Taxonomy of Nets

Michael O'Keeffe

Enumeration and classificaion of rystal nets

Taxonomy of nets and tilings: Classification by transitivity

Tiling a surface

1. Tiling of sphere (polyhedra, 0-periodic)
2. Tiling of cylinder (1-periodic nets)
3. Tiling of plane (2-periodic nets)

transitivity: 111 regular
112 quasiregular
21*r* other edge transitive

Tiling of space (3-periodic nets)

transitivity: 1111 regular
1112 quasiregular
11*rs* semiregular
21*rs* other edge transitive

Reminder

2-D tilings: transitivity = *pqr*

p kinds of vertex

q kinds of edge

r kinds of face (2-D tile)

3-D tilings: transitivity = *pqrs*

p kinds of vertex

q kinds of edge

r kinds of face

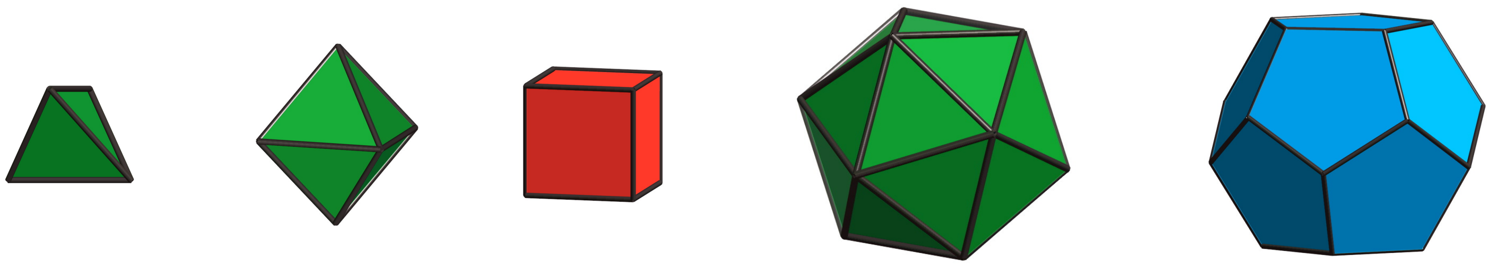
s kinds of tile

There are infinitely many polyhedra and nets
with one kind of vertex. But...

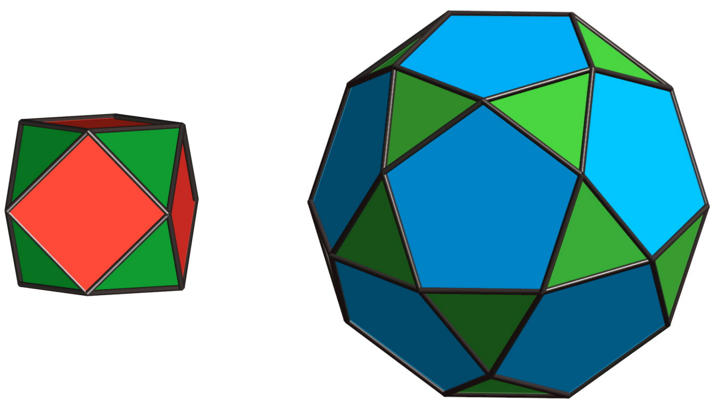
The are only a small number with one kind of edge

This has important implications for chemistry

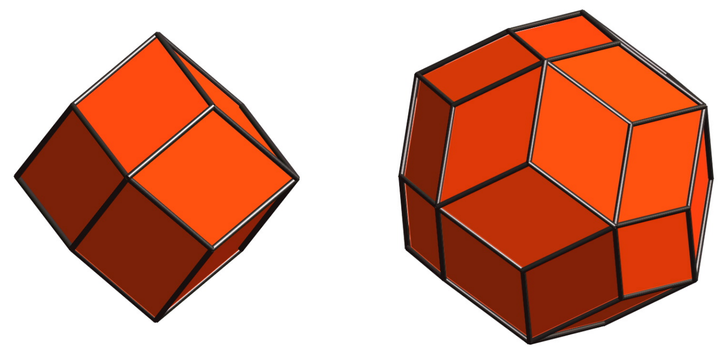
All edge-transitive polyhedra – tilings of $\mathbf{S}^2$



regular: transitivity 111

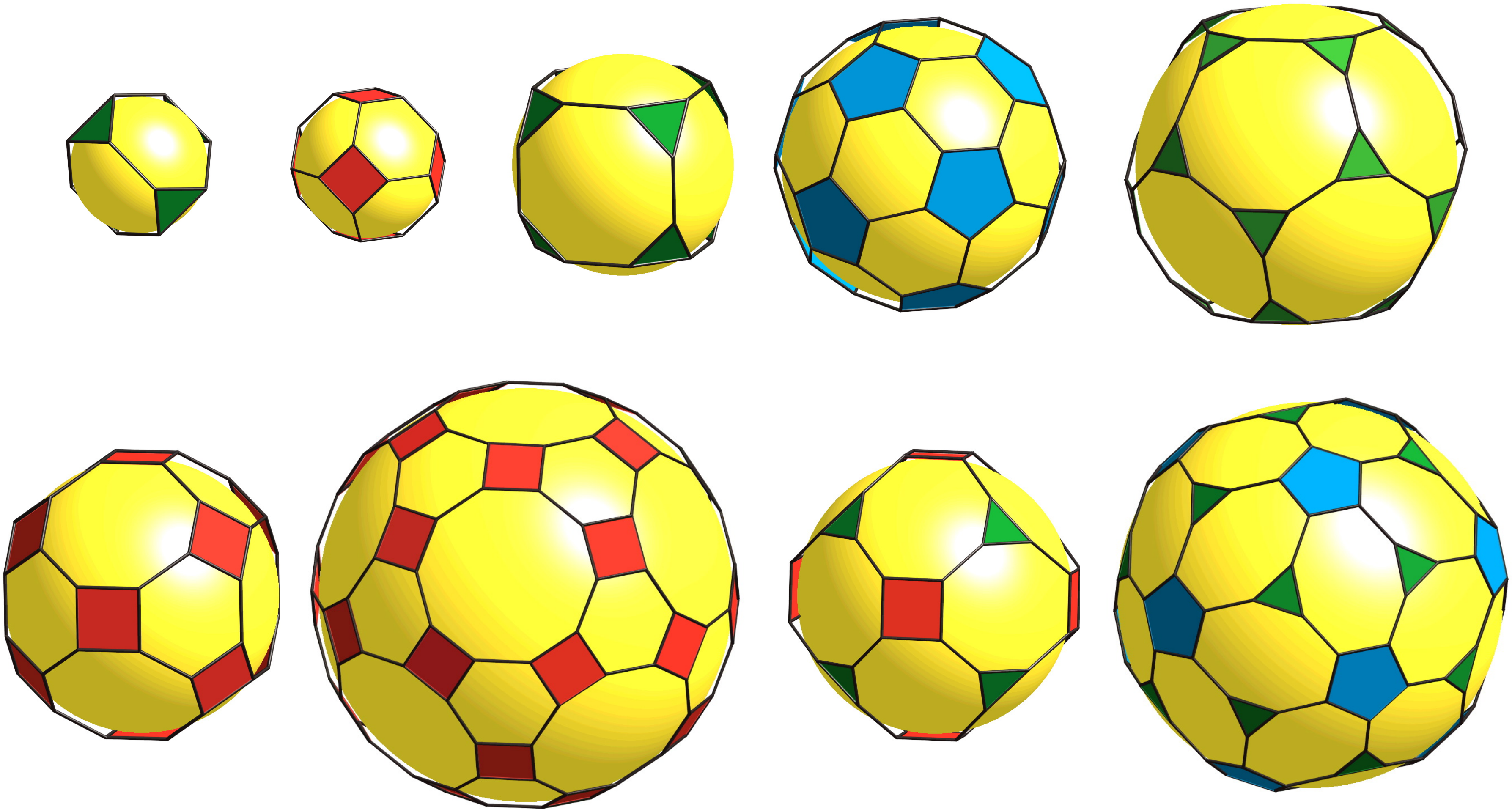


quasi-regular: transitivity 112



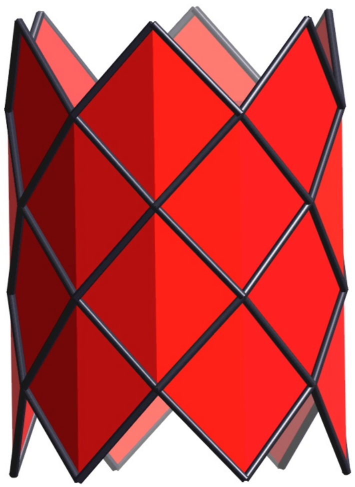
duals of quasi-regular:
transitivity 211

All possible ways of linking polygons with one kind of link to form 0-periodic structures



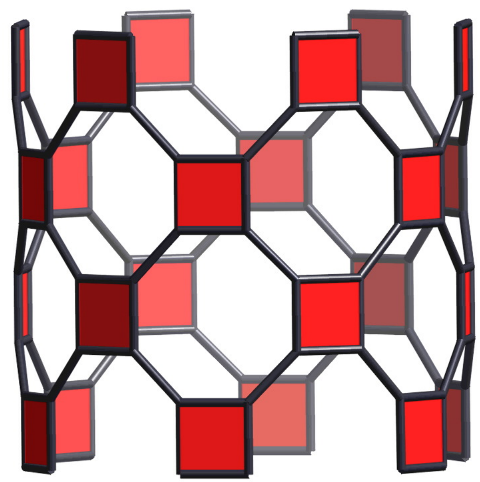
Augmented (truncated) edge-transitive polyhedra

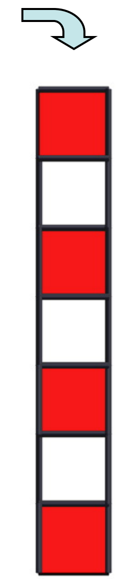
The only family of edge-transitive tilings of cylinder



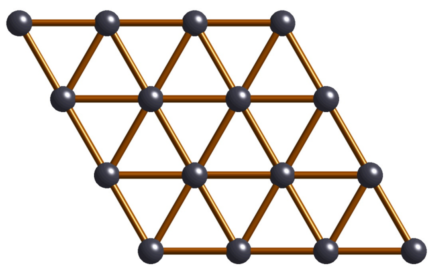
regular cylinder tiling:
transitivity 111

special case

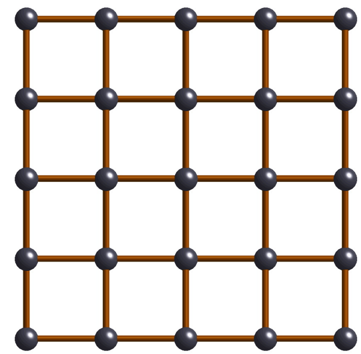




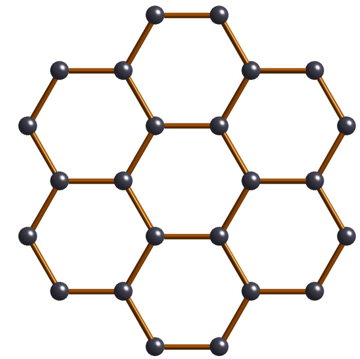
The augmented structure: The only 1-periodic structure of polygons joined by equal links all edge-transitive 2-periodic nets



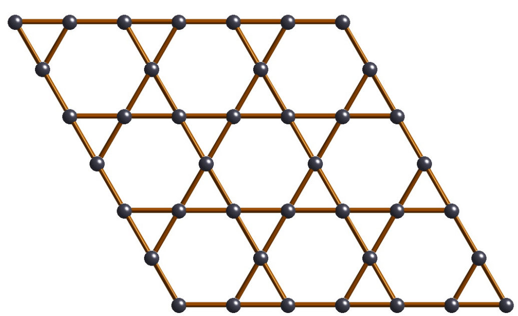
hexagonal lattice 111



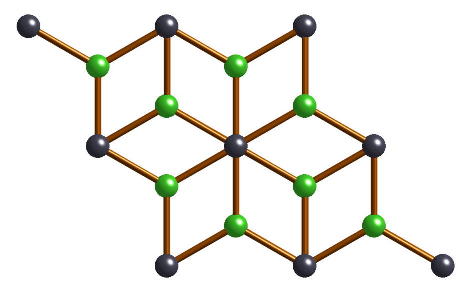
square lattice 111



honeycomb 111

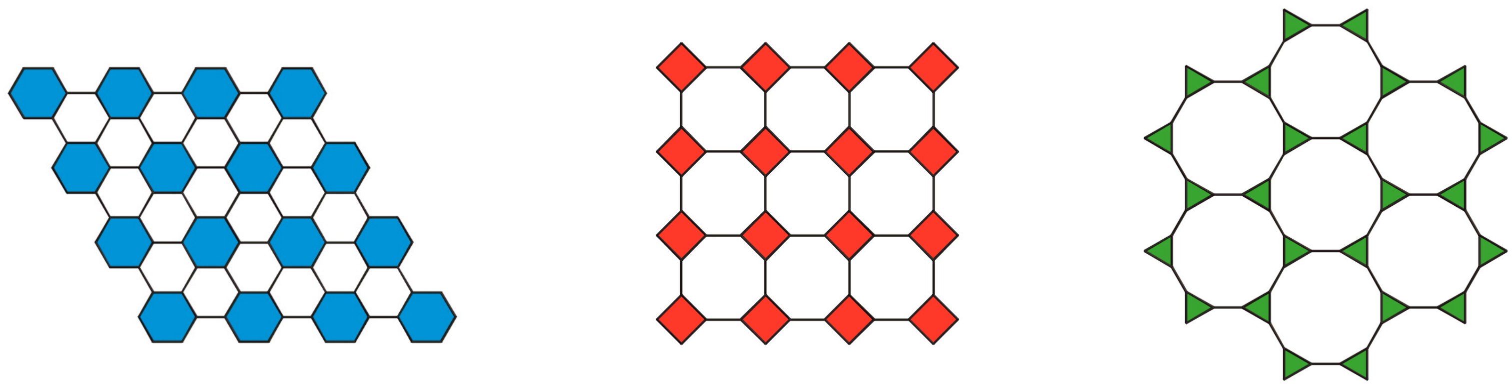


kagome 112 (quasiregular)

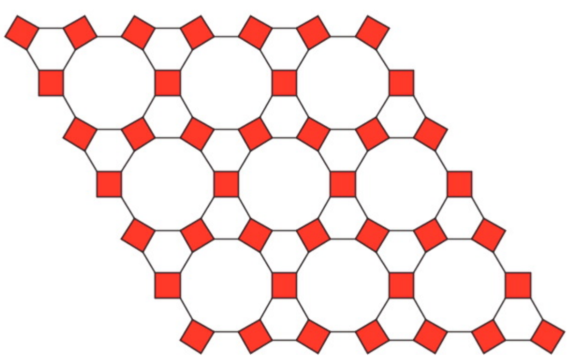


kagome dual 211

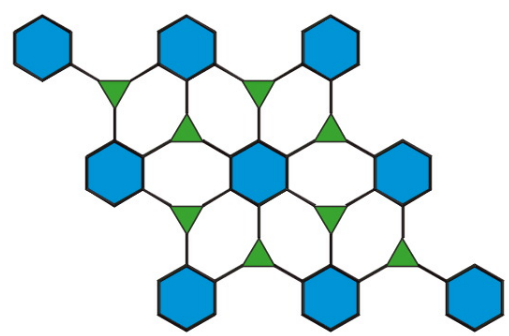
All possible ways of linking polygons with one kind of link to form 2-periodic structures



augmented regular nets



augmented quasiregular



augmented dual of quasiregular

Summary of tiling 2-surfaces. All edge-transitive structures

Sphere -> 111 = 5 regular polyhedra 112 = 2 quasiregular polyhedra 211 = 2 duals of above	9	
Plane -> 111 = 3 regular nets 112 = 1 quasiregular net 211 = 1 dual of above	5	15
cylinder->111 one family	1	

So there aren't too many
(but if we include hyperbolic surfaces the number becomes infinite – S. T. Hyde).

Regular 3-periodic nets

Vertex (coordination) figure is a regular polygon or polyhedron

As the net is periodic, the vertex figure can only have crystallographic symmetry (1-, 2-, 3-, 4- or 6-fold rotations)
So possibilities are

1. triangle
2. square
3. tetrahedron
4. octahedron
5. cube

(hexagon cannot lead to a 3-D structure as all 6-fold axes must be parallel)

There is only one possibility in each case → 5 regular nets

It turns out that:

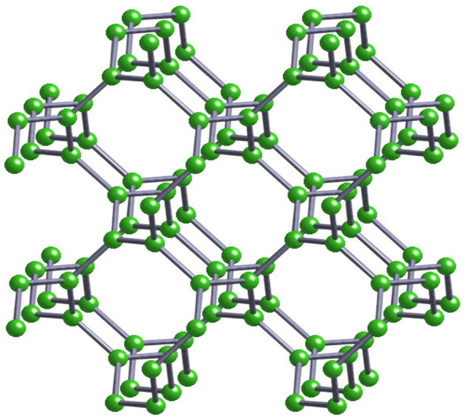
regular nets have transitivity 1111

For *natural* tilings there are no more with

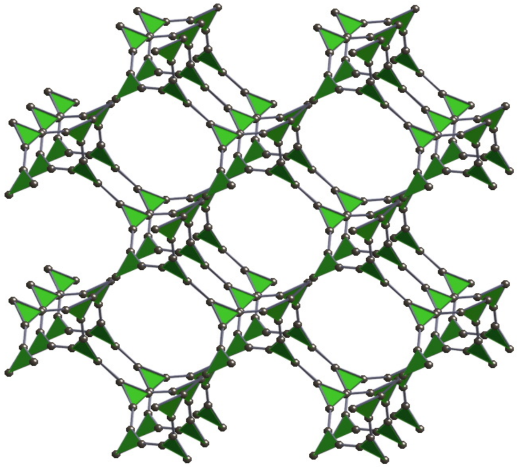
transitivity 1111

(this is rather nice)

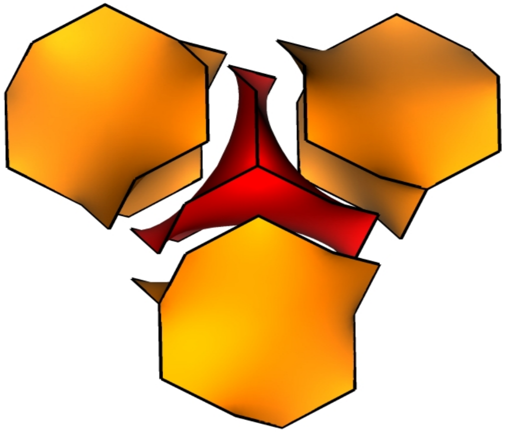
vertex figure: triangle



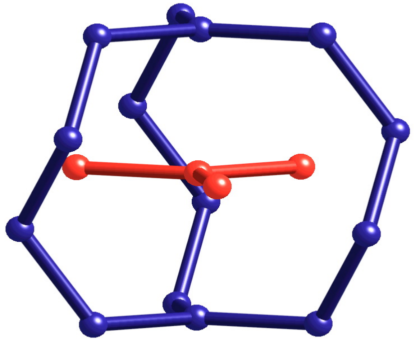
srs (the $SrSi_2$ net)



the augmented net **srs-a**



natural tiling $[10^3]$



skeleton of tile with dual (self)

BULLETIN
(NEW SERIES)
OF THE
AMERICAN MATHEMATICAL SOCIETY

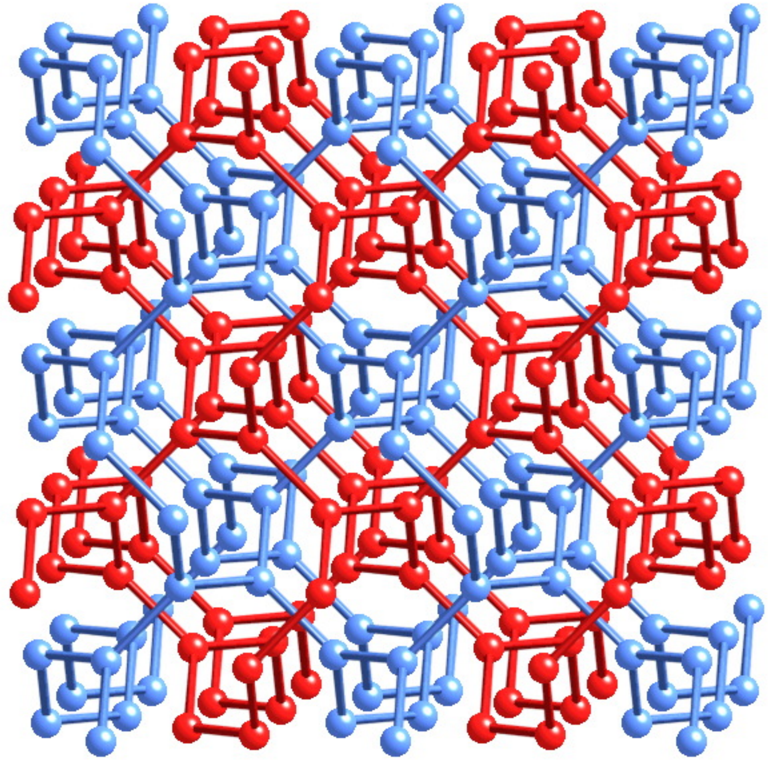
A Crystal that Nature May Have Missed

K_4 crystal. Created by Hisashi Naito.

January 3, 2008

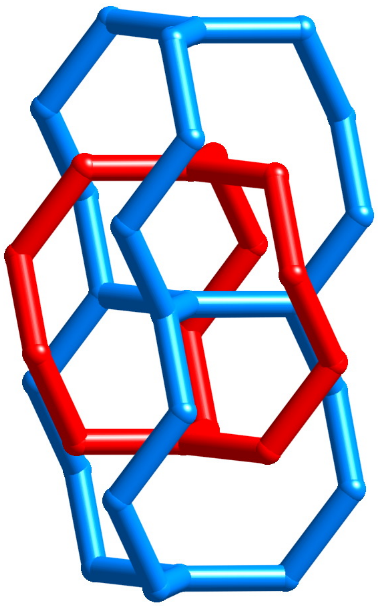
Providence, RI: For centuries, human beings have been entranced by the captivating glimmer of the diamond. What accounts for the stunning beauty of this most precious gem? As mathematician Toshikazu Sunada explains in an article appearing today in the Notices of the American Mathematical Society, some secrets of the diamond's beauty can be uncovered by a mathematical analysis of its microscopic crystal structure. It turns out that this structure has some very special, and especially symmetric, properties. In fact, as Sunada discovered, out of an infinite universe of mathematical crystals, only one other shares these properties with the diamond, a crystal that he calls the "K4 crystal". It is not known whether the K4 crystal exists in nature or could be synthesized.

"K4" = srs which is ubiquitous in nature from the structure of high-pressure nitrogen to butterfly wings

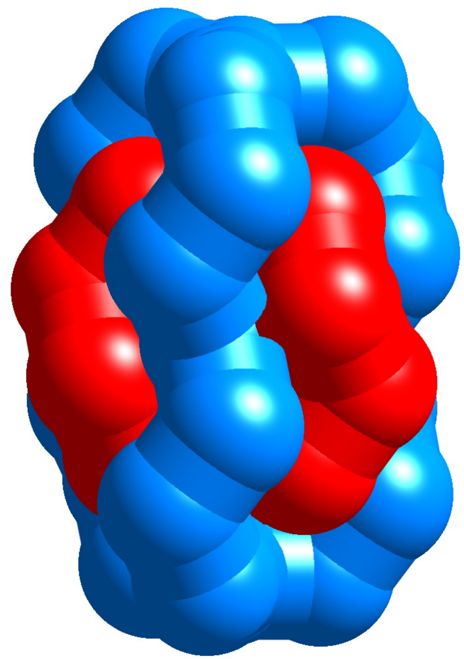


The **srs** net is chiral (symmetry $I4_132$).
The dual is the enantiomorph. Here two **srs** nets of opposite hand are intergrown to form a centrosymmetric structure (symmetry *Ia*-3*d*). The surface separating the two nets is the *G* minimal surface (*gyroid*)

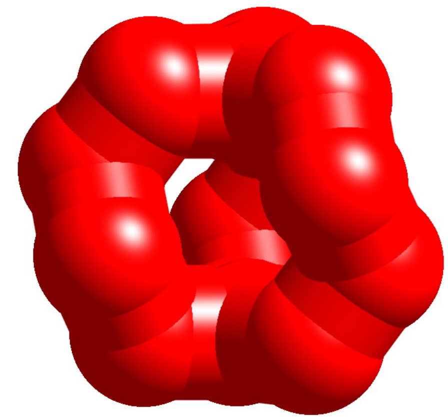
Alan Schoen's gyroid – periodic minimal surface *G*



Fragments of
two **srs nets**



The same –
"blown up"

