

# A tourist guide to the RCSR

Some of the sights, curiosities, and little-visited by-ways

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RCSR is a Reticular Chemistry Structure Resource available at <http://rcsr.net>. It is open every day of the year, 24 hours a day, and admission is free. It consists of data for polyhedra and 2-periodic and 3-periodic structures (nets). Visitors unfamiliar with the resource are urged to read the "about" link first. This guide assumes you have.

The guide is designed to draw attention to some of the attractions therein. If they sound particularly attractive please visit them. It can be a nice way to spend a rainy Sunday afternoon.

OKH refers to M. O'Keeffe & B. G. Hyde. *Crystal Structures I: Patterns and Symmetry*. Mineral. Soc. Am. 1966. This is out of print but available in .pdf form from: <http://www.public.asu.edu/~rosebudx/okeeffe.htm>,

## POLYHEDRA

Read the "about" for hints on how to use the polyhedron data to make accurate drawings of polyhedra using crystal drawing programs such as CrystalMaker (see "links" for that program). Keywords used in the search include:

**Simple.** Each vertex is trivalent (three edges meet at each vertex)

**Simplicial.** Each face is a triangle. The dual of a simplicial polyhedron is a simple polyhedron and *vice versa*.

**Regular polyhedra.** The five regular polyhedra should be well known. they are the: tetrahedron  $3^4$  **tet**, octahedron  $3^4$  **oct**, icosahedron  $3^5$  **ico** cube  $4^3$  **cub**, dodecahedron  $5^3$  **dod**. These are the only polyhedra with one kind of vertex, one kind of edge and one kind of face, i.e. *transitivity* 1 1 1

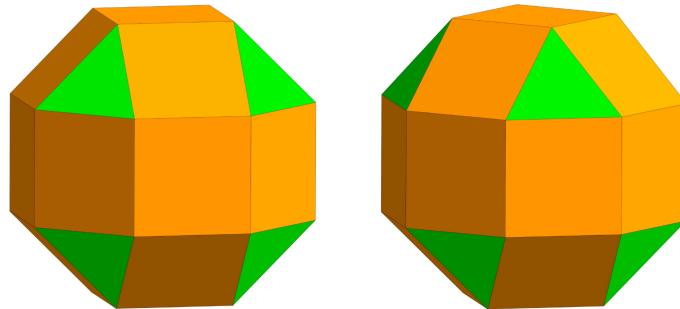
**Quasiregular polyhedra.** These have one kind of vertex and one kind of edge but two kinds of face so transitivity 1 1 2. Searching using these criteria will find the cuboctahedron 3.4.3.4 **cuo** and the icosidodecahedron, 3.5.3.5 **ido**. It is not hard to show that these are the only possibilities. Their duals have transitivity 2 1 1 and are the rhombic dodecahedron **rdo** and the rhombic triacontahedron **trc**. If you search for structures with two kinds of vertex, one kind of edge and one kind of face, you will retrieve three structures. The third is the adamantane cage **ada**; this is not a polyhedron in the strict sense as some vertices are divalent.

**Archimedean polyhedra.** These have one kind of vertex and more than one kind of face. By convention these do not include the infinite families of prisms and antiprisms which have one kind of vertex and two kinds of edge and face (transitivity 1 2 2). See e.g. the square antiprism **sap** and the hexagonal antiprism **hap** and the trigonal prism **trp**.

**Deltahedra.** These are convex polyhedra with faces that are equilateral triangles. There are eight of them.

**Frank-Kasper polyhedra.** These are simplicial polyhedra with 5- and 6- valent vertices such that no 6-valent vertices are adjacent. They are  $[3^{20}]$  **ico** (icosahedron),  $[3^{24}]$  **fkf**,  $[3^{26}]$  **zap** (not in RCSR!) and  $[3^{28}]$  **mcp**. You can find them as other name include "Frank-Kasper" [Hint; in searching using "name contains" just a few symbols suffice, in this case "k-k" would do.] These polyhedra are very important in the structural chemistry of intermetallic compounds. Their duals are simple polyhedra with 5- and 6-sided faces with no two 6-sided faces adjacent. They are **dod**, **fkf-d** (not in RCSR!), **zap-d** and **mcp-d**. for more polyhedra of related kinds relevant to intermetallic crystal chemistry see Bonneau, C.; O'Keeffe, M. *Inorg. Chem.* **2015**, *54*.

**Polyhedra with faces that are squares and equilateral triangles.** Those with one kind of vertex are triangular prism, **trp**,  $3.4^2$ ; rhombicuboctahedron, **rco**,  $3.4^3$ ; square antiprism, **sap**,  $3^3.4$ ; snub cube, **snc**,  $3^4.4$ ; cuboctahedron, **cuo**,  $3.4.3.4$ . Missing are  $3^2.4$  and  $3^2.4^2$ . It is easy to see that these are topologically impossible (draw a triangle and the other edges incident on those three vertices and label each angle "3" or "4" according to the vertex symbol. You will see it is impossible.) There is a second uninodal polyhedron (Miller's polyhedron)  $3.4^3$ . This the only example of more than one tiling with the same single vertex symbol for tilings of the sphere plane.



Two polyhedra  $3.4^3$ . On the left the Archimedean solid symmetry  $O_h$ . On the right symmetry  $D_{4d}$ .

## 2D NETS

**Source.** many nets come from the compilation in O'Keeffe, M.; Hyde, B. G. *Phil Trans. Roy. Soc. Lond. A* **1980**, *295*, 553-618. identified as OKHn. See also the next reference.

**Uniform tilings.** Uniform tilings are tilings by regular polygons. Strictly speaking if there are  $k > 1$  vertices they should be called  $k$ -uniform. With  $k = 1$  they are the familiar regular and Archimedean (or Kepler, who first enumerated them) tilings. All 20 for  $k = 2$  are also there. For all  $k = 1-3$  see Chavey, D. *Computers Math. Applic.* **1989**, *17*, 147-165.

**5-6-7 nets.** The regular 3-coordinated net **hcb** is a tiling by hexagons (honeycomb, graphene layer). There are related 3-coordinated nets containing 5- and 7-gons as well as 6-gons. The 5-gons and 7-gons must occur in equal numbers (and it appears that there must be at least two of each in the unit cell). See **hnc**, **hnd**, **hne**

**4-5-6-7-8 net.** The 3-coordinated net **ply** is a pretty example of tiling by almost regular polygons of different sizes. It would be nice if it came from a crystal structure but in fact I found it in D. Wells, *The Penguin Dictionary of Curious and Interesting Geometry*, Penguin 1991 page 249.

