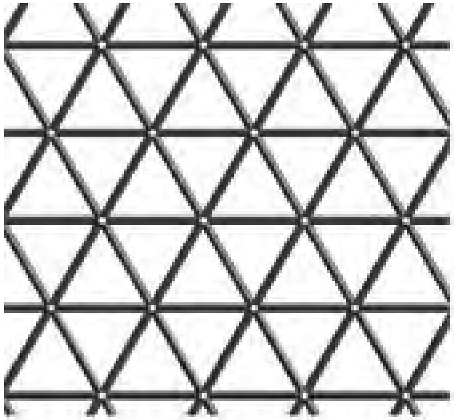
{3,3} tetrahedron
{3,4} octahedron
{3,5} icosahedron
{4,3} cube
{5,3} dodecahedron



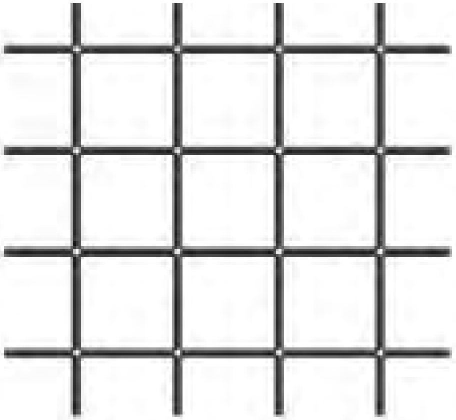
Two dimensions. The symbol is {p,q}
which means that q {p} meet at a point
three cases:

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

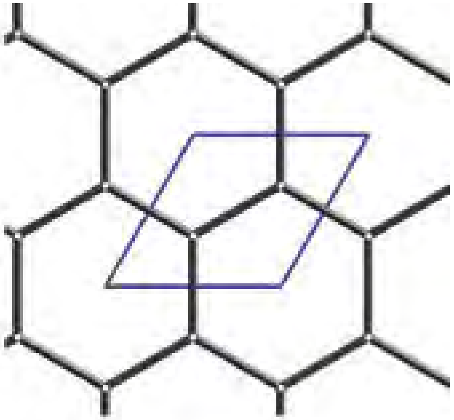
{3,6} hexagonal lattice
{4,4} square lattice
{6,3} honeycomb lattice complex



hxl =
hexagonal lattice



sql =
square lattice

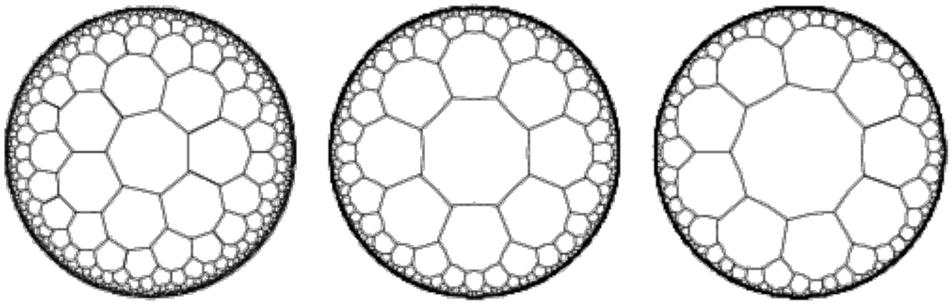


hcb =
honeycomb

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

case (c) $1/p + 1/q < 1/2$ → 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)

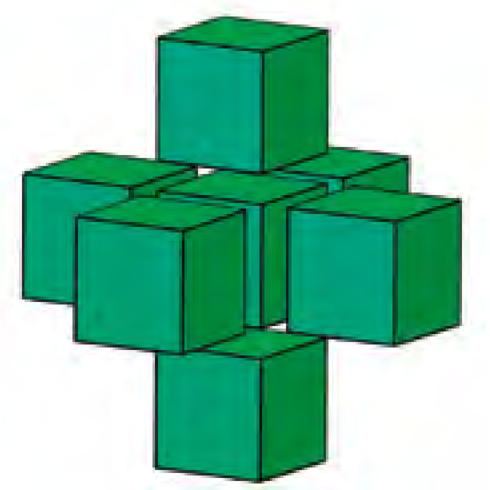
Three dimensions. Schläfli symbol {p,q,r} which means r {p,q} meet at an edge.

Again 3 cases

case (b) Tilings of E^3

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

Only regular tiling of E^3

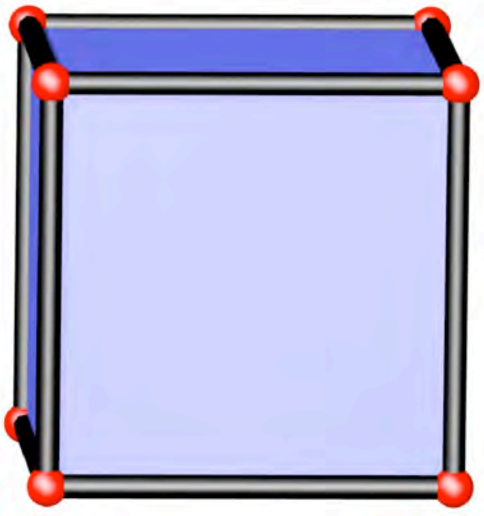


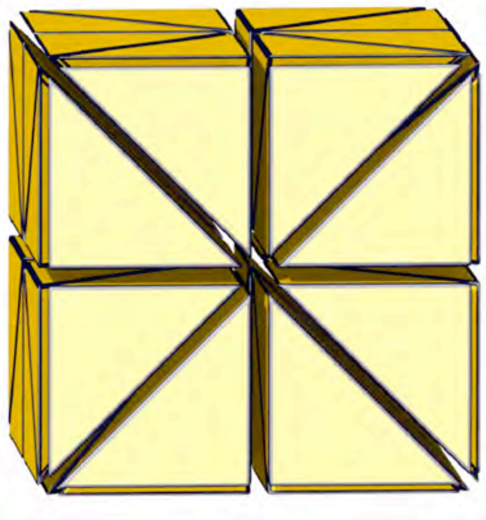
So what do we use for tilings that aren't regular?

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

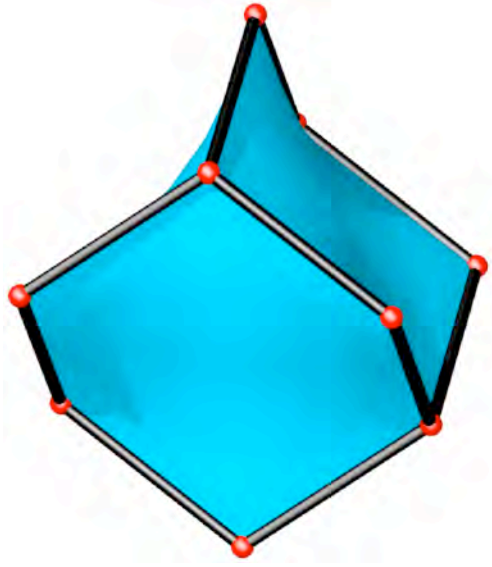
Introduced by Andreas Dress (Bielefeld) in
combinatorial tiling theory.