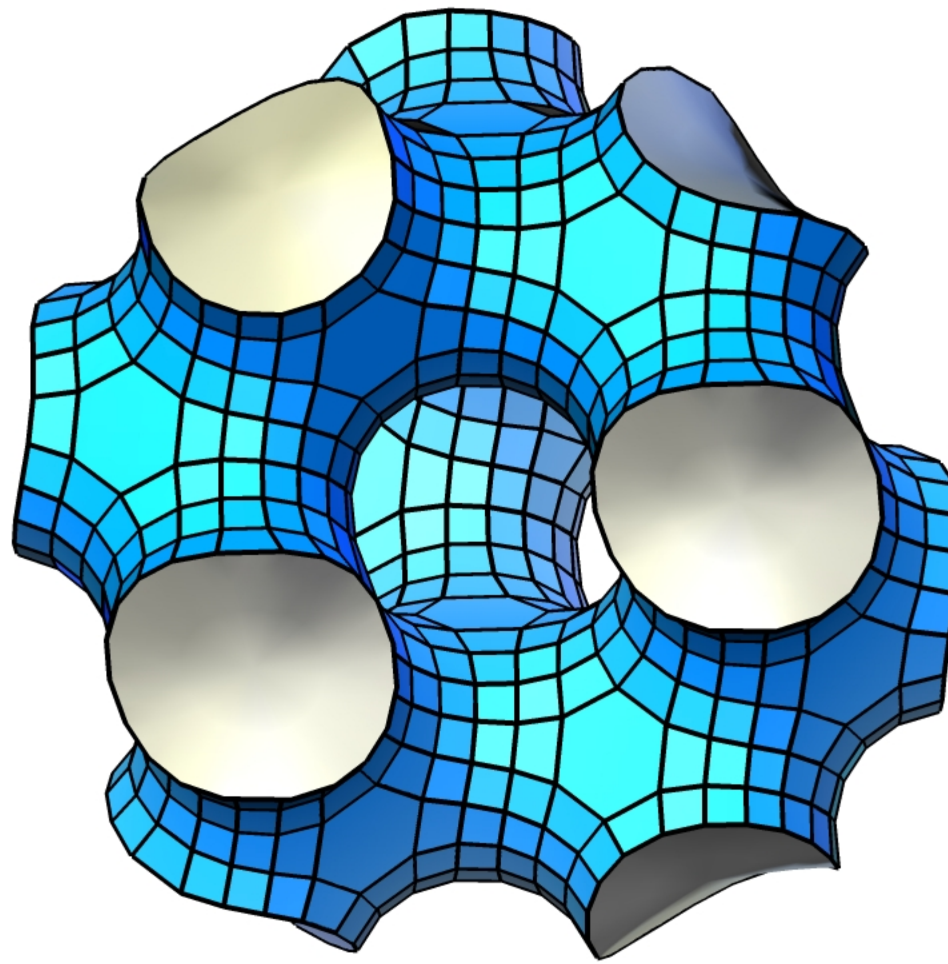


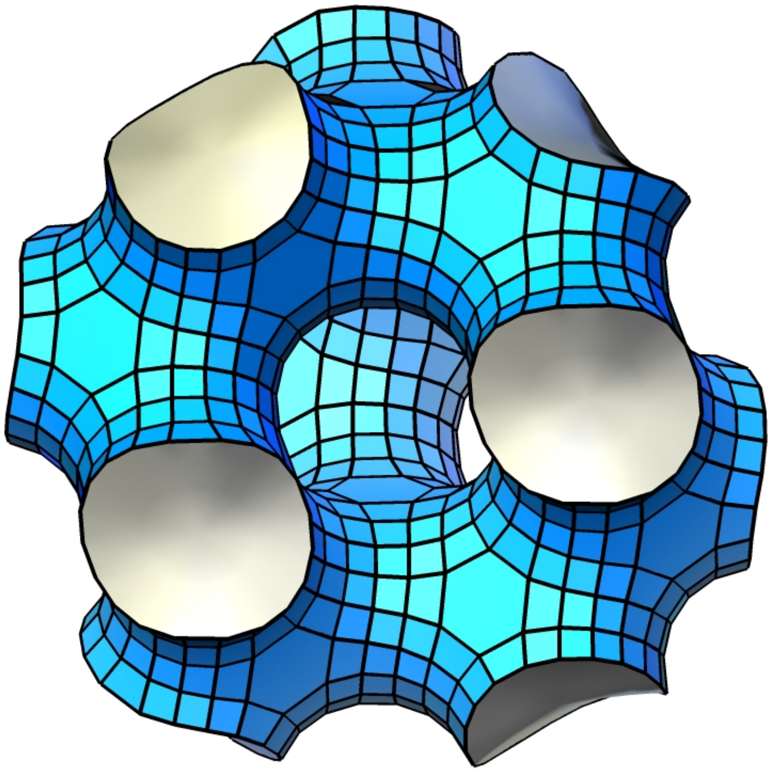
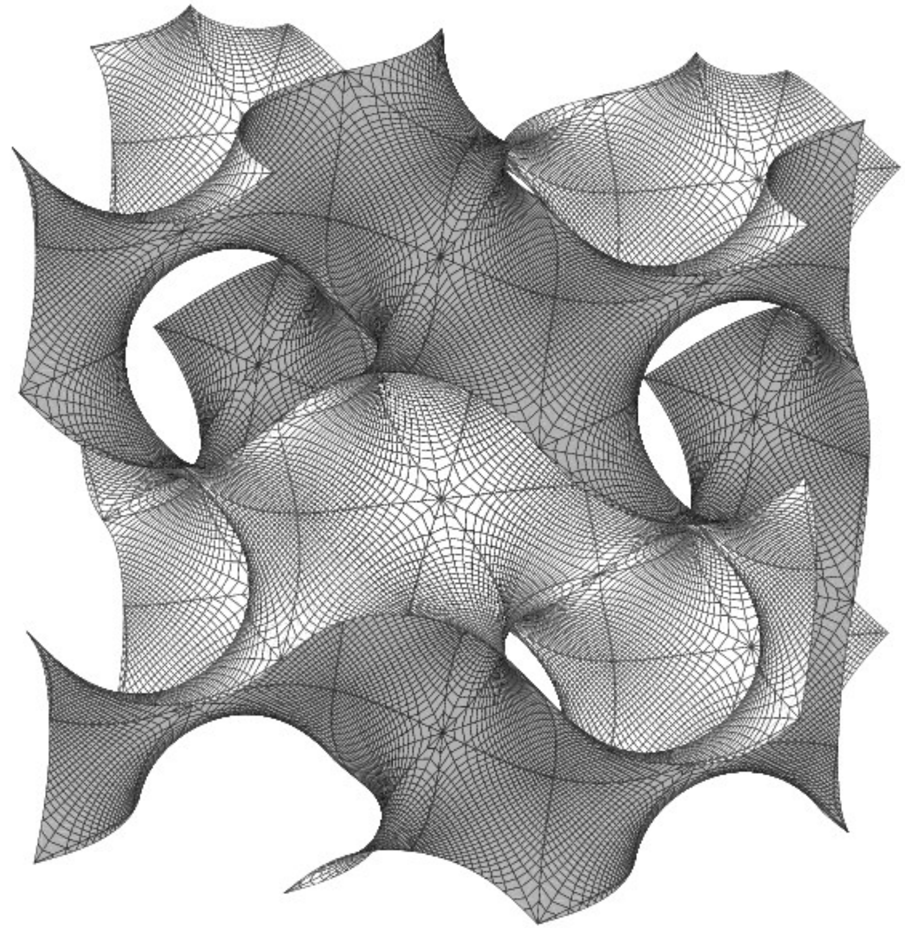
A "tile" of
the *G* surface

G surface of Alan Schoen

bicontinuous surfactant/water phases =>
mesoporous silicates, etc

Reminder: a minimal surface has positive and negative principal curvatures, k_1 and k_2.
Mean curvature = $(k_1 + k_2)/2 = 0$
Gaussian curvature $k_1 k_2 < 0$

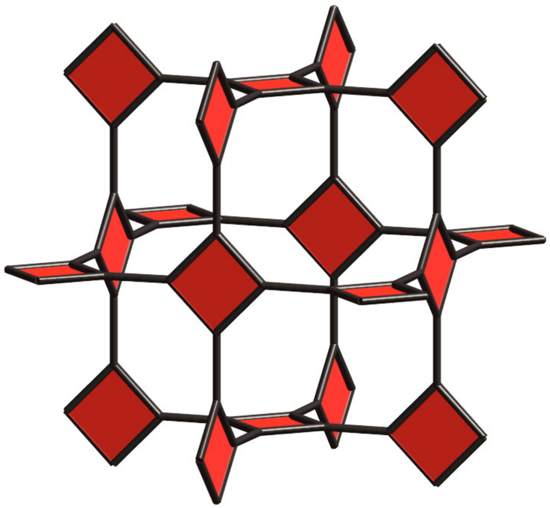


the gyroid is a surface !

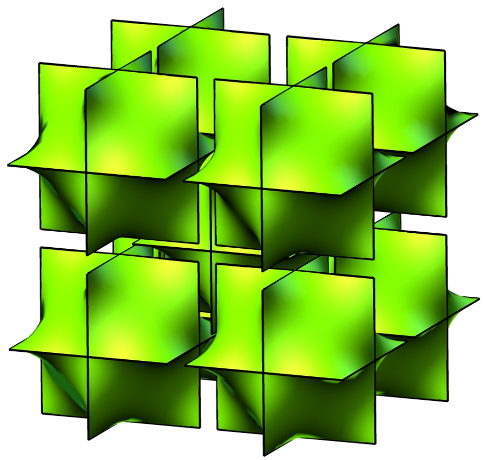
vertex figure: square

The **nbo** net



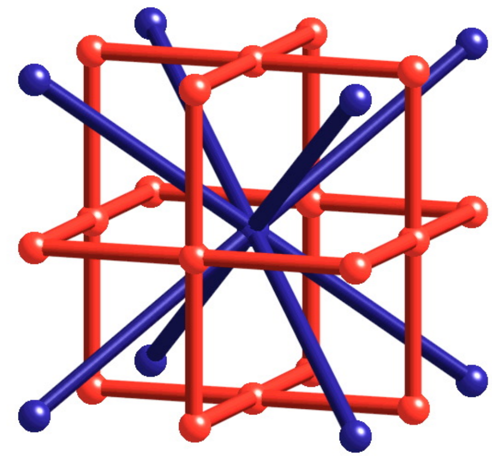
augmented net

nbo-a



natural tiling

$[6^8]$

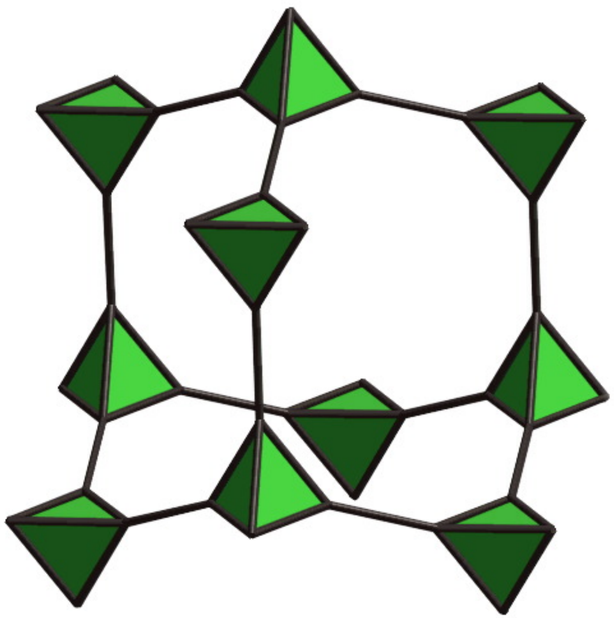


dual is 8-coordinated

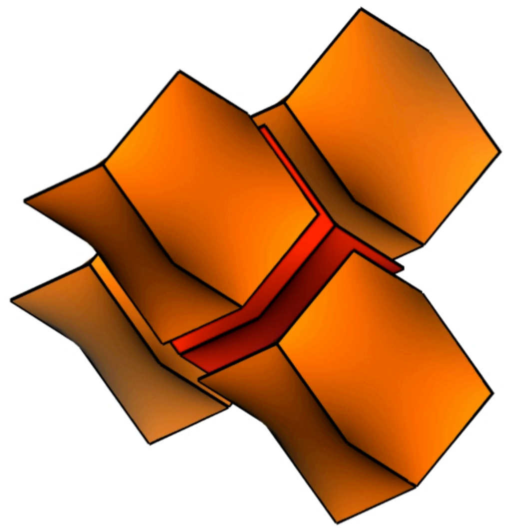
bcu net (bcc, blue)

vertex figure: tetrahedron

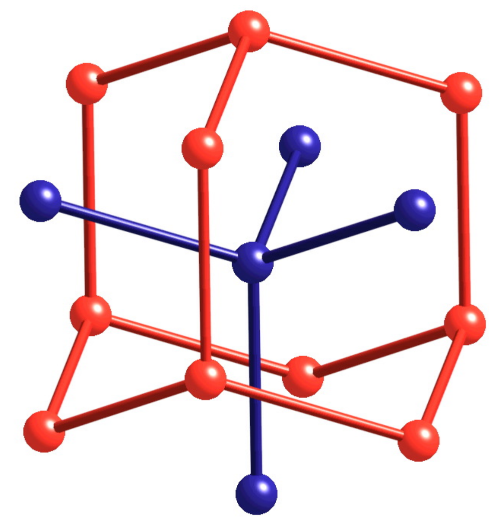
dia (diamond) net



augmented net
dia-a

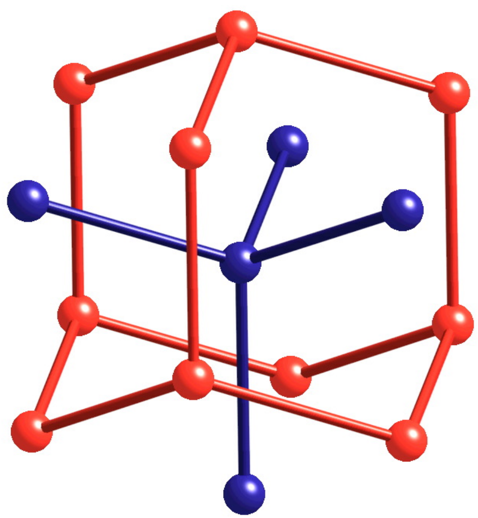


tiling
$[6^4]$

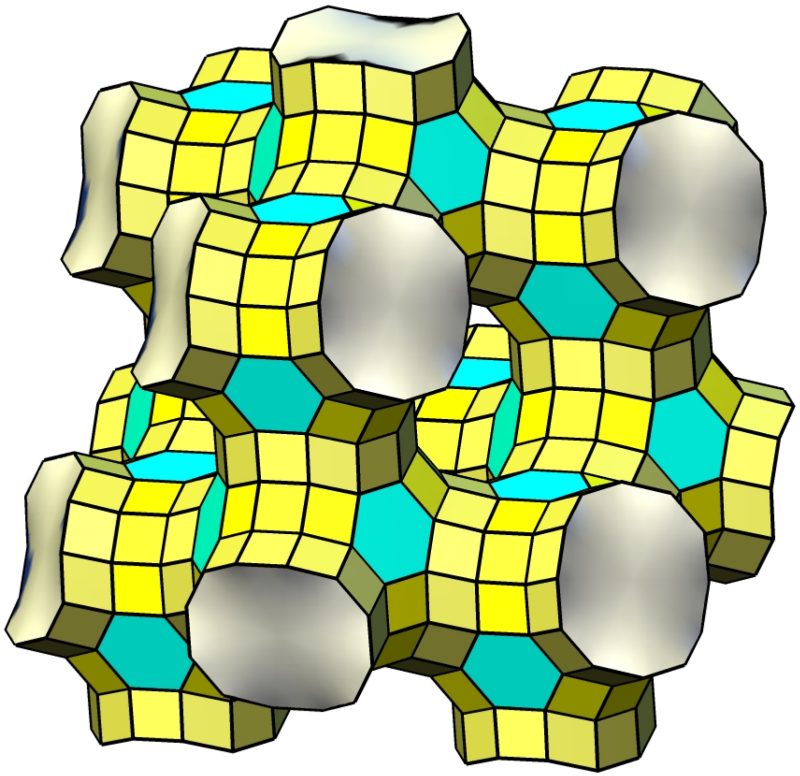


tile with dual
(self dual)

D minimal surface separates two **dia** nets

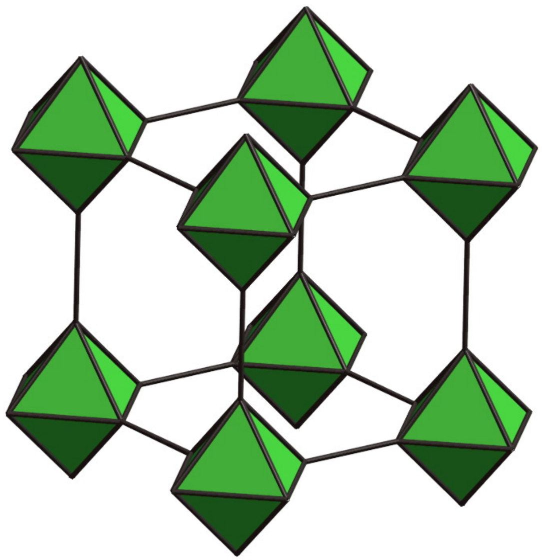


Red is skeleton of tile
of **dia**

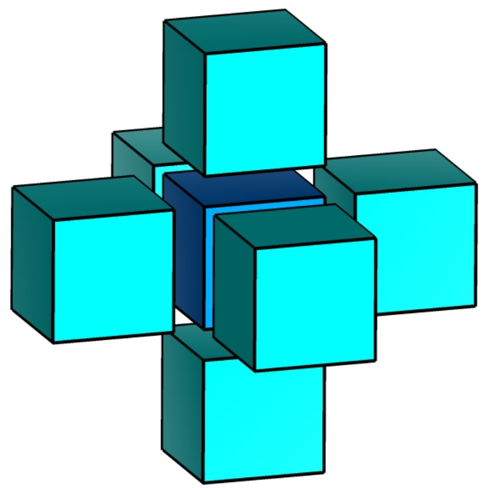


approximation to the D
surface (should be smooth)

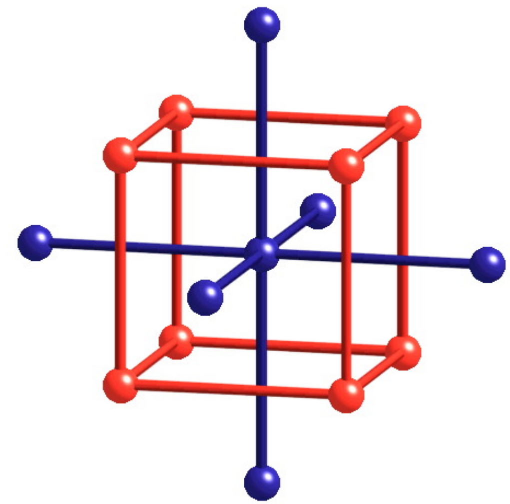
vertex figure: octahedron
pcu (primitive cubic) net



augmented net
pcu-a = cab
(B in CaB_6)

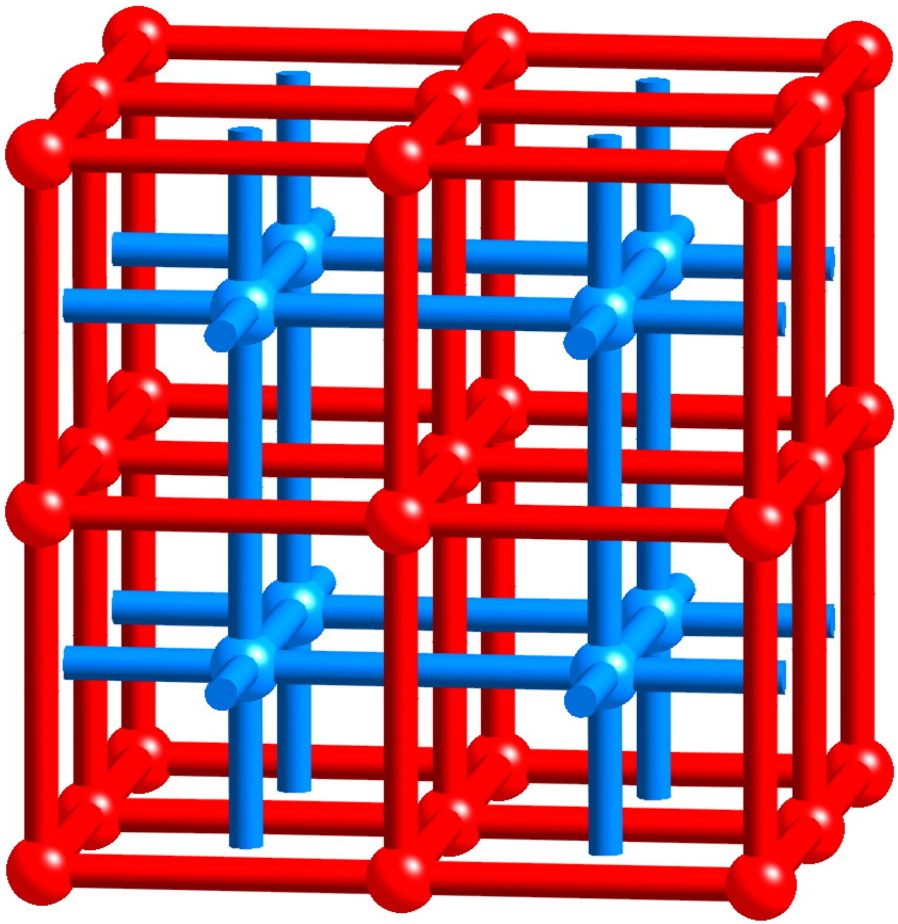


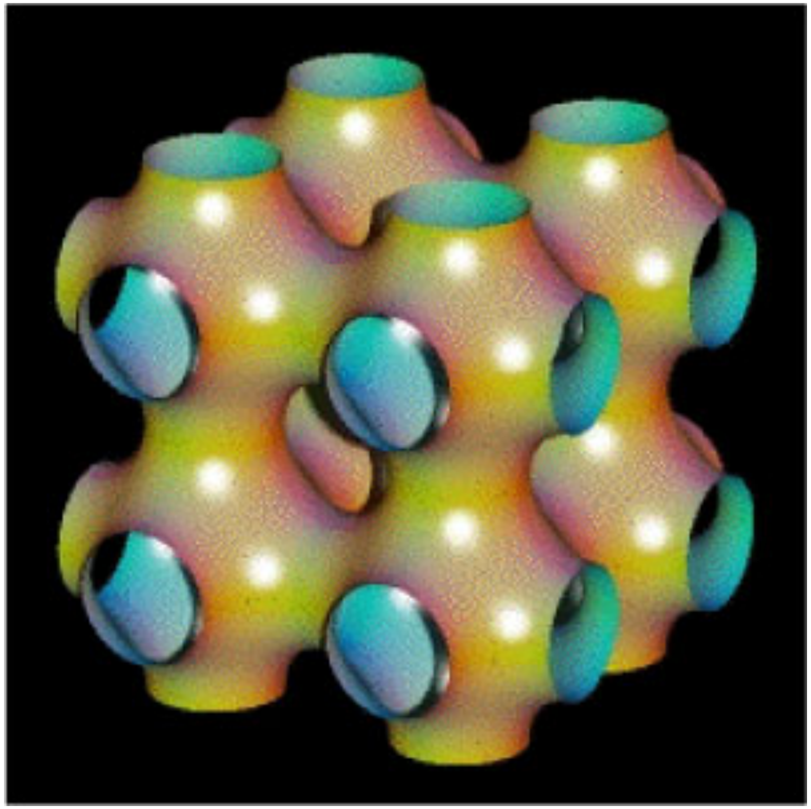
tiling
$[4^6]$



tile with dual
(self dual)

P minimal surface separates two **pcu** nets



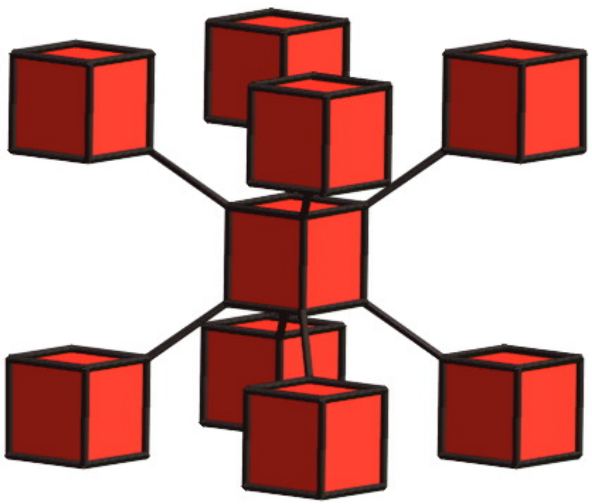


Two interpenetrating **pcu** nets
(notice that the nets are self-dual)

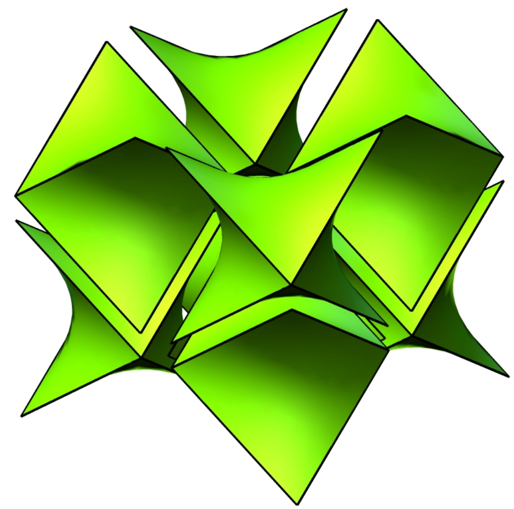
The *P* minimal surface
separates the two nets.
Average curvature zero
Gaussian curvature neg.

vertex figure: cube

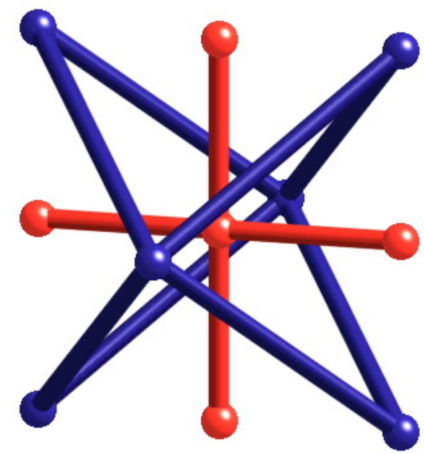
bcu (body-centered cubic) net



augmented net
bcu-a = pcb
(polycubane)



tiling
$[4^4]$

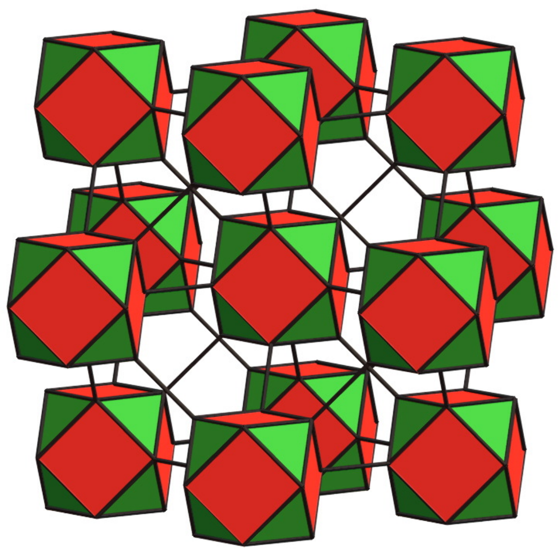


tile with dual
(dual is **nbo**)

Quasiregular net: *vertex figure cuboctahedron*

fcu (face-centered cubic) net

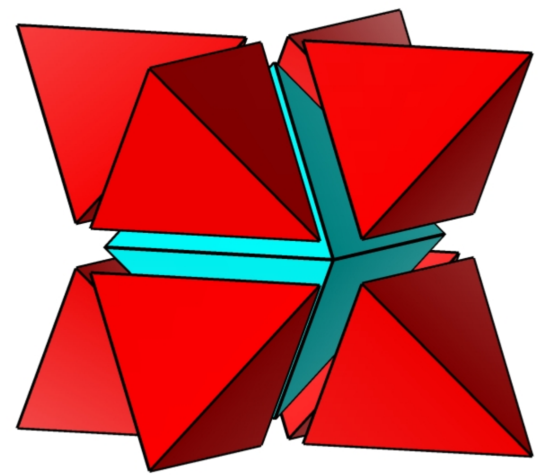
transitivity 1112



augmented net

fcu-a = ubt

(B in UB_{12})

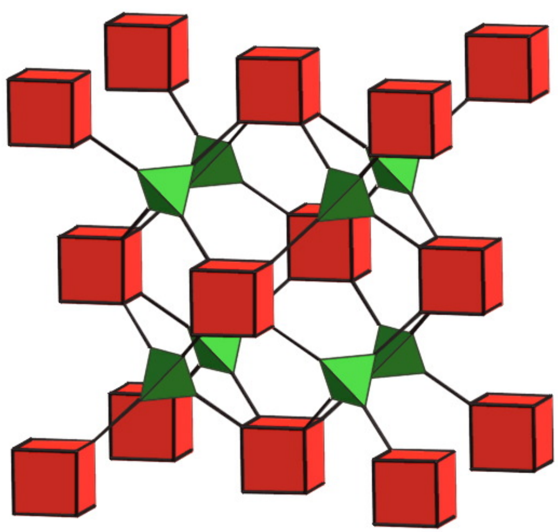


tiling

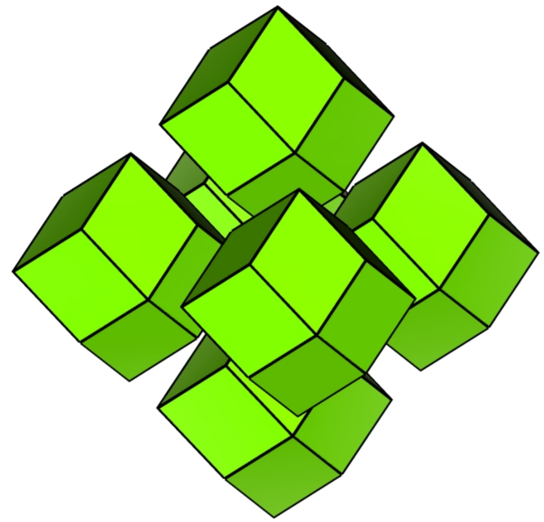
(note dual has two vertices)

$2[3^4] + [3^8]$

Normal dual of the **fcu** net. **flu** (fluorite)
transitivity 2111



augmented net
flu-a



tiling
$[4^{12}]$

3-periodic nets. The story so far:

The Regular Nets. Transitivity 1111

1. **srs,** triangle, $I4_132$, Si net of $SrSi_2$ (self-dual)
2. **nbo,** square, *Im*-3*m*, all atoms of NbO (dual = **bcu**)
3. **dia,** tetrahedron, *Fd*-3*m*, diamond net (self-dual)
4. **pcu,** octahedron, *Pm*-3*m*, primitive cubic (self dual)
5. **bcu,** cube, *Im*-3*m*, body-centered cubic (dual = **nbo**)

Quasiregular. Transitivity 1112

6. **fcu,** cuboctahedron, face-centered cubic dual is …

7. **flu,** cube and tetrahedron, net of fluorite (CaF_2)
(transitivity 2111)

there are 14 more vertex and edge transitive nets 11*rs*:

What 11*rs* structures are there?