**dense square nets.** **esq** and **suz** are of interest as dense nets with square symmetry. The vertices are the centers of unit circles in a dense circle packing. O’Keeffe, M.; Treacy, M. M. J. *Acta Cryst.* **2010**, A66, 5-6 for related quasicrystalline layers.

**Tetragonal tungsten bronze.** net **pnc** is the net of O atoms in a layer of the celebrated tetragonal tungsten bronze (TTB) structure.

**Cairo tiling.** The net **mcm** is an example of a tiling by congruent pentagons. It is a conspicuous feature of Cairo, Egypt sidewalks, hence the name. It is the dual of  $3^2.4.3.4$  (**tts**). It is also called MacMahon's net for the distinguished mathematician who called attention to it.

**Pentagon tilings.** Another example of tiling by pentagons is **fsz-d** the dual of  $3^4.6$ . If we want tilings by pentagons all related by symmetry (*isohedral* tilings) then there are only one more other than **mcm** – **cen-d** the dual of  $3^3.4^2$  (**cem**). One often sees stated that there are 14 tilings of the plane by congruent pentagons. Most of these are not *edge-to-edge* (i.e. each edge common to exactly two tiles) in contrast to all 2D tilings in RCSR, and for some of the others the tiles are congruent but not related by symmetry (and now called *monohedral*). Other pentagon tilings are the duals of 5-c tilings by triangles and squares. These are rather rare only two with each of 2 and 3 vertices. they have symmetries  $p2$  or  $p2gg$ . See the O’Keeffe & Hyde reference at the beginning of this section.

**Circle-packing nets.** A circle packing is a packing (on the Euclidean plane in this instance) of equal diameter circles in contact. The centers of the circles are nodes of a net and contacts correspond to links. A circle-packing net is then one that has an embedding with equal-length links that are the shortest distance between nodes.

**Self-dual tilings.** These are of interest for several reasons. In chemistry a number of the most-common crystal structures can be described as a stacking of self-dual tilings with the vertices of one layer being in the position dual to the layers above and below. A dozen such were described by O’Keeffe, M. *Aust. J. Chem.* **1992**, 45, 1489-1498. More are in O’Keeffe, M.; Hyde, B. G. *Crystal Structures I. Patterns and symmetry*. Amer. Min. Soc. 1996. The name of these tilings corresponds to the name of the crystal structure

type in the cited reference. Self-dual tilings are also of interest in mathematical physics. See Kotecky, R.; Sokal, A. D.; Swart, J. M. *Commun. math. Phys.* **2014**, *330*, 1339-1394. For a self-dual tiling the average ring size must be 4 so that, except for  $4^4$ , there must be triangular tiles. In RCSR they have symbols beginning with **sd**.

### 3D NETS

**Regular nets.** Starting in 2003 (Delgado-Friedrichs et al. *Acta Crystallogr. A* **2003**, *A59*, 22-27) a systematic classification of three-periodic nets was attempted. The five regular nets have regular coordination figures<sup>1</sup> (regular polygon or polyhedron). They have one kind of vertex and one kind of edge and their natural tiling has one kind of face and one kind of tile (transitivity 1111). These can be retrieved using the keyword "regular". They are: 3-coordinated **srs**, square 4-coordinated **nbo**, tetrahedral 4-co-ordinated **dia**, octahedral 6-coordinated **pcu**, cubic 8-coordinated **bca**. There is also one *quasiregular* net **fcu** whose vertex figure is a cuboctahedron (a quasiregular polyhedron) and the structure is 12-coordinated. This has transitivity 1112 (the 12-coordinated **fcu** is the net of face-centered cubic lattice whose natural tiling consists of tetrahedra and octahedra).

**Semiregular nets.** these have one kind of vertex and one kind of edge. transitivity 1 1 r s. Example **qtz** (quartz) **sod** (sodalite).

**What every child should know about nets.** Everyone should be familiar with these nine nets. They all have a unique proper tiling (one with the full symmetry of the net). The “dual” net is the net of the dual of the proper tiling. A net and its dual define a periodic surface that separates the two nets. The surfaces below are *minimal* surfaces – they have embeddings with everywhere zero mean curvature. **flu** is the only net with transitivity 2 1 1 1. **sod** is the net of the only uninodal and isohedral simple tiling. The dual, **bca-x**, is body-centered cubic with the 8 first and 6 second neighbor links as edges (14-c). It is the only uninodal isohedral tiling by  $[3^4]$  tetrahedra.

net	symm	CN	transitivity	dual	surface	genus
<b>srs</b>	$I4_132$	3	1 1 1 1	<b>srs</b>	<i>G</i>	3
<b>nbo</b>	$Im\bar{3}m$	4	1 1 1 1	<b>bca</b>	<i>I-WP</i>	4
<b>dia</b>	$Fd\bar{3}m$	4	1 1 1 1	<b>dia</b>	<i>D</i>	3
<b>pcu</b>	$Pm\bar{3}m$	6	1 1 1 1	<b>pcu</b>	<i>P</i>	3
<b>bca</b>	$Im\bar{3}m$	8	1 1 1 1	<b>nbo</b>	<i>I-WP</i>	4
<b>fcu</b>	$Fm\bar{3}m$	12	1 1 1 2	<b>flu</b>	<i>F-RD</i>	6
<b>flu</b>	$Fm\bar{3}m$	4,8	2 1 1 1	<b>fcu</b>	<i>F-RD</i>	6
<b>sod</b>	$Im\bar{3}m$	4	1 1 2 1	<b>bca-x</b>	<i>O,C-TO</i>	7
<b>bca-x</b>	$Im\bar{3}m$	14	1 2 1 1	<b>sod</b>	<i>O,C-TO</i>	7

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<sup>1</sup> In the present context we can define the vertex figure as the figure defined by (better, the convex hull of) here).

**Other tilings** **1111**. the net **lcy** has a not natural, but proper tiling of this sort (tiling ignores the 3-rings of the structure. **fcu** also has a tiling 1 1 1 1 with symmetry  $P\bar{a}\bar{3}$ . See Bonneau, C; O'Keeffe, M. *Acta cryst. Ab* **2014**, *71*, 82-91. If one allows tiles that are infinite in one direction (rods) then **lcs** also has tiling 1 1 1 1. Delgado Friedrichs, J. Plévert and M. O'Keeffe . *Acta Crystallogr. A*58, 77-78 (2002).