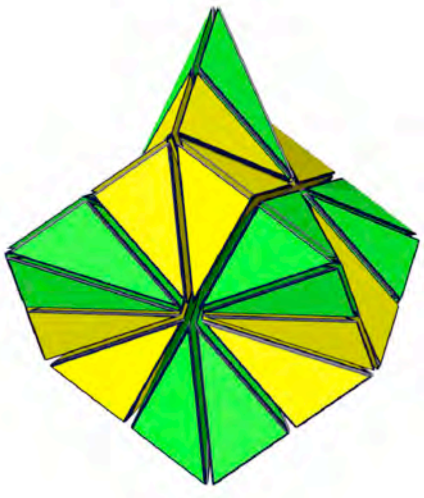
Developed by Daniel Huson
and Olaf Delgado-Friedrichs.





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>

How do you find the natural tiling for a net?

Use TOPOS

How do you draw tilings?

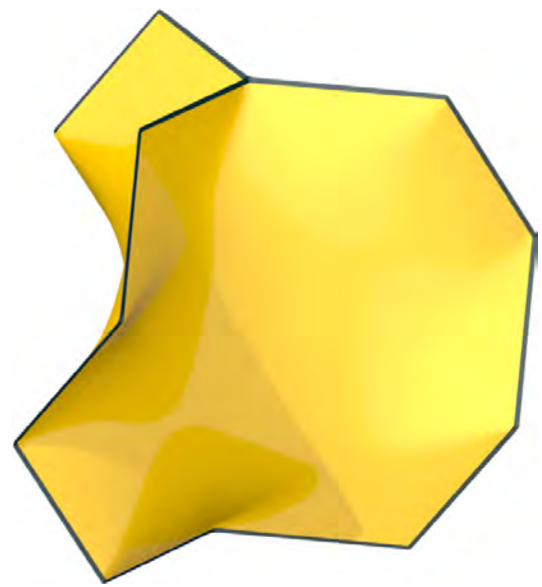
Use 3dt

We ordinary people use face data for tilings
3dt converts them to D symbols.
See next slide:

```
TILING
NAME "srs”
GROUP I4132
FACES 10
0.12500 0.12500 0.12500
-0.12500 0.37500 0.12500
-0.12500 0.62500 0.37500
-0.37500 0.62500 0.62500
-0.37500 0.37500 0.87500
-0.12500 0.37500 1.12500
0.12500 0.12500 1.12500
0.37500 0.12500 0.87500
0.37500 -0.12500 0.62500
0.12500 -0.12500 0.37500
END
```

D-symbol

```
<1.1:10 3:2 4 6 8 10,10
 3 5 7 9,6 5 4 10 9,2
 10 9 8 7:10,2 2 3,10>
```



tile for **srs** net

To calculate D-size

The number of chambers in each tile = 4 x number of edges / order of point symmetry

Tiling by cubes with 12 edges and symmetry *m*-3*m* (order 48)
D-size = 4x12/48 = 1

Diamond tile has 12 edges, symmetry -43*m*
D-size = 4x12/24 = 2

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)

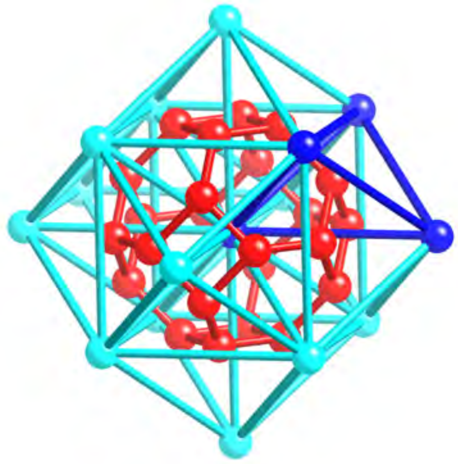
Duals

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



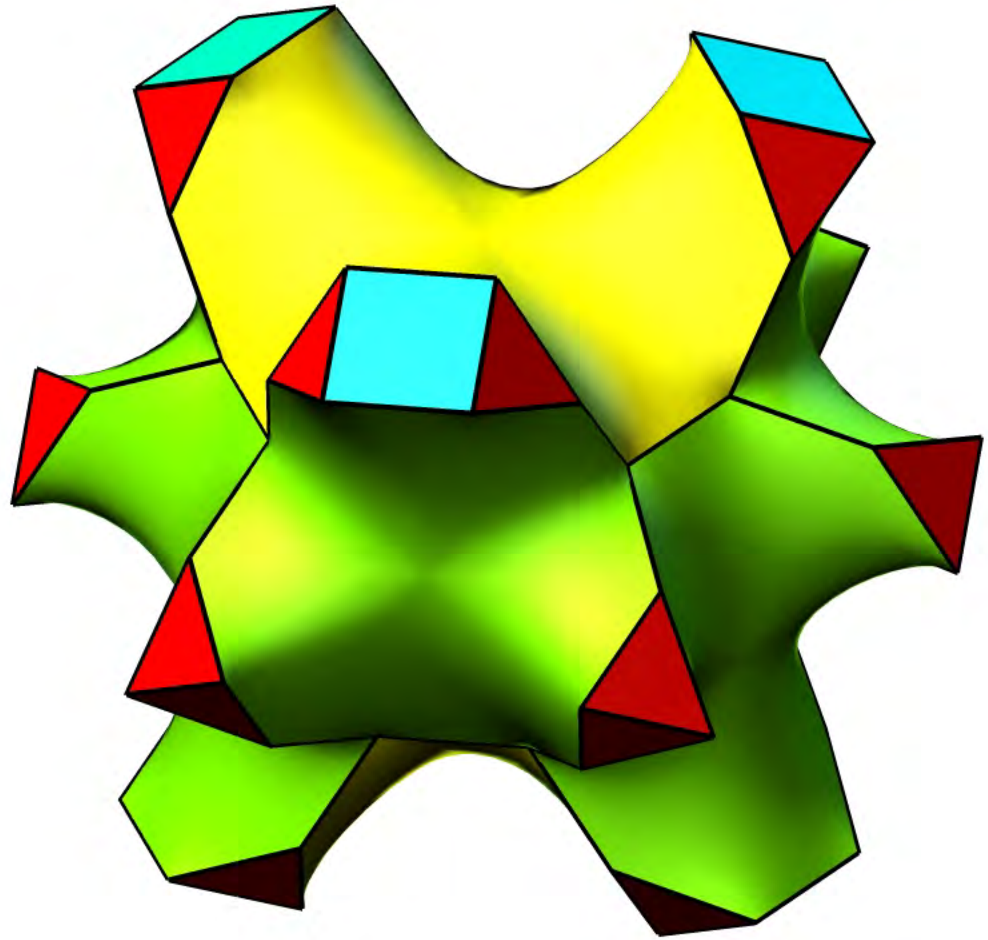
Dual tiling (blue) is **bcu-x** 14-coordinated body-centered cubic. A tiling by congruent tetrahedra

Simple tiling again

The dual of a tiling by tetrahedra may not be a simple tiling by simple polyhedra.

Here is an example – the graph of the tile is 2-connected.
(3-coordinated, but not 3-connected!)