1111 5 regular

1112 1 quasiregular

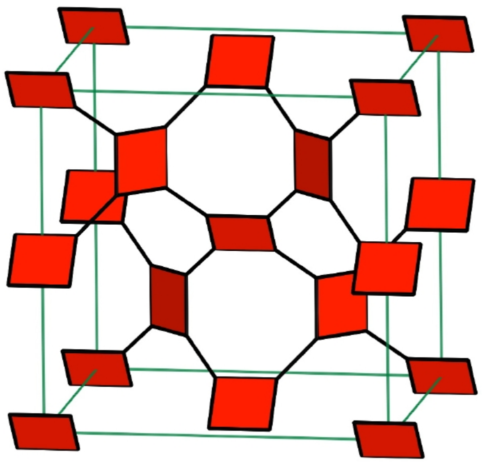
11*rs* 14 semiregular

(these have embeddings in which there is

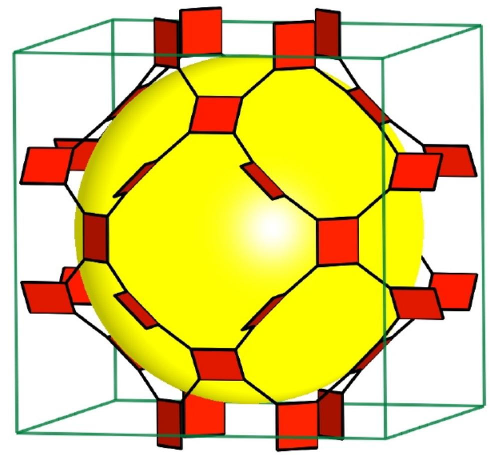
no intervertex distance shorter than edges)

The augmented regular, quasiregular, and semiregular nets are ways of linking polygons or polyhedra with one kind of link.

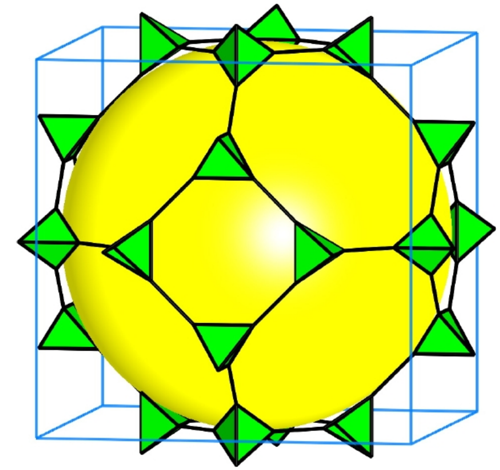
augmented semiregular nets -1



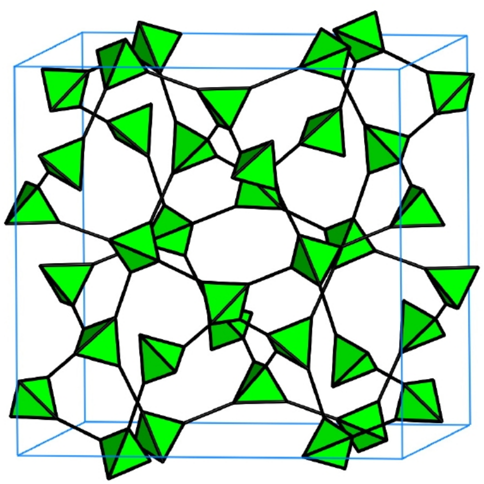
lvt-a



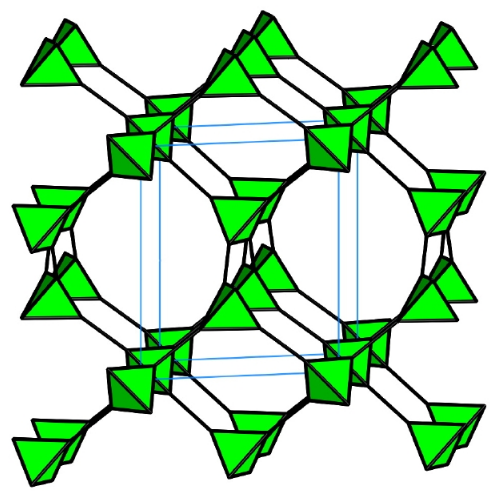
rhr-a



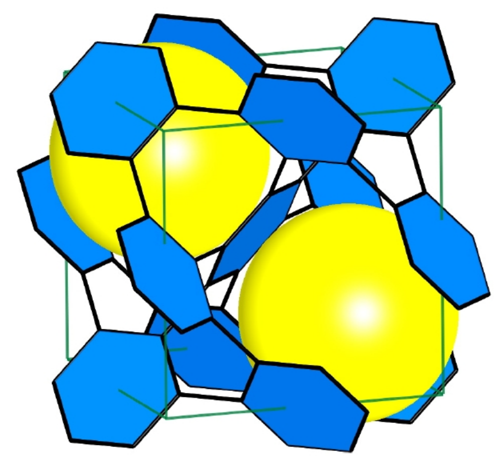
sod-a



lcs-a

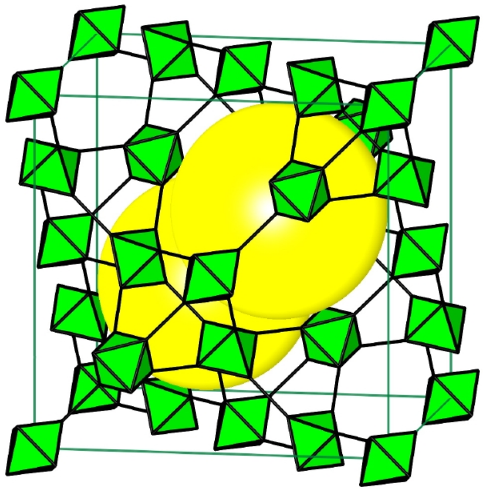


qtz-a

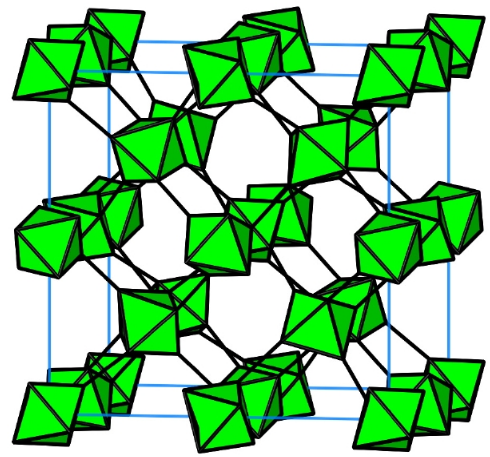


hxg-a = pbz

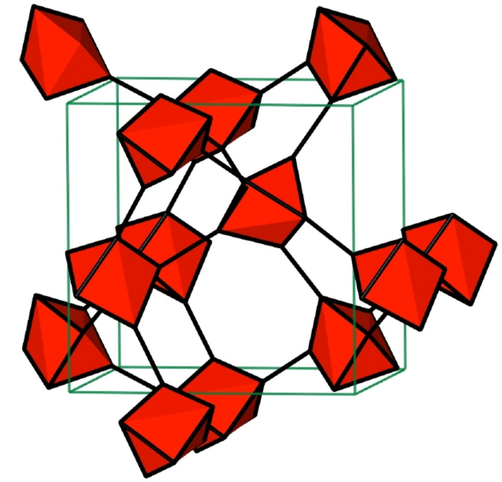
augmented semiregular nets -2



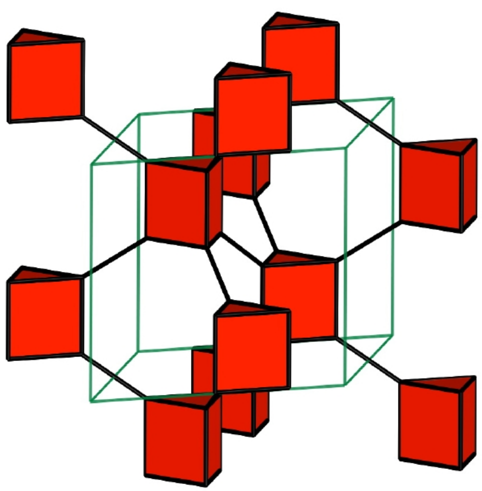
crs-a



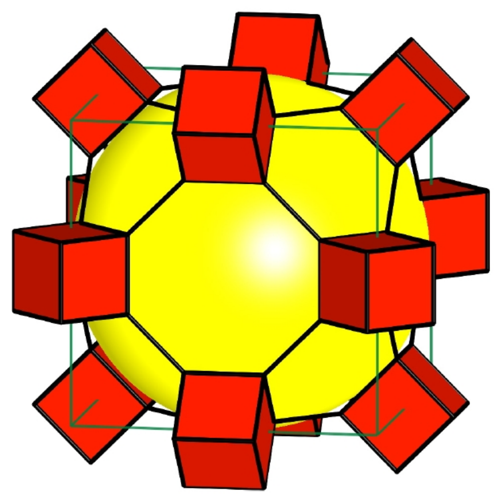
bcs-a



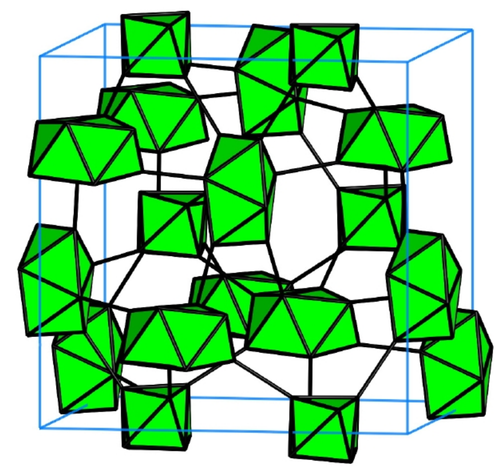
lcy-a



acs-a



reo-a = lta

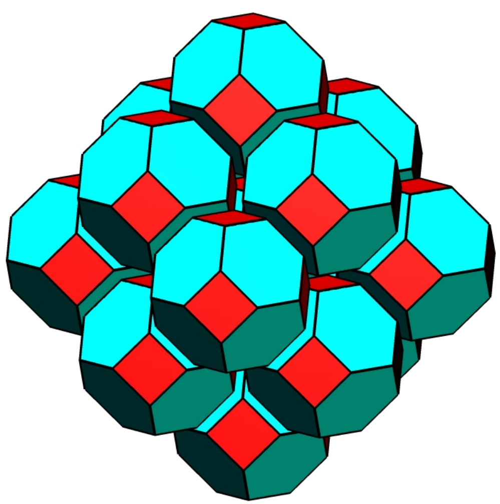


thp-a

the net **sod**, symmetry *Im*-3m with transitivity 1121

atomic positions
1/2, 1/4, 0 etc

"imvariant lattice complex" *W**



tiling has transitivity 1121
simple tiling

Cubic invariant lattice complexes. O'K&H p. 281
International Tables for Crystallography, ol. A

RCSR symbol	lattice complex	space group		coordination
fcu	*F*	*Fm*-3*m*	4 *a*	12
bcu	*I*	*Im*-3*m*	2 *a*	8
reo	*J*	*Pm*-3*m*	3 *c*	8
lcs	*S*	*I*-43*d*	12 *a* or 12 *b*	8
crs	*T*	*Fd*-3*m*	16 *c* or 16 *d*	6
lcy	^{+}Y	$P4_332$	4 *a*	6
lcy	^{-}Y	$P4_132$	4 *a*	6
dia	*D*	*Fd*-3*m*	*8 a* or 8 *b*	4
lcv	^{+}V	$I4_132$	12 *d*	4
lcv	^{-}V	$I4_332$	12 *d*	4
nbo	*J**	*Im*-3*m*	6 *b*	4
sod	*W**	*Im*-3*m*	12 *d*	4
lcs	*S**	*Ia*-3*d*	24 *c*	4
srs	^{+}Y*	$I4_132$	8 *a*	3
srs	^{-}Y*	$I4_132$	8 *b*	3
srs-c	*Y***	*Ia*-3*d*	16 *b*	3
lcw	*W*	*Im*-3*m*	6 *c* or 6 *d*	2

Structures based on edge-transitive nets with two kinds of vertex (transitivity 21*rs*)

These are of two kinds

1. Structures based on coloring of nets with one kind of vertex (e.g. the NaCl structure is derived from **pcu** (primitive cubic) by alternating Na and Cl at the vertices.

2. Structures in which the vertices have different vertex figures (e.g. tetrahedron + square or triangle + octahedron)

Edge-transitive binodal nets

These form the basis for structures formed by joining two shapes by one kind of link.

O. Delgado-Friedrichs, M. O'Keeffe, O. M. Yaghi, *Acta Cryst*. ***A*62**, 350-355 (2006)

Edge-transitive 3-periodic nets

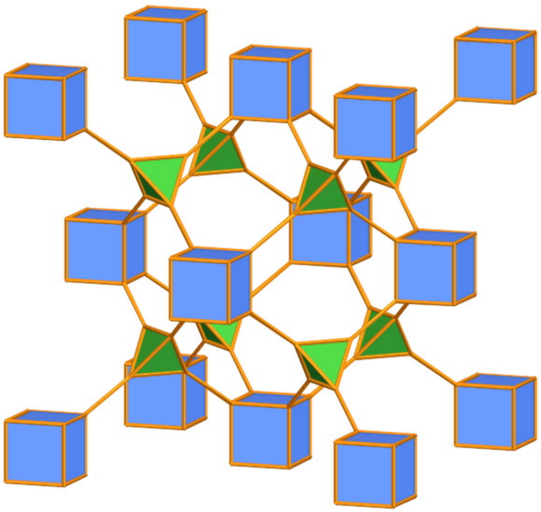
11*rs*	20
21*rs*	13 binary versions of above
	34 others

Note:

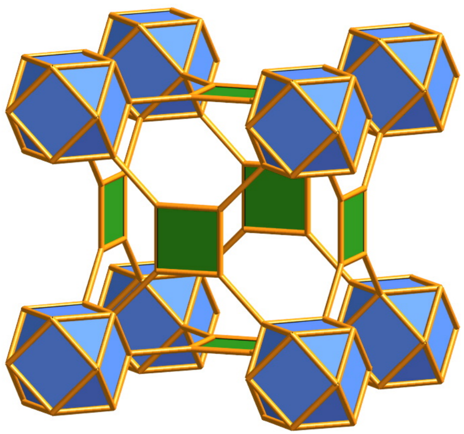
These are nets that have embeddings with edge lengths equal to the shortest distance between vertices.

Without this restriction there are infinitely many

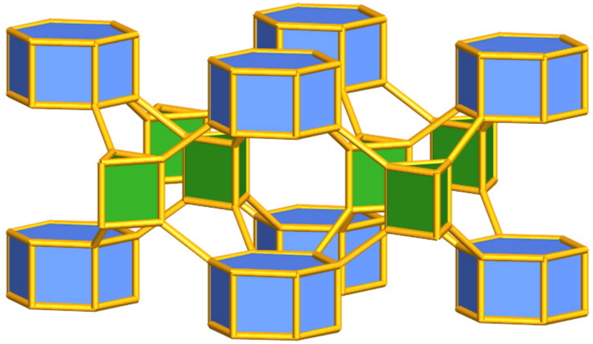
Edge-transitive binodal nets



flu-a $o/z = 6$



ftw-a $o/z = 4$



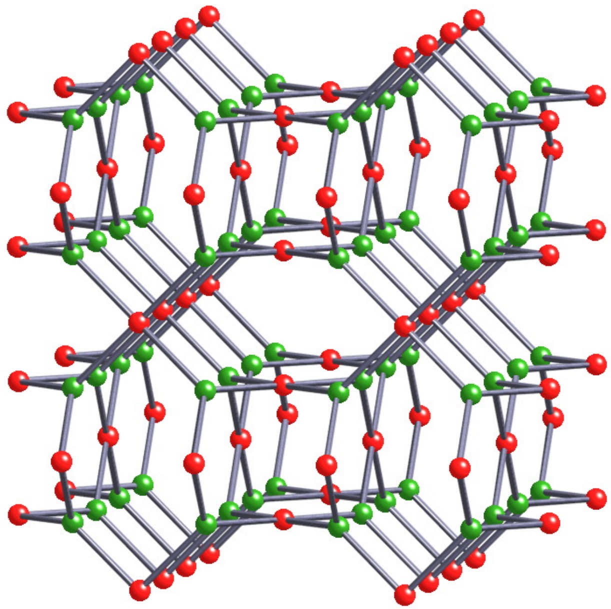
alb-a $o/z = 2$

Possible ways of linking polyhedra with full symmetry

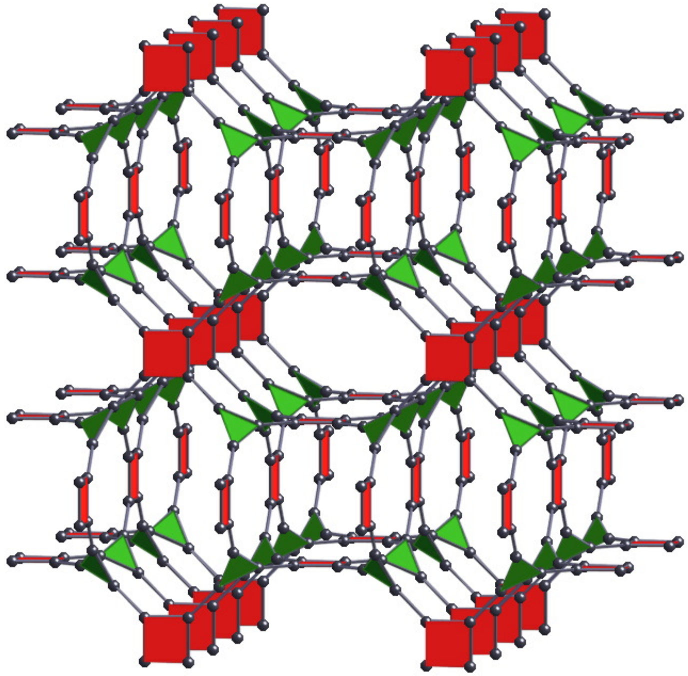
Edge-transitive binodal nets

triangle - square; order 6 - 8

this is the order of the point symmetry of the vertices



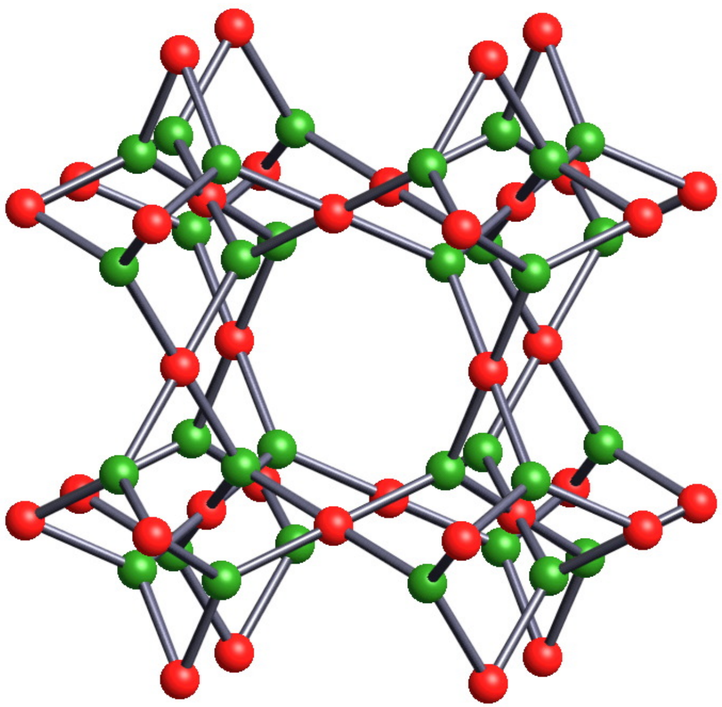
the Pt_3O_4 net,
pto



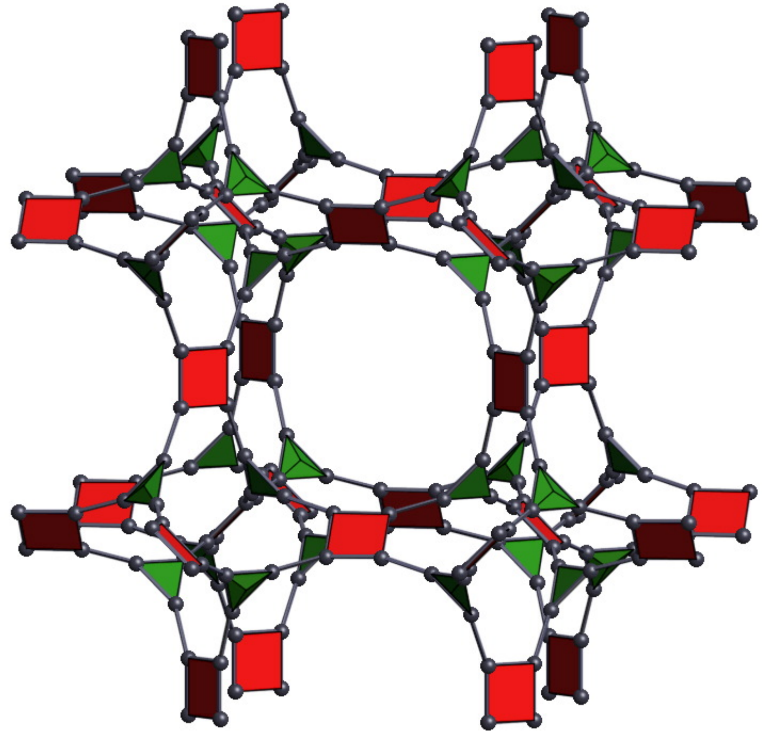
the augmented structure
pto-a

Edge-transitive binodal nets

triangle - square: order 6 - 8



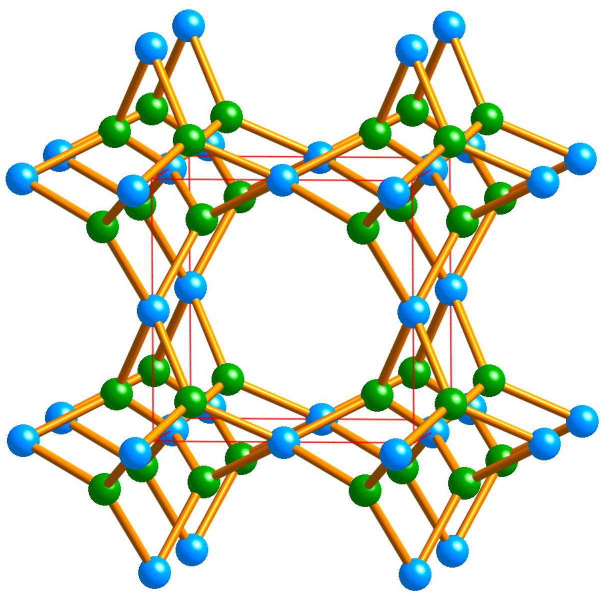
the "twisted boracite" net
tbo *Fm*-3*m*