**Isohedral tilings by tetrahedra.** there are exactly nine. The duals are the nine uninodal simple tilings (look for keyword “simple tiling” and no. vertices = 1). Delgado-Friedrichs, O; Huson, D. H. *Discrete Comput. Geom.* **1999**, *21*, 299-305.

**hidden keywords.** There are certain "names" that act as keywords, but are invisible to the user. You just have to know them. Some are:

*square*. This will retrieve nets with planar 4-coordination at every vertex.

*icosahedron*. this will retrieve nets with icosahedral groups of twelve vertices.

*silica*. this will retrieve nets of framework silicates etc. that are not zeolite nets (e.g. that of quartz, **qtz**).

*iso14*. This will retrieve the isohedral simple tilings by tiles with 14 faces

*alpha cage*, *FAU cage*, *C60*, *hexagonal barrel*, *tennis ball* will retrieve structures with one of these cages. There are four structures with  $C_{60}$  (truncated icosahedra) tiles: **csi**, **csp**, **fvh**, and **fvi**.

*ST-net* (note the hyphen) will retrieve nets with mixed square and tetrahedral coordination

**Structures with transitivity  $n+1$  n r s.** “minimal transitivity nets”. For a discussion of the minimal transitivity principle in crystal chemistry see Li, M. *et al. Chem. Rev.* **2014**, *114*, 1343-1340. **viv** is a sphere packing net with transitivity 5 4

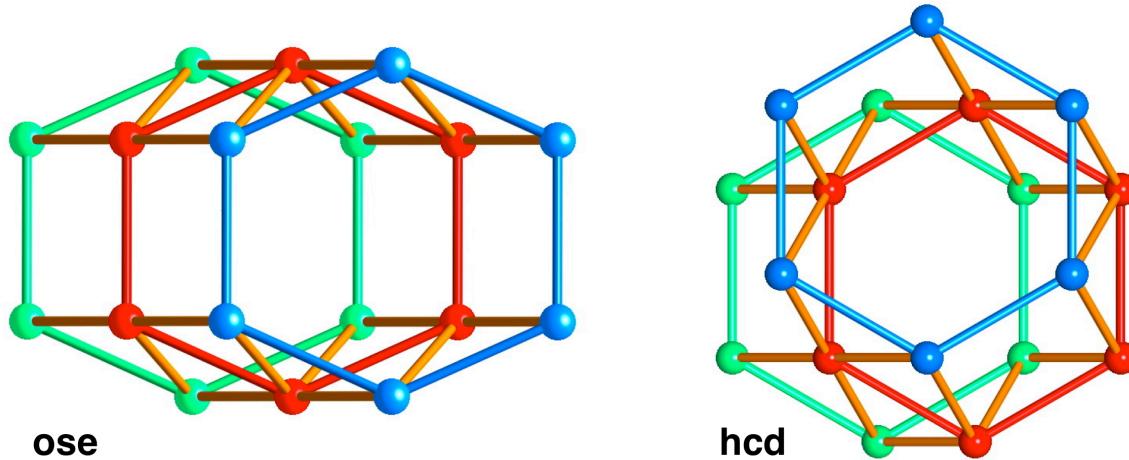
**Bipartite nets.** In bipartite nets the vertices can be divided into two groups say “cations” and “anions” so that all edges join a cation to an anion.

**Closest packings.** The closest sphere packings are familiar 12-coordinated structures. Most notably **fcu** cubic closest packing in which the sphere centers are at the points of the face-centered cubic lattice. This is the only lattice packing with maximum density but there are infinitely more with the same density known as Barlow packings. The only one of these with one kind of sphere (nets with one kind of vertex) other than **fcu** is hexagonal closest packing **hcp**. Other closest packings can be described as composed of *h* layers and in **hcp** and *c* layers as in **fcu**. Those with two kinds of vertex are **tcj** (*hc*), **tck(hcc)**, **tcl(hhc)**, **tcm(hhcc)**. See OKH Chapter 6.

**The -6 family.** The closest packed structures other than **fcu** (cubic closest packing!) are trigonal or hexagonal and the axial ratio is  $c/a = N\sqrt{(2/3)}$  where *N* is the number of layers normal to **c** in the repeat unit. If the value of  $c/a$  is reduced by a factor of 2 while keeping the other structural parameters the same, one gets a 6-coordinated family of structures. Vertices in *c* layers now have octahedral coordination and vertices in *h* layers have trigonal prismatic coordination. The structure thus derived from **fcu** is **pcu** (vertices on a

primitive cubic lattice) and that from **hcp** is **acs** (the only semiregular net with trigonal prismatic coordination). Those with two kinds of vertex are **hc-6 nia** (the idealized NiAs structure), **hcc-6 sta**, **hhc-6 stb**, **hhcc-6 ste**. Just as NaCl is the binary version of **pcu**, so WC is the binary version of **acs**. TiP has the **ste** (**hccc-6**) structure – actually ternary. MOFs (cobalt formates) based on these structures were reported by Shang *et al.* *APL Materials* **2014**, 2, 124104.

**Stacked  $6^3$  (honeycomb) nets.**  $6^3$  nets can be packed in the same way as  $3^6$  nets in close packing so that each vertex has seven nearest neighbors. The density is ideally  $2/3$  that of closest-packing, but for some configurations there is a slightly lower density embedding with the same symmetry and seven equal edges. For *AB* (*h*) packing there are two uninodal packings **osf** and **wkv**. For *ABC* (*c*) packing there is one uninodal net **ose** and one binodal structure **hcd**. See figure below. Other binodal structures are: **hci** (*hcc* packing), **hcj** (*hhc*) and **a<sub>2</sub>hck** (*hhcc*). For a reason why these nets might be interesting see: *J. Appl. Phys.* **102**, 093511 (2008). In RCSR search by “name contains” = “ $6^3$ ”.



**Uniform tiling.** If you click on the "keyword" in the nets search page you will find the following information for the 28 uniform tilings:

In a uniform tiling, all the vertices are the same (uninodal or vertex transitive) and the tiles are all uniform polyhedra (vertex transitive with regular polygonal faces). Grünbaum, B. *Geombinatorics* **1994**, 4, 49-56. Deza, M.; Shtogrin, M. *Eur. J. Combinatorics* **2000**, 21, 807-814.