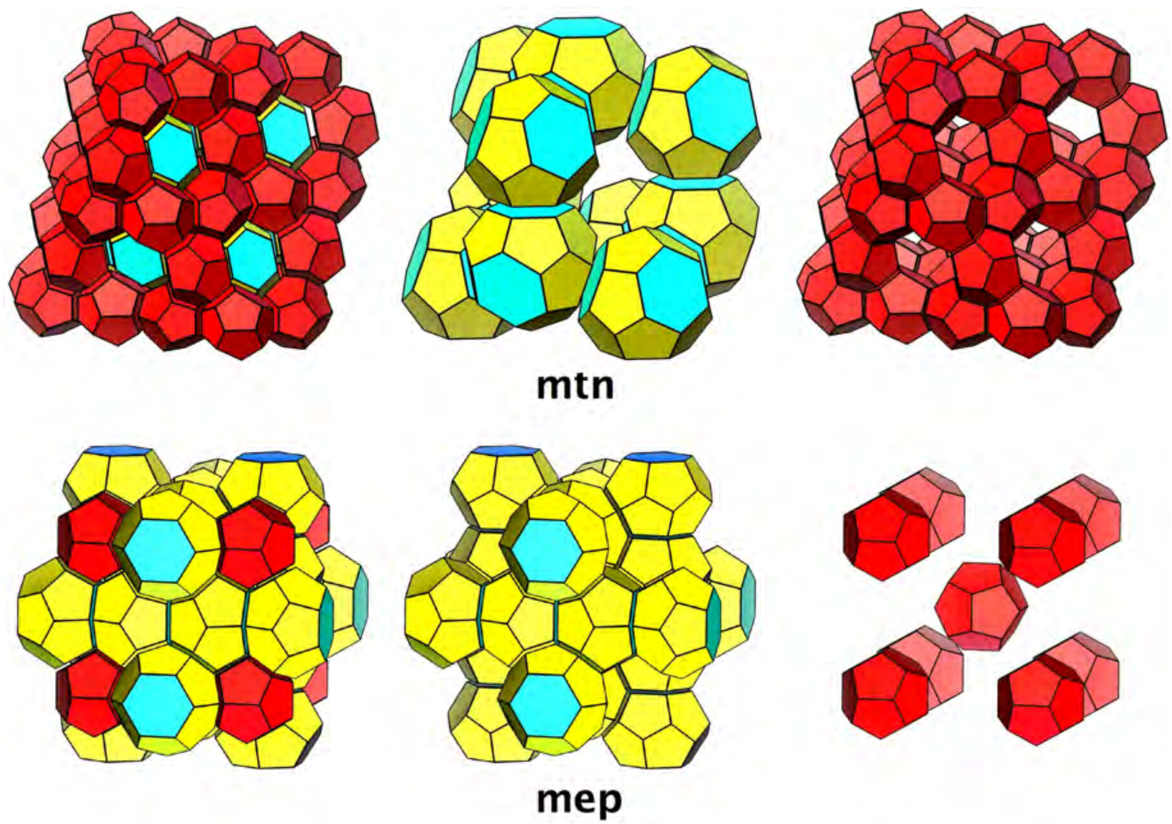
net is **bcr**

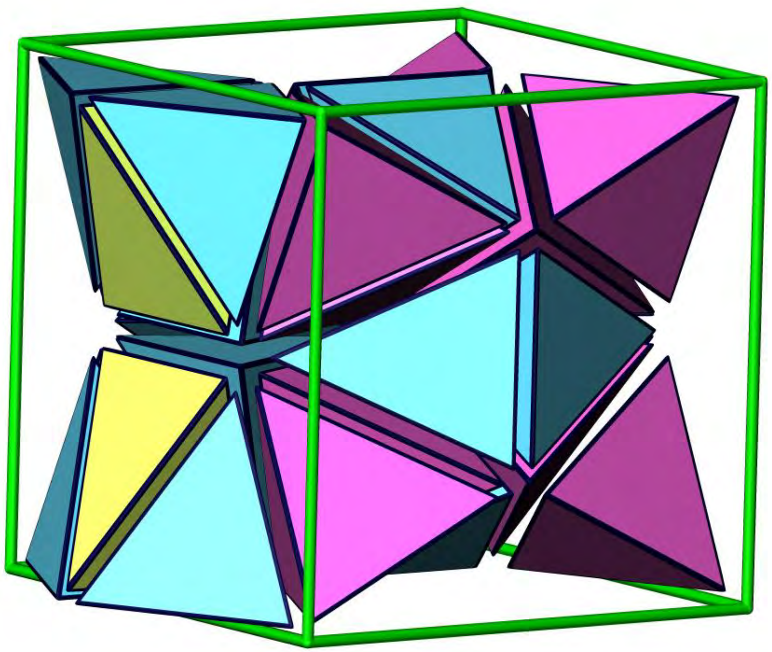


This tiles fills space just by translations alone.
Tiling symmetry is *R*-3.

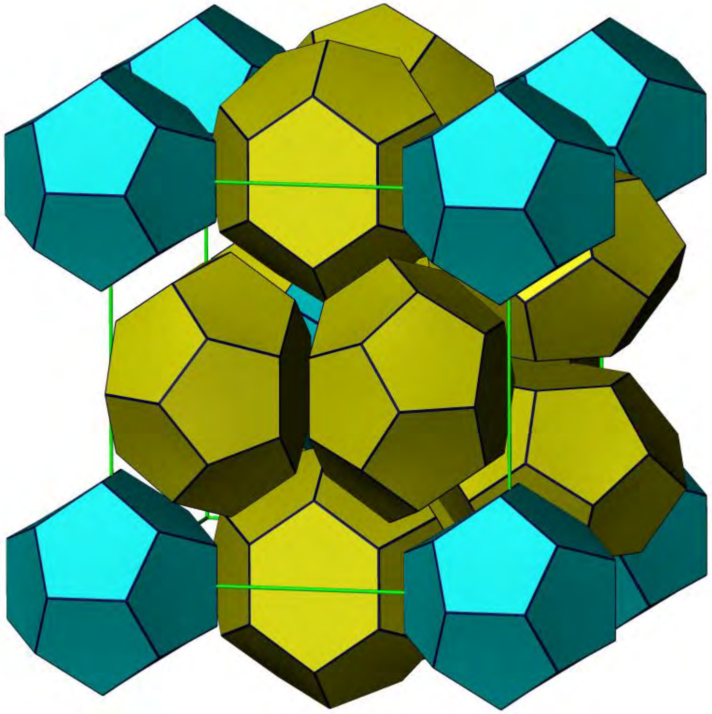
Some examples of dual structures

simple tiling	tiling by tetrahedra
sodalite (**sod**)	body-centered cubic
type I clathrate (**mep**)	A15 (Cr_3Si)
type II clathrate (**mtn**)	$MgCu_2$