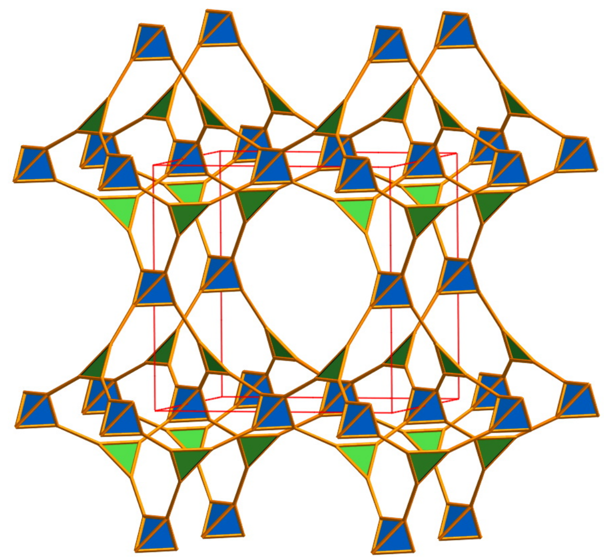
the augmented structure
tbo-a

Edge-transitive binodal nets

triangle - tetrahedron: order 6 - 8



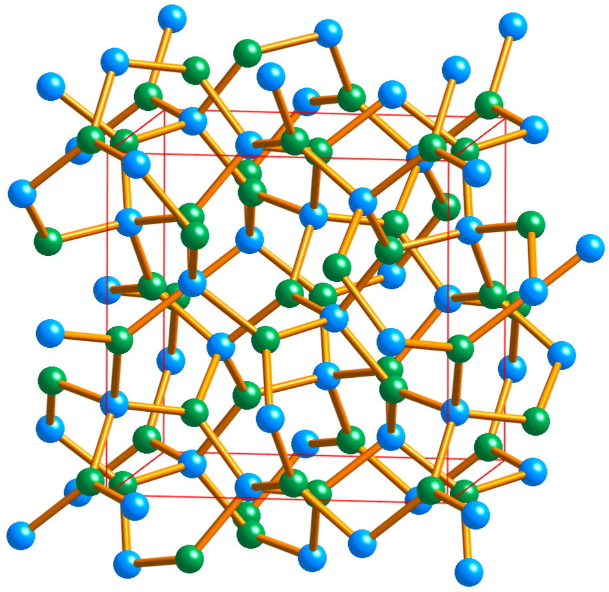
the boracite net
bor, *P*-43*m*



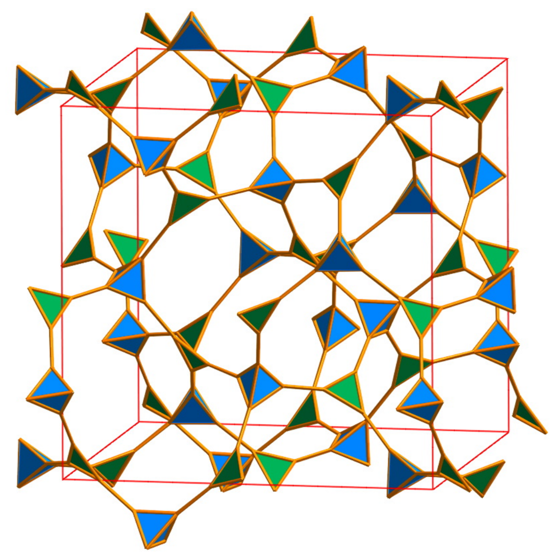
the augmented structure
bor-a

Edge-transitive binodal nets

triangle - tetrahedron: order 3 - 4



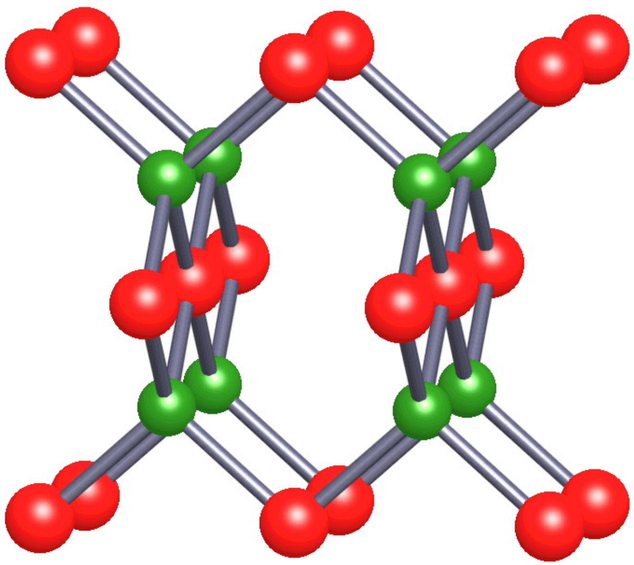
The "C_3N_4" net
ctn, *I*-43*d*



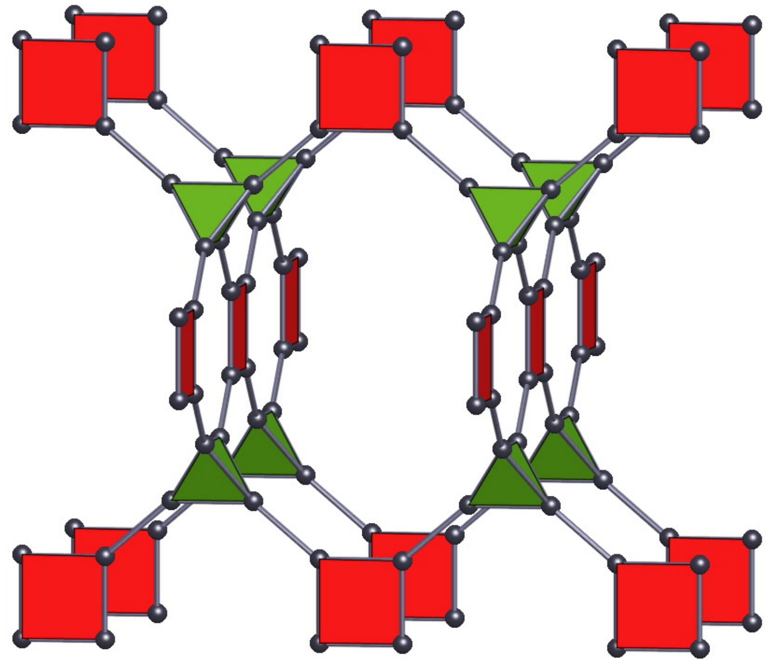
the augmented structure
ctn-a

Edge-transitive binodal nets

square - tetrahedron: order 8 - 8



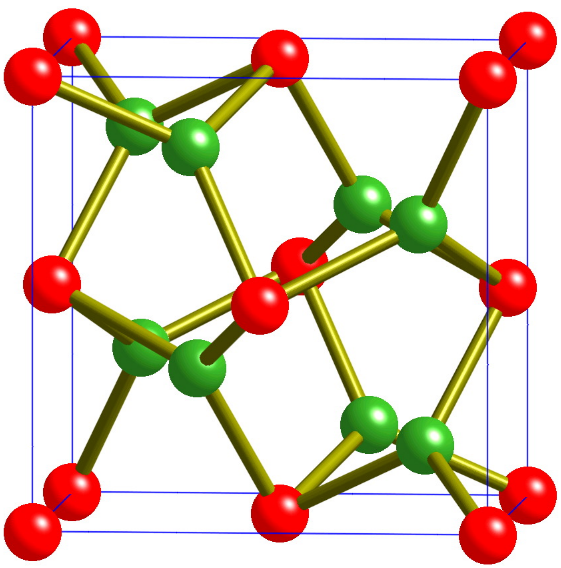
the PtS net
pts P4_2/*mmc*



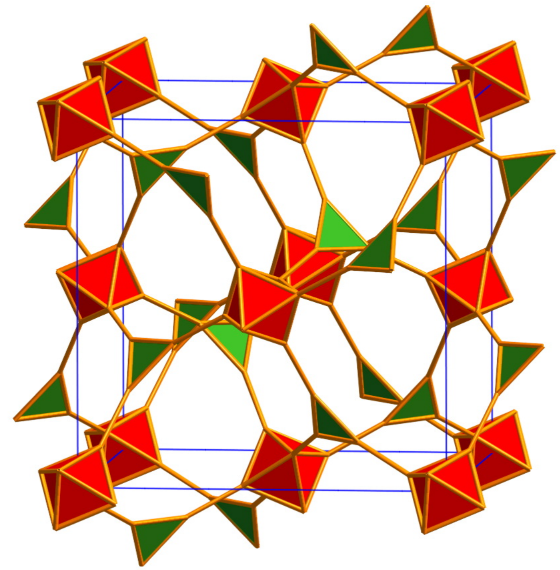
the augmented structure
pts-a

Edge-transitive binodal nets

triangle - octahedron: order 3 - 6



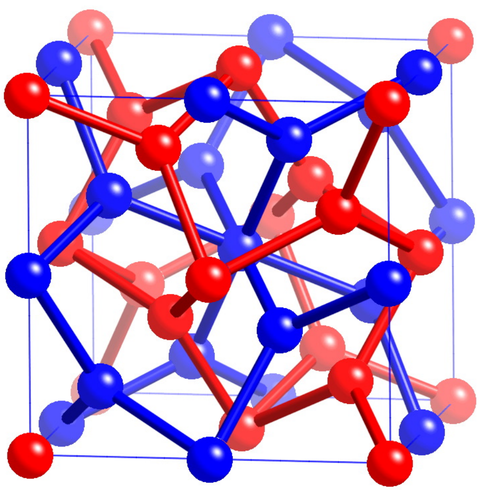
the pyrite (FeS_2) net
pyr *Pa*-3



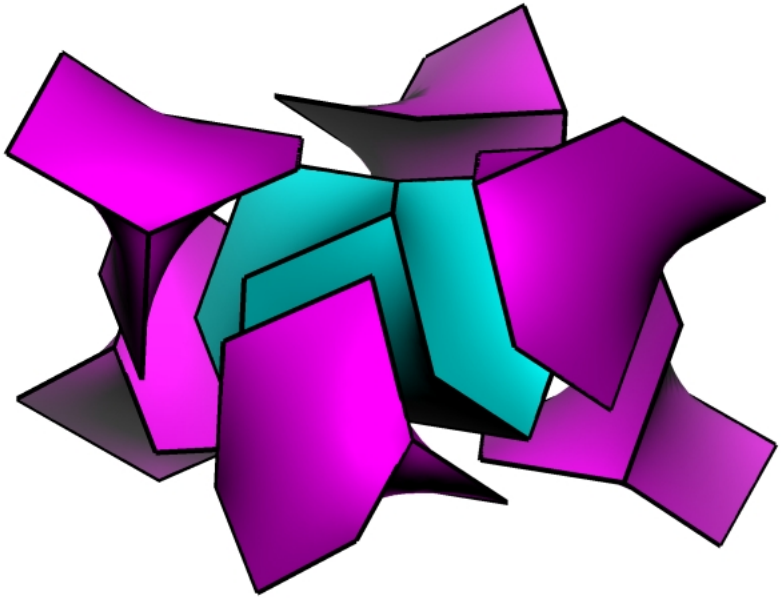
the augmented structure
pyr-a

Edge-transitive binodal nets

The **pyr** structure is naturally self dual transitivity 2112. Tiles 2[6^3] + [6^6]



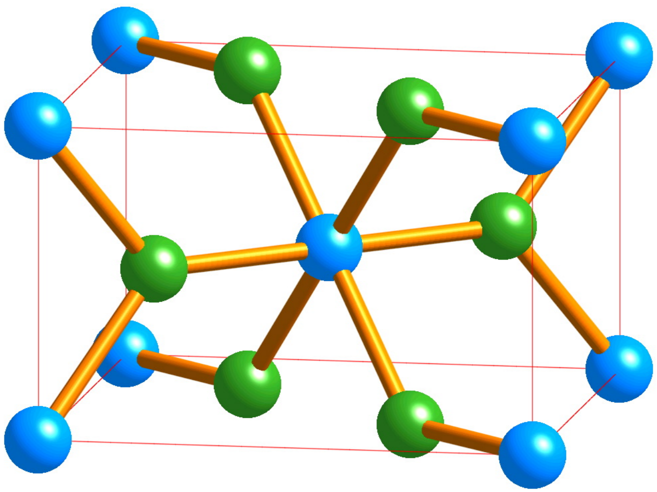
two fully catenated **pyr** nets



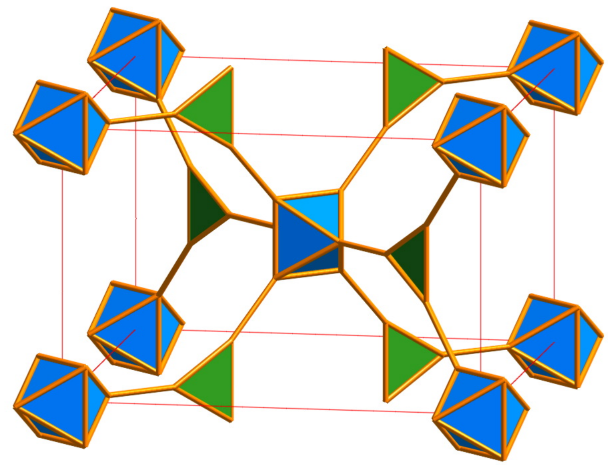
tiling

triangle - octahedron: order 4 - 8

the rutile structure symmetry $P4_2/mnm$



rtl



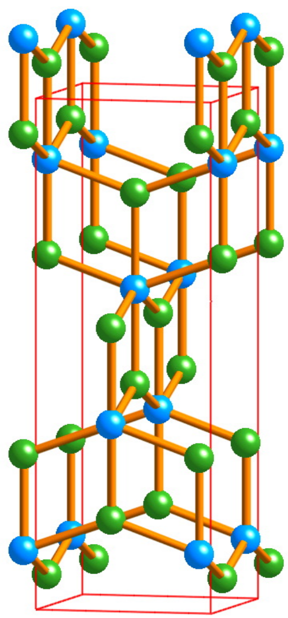
rtl-a

although the vertices here have higher site symmetry than in **pyr**,

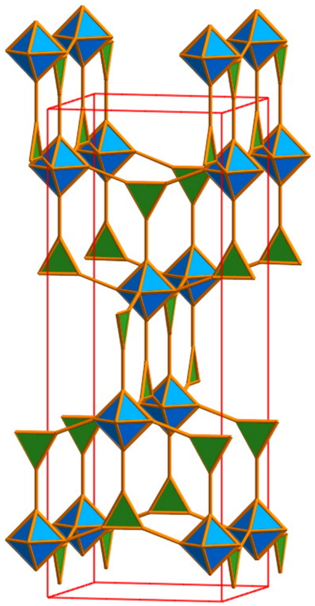
this is *not* an edge-transitive structure triangle - octahedron: order 4 - 8

the anatase structure symmetry $I4_1/amd$

ant



ant-a

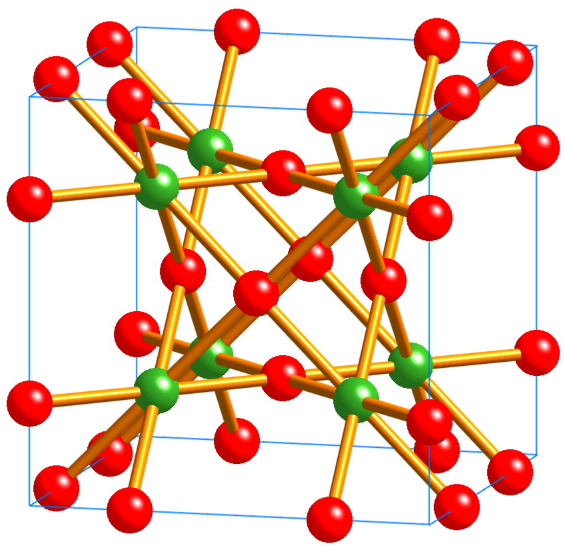


although the vertices here have higher site symmetry than in **pyr**,

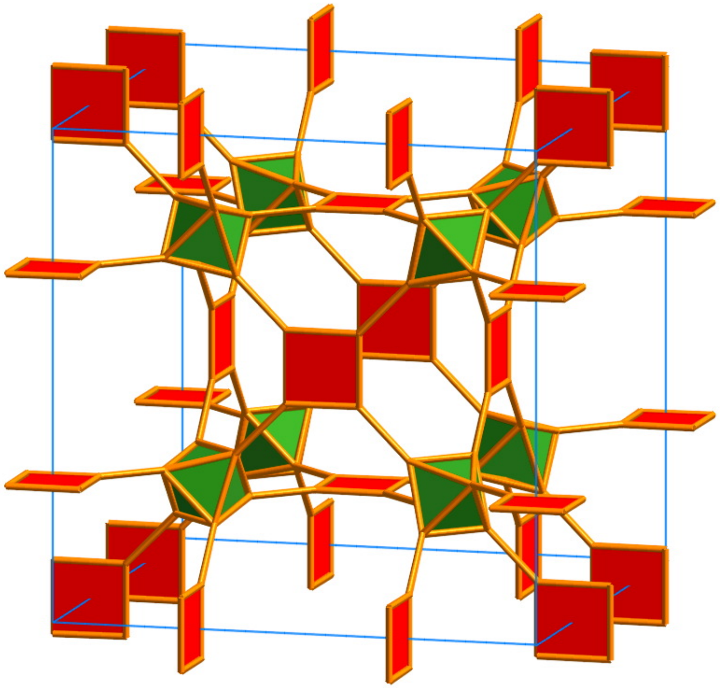
this is *not* an edge-transitive structure

Edge-transitive binodal nets

square - octahedron: order 8 - 12



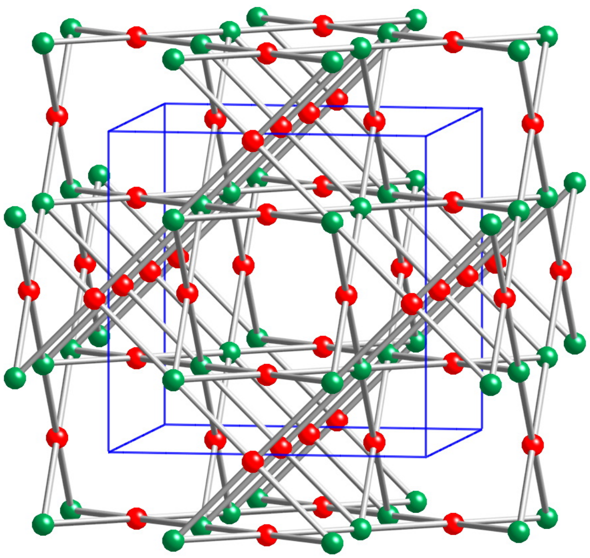
soc *Im*-3*m*



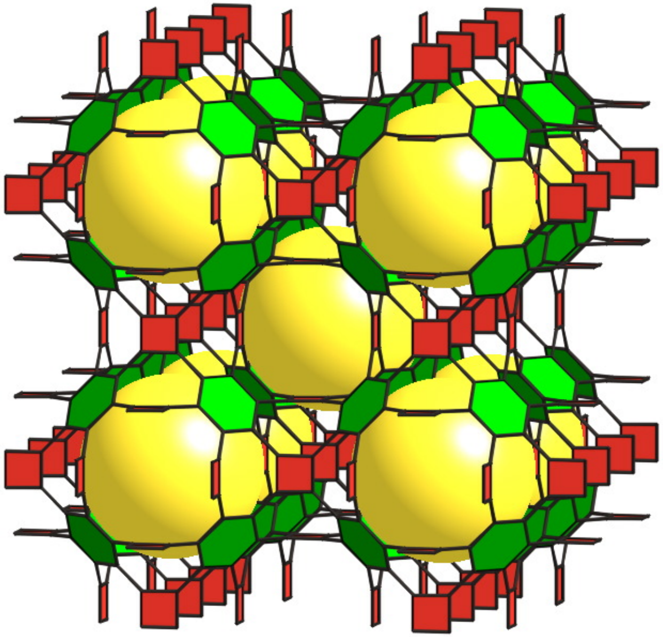
soc-a

Edge-transitive binodal nets

square - hexagon: order 8 - 12



she



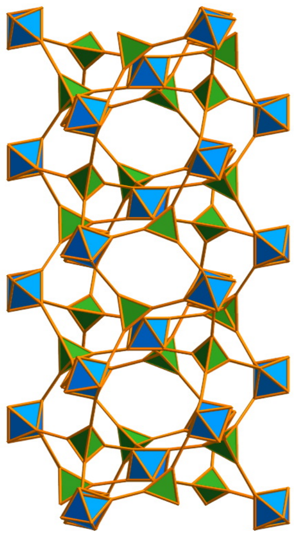
the augmented structure
she-a

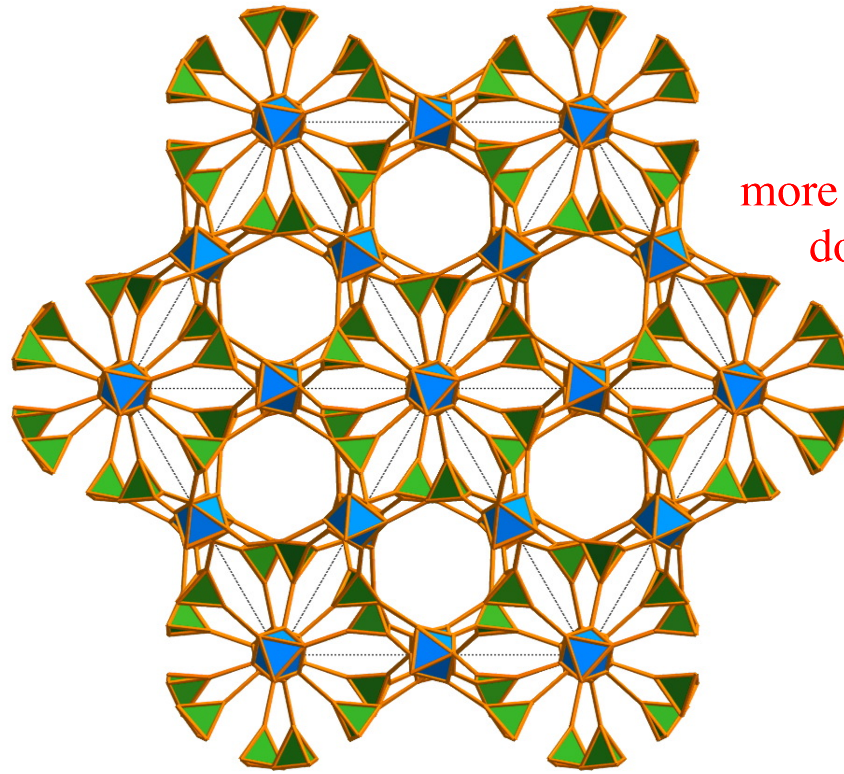
Edge-transitive binodal nets

tetrahedron - octahedron: order 4-6

augmented garnet net: **gar-a**. symmetry *Ia*-3*d*

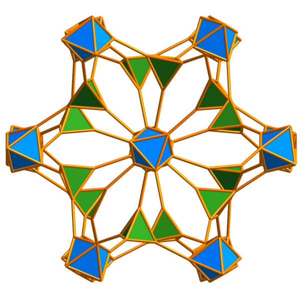
a fragment normal to [111]





more projected down [111]

the same fragment down [111]



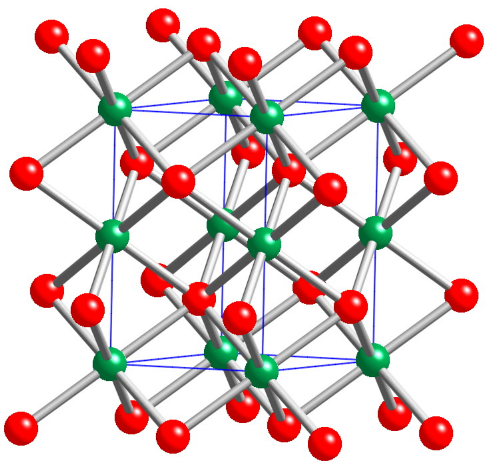
the garnet structure is notoriously difficult to illustrate!

Edge-transitive binodal nets

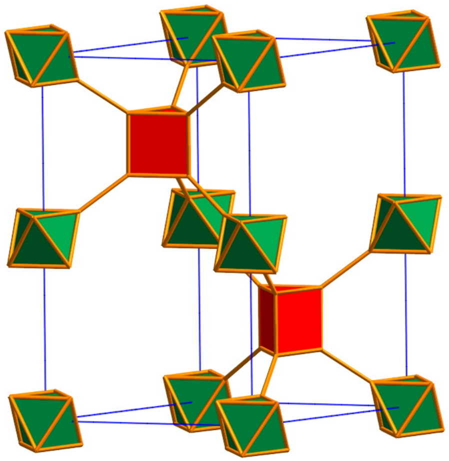
trigonal prism - octahedron: order 12-12

NiAs **nia**, symmetry $P6_3/mmc$

nia



nia-a

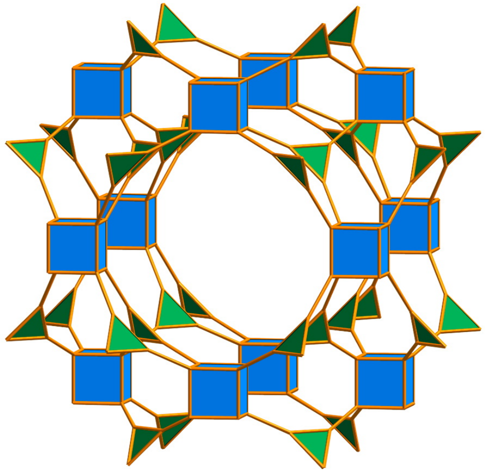


The green balls ("Ni") are in trigonal prismatic coordination and at the points of a hexagonal lattice. The red balls ("As") are in octahedral coordination and arrangeds as in hexagonal closest packing.