The correspondence with Grünbaum's numbers are: 1: **fcu** 2: **hcp** 3: **tc** 4: **tca** 5: **flu-e** 6: **crs** 7: **reo** 8: **cab** 9: **reo-e** 10: **ubt** 11: **hex** 12: **tsi** 13: **svk** 14: **sve** 15: **svh** 16: **tfs** 17: **svj** 18: **kag** 19: **ttw** 20: **pcu-i** 21: **hal** 22: **pcu** 23: **fst** 24: **fee** 25: **ita** 26: **hex** 27: **rho** 28: **sod**

**Tiling with regular polygon faces.** The uniform tilings are vertex-transitive ND all faces are regular polygons. additional tilings of this sort are those of **nia-e** and **wng**. These contain isomeric Johnson polyhedra (polyhedra with regular faces) with 18 faces; not in

themselves vertex transitive, but the tilings are. It might be nice to know all such tilings (*hint*).

A remarkable tiling that “almost” has faces that are regular polygons is that of the binodal net **bon** in which the tiles are rhombicuboctahedra, cuboctahedra, octahedra and square antiprisms. It is easy to see that the faces aren’t exactly regular. (a) square antiprisms have non-crystallographic symmetry and (b) the structure has four edges but only three degrees of freedom. A more subtle case is **fub** = **sod-e-a**. This is a tiling by trigonal prisms, truncated tetrahedra and a large polyhedron with 4-, 6-, 8-, and 12-sided faces. The coordinates are fixed by the requirement of equal edges, but it will be found that the polygons, other than the square, are not quite regular or even planar,

**mog-e-x-z**. This is the idealized net (regular tetrahedra) of the anions in the moganite form of silica (also in BeH<sub>2</sub>). Why the bizarre symbol? **mog** is the topology of the 4-coordinated net of the Si atoms. In the maximum symmetry (*Cmmm*) embedding of the net **mog-e** (*q.v.*) some of the tetrahedra collapse to squares. To get the topology of the tetrahedra we need to add the diagonals of the squares as edges and the net symbol would be **mog-e-x** (*extended structure*) but now we have edges intersecting and tetrahedra of zero volume so we go to a lower symmetry (*Ibam*) embedding which allows regular tetrahedra and add **-z** to the net symbol. Incidentally *Ibam* is the symmetry of crystalline BeH<sub>2</sub>. Moganite is even lower symmetry (monoclinic) to allow the Si-O-Si angles to come to preferred values (about 145°). See *Phil/ Trans. 2014*, 372, 20120034.

**Uninodal 3-coordinated tilings of D, P and G surfaces.** Possibly the only uninodal structures of this type are the polybenzene family 6.8<sup>2</sup> **pbz**, **pbp** and **pbg** which have the full symmetry of the surfaces (*Pn*  $\bar{3}m$ , *Im*  $\bar{3}m$ , *Ia*  $\bar{3}d$ ) and the 9<sup>3</sup> family **uta**, **utb** and **utc** which however have lower symmetries (*Fd*  $\bar{3}m$ , *I432* and *I4\_132*). For a 7<sup>3</sup> tiling (not uninodal) of *P* see **kgn**. For more such search for e.g. name contains 9<sup>3</sup>.

**4-coordinated tilings of D, P and G surfaces.** There are many of these. A good example is the trio **ukd**, **rho** and **gie** which are 4<sup>3</sup>.6 tilings of *P*, *D* and *G* respectively. There are two distinct uninodal 4<sup>3</sup>.6 tilings of the hyperbolic plane, the second gives **fau** as a tiling of *D*. (what are *P* and *G* structures?), See *J. Solid State Chem. 2005*, 178, 2533-2554. The net, **tsc**, of the zeolitic mineral *tschortnerite*, is a tiling of the *F-RD* surface.

**5-coordinated tilings of the P surface.** There are infinitely many 3.4<sup>4</sup> tilings of the *P* surface with regular polygons. **pcu-i** is the only uninodal one, See **mjy** and **mjz** for other examples. **fcp** is 5<sup>5</sup> self-dual tiling of *I-WP* (vertex and face transitive as 2D tiling)

**Two 3<sup>2</sup>.4.3.6 tilings of G.** These are the nets **fcy** and **fcz**. Although there is only one hyperbolic tiling 3<sup>2</sup>.4.3.6 there are two distinct projections on the *G* surface. This property arises for an chiral hyperbolic tiling; see *Eur. Phys. J. 2004*, B39, 365. **fcz** is the underlying topology of a porous germanate with a giant cubic cell (see references).

**Tilings of CLP.** This tetragonal minimal surface of genus 3 has **cds** as its labyrinth graph. **abr** is a tiling of the surface by quadrilaterals and hexagons with 4.6.4.6, 4<sup>2</sup>.6<sup>2</sup>, and 4<sup>4</sup> vertices.

**Subnets of bcu.** Nets of embed type 2 can be derived from **bcu** by systematically deleting links to produce *subnets* (or *subgraphs*). Examples are **bcs**, **rob**, **sxa**, **loh**, **lom**. **dia-c** has two disjoint subnets, linking them with one extra link gives the 5-coordinated structures **fnu** and **fnx**. See V. A. Blatov. *Acta cCryst. A*63, 239 (2007).

**Subnets of fcu.** Nets of embed type 2 can be derived from **fcu** by systematically deleting links to produce subnets. Examples are **hxg**, **lsz**. **srs-c4** has four disjoint subnets as does **srs-c4\***.

**Subnets of pcu.** Nets of embed type 2 can be derived from **pcu** by systematically deleting links to produce subnets. Examples are **cds**, **cdl**, **cds-f**, **fsc**, **fsg**, **pto-d**.

**Vertices with the same vertex symbol and coordination sequence.** See **ana-f**, **ana-a** **edq cdj**, **ffi tff**, **ffg ffj**. **bwt** is a binodal net with the same vertex symbol and coordination sequence for each node.

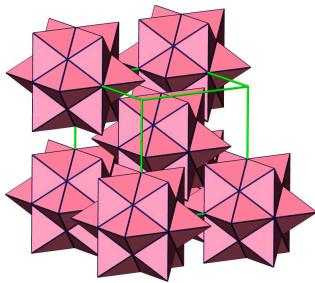
**Monoclinic with  $\beta = 90^\circ$ .** Some monoclinic crystals have  $\beta$  very close to  $90^\circ$  ( $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is a good example). The net **vna** has  $\beta$  also very close to (exactly equal to?)  $90^\circ$  in its minimum density embedding.