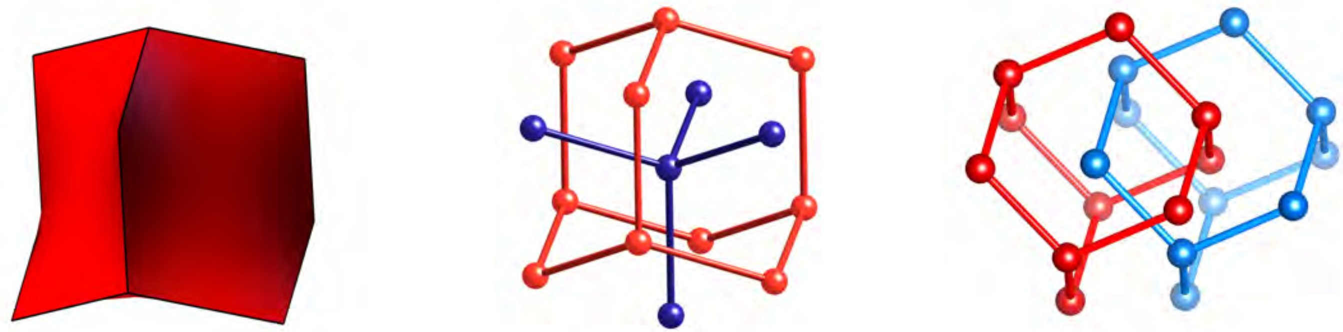


Cr_3Si (A15)

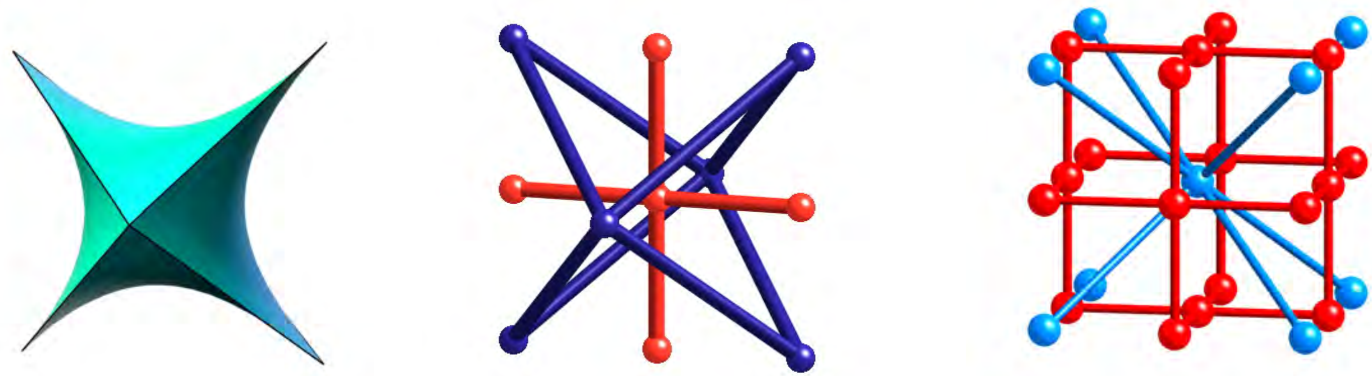


Type I clathrate
melanophlogite (**MEP**)
Weaire-Phelan foam

examples of duals



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



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

Tilings by tetrahedra: there are exactly

9 topological types of isohedral (tile transitive) tilings

117 topological types of 2-isohedral (tile 2-transitive)

In all of these there is at least one edge where exactly 3 or 4 tetrahedra meet. Accordingly none of them have embeddings in which all tetrahedra are acute (dihedral angles less than $\pi/2$).

Olaf Delgado Friedrichs and Daniel Huson, *Discr. Comput. Geom.* 21, 299 (1999)

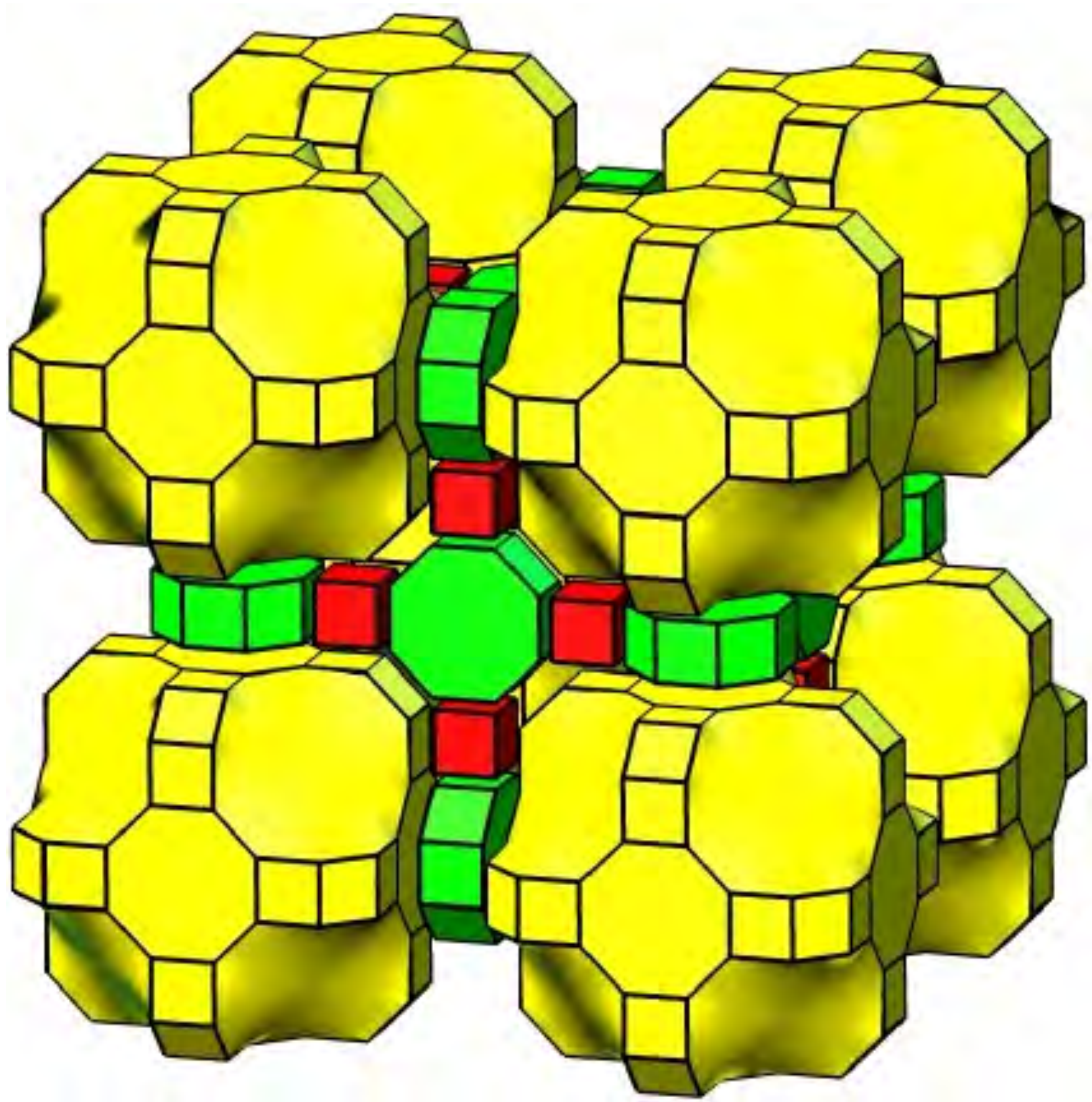
What do we know about tilings?