Edge-transitive binodal nets

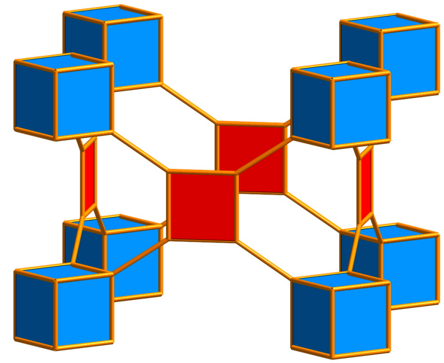
triangle - cube 6 - 16

the-a
Pm-3*m*



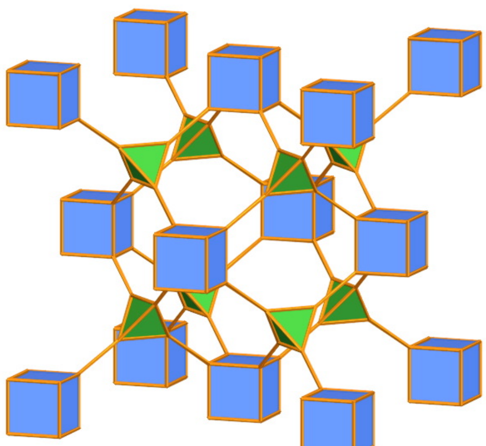
square - cube 8 - 16

scu-a
*P*4/*mmm*



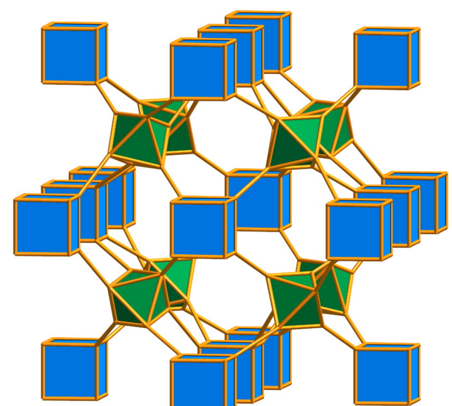
tetrahedron - cube 24 - 48

flu-a
Fm-3*m*

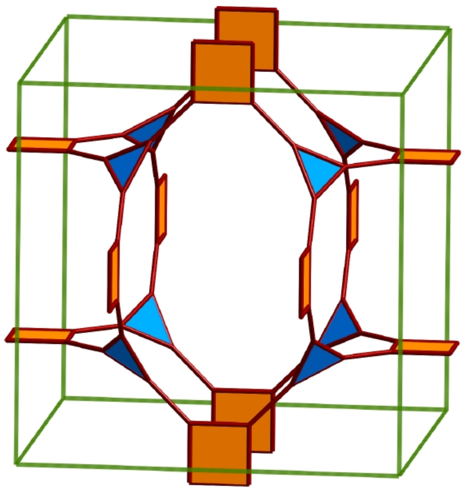


octahedron - cube 12 - 16

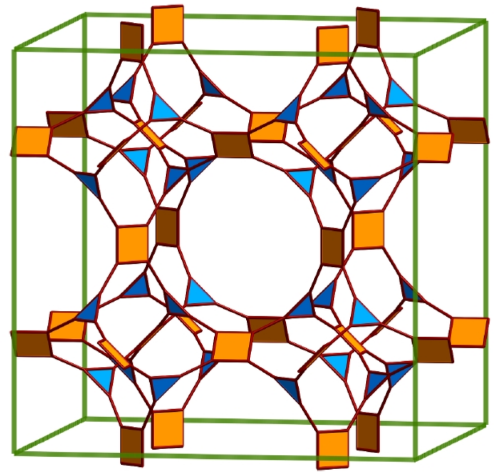
ocu-a
Im-3*m*



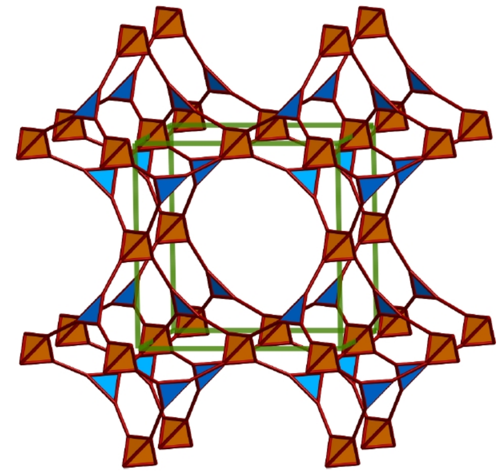
Edge-transitive binodal nets - summary 1



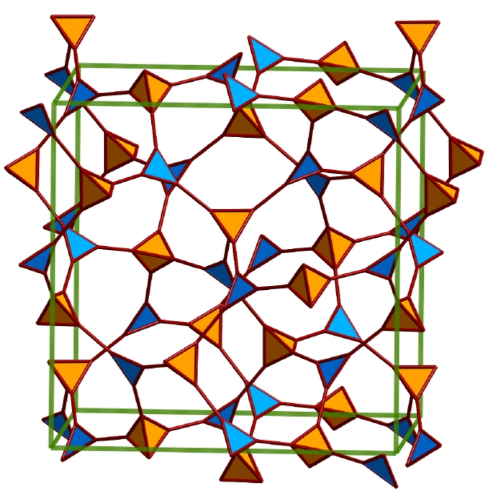
pto-a



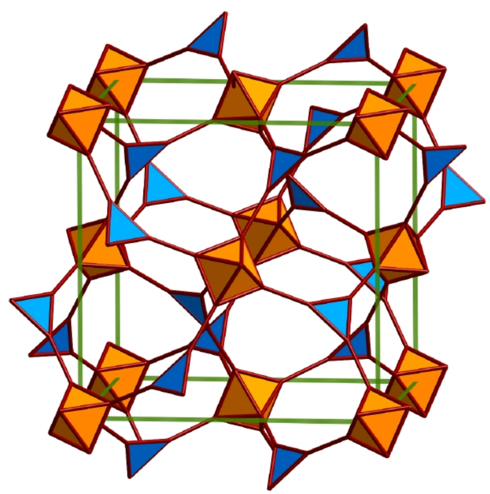
tbo-a



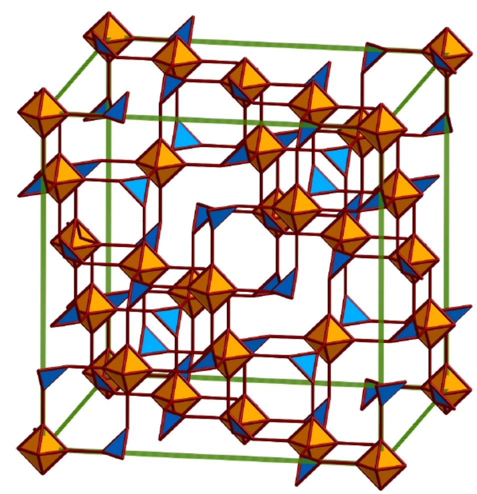
bor-a



ctn-a

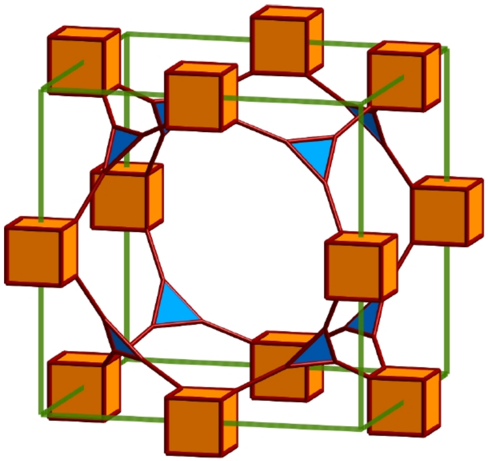


pyr-a

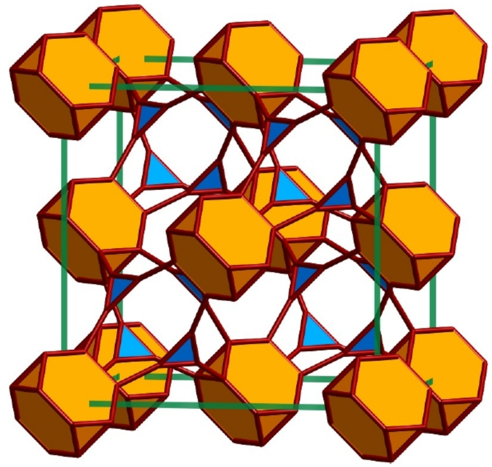


spn-a

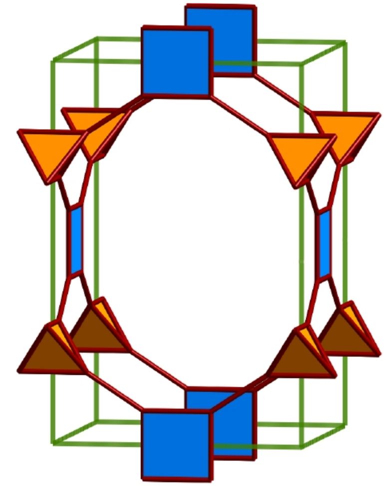
Edge-transitive binodal nets - summary 2



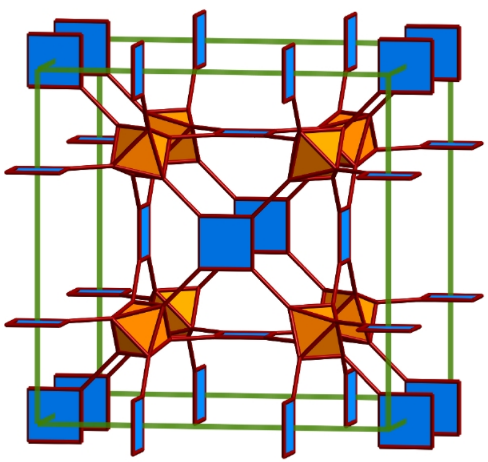
the-a



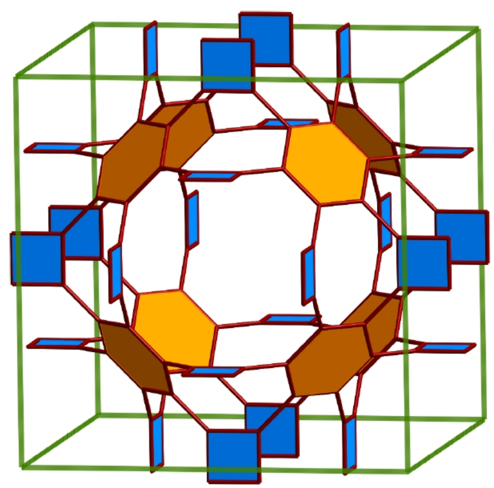
ttt-a



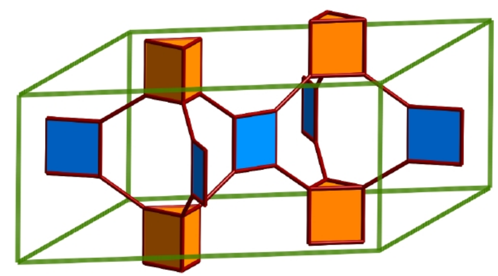
pts-a



soc-a

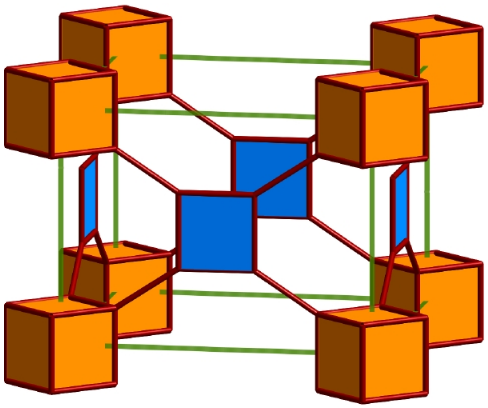


she-a

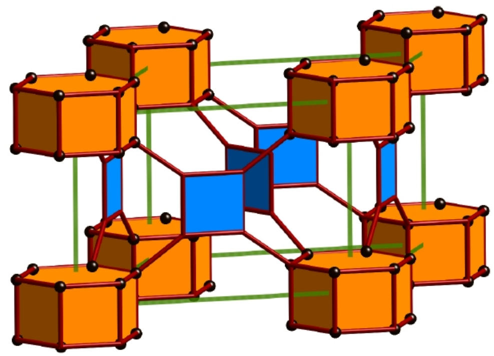


stp=a

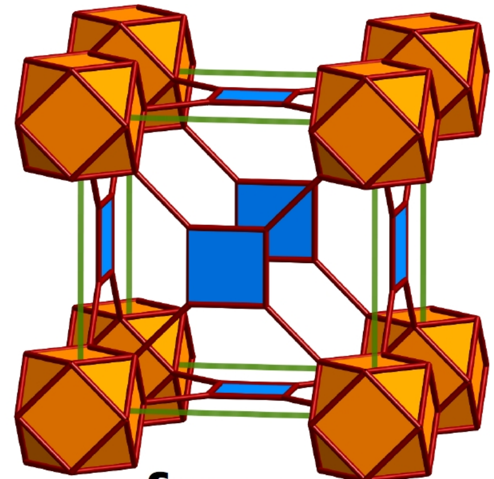
Edge-transitive binodal nets - summary 3



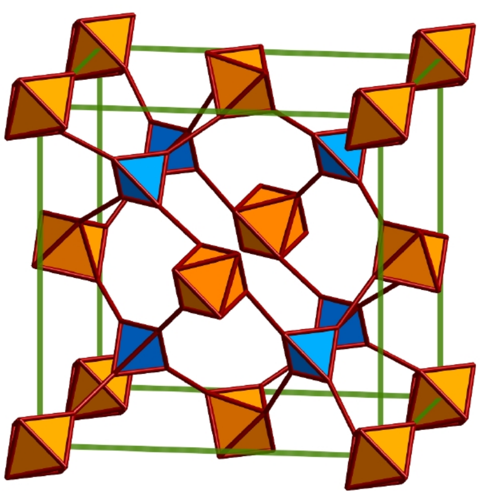
scu-a



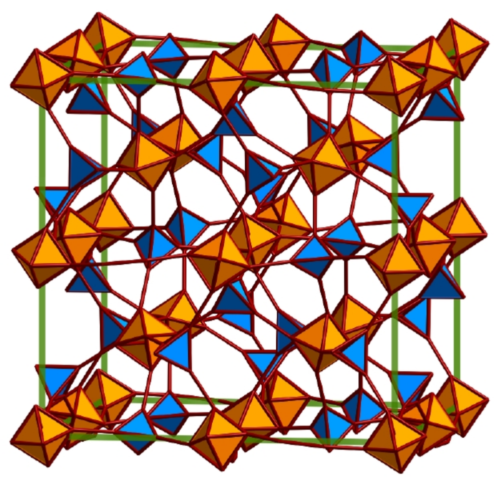
shp-a



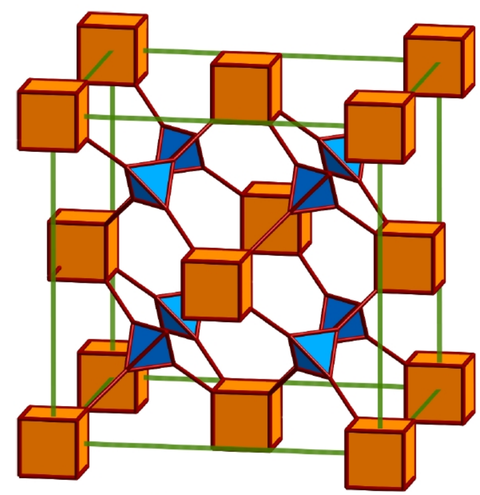
ftw-a



toc-a

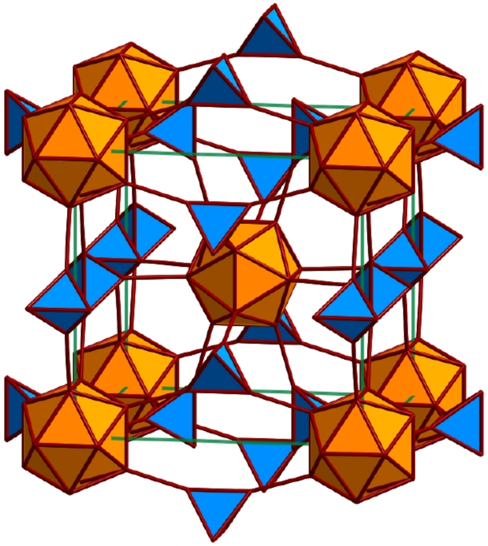


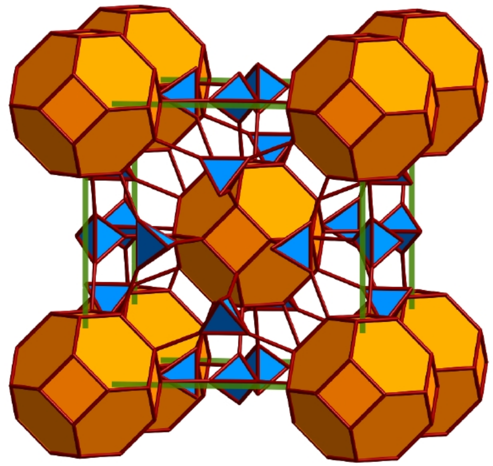
gar-a

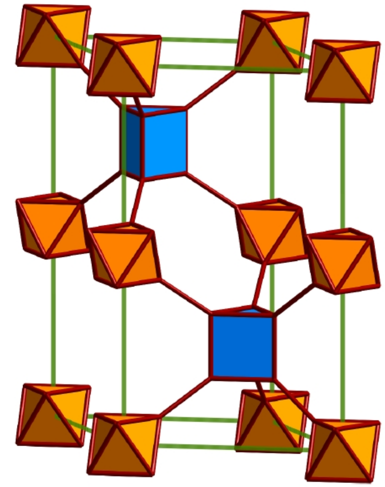


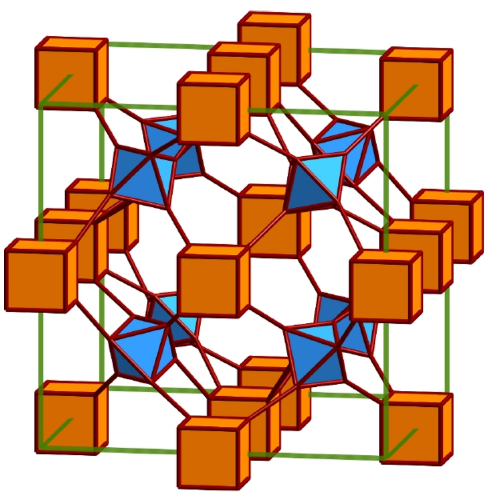
flu-a

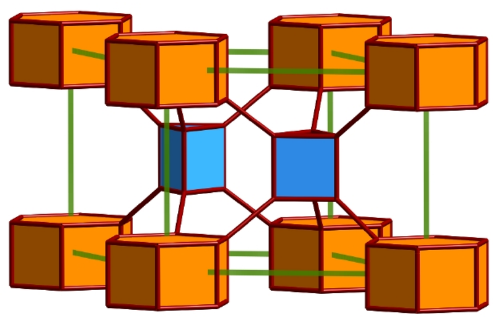
Edge-transitive binodal nets - summary 4

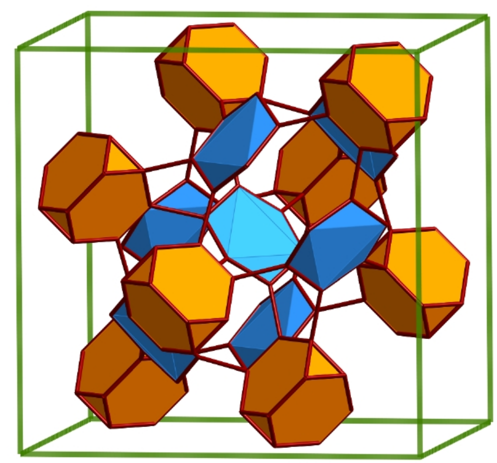

ith-a


twf-a

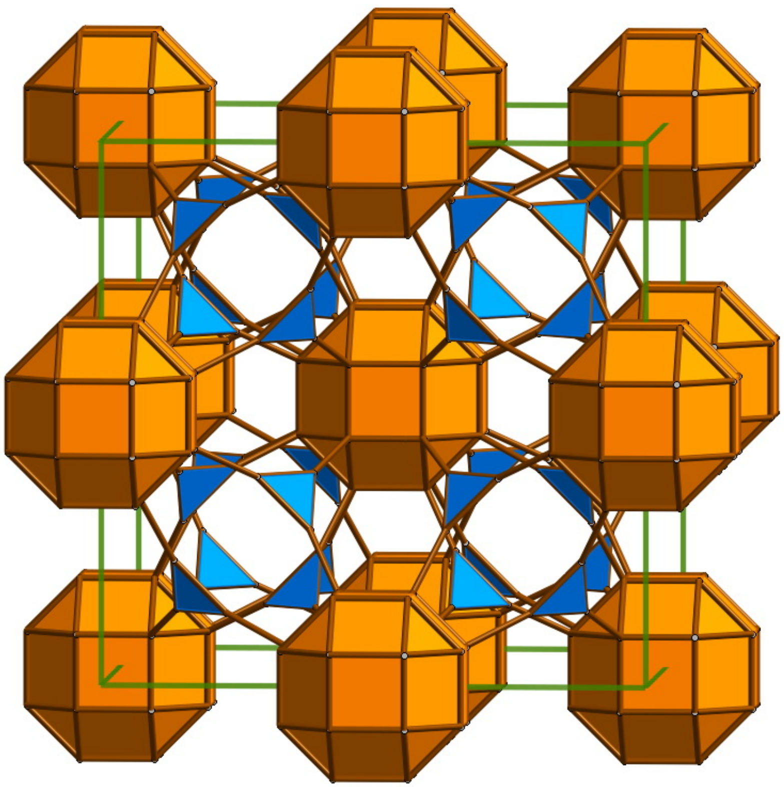

nia-a

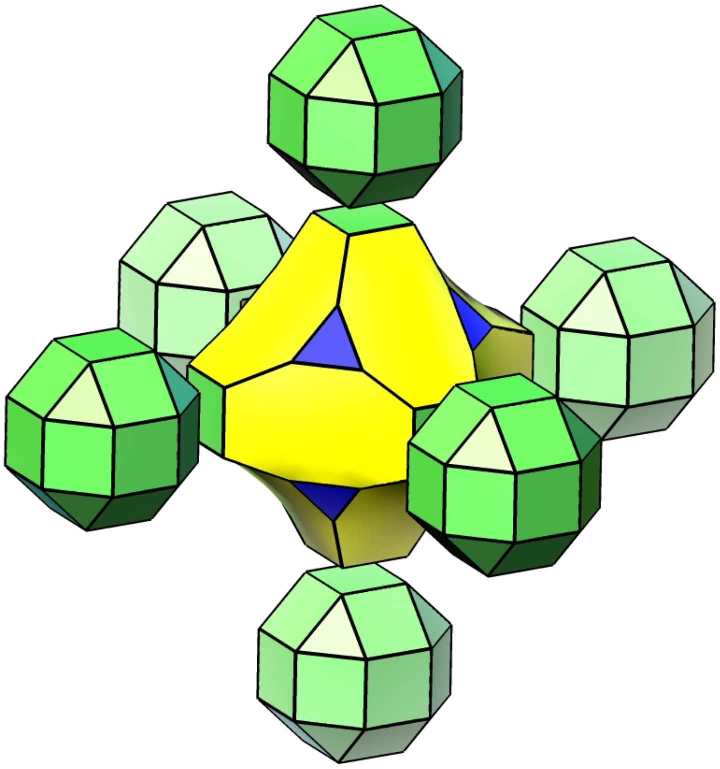

ocu-a


alb-a


mgc-a

oops





forgot (24,3)-connected **rht** (shown here as **rht-a**)

Results of enumerating face-transitive tilings

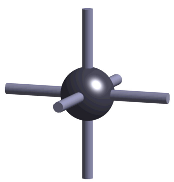
Table 1. Edge-transitive nets retrieved in this study listed by size of the Delaney-Dress symbol (D-symbol) of the proper tiling with smallest size. The 3-letter symbols are the RCSR (http://rcsr.anu.edu.au/) symbols.

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**

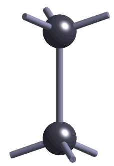
← **pcu** only regular tiling!

next: more nets

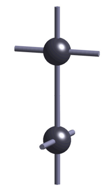
Minimal nets (genus 3). There are 15, of which 7 have collisions. The collision-free nets are:



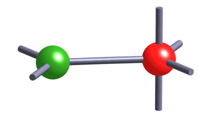
pcu self-dual
net of P



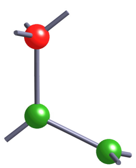
dia self-dual
net of D



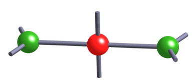
cds self-dual
net of CLP



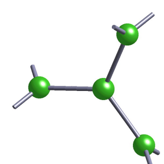
hms self-dual
net of H



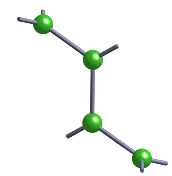
tfa
dual is **dia**



tfc
dual is **pcu**



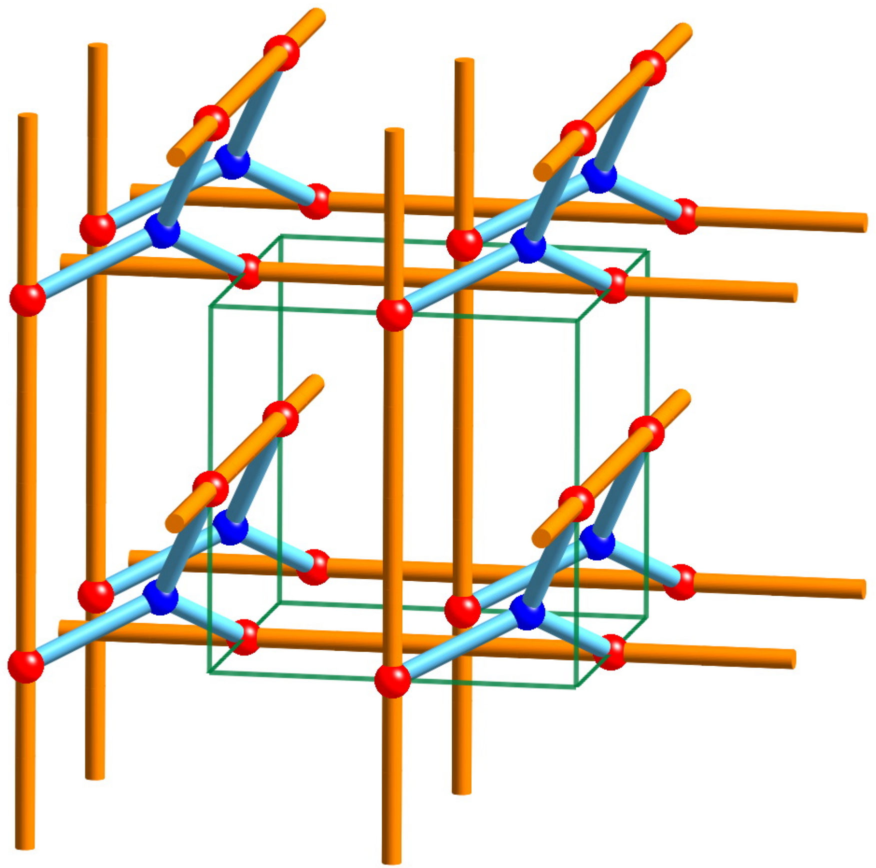
srs self-dual
net of G

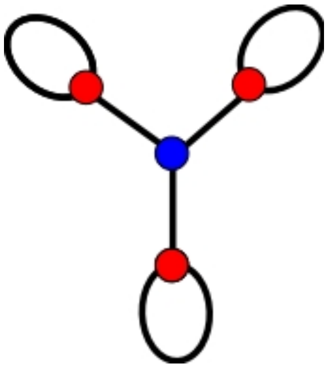


ths
dual is **dia**

C. Bonneau *et al*. *Acta Cryst* **A** **60**, 517 (2004). A. Beukemann & W. E. Klee, Z. Krist. **201**, 37 (1992).

a minimal net with collisions.





quotient graph

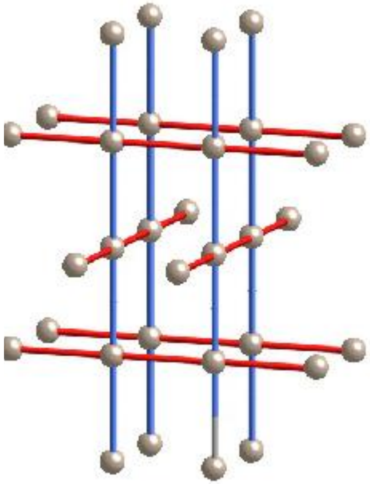
Vertex-transitive naturally self-dual nets:

srs	1111
dia	1111
pcu	1111
cds	1221

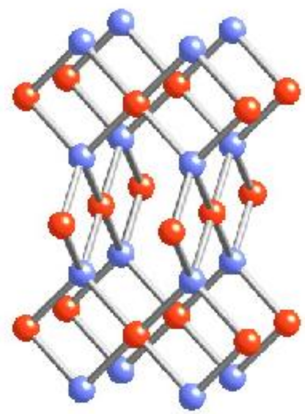
These account for most topologies found in crystal structures based on interpenetrating nets.