**Rod packing and Diamond/quartz relation.** There are four distinct 2-way (rods running in two different directions) packings of equivalent rods. There are two pairs in which there is a tetragonal and a hexagonal packing. nets based on these packings come in pairs. The following pairs have symmetry *I4<sub>1</sub>/amd*, *P6<sub>2</sub>22*: **ant**, **anh**; **ths**, **bto**  
The following pairs have symmetry *P4<sub>2</sub>/mmc*, *P6<sub>2</sub>22*: **cds**, **qzd**; **pts**, **pth**

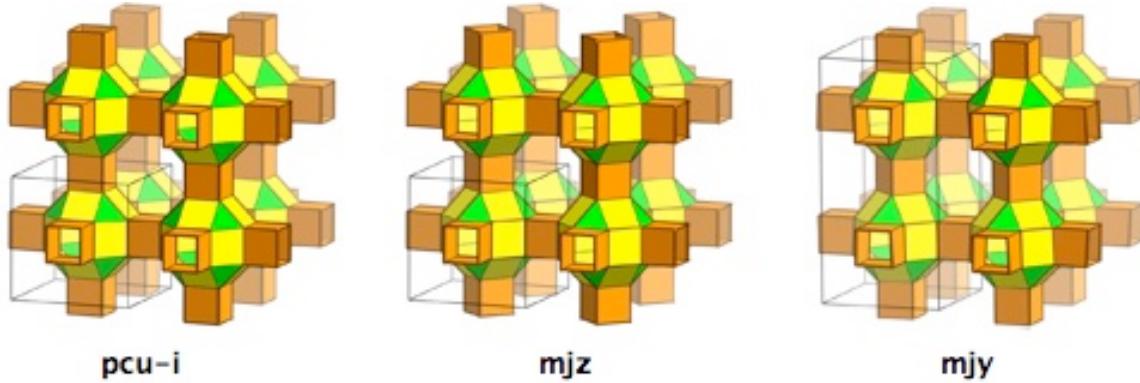
**1/2 transitive graphs.** A vertex-transitive graph is said to be 1/2 transitive if it is also edge-transitive, but not arc transitive (an arc is an edge with a direction). The nets of RCSR are graphs and there are just two that are 1/2 transitive, or, in other words, that have polar edges. They are **ana** and **thp**.

**Edge but not vertex transitive graphs.** In graph theory they are sometimes called semisymmetric graphs. Nets that are edge transitive but not vertex-transitive must have two kinds of vertex. Ignoring nets with symbols having extension **-b** there are just four nets of this type in RCSR with the same coordination number for each vertex. They are **pth**, **pts**, **ssb** and **ssc** - all 4-coordinated.

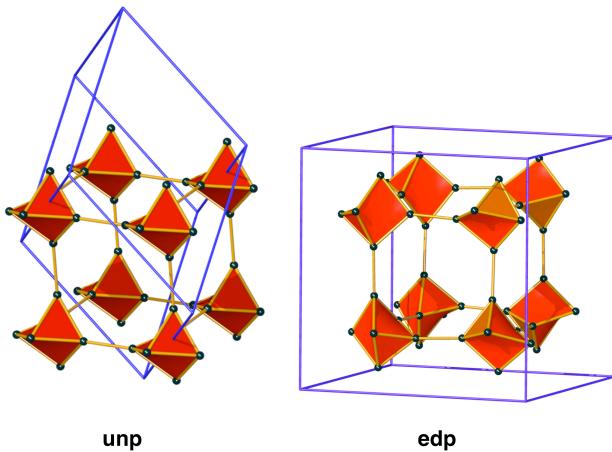
**A [3<sup>48</sup>] tiling (xom) with transitivity 2211.** What is the dual? The answer is **bcu** (body-centered cubic lattice with 6-fold edges). Pairs of tiles have six faces in common.



**$3.4^4$  tilings of  $P$ .** The structure **pcu-i** is the net of a uniform tiling (q.v.) – the tiles are cubes, truncated cubes, octagonal prisms and rhombicuboctahedra. It can also be thought of as a uninodal  $3.4^4$  tiling of the  $P$  surface using equilateral triangles and squares. There are infinitely many variants of this  $3.4^4$  tiling using regular triangles and squares. Two simple examples are shown by **mjz** (see reference) and **mjy**.



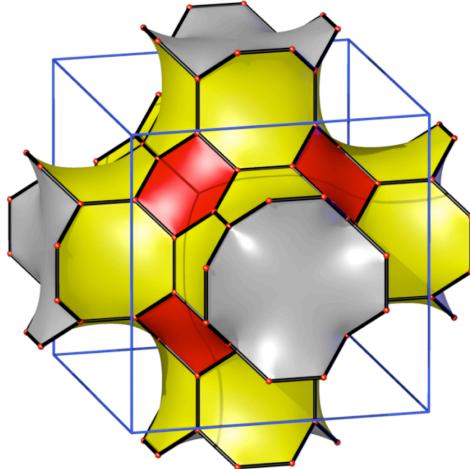
#### Linking trigonal prisms with pcu topology



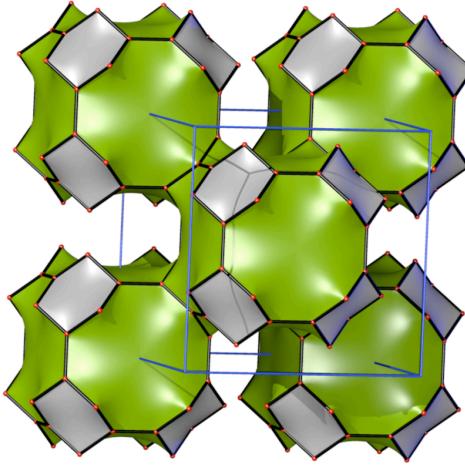
There are more than one way of doing this. In Chem. Rev. 112, 675 (2012) figure 24 the binodal **edp** (symmetry  $Pa\text{-}3$ ) is misidentified as the uninodal **unp** (symmetry  $R\bar{3}2$ )