1. Exactly 9 topologically-different ways
of tiling space by one kind of tetrahedron

Duals are simple tilings with one kind of vertex
These include the important zeolite framework
types **SOD**, **FAU**, **RHO**, **LTA**, **KFI** and **CHA**

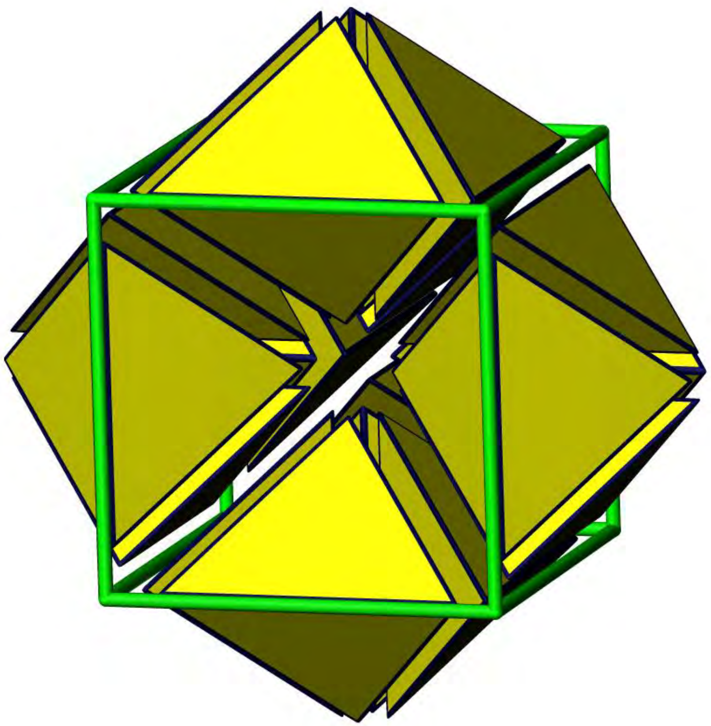
Two of the remaining three (**sod-a** and **hal**) have
3-membered rings. The other has many 4-rings

O. Delgado-Friedrichs *et al. Nature*, **400**, 644 (1999)

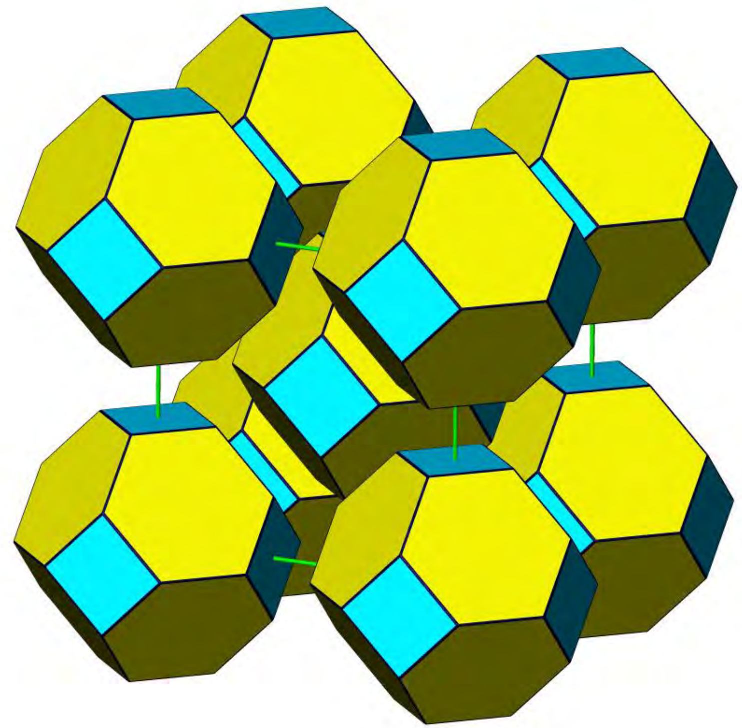


wse not suitable for a silica zeolite

Example of isohedral tiling by tetrahedra (Somerville tetrahedra). Only one that is also vertex transitive
So the dual structure is the only vertex- and tile-transitive simple tiling (transitivity 1121)