~ 80% see V. A. Blatov *et al*. *CrystEngComm*. 2004, *6*, 377.

These are all minimal (genus 3) nets

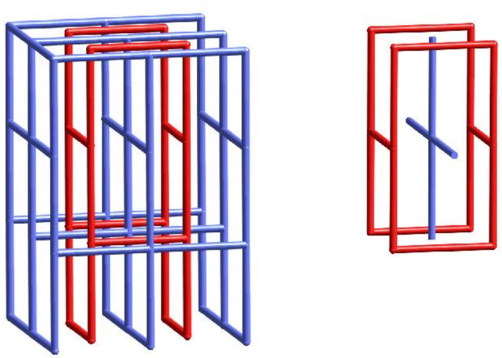


$CdSO_4$ net

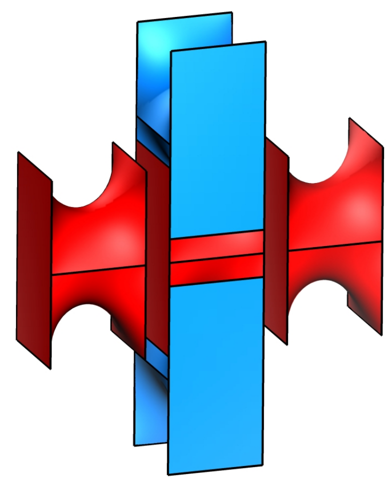


PtS net (edge net)

Aspects of the $CdSO_4$ net:
A self-dual minimal net.
Labyrinth of CLP surface.
Transitivity 1221.

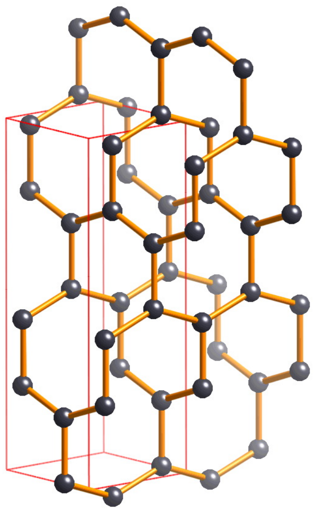


Two interpenetrating $CdSO_4$ nets

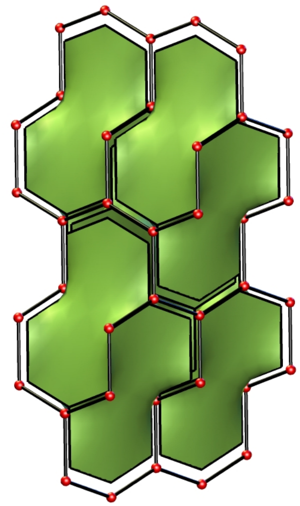


natural tiling $[6^2.8^2]$

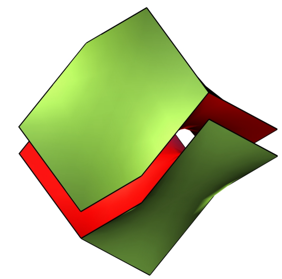
Aspects of the $ThSi_2$ (**ths**) net, symmetry $I4_1/amd$

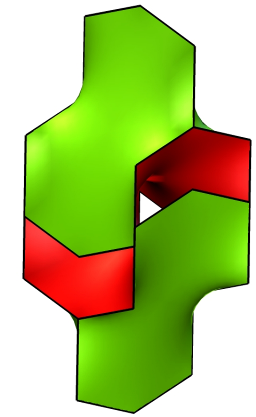


Net with unit cell



Natural tiling [10^4] transitivity 1211

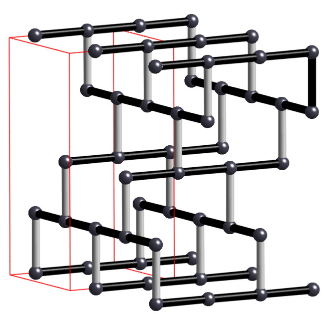




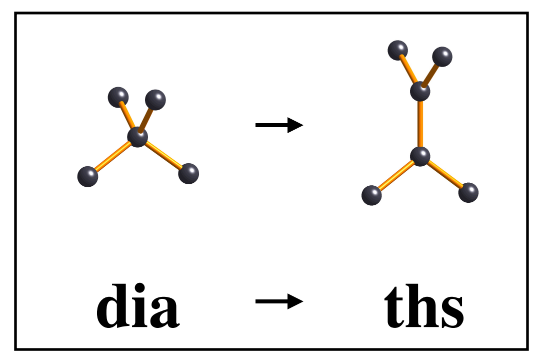
red faces are not formed by strong rings

Dual tiling is diamond tiled by half-adamantane tiles. Transitivity 1121

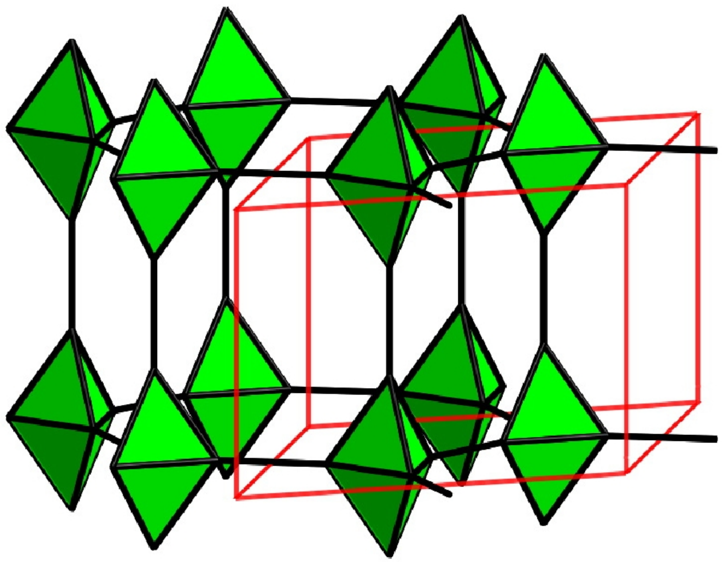
Self-dual tiling of **ths**. Transitivity 1221 (*not* natural)



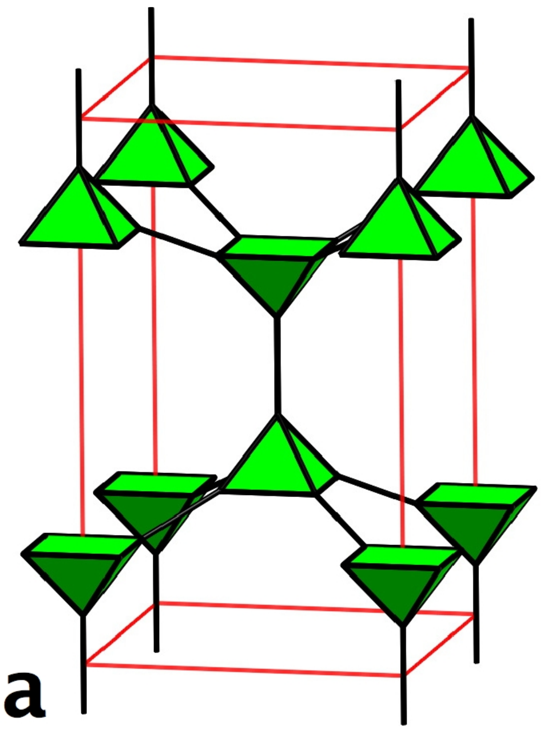
As the net of a rod packing (**ths-z**)



Simple nets for 5-coordination. Vertex figure must be square pyramid or trigonal bipyramid. Must be at least two kinds of edge.



bnn-a



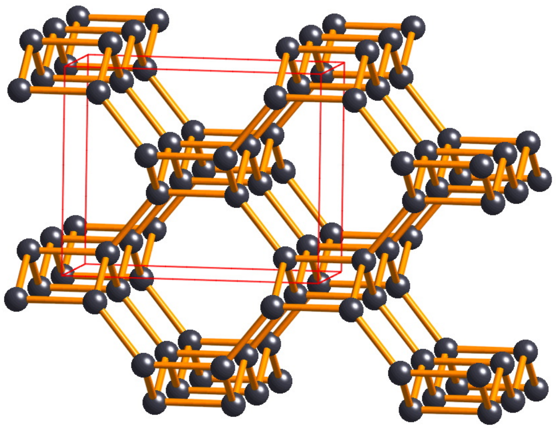
sqp-a

bnn transitivity 1221

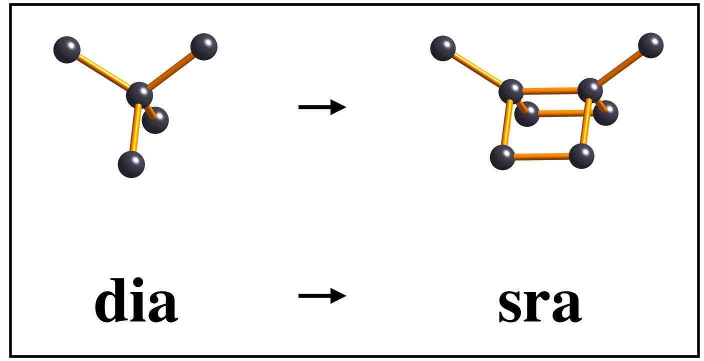
sqp transitivity 1222

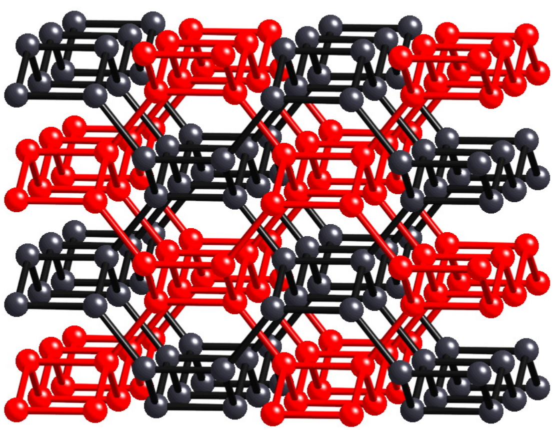
Aspects of the $SrAl_2$ (**sra**) net, symmetry *Imma*
The simplest way of linking ladders

sra

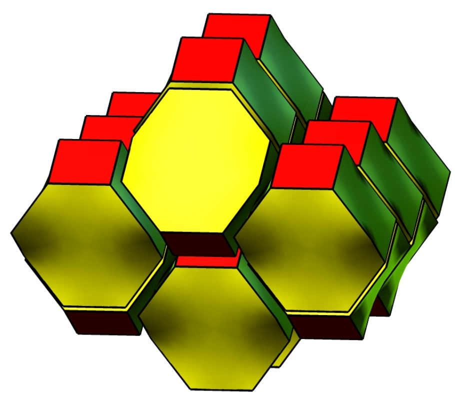


zig-zag ladder

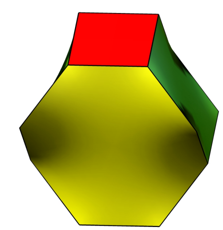




sra-c, symmetry *Cmma*

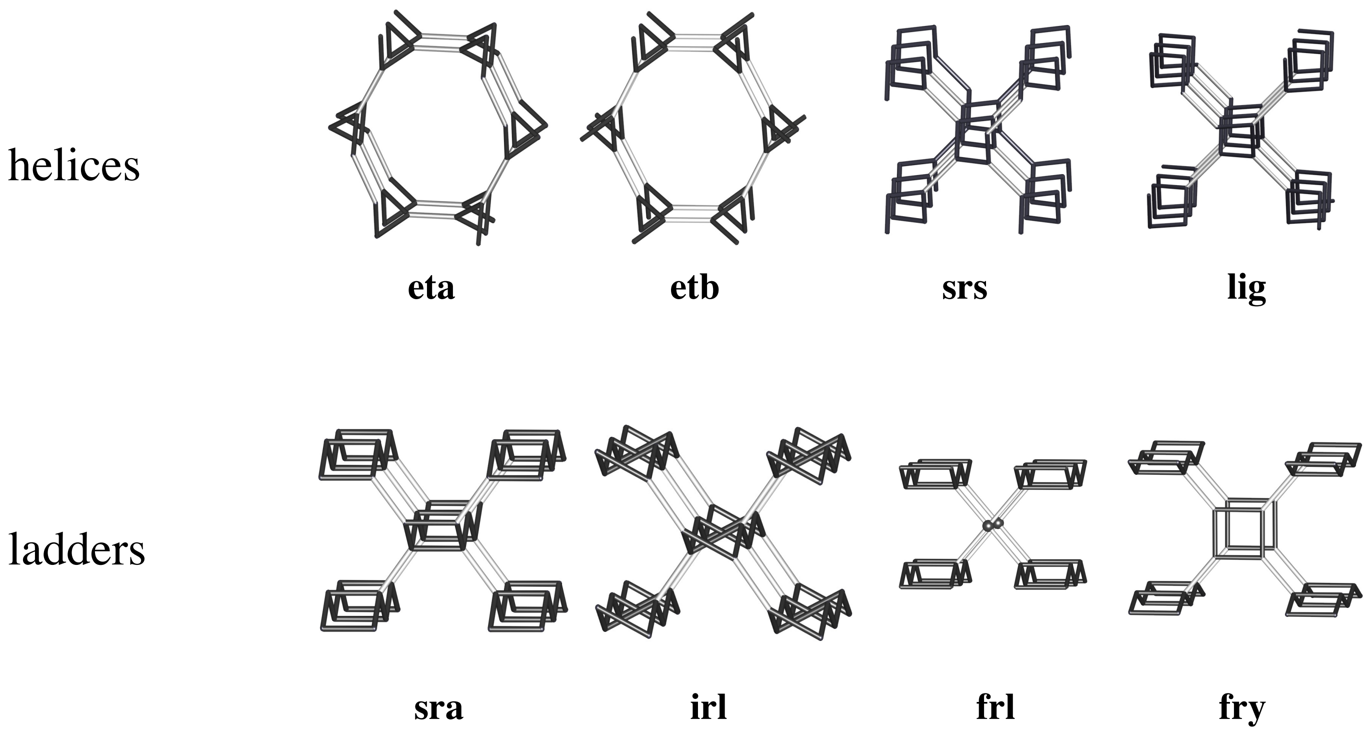


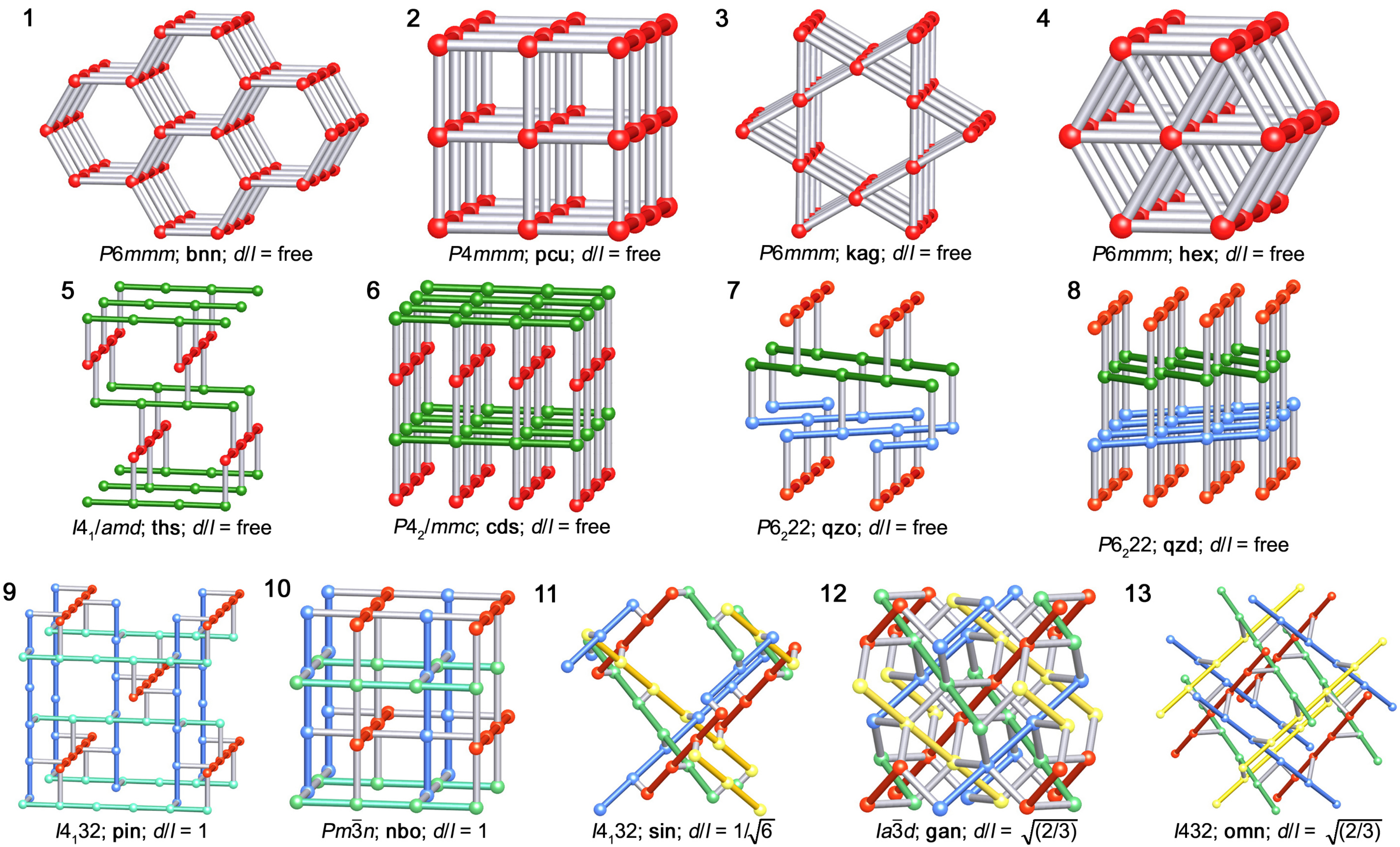
tiling, 1331
(not self-dual)



tile is an expanded version of adamantane with 4 inserted edges

simple nets formed by linking helices and ladders.

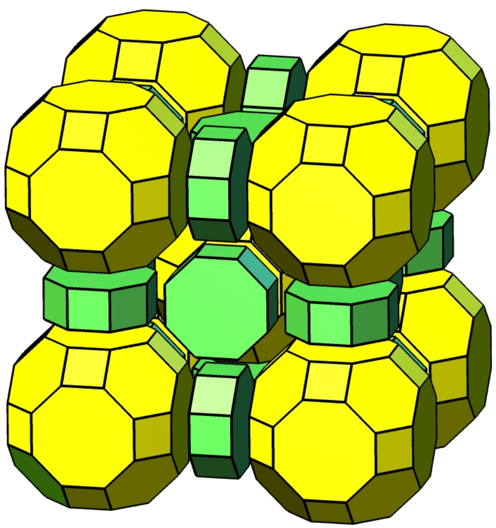




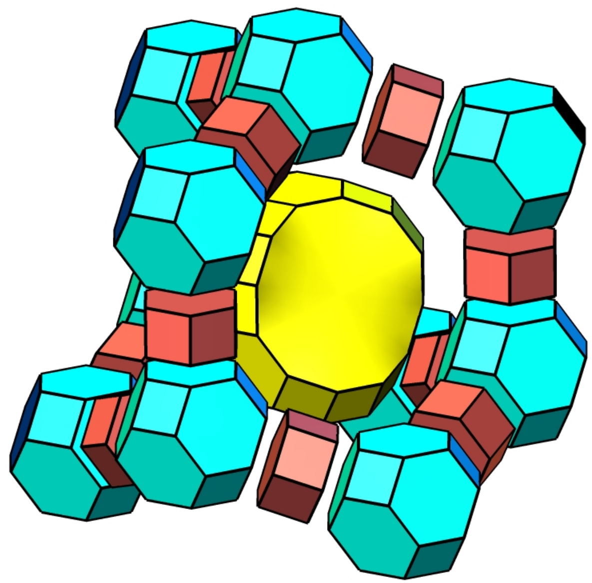
the invariant rod (cylinder) packings as nets JACS **2007**, *127*, 1504

Nets of simple tilings (duals of tlings by tetrahedra)

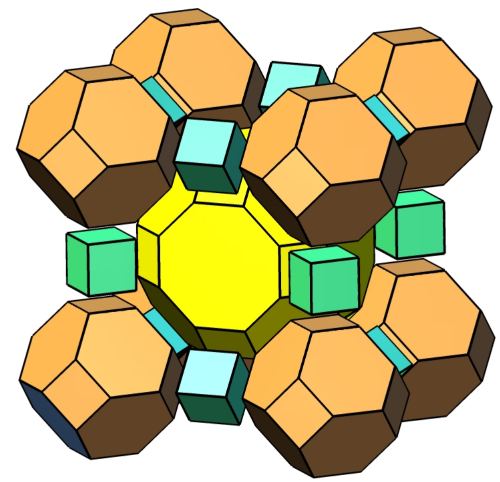
There are 9 vertex-transitive simple tilings (Delgado, Huson)
We have met **sod** (sodalite) already. Some of the others are important zeolite nets:



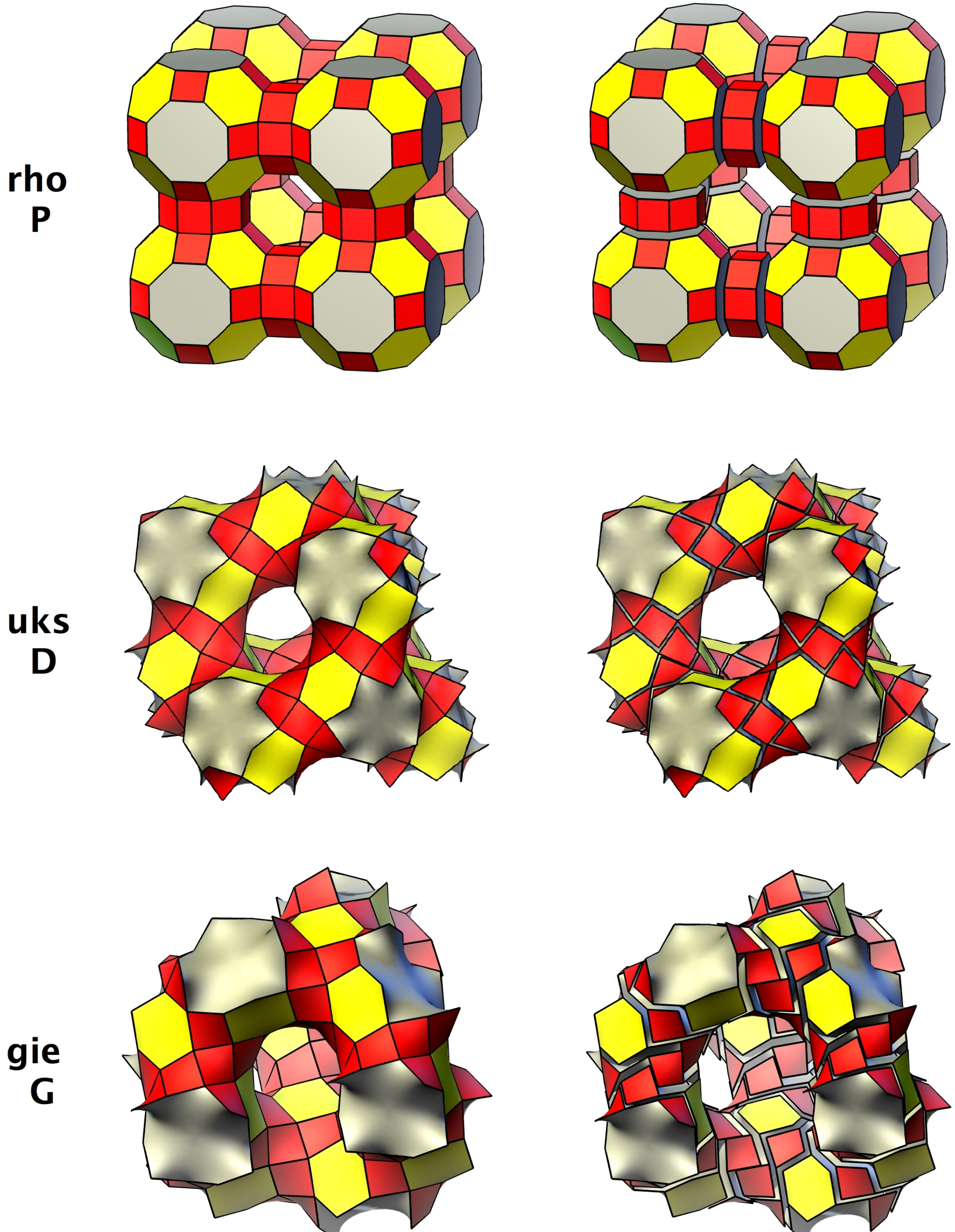
rho



fau (faujasite)

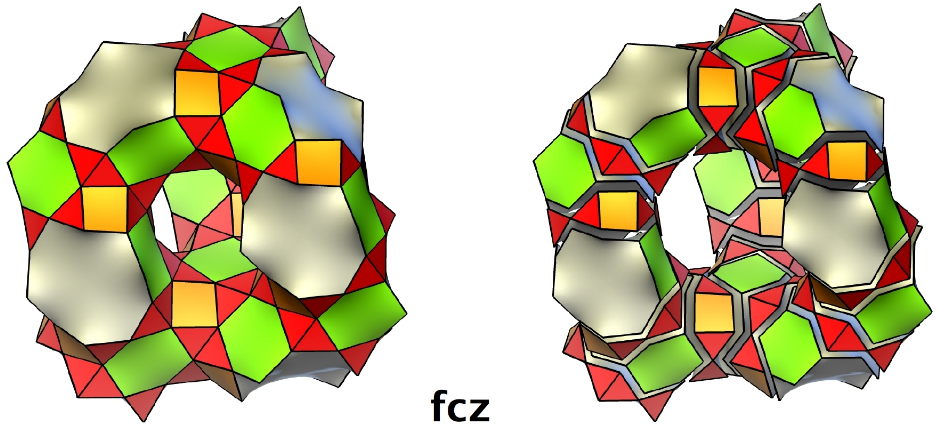


lta

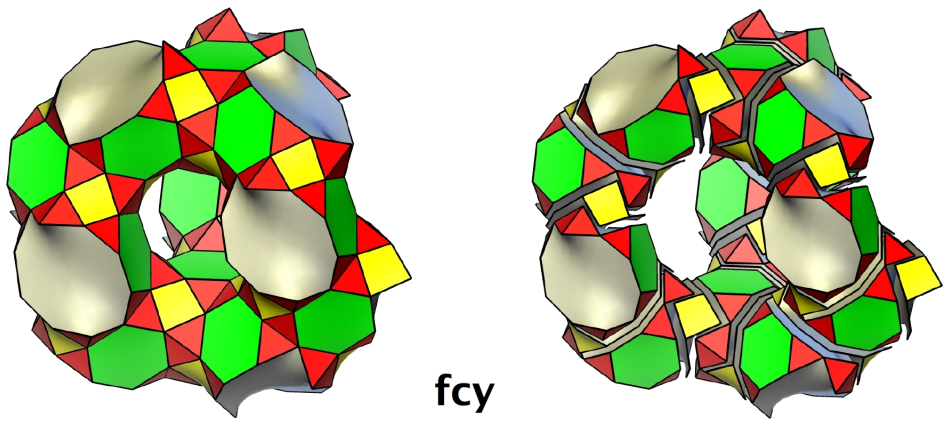


Nets as tilings of minimal surfaces.
On the left $4^3.6$ tilings of P, D and G surfaces.
On the right as tilings E^3.