### Nets with collisions

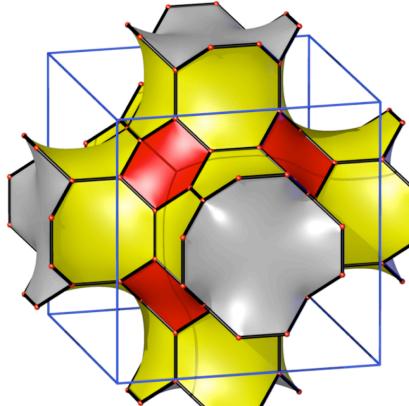
nets with collisions are those in which two or more vertices have the same coordinates in



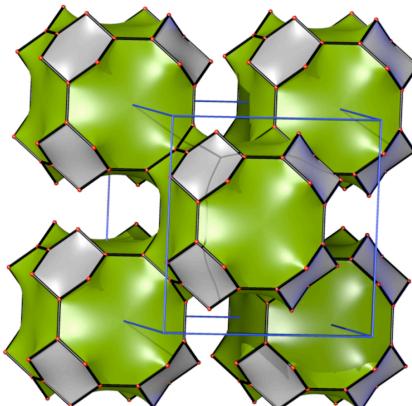
**pbp** as  $6,8^2$  tiling of P



and as  $12^3$  tiling if I-WP



**pbp** as  $6,8^2$  tiling of P



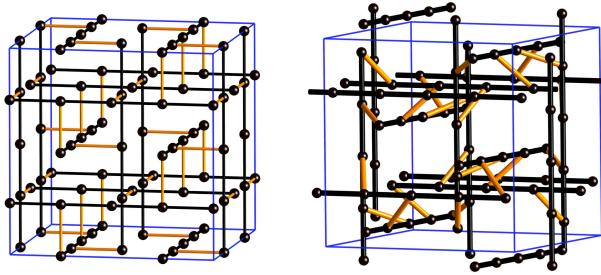
and as  $12^3$  tiling if I-WP

**Triclinic nets.** There are only two triclinic nets in RCSR. **nch** is the unique triclinic uninodal sphere packing (Werner Fischer). **rug** is a remarkable simple tiling by one topological kind of 14-face simple polyhedron with four topologically-distinct polyhedra in the packing (monohedral but not isohedral tiling). Discovered by Ruggero Gabbrielli. See references provided in RCSR. **rug** is one of the most complex nets in RCSR. Transitivity 24 48 32 4. (Slightly more complex are **tei** and **tep** of interest as theoretical Frank-Kasper phases). See also occurrence of space groups (below).

**Uninodal polar nets.** It is interesting that it is possible to have uninodal polar 3-periodic structures. Note that to have a polar *finite* structure (molecule) there must be at least two kinds of vertex (atom). But for infinite periodic point sets, uninodal polar structures are possible in 14 of the 58 polar space groups (this includes four enantiomorphous pairs).

These are  $Fdd2$ ,  $P4_1$ ,  $P4_3$ ,  $I4_1md$ ,  $I4_1cd$ ,  $P3_1$ ,  $P3_2$ ,  $R3$ ,  $R3m$ ,  $R3c$ ,  $P6_1$ ,  $P6_5$ ,  $P6_2$ ,  $P6_4$ . Indeed the RCSR lists 21 polar uninodal nets. But note that when we consider uninodal *connected* point sets (nets) all symmetries other than  $P1$  are possible

**Minimal density.** The embedding of a net in RCSR is that for equal edge if possible and for those which still have degrees of freedom the density is minimized. The binodal 3-c net **bwt** is unusual in not having a single configuration of minimum density. 2/3 of the links of the net fall on rods along  $\langle 100 \rangle$ . At minimum density the rods are straight, and for links of nit edge the unit cell edge is 4.0. For this (symmetry  $Pa\bar{3}$ ) the vertices are at  $x, y, 1/4$  and  $x+1/4, y, 1/4$ . for straight rod (minimum density)  $y = (1+2x \pm \sqrt{(1+2x)^2 - 1 - 16x^2})/4$ . the picture n the left below is for  $x = y = 1/4$ . in the middle of the sphere packing range. on the right another minimal density arrangement.



Note that this is not a sphere-packing net – the vertices of the embedding on the left above are in the positions of the 4-c net **nbo**. So the net is derived from NbO by systematically deleting  $1/4$  of the edges. Another net derived in the same way from **nbo** is the lovely uninodal **vab** (q.v.). Many nets in RCSR have been derived in this way by V. A. Blatov. *Acta Cryst.* **2007**, A63, 29-343; **2009**, A65, 202-212.

**Net of girth 16.** The girth of a net is the size of its shortest ring. The largest girth of any net in RCSR is in **sxt** which has girth 16. Another Blatov net (see abve). The largest rings in a uninodal net are the 26-rings in **sin**.

**Largest ring in a uninodal net.** This question only makes sense if we ask for strong rings (which are not the sum of smaller rings). Even then one can make arbitrarily large rings by, for example, replacing vertices of a net by groups of vertices. See nets whose symbol begins with “**sod-a**”. Each “-a” doubles the largest ring size. But for a uninodal net the record appears to be held by **sin** which contains 26-rings (370 meet at each vertex!..)

**-t nets.** The extension  $-t$  refers to a net derived from a tiling of a net. In the Dress approach to tiling, each tile is divided into *chambers* formed by (in 3-D) a vertex, the center of an incident edge, the center of an incident face and the center of the tile. The number of distinct chambers is the tiling size (given under “D-symbol” at the bottom of an RCSR page). The dual of the tiling by those chambers gives the  $-t$  net. That net has its vertices on the surface associated with the net (see e.g. **srs-t**). See de Carpo, L. et al. *Acta Cryst.* **2013**, A65, 483-489. The number of vertices in the  $-t$  net is the same as the

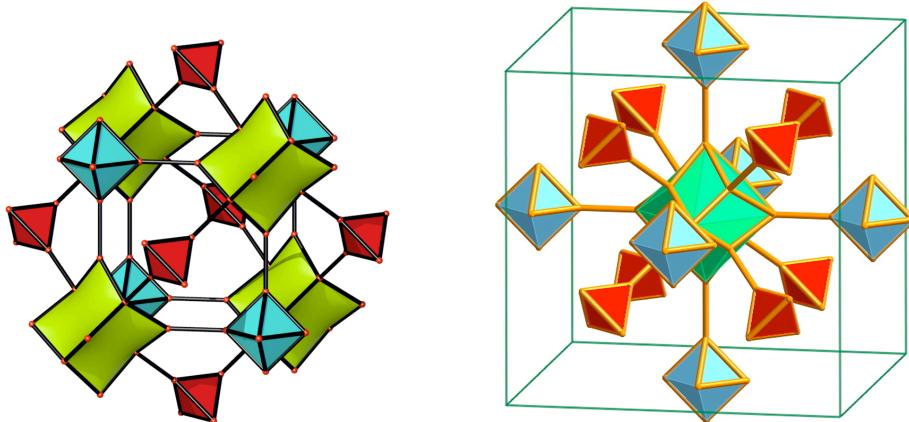
number of chambers (size) of the original; for qtz-t this is 14. Try searching for symbol contans “-t”; the nets are pretty – ans some surprises.