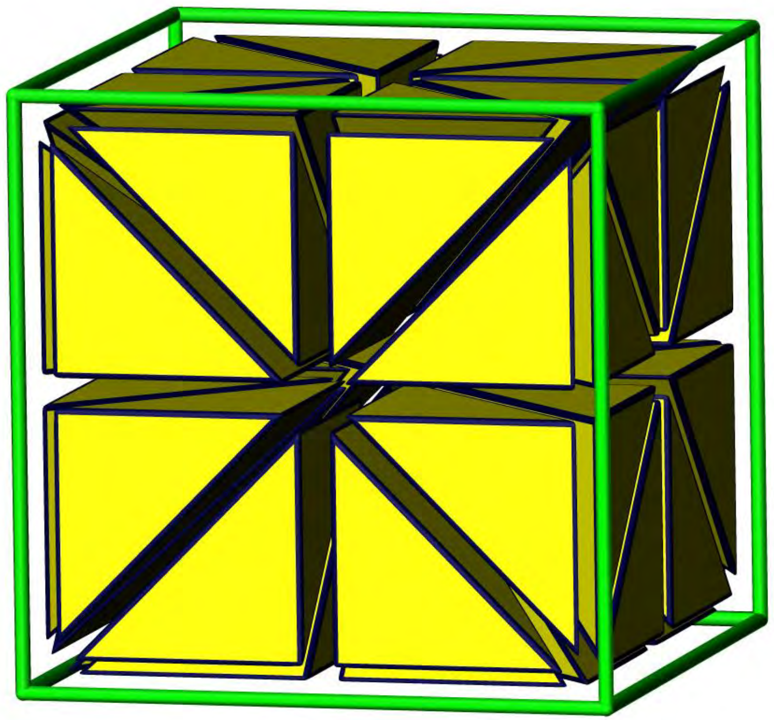


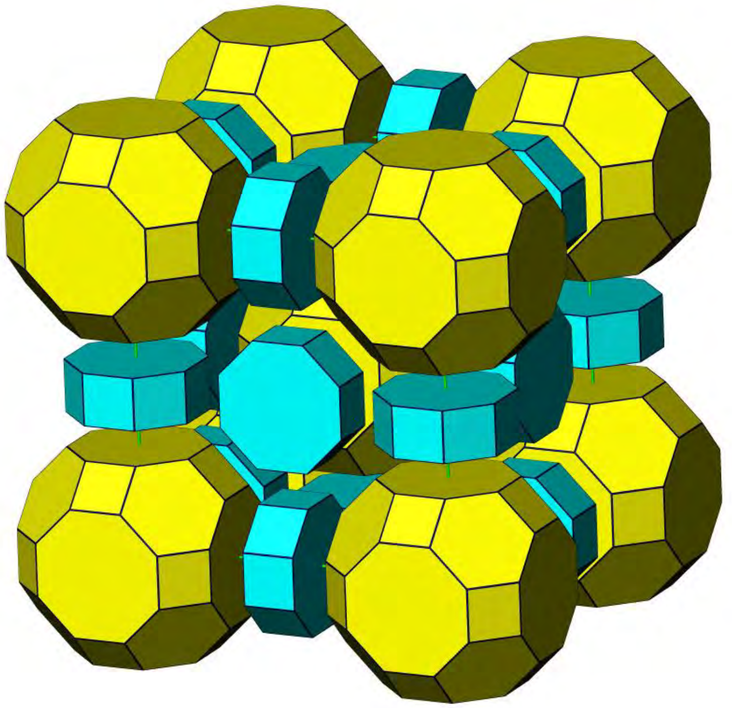
vertices are body-centered cubic



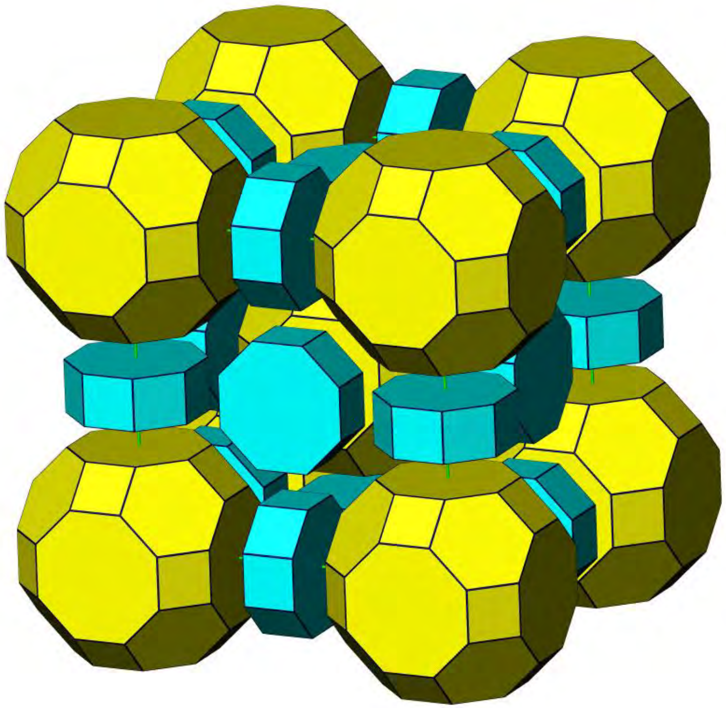
Dual structure (sodalite).
"Kelvin structure"

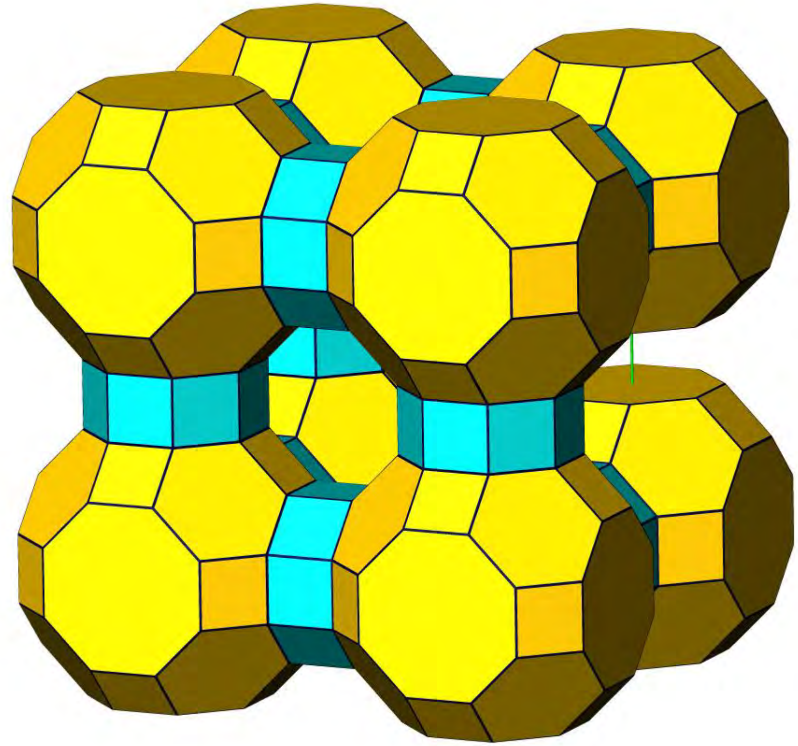
Another example: isohedral tiling by half-Somerville tetrahedra

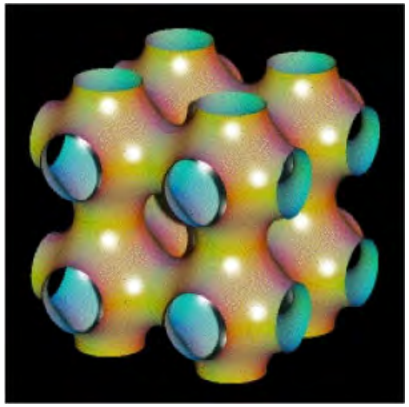




Dual structure -zeolite **RHO**

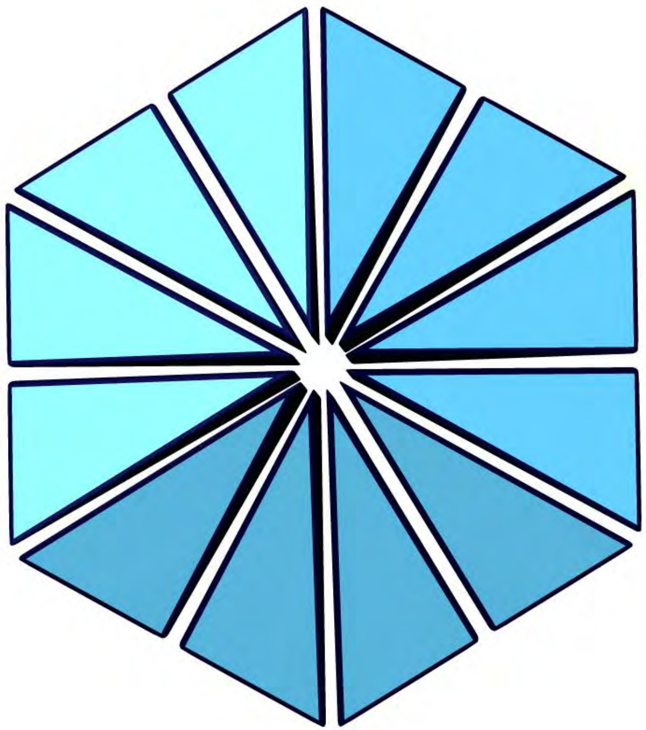




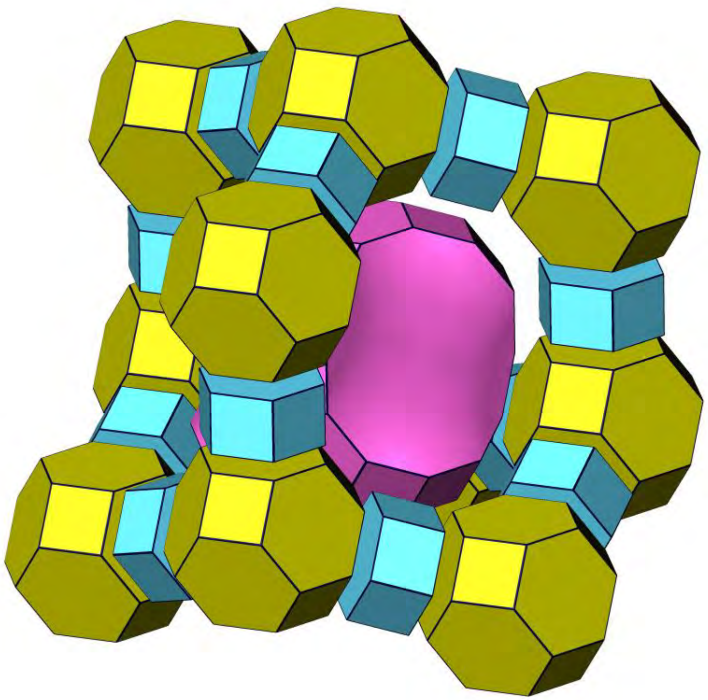


The 1-skeleton (net) of **RHO**
is also the 1-skeleton of a
$4^3.6$ tiling of a 3-periodic surface.