The epinet project
epinet.anu.edu.au
of S. T. Hyde et al. derives net as projections from H^2 onto P, G, and D.



fcz



fcy

There are two distinct $3^2.4.3.6$ tilings of G

One of these (**fcz**) is the underlying topology of a germanium oxide with a giant unit cell (a = 53 Å)
X. Zou, T Conradsson. M. Klingstedt. M. S. Dadachov, M. O'Keeffe, *Nature*, **437**, 716 (2005)

how many 3-periodic structures are there?

minimal-density vertex-transitive sphere packings:

49 3-coordinated*
~160 4-coordinated
probably ~2000 in total

For symmetry *P*6/*mmm* and 6 kinds of vertex, there are 18,400,408 nets that are potential zeolite frameworks. Treacy & Foster, 2004
The most complicated zeolite has 24 kinds of vertex.

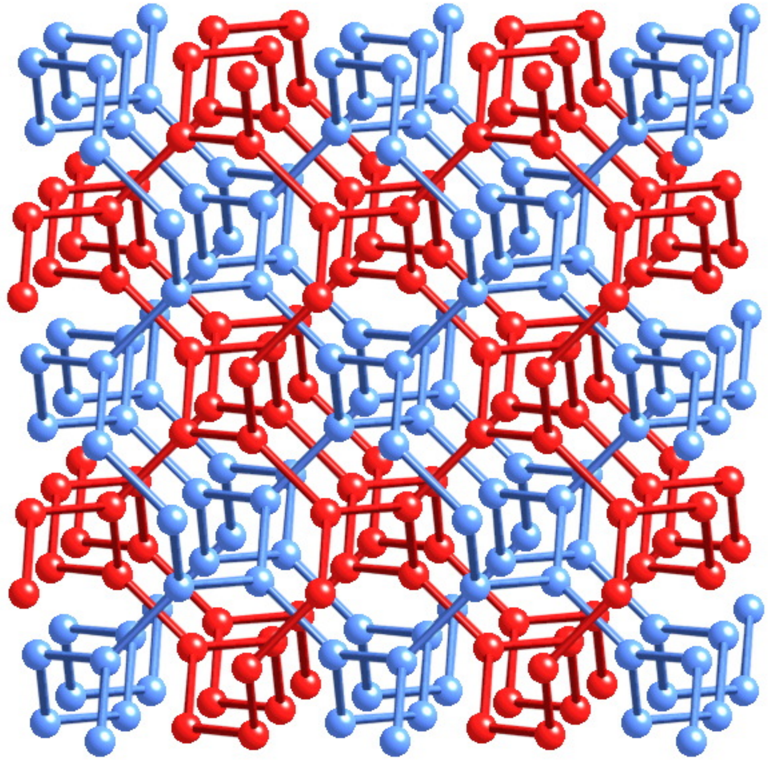
* Koch & Fischer, 1995 (+ 2005)

Interpenetrating nets

in special cases there are extra symmetry elements

these can be extra translations

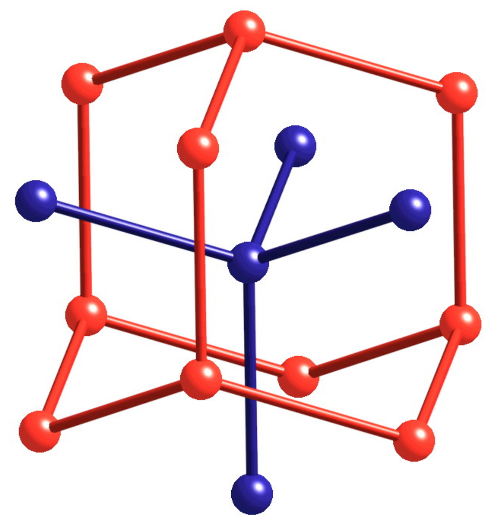
or point operations such as inversion

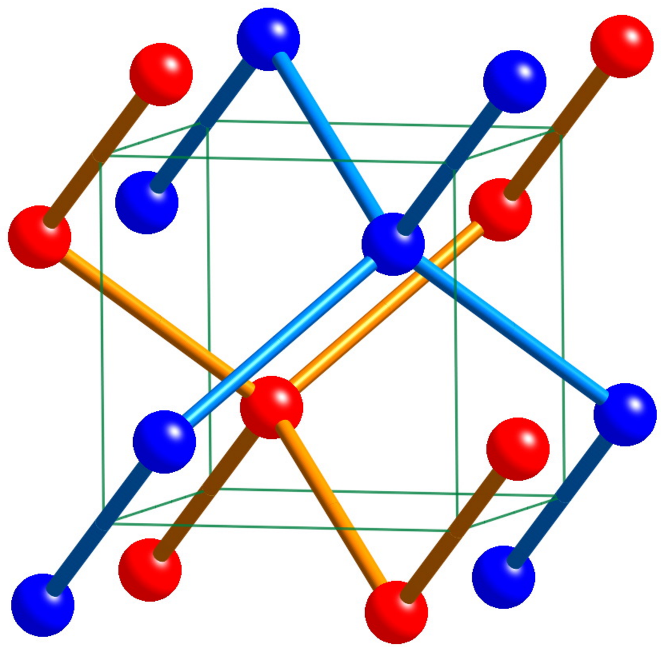


The **srs** net is chiral (symmetry $I4_132$).
The dual is the enantiomorph. Here two **srs** nets of opposite hand are intergrown to form a centrosymmetric structure (symmetry *Ia*-3*d*). The surface separating the two nets is the *G* minimal surface (*gyroid*)

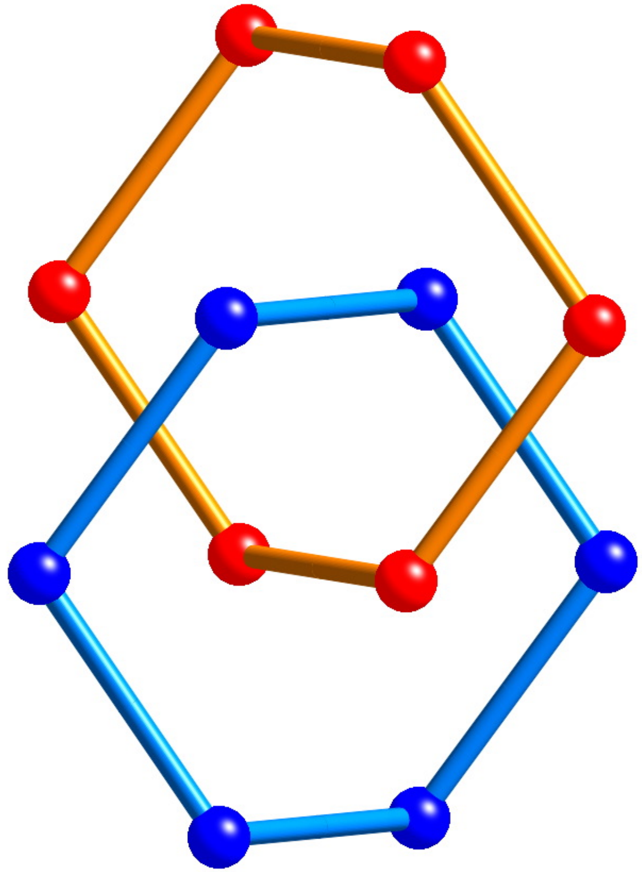
diamond (**dia**) symmetry *Fd*-3*m*
two vertices in primitive cell

dia-c symmetry *Pn*-3*m*
two vertices in primitive cell
two nets related by translation





dia-c symmetry *Pn*-3*m*
two vertices in primitive cell
two nets related by translation

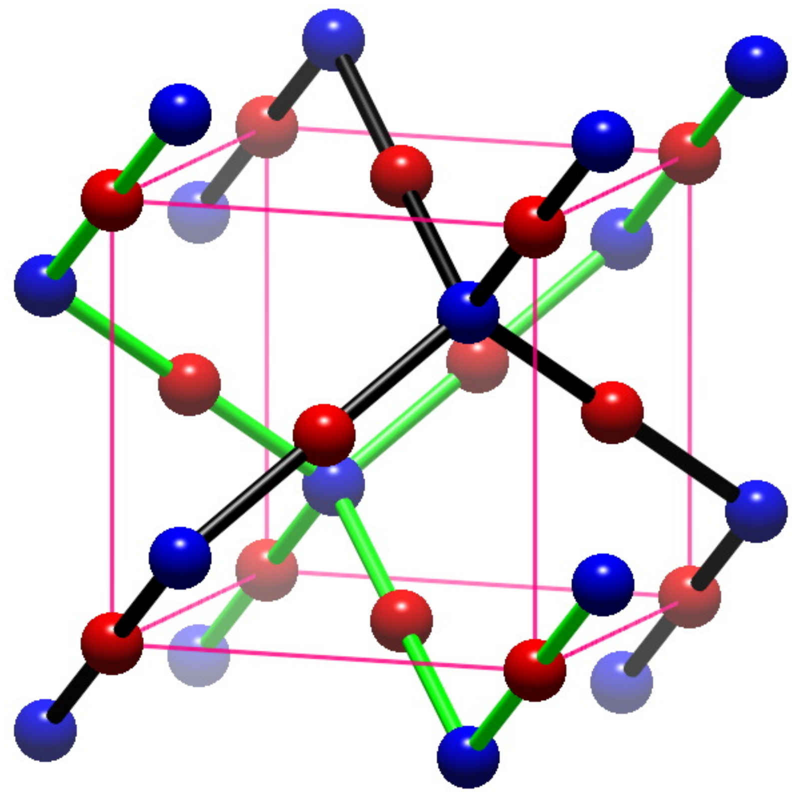


rings are catenated

Cuprite (Cu_2O) - one of the very first crystal structures Bragg (1915)

Note the two nets related by a unit cell edge (a translation)

Blue spheres are Cu at vertices of **dia** nets edges are -O- links (O red)



Multiple **dia** nets related by translation

Table 1. Crystallographic Data for the Ideal Geometry of *N*-Fold Interpenetrated Diamond Nets

N^a	crystal system	space group	a^b	c^b	a/c
1	cubic	$Fd\bar{3}m$	$4/\sqrt{3}$	a	1
2	cubic	$Pn\bar{3}m$	$2/\sqrt{3}$	a	1
$2n+1$	tetragonal	$I4_1/amd$	$\sqrt{8}/\sqrt{3}$	$4/\sqrt{3}N$	$N/\sqrt{2}$
$4n$	tetragonal	$P4/nbm$	$2/\sqrt{3}$	$4/\sqrt{3}N$	$N/2$
$4n+2$	tetragonal	$P4_2/nnm$	$2/\sqrt{3}$	$4/\sqrt{3}N$	$N/2$

[a] N = Interpenetration number, n is any integer > 1. [b] Cell parameters are in units of the edge length (distance between linked vertices).

see **dia-3***, **dia-c4**, **dia-c6** in RCSR.
Primitive cell in each case contains 2 vertices

F. Uribe-Romo, M. O'Keeffe, O. M. Yaghi, *et al*. *J*. *Am*. *Chem*. *Soc*. **131**, 4570 (2009)

Interpenetrating quartz (**qtz**) nets - non-intersecting edges

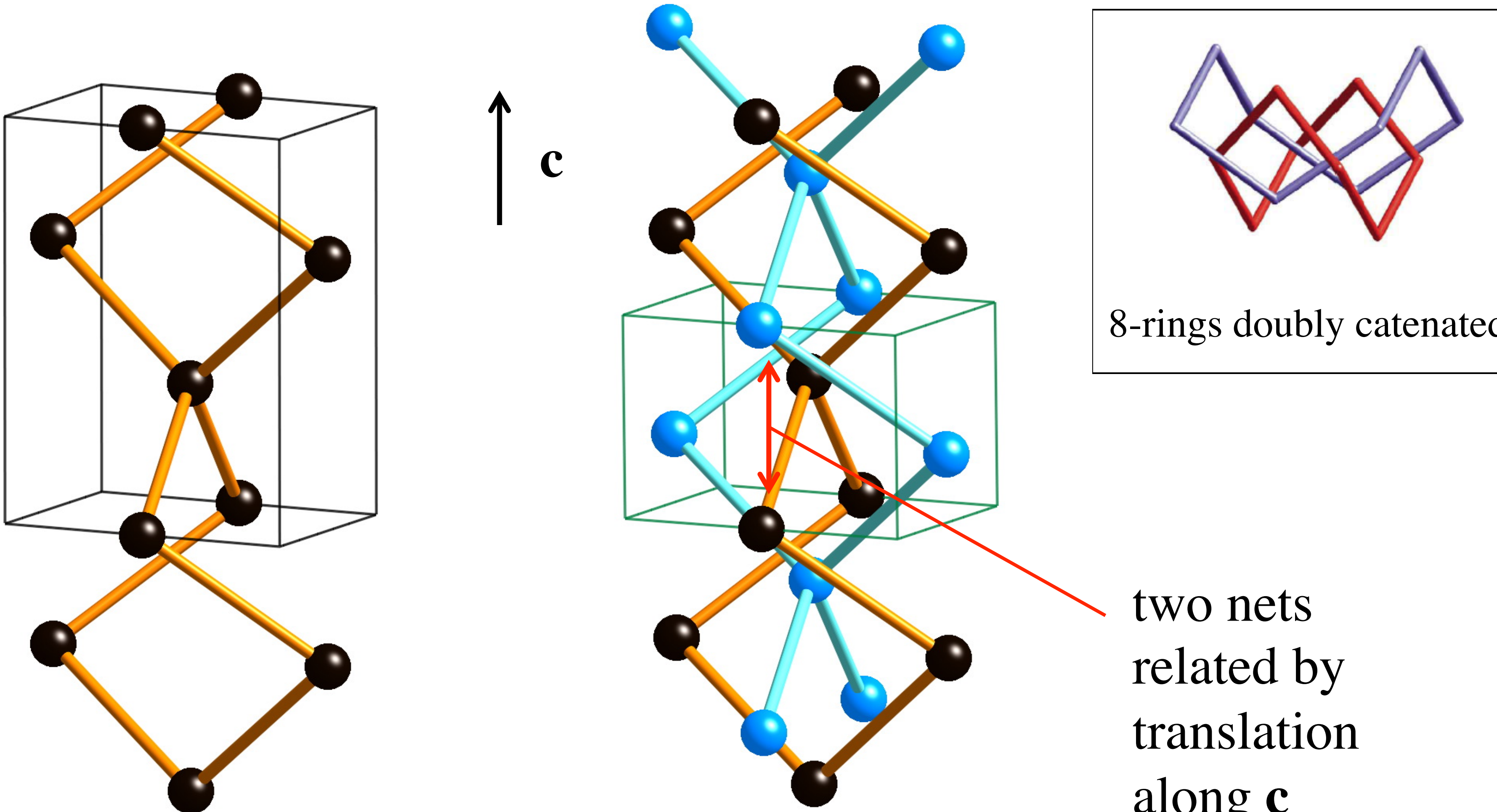
"ideal" **qtz** net $P6_222$ (or $P6_422$) $a = a_q = \sqrt{(8/3)}$, $c = c_q = \sqrt{3}$

a. qtz-n, *n* not a multiple of 3, related by translations along *c*
$a = a_q$, $c = c_q/n$

b. qtz-n, $n = 3$, related by translations along *a*.
$a = a_q/\sqrt{3}$, $c = c_q$

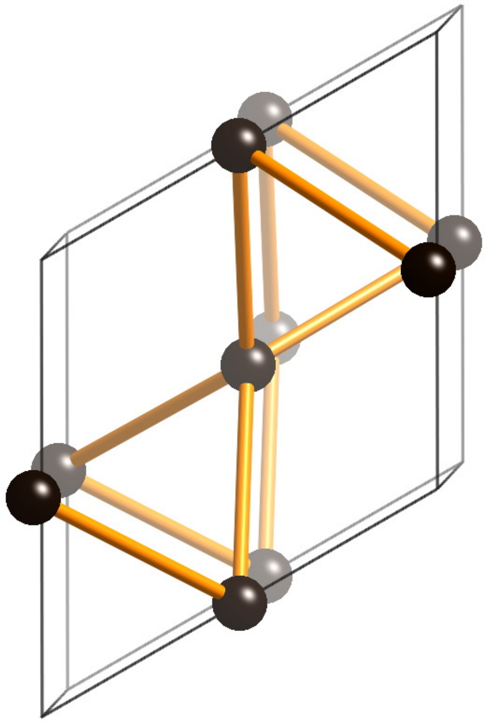
c. qtz-n, $n = 3$ times (not a multiple of 3),
related by translations along *a* and *c*
$a = a_q/\sqrt{3}$, $c = 3c_q/n$

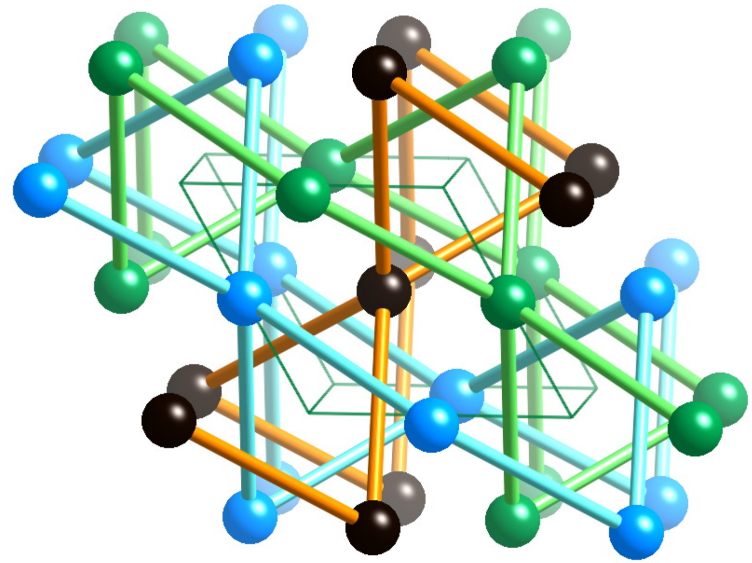
possibilities for *n*: 2(a),3(b),4(a),5(a), 6(c),7(a),8(a),9 (not possible)



qtz $P6_222$ **qtz-c** $P6_422$

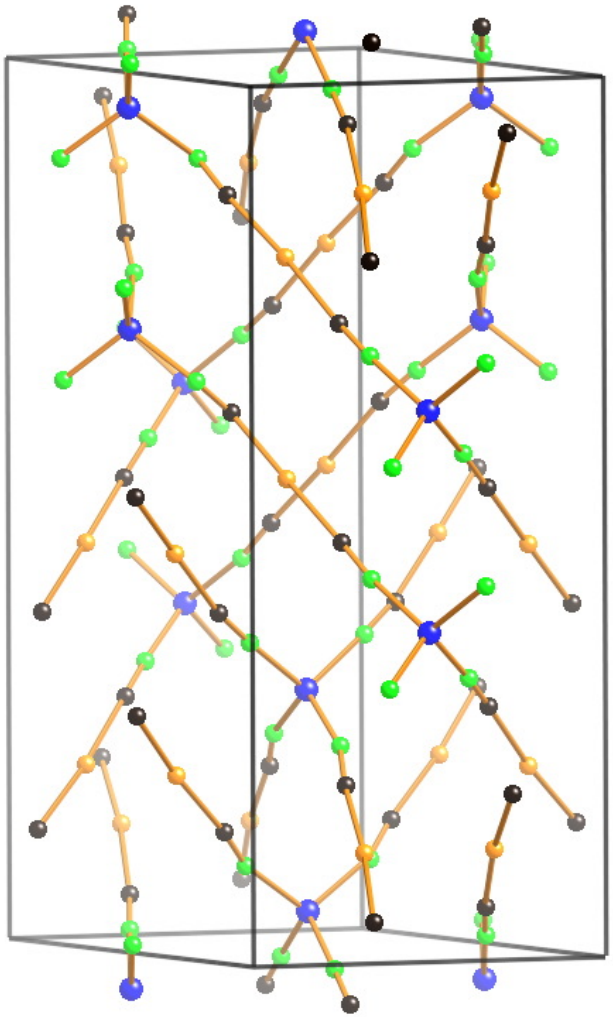
note that space group changes "hand", not the net!



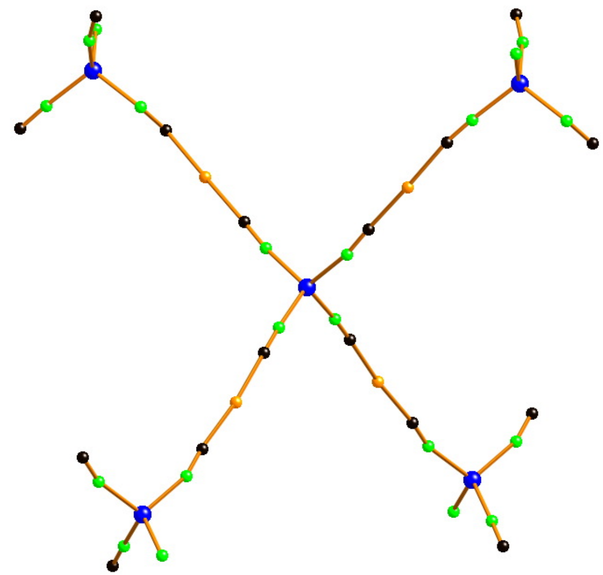


qtz - view down **c**
$P6_222$

qtz-c3 - view down **c**
$P6_222$, $a' = a/\sqrt{3}$
nets related by **a'**

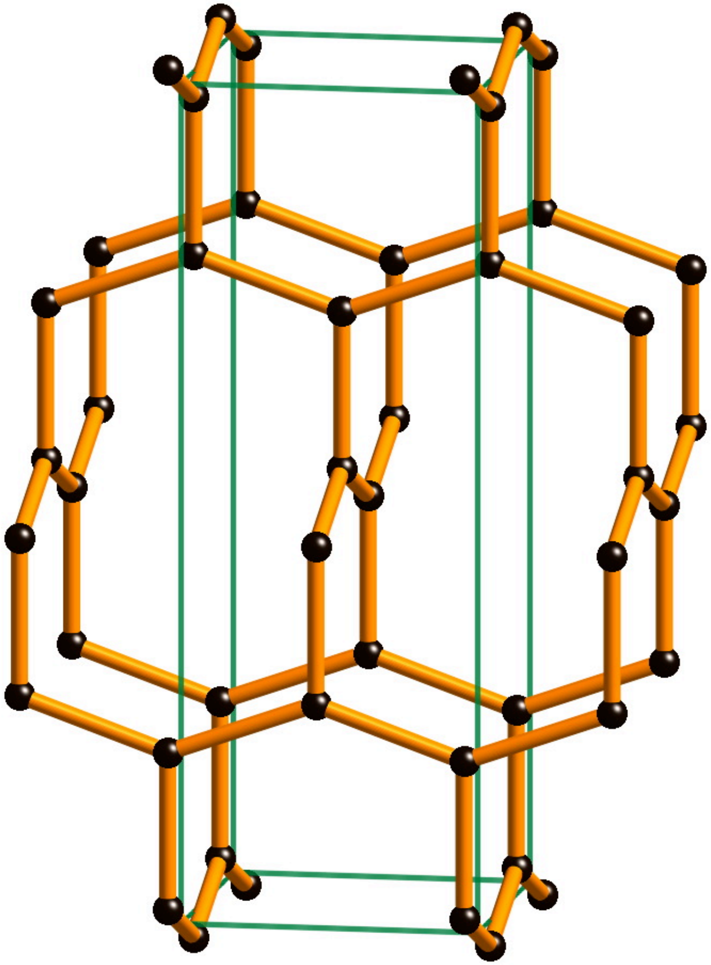


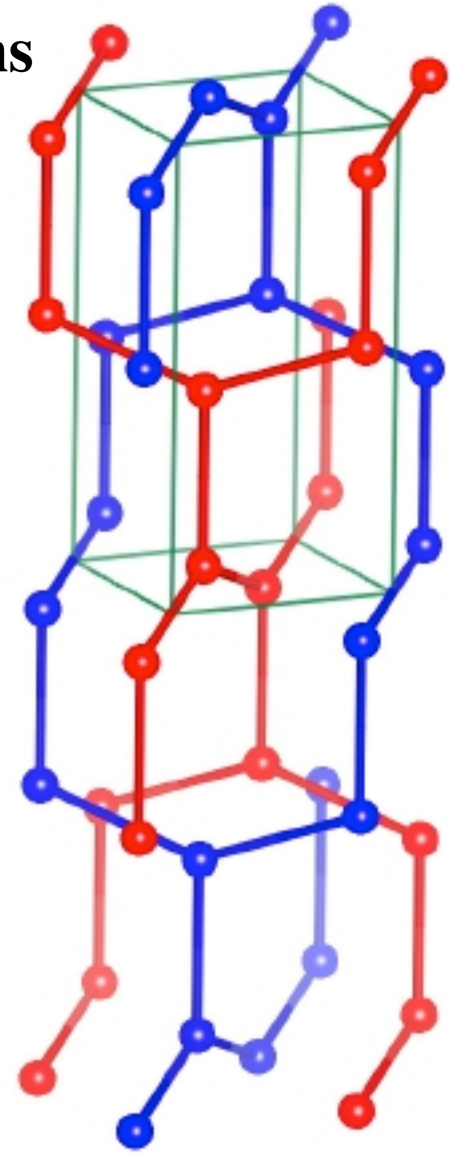
example of **qtz-c6** (both modes of interpenetration)

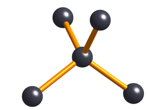


$Co[Au(CN)_2]_2$ S. C. Abrahams et al. *J. Chem. Phys.* **76**, 5458 (1982)