**-l nets.** The extension **-l** is another specialized one referring explicitly to 3-c tilings of 2-D surfaces. For a given 3-c tiling center every tile and form triangles from that vertex and each edge of the tile. Now one has a tiling by triangles. The dual of that is a new 3-c tiling with three times as many vertices as the original. The procedure was introduced as “leap-frog” by Patrick Fowler for fullerenes. In RCSR it is applied to some “Schwartzites” (hypothetical 3-c carbons formed by tiling periodic surfaces)

**Tilings with 5-sided faces.** sadly pentagonal dodecahedra do not tile Euclidean space in a tiling in which at least three faces meet at each edge. For a tiling with “two-face” edges see **cdh**. For a lovely tiling of pentagonal dodecahedra with a larger polyhedron with all 5-sided faces see **fiv**. A tiling by pentagonal dodecahedra and pentagonal tetrahedra(not polyhedra is the equally beautiful **ith-d**. [It seems likely that there is no uniform 4-c net of girth 5 – i.e. all shortest rings at each angle 5-rings]. There is a uninodal uniform 5-c net **gan** with isohedral tiling  $[5^4]$

**Tilings with 7-sided faces.** **itv** (the net of ice-XII) has an isohedral tiling by  $[7^8]$  tiles.

**A nets with high-symmetry 10 and 14 coordination.** The net **xbp** is a minimal transitivity (3 vertices, two edges) (4,6,10)-c net. The 10-c vertex has  $\bar{4}3m$  (tetrahedral) symmetry and the coordination figure is an adamantane cage with 6 vertices arranged as a regular octahedron and 4 as a regular tetrahedron. The “octahedral” vertices are linked to octahedral vertices and the “tetrahedral” vertices are linked to tetrahedral vertices. See **xbp-a** shown below left. The net **wzz** is (4,6,14)-c again with minimum transitivity (3 2) and the 14-c coordination figure is a rhombic dodecahedron –see **wzz-a** below right.



**Homometric structures.** In the early days of x-ray diffraction (before direct methods) there was discussion of whether two different crystal structures could have the same diffraction pattern (and thus the same Patterson map). Such structures, called homometric, are rare but do exist. The simplest homometric pair of closest (Barlow) packings have 15 layer sequences [Mardix, S. *Acta Cryst.* **1990**, *A46*, 133-138. A good place to learn about descriptions of close packings.]. Two simple structures in RCSR are

homometric **Ics** and **Icv-c**. The nodes of these in the most symmetric embedding are the invariant lattice complexes  $S$  and  $V^*$ . They are obviously different patterns (one contains 3-rings, the other doesn't) but they are homometric (have the same sets of inter-node vectors). *Homeometric* has a different meaning - thought you might like to know.

### Simple tilings and foams

A *simple* polyhedron has two faces meeting at an edge and three faces meeting at a vertex (3-c). In a *simple tiling* of 3-D Euclidean space, two tiles meet at a face, three at an edge and four at a vertex. It is the dual of tiling by tetrahedra. A *foam* has the topology of a simple tiling but the dihedral angles at the edges are  $\cos^{-1}(-1/2) = 120^\circ$  and the angles at the vertices are  $\cos^{-1}(-1/3) = 109.5^\circ$ . Accordingly, the faces and edges are curved and the faces have constant mean curvature.

We know of two duals of tilings by tetrahedra (**bcr** and **bda**) in which the tiles are not polyhedra in the strict sense as their 1-skeleta (graphs) are not 3-connected. See Delgado-Friedrichs, O.; O'Keeffe, M. *Acta Cryst.* **2005**, *A65*, 58-62. In general simple tilings will not be realizable with convex polyhedra anyway (see below).

### Space-filling solids: Isohedral and monohedral tilings and parallelohedra. A

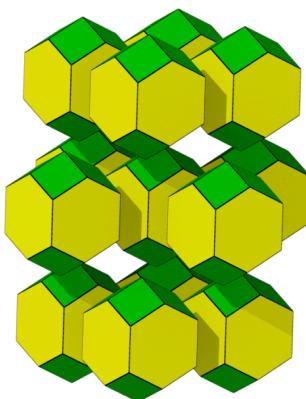
A good reference is *Tiling with congruent tiles*, Grünbaum, B.; Shephard G. C. *Bull. Am. math. Soc.* **1980**, *3*, 951-973.

A *monohedral tiling* is one in which all tiles are topologically the same. For example tilings by tetrahedra [ $3^4$ ].

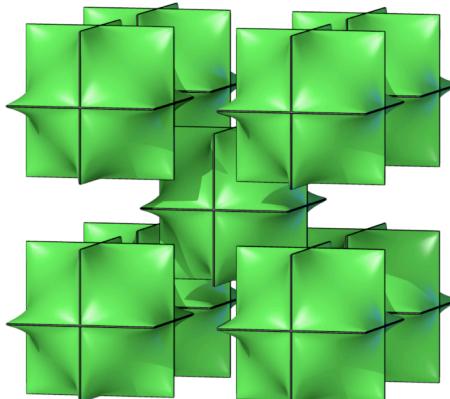
An *isohedral tiling* is one in which all tiles are related by symmetry ("kinds of tile" = 1 in RCSR). RCSR lists all isohedral simple tilings by tiles with 14 faces (the smallest possible number of faces) See Delgado-Friedrichs, O.; O'Keeffe, M. *Acta Cryst.* **2005**, *A65*, 58-62. There is only one uninodal isohedral simple tiling (**sod**). There are 11 binodal isohedral simple tilings all in RCSR (keyword "simple tiling", "kinds of vertex" = 2, "kinds of tile" = 1).