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 $4^3.6$ tiling of a surface

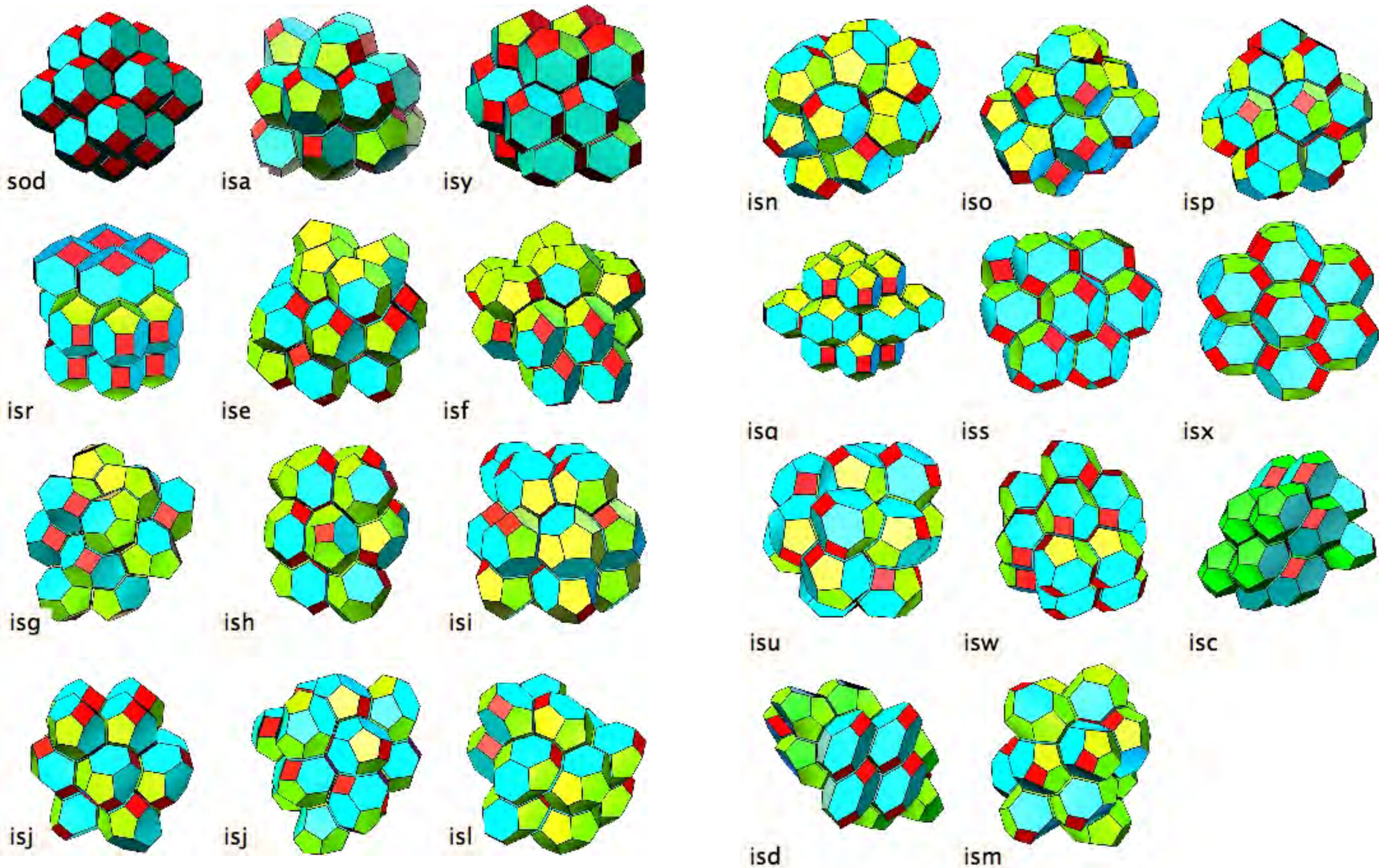
Isohedral simple tilings.

1. Enumerate all simple polyhedra with N faces
(plantri - Brendan McKay ANU, Canberra)

2. Determine which of these form isohedral tilings

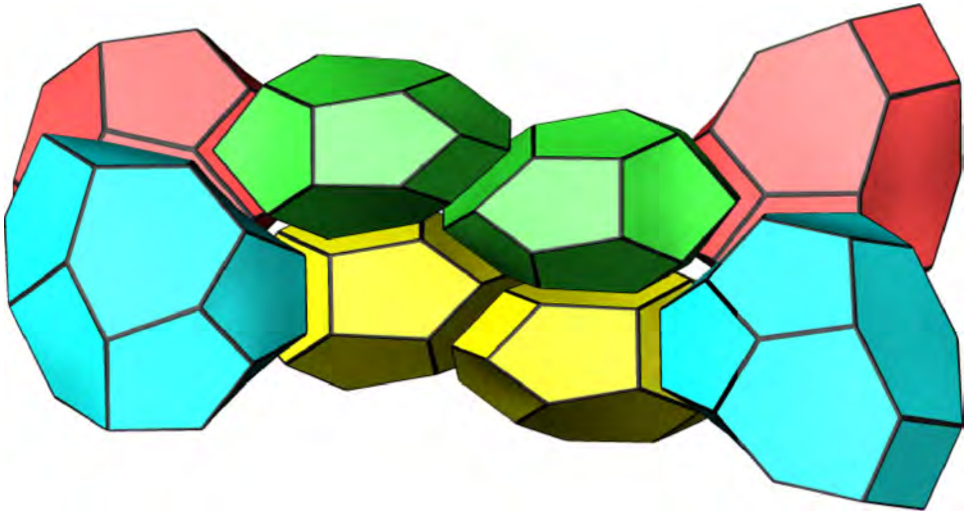
Faces	tilers	tilings
<14	0	0
14	10	23
15	65	136
16	434	710

O. Delgado-Friedrichs & M. O'Keeffe, *Acta Cryst. A*, **61**, 358 (2005)



The 23 isohedra simple tilings with 14-face tiles

What's this?