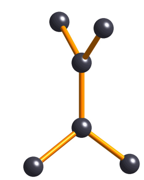
Another common intergrowth **ths**







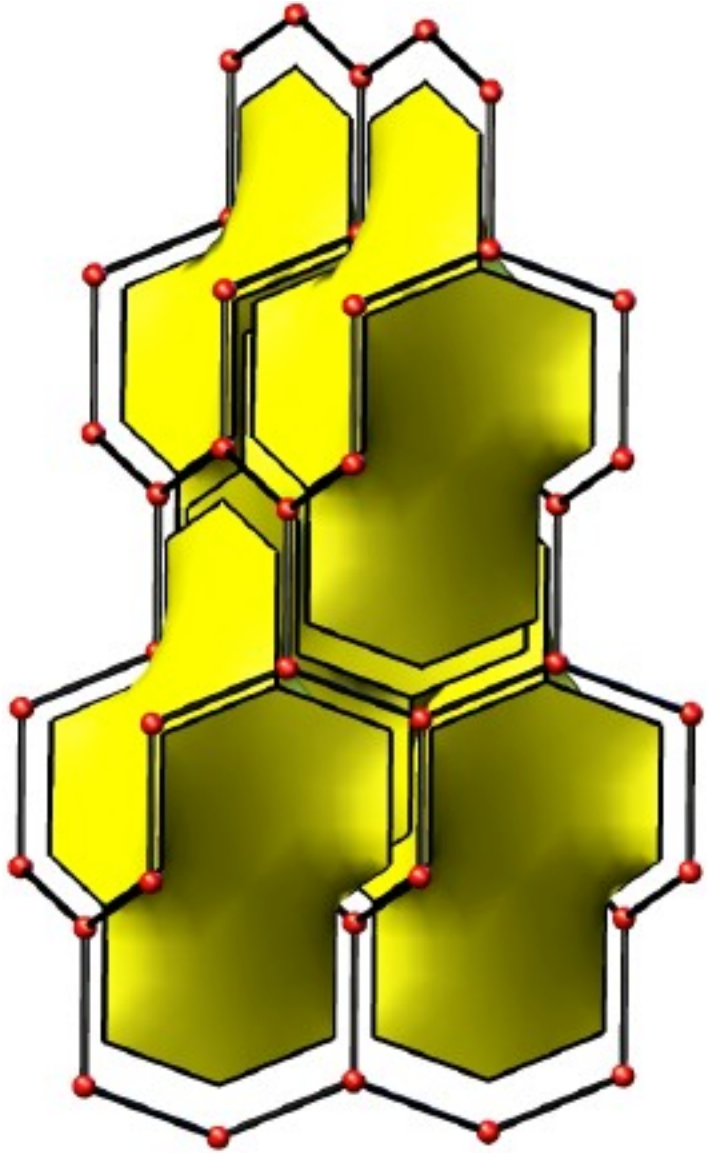
dia



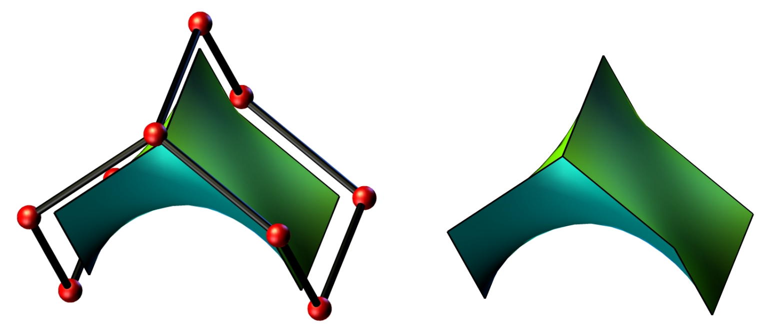
ths

ths $I4_1/amd$
4 vertices in primitive cell

ths-c $P4_2/nnm$, $a' = a/\sqrt{2}$, $c' = c/2$
4 vertices in primitive cell



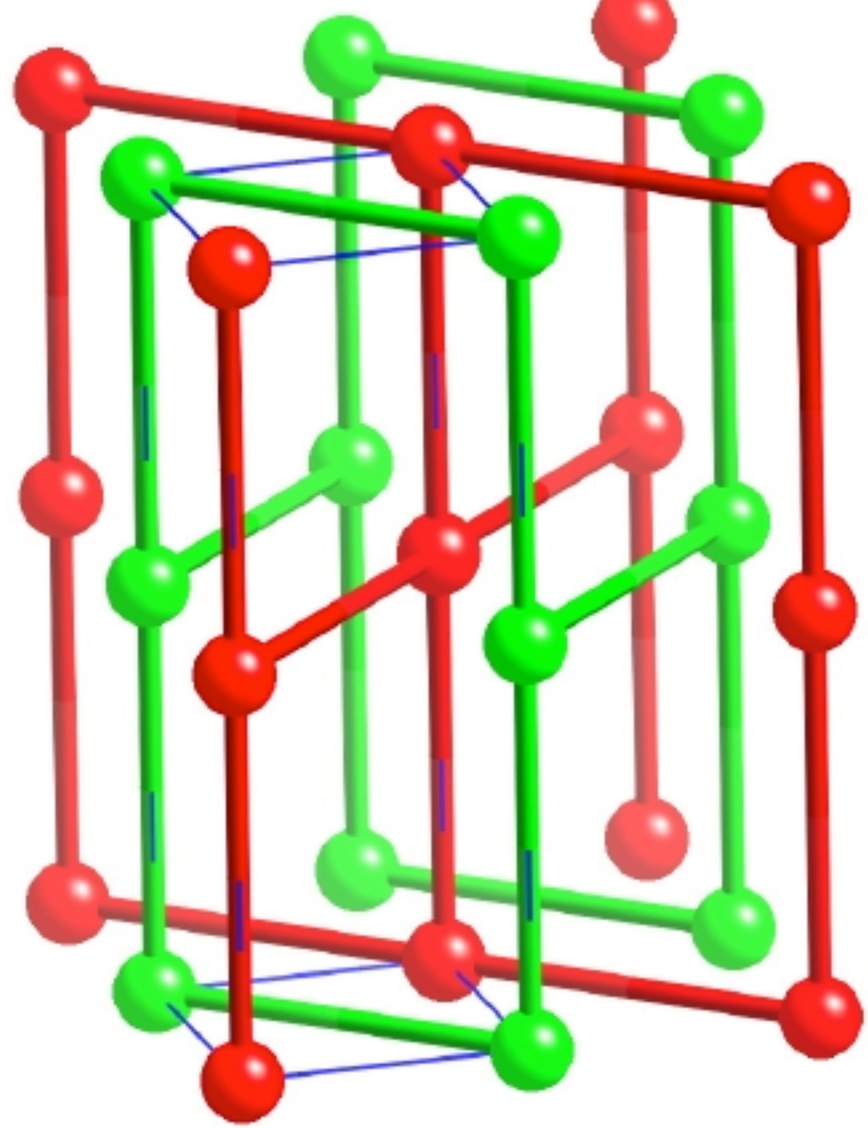
note that **ths** has a natural tiling [10^4]. So dual is 4-coordinated and is in fact **dia**. But the dual tile must have only 3 faces and is the "half-adamantane"tile [6^2.8]



cds is naturally self-dual

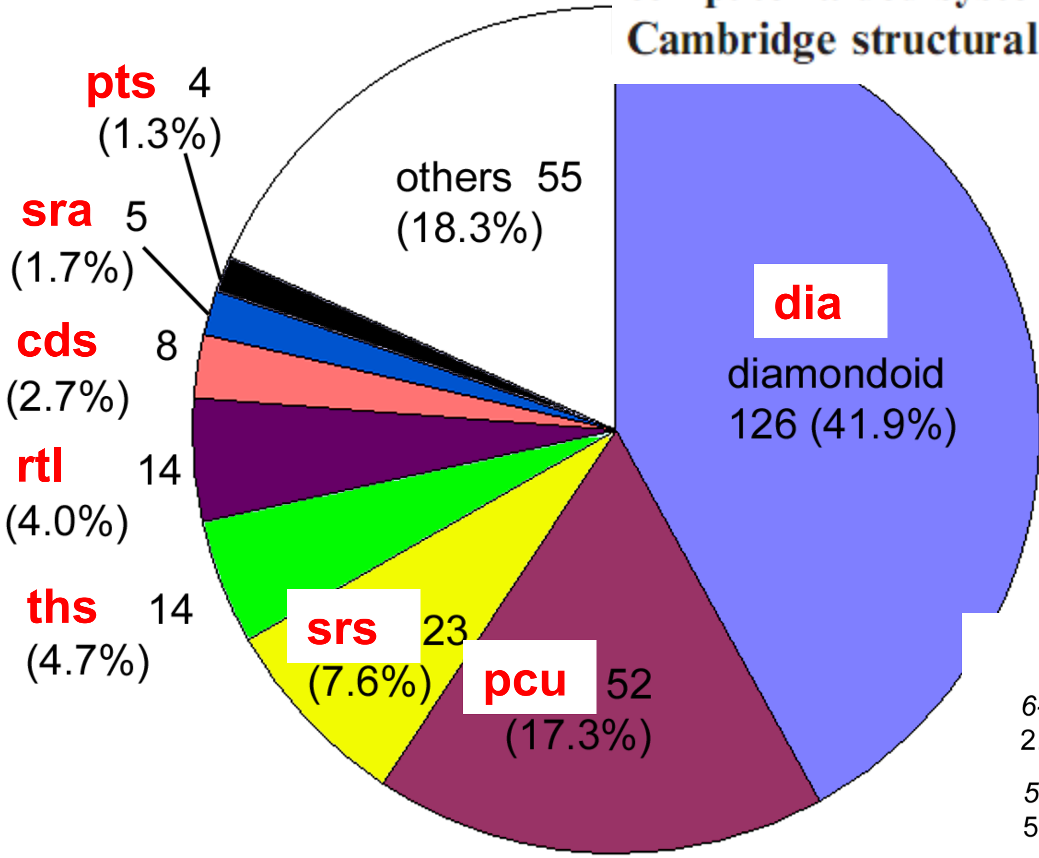
cds $P4_2/mmc$

cds-c $P4_2/mcm$.
$a' = a/\sqrt{2}$
nets related by a'



Interpenetrating metal–organic and inorganic 3D networks: a computer-aided systematic investigation. Part I. Analysis of the Cambridge structural database†‡

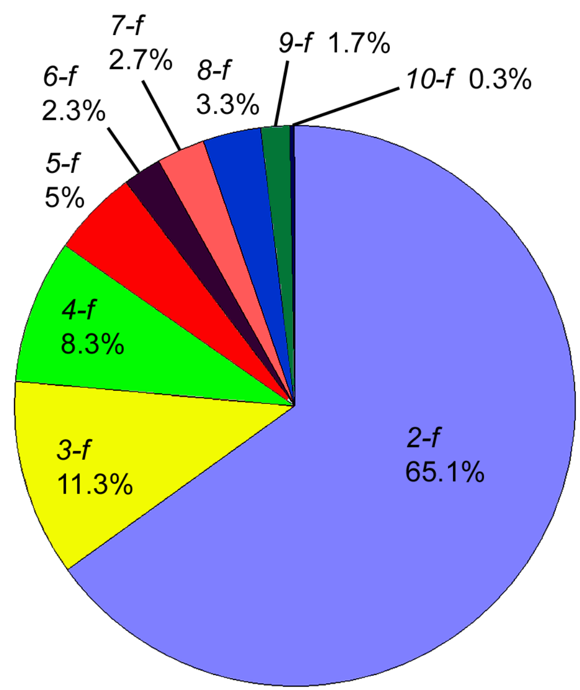
CEC 2004



301 cases
CSD 2004/1

Distribution of the topologies and degree of interpenetration Z

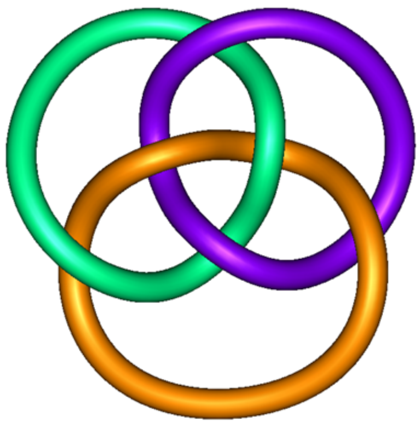
551 cases
CSD 2006 nov
same trends



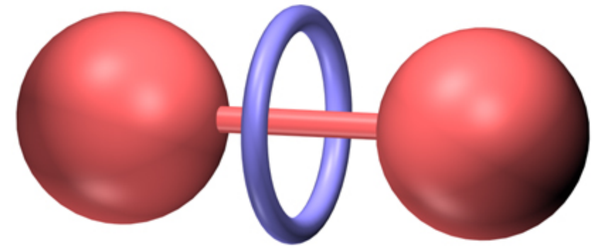
	diam	others	Total
2-f	53	143	196
3-f	18	16	34
4-f	15	10	25
5-f	13	2	15
6-f	5	2	7
7-f	8	0	8
8-f	7	3	10
9-f	5	0	5
10-f	1	0	1

Geometrical requirement for Inextricable Entanglement

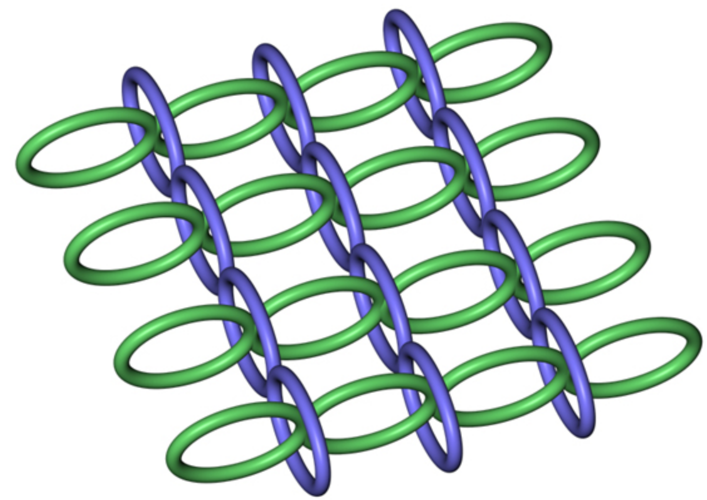
Hopf link



Borromean

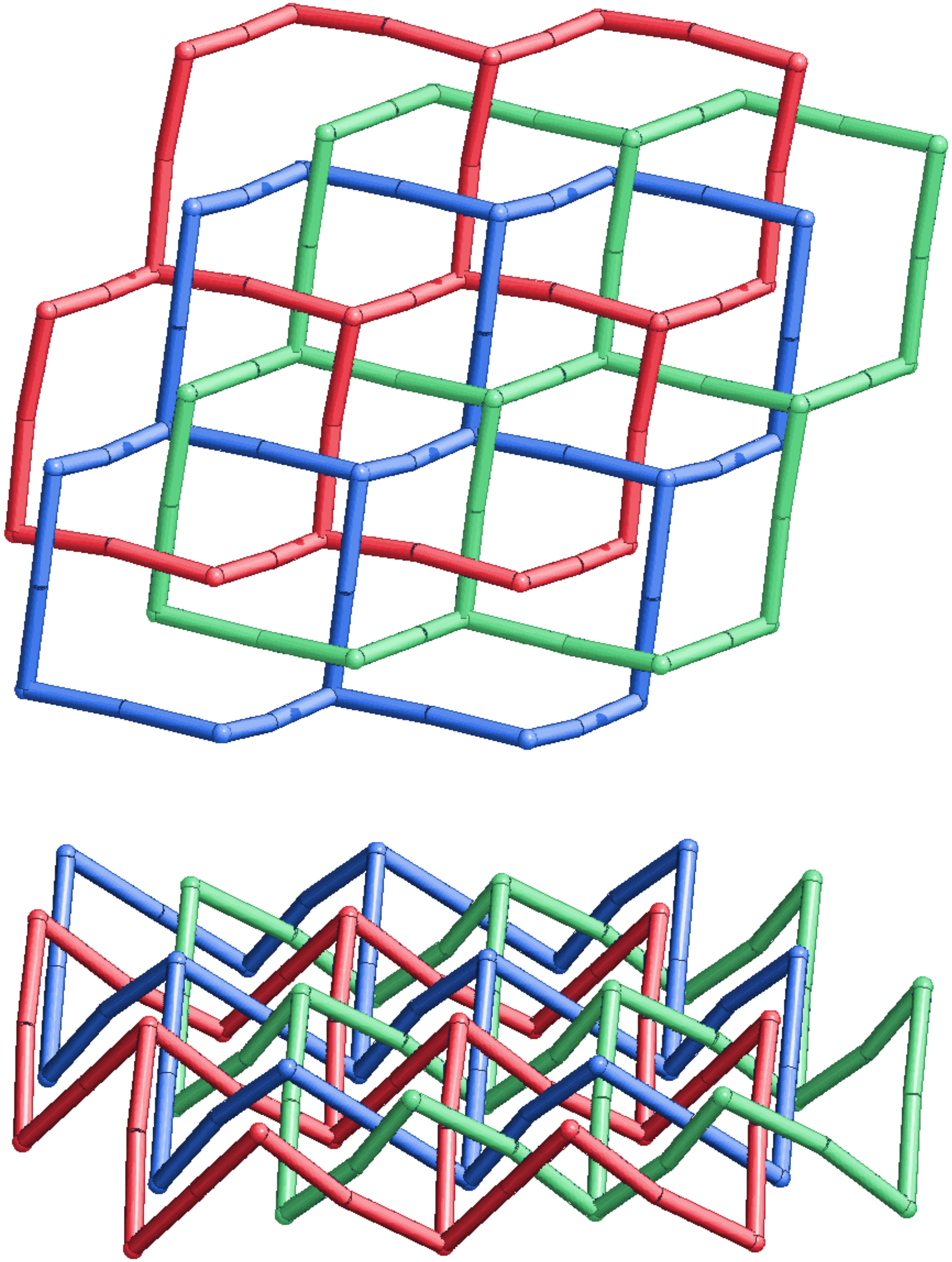


[2]-rotaxane



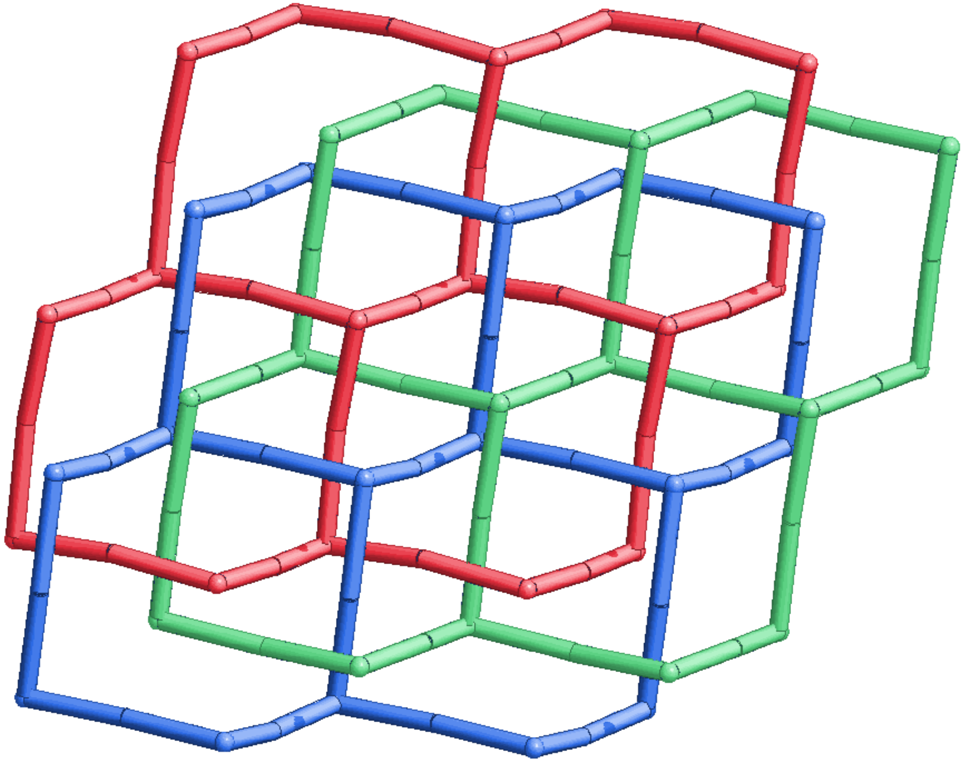
"Topological" Entanglement

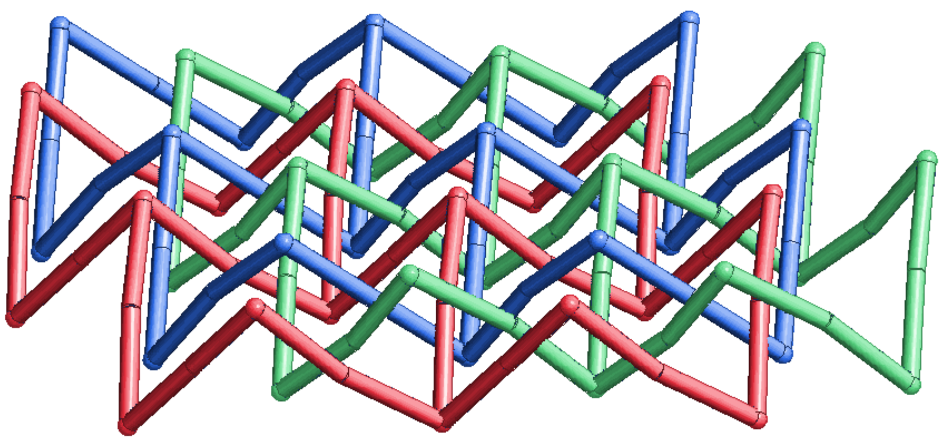
"Euclidean" Entanglement



Borromean

red > green
green > blue
blue > red





2D // 2D ⇒ 2D

NOT

interpenetrated

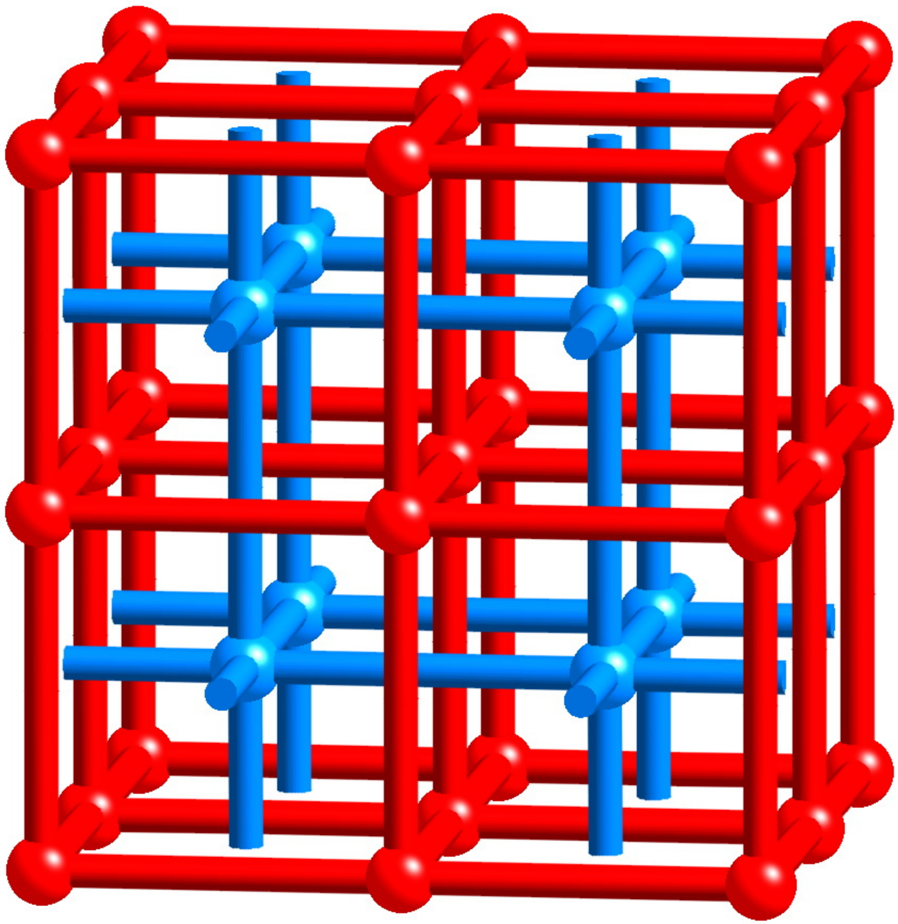
nor catenated

Borromean Entanglements

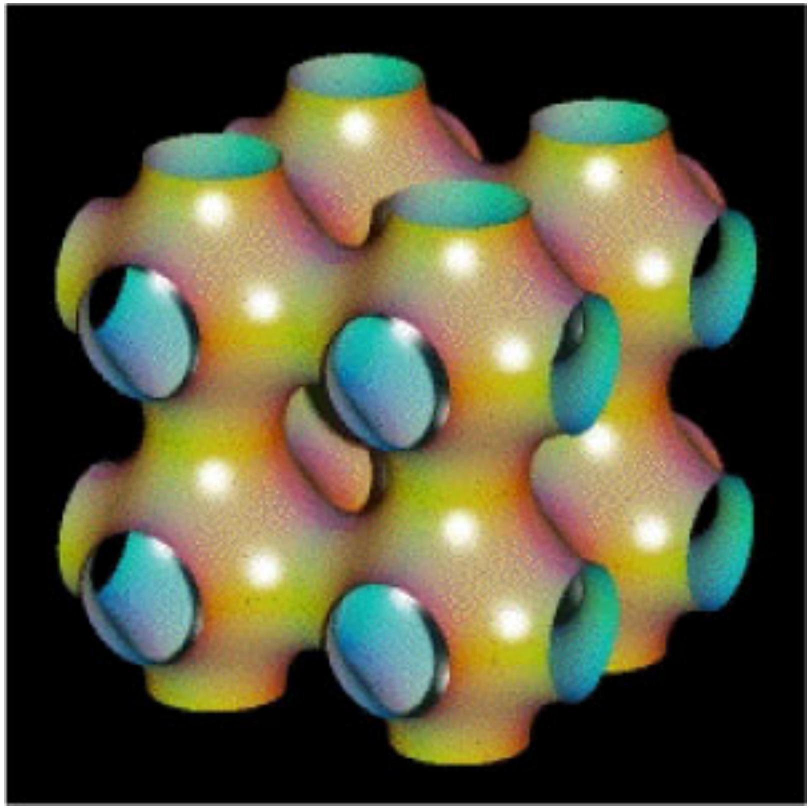
nets as surfaces - minimal surfaces

periodic minimal surface (PMS) divides space into two parts. The surface has zero mean curvature ($(k_1 + k_2) = 0$), but negative Gaussian curvature ($k_1 k_2 < 0$).
There are 5 PMS of genus 3. They divide two interpenetrating nets of genus 3

net	transitivity	surface
srs	1111	*G*
dia	1111	*D*
pcu	1111	*P*
cds	1221	*CLP*
hms	2222	*H*



Two interpenetrating **pcu** nets



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

don't confuse two usages of the term "minimal"

Minimal surface has zero mean curvature $(k_1 + k_2) = 0)$

Minimal net has genus = 3.

There are 5 Periodic Minimal Surfaces of genus 3
but more than five nets of genus 3

end