A convex isohedral tile is known as a *stereohedron*.

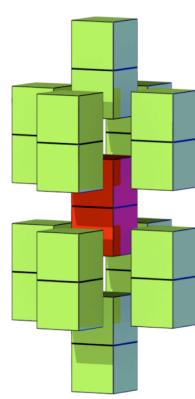
A remarkable monohedral simple tiling by 14-face tiles with tile transitivity 4 was discovered by Ruggero Gabrielli. See **rug** in RCSR. This polyhedron has no isohedral tiling.



**tcs**



**nbo**



**bct-d**

A *parallelohedron* is a space-filling polyhedron with a tiling in which all tiles are related by translations. It has long been known (Fedorov, 1885) that there are only five topologically-distinct such tilings by convex poluhedra. By cubes [ $3^3$ ] **pcu**, by hexagonal prisms [ $3^6 \cdot 6^2$ ] **bnn**, by rhombic dodecahedra [ $4^{12}$ ] **flu**, by truncated octahedra [ $4^6 \cdot 6^8$ ] **sod**, and by elongated dodecahedra ("hexarhombic dodecahedra" = [ $4^8 \cdot 6^4$ ]). Net = **tcu**. The centers of the tiles form a lattice (in the strict sense of one point per primitive cell). These are respectively: primitive cubic, hexagonal, face-centered cubic, body-centered cubic (considered as 14-coordinated) and tetragonally-distorted face-centered cubic. The **nbo** tile [ $6^8$ ] is a generalized parallelohedron (not strictly a polyhedron as it has 2-c vertices) with centers forming the 8-c **bcu** structure. The 10-c body-centered tetragonal lattice net **bct** is generated as the dual of a  $94^{10}$ ] "double cube" tiling as shown above. Having contiguous faces co-planar excludes convexity. Of course, **bct-d** has the same net at **pcu**.

An interesting paper Fortes, M. A.; Ferro, a. c. Z. *Kristallogr.* **1985**, *173*, 41-57 showed how to generate simple (3-c) parallelohedra of arbitrarily number of faces. Crystallographic data for some of these were given by O'Keeffe, M. *Kristallogr.* **1999**, *214*, 438-442. Two in RCSR are **kto** (20 faces) and **kts** (26 faces). Clearly these tilings can't be realized with convex tiles.

**Occurrence of space groups.** Some symmetries are more suitable than others for crystal structures. There is a large literature on the subject. Organic crystals (of the order of  $10^6$  known) are composed of molecules with generally only trivial symmetry (1) and the most common symmetries are first  $P2_1/c$  and next  $P\bar{1}$ . Brock, C. P.; Dunitz, J. D. *Chem. mater.* **1994**, *5*, 1118. For inorganic crystals the most common symmetry is *Pnma* followed by  $P2_1/c$  again. Baur, W. H.; Kassner, D. *Acta Cryst.* **1992**, *B48*, 356. We have noted that the intermetallic structures have high symmetry generally tetragonal, hexagonal or cubic in classes  $4/mmm$ ,  $6/mmm$  and  $m\bar{3}m$ . Bonneau, C.; O'Keeffe, M. *Inorg. Chem.* **2015**, . What about RCSR? The results are skewed by the propensity of certain space groups to have many uninodal sphere packings but generally the "interesting" nets (the aim of RCSR is to collect these) have high symmetry. In RCSR the most-common symmetries are  $I\bar{m}\bar{3}m$  and  $P6_3/mmc$  (about 6% each). These are followed closely by  $I4_1/amd$  and  $I4/mmm$ . Next is  $P6_222$ , by far the most common chiral symmetry in RCSR. By contrast for organic and organic crystals it is  $P2_12_12_1$  which has no entries in RCSR. About one half of the space groups have 0 or 1 entry in RCSR.

### Quotient graph, genus, and complete graphs

The quotient graph of a net is a finite graph in which a vertex replaces all translationally-equivalent vertices of the net. The edges are labeled to denote the translation between connected vertices. Thus vertex 1 might be connected to vertex 2 in the unit cell displace by a translation  $100$ , and the edge is labeled accordingly. [Chung et al. *Acta Cryst.* A40, 42 (1984). The number of numberings and labelings for the quotient graph of a given net is infinite but there is a canonical form ("Systre key") used by Systre to identify nets. (Export from Systre as "abstract topology").

A complete graph  $K_n$  is a finite graph with  $n$  vertices in which every vertex is connected to every other. For a given number of vertices it is the most "symmetrical". "Symmetry"

in this context, better “automorphism”, means permutations of the vertices that leave the adjacencies (edge) unchanged. In the case of  $K_n$ , the automorphisms form a group of order  $n!$ . The cyclomatic number,  $g$ , of  $K_n$  is the number of independent cycles:  $g = 1 + e - v = (n-1)(n-2)/2$

In RCSR the chromatic number of the quotient graph is called the genus. For a 3-periodic graph the minimal genus is 3 and each net of genus 3 (“minimal net”) has a unique quotient graph. Famously, **srs** is the unique graph with  $K_4$  as quotient graph. For more on Minimal nets see de Campo et al. *Acta Cryst. A* 69, 483 (2013) and references therein.

Not very useful information: In RCSR there are five graphs with  $K_5$  and five with  $K_6$  as quotient graph. None with  $K_7$  and two with  $K_8$ . [look for name – “K5 net” etc].

### Some additional references

Many oddities about nets can be found in Delgado-Friedrichs, O. *et al.* What do we know about three-periodic nets? *J. Solid State Chem.* **2005**, *178*, 2522-2554.

For sphere packings see O’Keeffe, M. Some properties of three-periodic sphere packings. *Struct. Chem.* **2012**, *23*, 1079-107.

Nets with one vertex in the repeat unit (“lattice nets”). Delgado-Friedrichs, O.; O’Keeffe, M. Edge-transitive lattice nets *Acta Cryst.* **2009**, *A65*, 360-363. Eon, J.-G. Topological density of lattice nets. *Cryst.* **2013**, *A69*, 119-121.

Interpenetrating nets: Bonneau, C.; O’Keeffe, M. High-symmetry embeddings of interpenetrating periodic nets. Essential rings and patterns of catenation. *Acta Cryst.* **2015**, *A71*, 82-91. See also I. Baburin *Acta Cryst.* **2016**, *A72i*, 366-375.