A monotypic (but tile 4-transitive) simple tiling by a 14-face polyhedron. Triclinic! P-1 RCSR symbol **rug**

R. Gabrielli and M. O'Keeffe, Acta Cryst A64, 430 (2008)

D symbol
for **rug**

D-size = 576
4.36.4

transitivity
24 48 32 4

<1.1:576 3:2 4 6 8 10 12 14 16 18 20 22 24 26 28 30 32 34 36 38 40 42 44 46 48 50 52 54 56 58 60 62
64 66 68 70 72 74 76 78 80 82 84 86 88 90 92 94 96 98 100 102 104 106 108 110 112 114 116 118 120
122 124 126 128 130 132 134 136 138 140 142 144 146 148 150 152 154 156 158 160 162 164 166 168 170
172 174 176 178 180 182 184 186 188 190 192 194 196 198 200 202 204 206 208 210 212 214 216 218 220
222 224 226 228 230 232 234 236 238 240 242 244 246 248 250 252 254 256 258 260 262 264 266 268 270
272 274 276 278 280 282 284 286 288 290 292 294 296 298 300 302 304 306 308 310 312 314 316 318 320
322 324 326 328 330 332 334 336 338 340 342 344 346 348 350 352 354 356 358 360 362 364 366 368 370
372 374 376 378 380 382 384 386 388 390 392 394 396 398 400 402 404 406 408 410 412 414 416 418 420
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522 524 526 528 530 532 534 536 538 540 542 544 546 548 550 552 554 556 558 560 562 564 566 568 570
572 574 576,8 3 5 7 18 11 13 15 17 28 21 23 25 27 40 31 33 35 37 39 52 43 45 47 49 51 64 55 57 59 61
63 74 67 69 71 73 84 77 79 81 83 94 87 89 91 93 104 97 99 101 103 114 107 109 111 113 124 117 119
121 123 134 127 129 131 133 144 137 139 141 143 154 147 149 151 153 166 157 159 161 163 165 176 169
171 173 175 186 179 181 183 185 198 189 191 193 195 197 208 201 203 205 207 218 211 213 215 217 228
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271 273 275 277 288 281 283 285 287 298 291 293 295 297 308 301 303 305 307 318 311 313 315 317 328
321 323 325 327 340 331 333 335 337 339 350 343 345 347 349 360 353 355 357 359 372 363 365 367 369
371 382 375 377 379 381 392 385 387 389 391 402 395 397 399 401 412 405 407 409 411 424 415 417 419
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521 523 525 536 529 531 533 535 548 539 541 543 545 547 558 551 553 555 557 566 561 563 565 576 569
571 573 575,9 10 19 20 29 30 41 42 28 27 53 54 65 66 44 43 40 39 75 76 63 64 52 51 85 86 95 96 83 84
67 68 105 106 93 94 74 73 115 116 125 126 78 77 114 113 123 124 127 128 98 97 104 103 135 136 108
107 129 130 143 144 137 138 121 122 134 133 140 139 142 141 155 156 167 168 177 178 187 188 199 200
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486 485 472 471 515 516 501 502 482 481 527 528 525 526 492 491 537 538 535 536 505 506 547 548 514
513 549 550 518 517 546 545 559 560 557 558 551 552 567 568 530 529 569 570 540 539 571 572 565 566
576 575 562 561 574 573,5 6 7 8 95 96 97 98 99 100 101 102 103 104 145 146 147 148 149 150 151 152
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275 276 277 278 267 268 289 290 291 292 293 294 295 296 297 298 203 204 205 206 207 208 199 200 201
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300 231 232 233 234 235 236 237 238 229 230 193 194 195 196 197 198 309 310 311 312 313 314 315 316
317 318 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 263 264 265
266 348 347 346 345 344 343 342 341 350 349 484 483 492 491 490 489 488 487 486 485 513 514 503 504
505 506 507 508 509 510 511 512 463 464 465 466 467 468 469 470 471 472 518 517 516 515 526 525 524
523 522 521 520 519 402 401 400 399 398 397 396 395 394 393 572 571 570 569 568 567 576 575 574 573
533 534 535 536 527 528 529 530 531 532 419 420 421 422 423 424 429 430 431 432 550 549 558 557 556
555 554 553 552 551 543 544 545 546 547 548 563 564 565 566:4 5 5 6 6 6 5 5 5 5 5 5 5 5 6 5 5 6 5
5 5 5 5 5 4 6 5 5 5 5 5 6 5 5 6 5 5 5 5 6 4 5 5 5 5 5 5 6 6 5 6 5 4 5,3 3 3 3 3 3 3 3 3 3 3 3 3 3
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3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3,3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3>

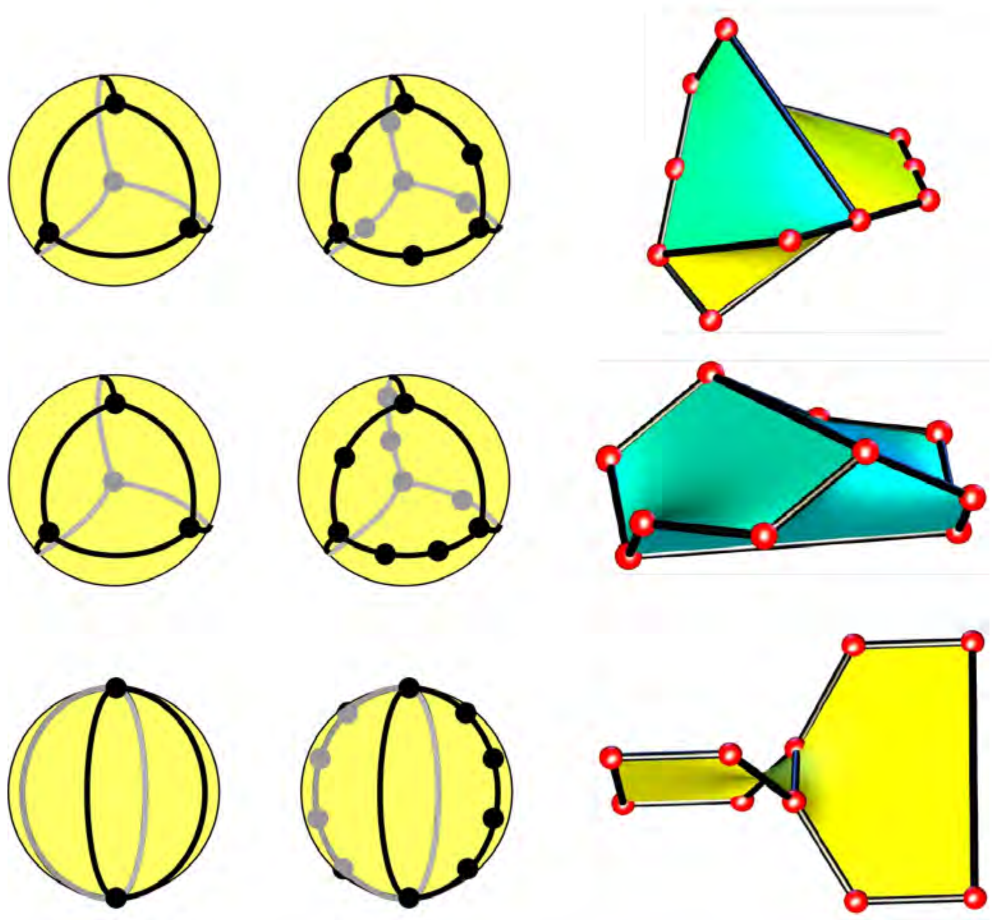
How to find edge-transitive nets?

A net with one 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