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Three-periodic nets and tilings: regular and related infinite polyhedra

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The six infinite regular (flag-transitive) polyhedra with finite faces of Grünbaum and Dress are described as tilings of the *P* and *D* periodic minimal surfaces. The three polyhedra formed by analogous tiling of the *G* surface are also described. The nets of these polyhedra are identified. It is shown how these polyhedra, and the nets they carry, could be found by mining the EPINET database of structures. The nets of regular three-periodic polyhedra with infinite helical or zigzag faces are also identified.

1. Introduction

Regular polyhedra play a special role in descriptive crystal chemistry and they feature prominently in chemistry text books. In this context, they are usually confined to the Platonic solids: the regular tetrahedron {3,3}, octahedron {3,4}, icosahedron {3,5}, cube {4,3} and dodecahedron {5,3}. Here the notation $\{p,q\}$ indicates that q regular p-gons meet at each vertex. The modern definition of regularity requires that the group of symmetries of the polyhedron act transitively on the flags – a flag being a triplet of a mutually incident vertex, edge and face.

Many years ago, the infinite polyhedra {4,6}, {6,4} and {6,6} with faces that are regular plane polygons were added to the list (Coxeter, 1937); these are sometimes known as the Petrie–Coxeter polyhedra. Later, Grünbaum (1977) enlarged the family of regular polyhedra by allowing faces that were skew polygons that could even be infinite (helices or zigzags). Shortly thereafter, Dress (1981, 1985) added to Grünbaum's list and showed that the enumeration was complete. These generalized polyhedra are known as the Grünbaum–Dress polyhedra. A good account of the theory of them has been given by McMullen & Schulte (1997) and I follow their notation and nomenclature. There are also related polyhedra, flag-2-transitive, that have been discussed by Schulte (2004, 2005). Infinite polyhedra are also called apeirohedra (McMullen & Schulte, 1997).

The motivation for this work is that what appear at first to be exercises in mathematics often turn out later to be of relevance to crystallography. For example, periodic structures such as sphere packings, tilings and minimal surfaces were first topics in 'pure' mathematics but now play an essential role in crystal chemistry and materials science. Often the transition to crystallography is hindered by the abstract style preferred by mathematicians and by the lack of illustrations and information such as space-group symmetry and coordinates. This paper is designed to ameliorate that transition for the regular periodic polyhedra which are not well known to crystal chemists. The treatment is informal and no new mathematical results are presented.

It is instructive first to consider the finite regular polyhedra. In addition to the planar faces, each polyhedron has Petrie polygons determined as follows. Take two adjacent edges of a face. The second edge is common to a second face and continue for the next edge along that new face. Repeat until one gets back to the starting vertex. Petrie polygons of a regular tetrahedron, octahedron and cube are shown in Fig. 1; these are skew quadrangles, hexagons and hexagons with angles of 60, 60 and 90°, respectively.

Now, if we don't mind faces intersecting, we can make five new polyhedra with the same edges and vertices as the Platonic solids but with faces that are Petrie polygons. These new polyhedra are the *Petrials* of the original and their Petrials recover the originals. In other words, Petrials are like duals in that just as the dual of a dual is the original so is the Petrial of a Petrial. The symbol for the Petrial of $\{p,q\}$ is $\{r,q\}_p$ in which r is the number of edges of the Petrie polyhedron.

In the same way, the regular tilings of the plane {3,6}, {4,4} and {6,3} have Petrials whose faces are infinite zigzags. Their symbols are $\{\infty,6\}_3$, $\{\infty,4\}_4$ and $\{\infty,3\}_6$.

Recall the basic definition of a polyhedron in the present context as a family of polygons such that any two polygons

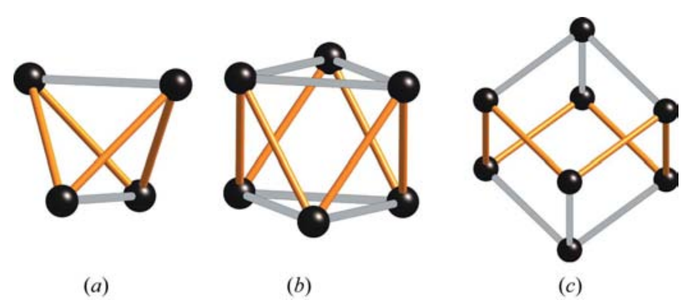

Figure 1
Petrie polygons (orange) of (*a*) a tetrahedron, (*b*) an octahedron and (*c*) a cube.

have in common either one vertex or one edge (two adjacent vertices) or have no vertices in common, and each edge is common to exactly two polygons.

2. Identification of infinite polyhedra (apeirohedra) with finite faces

In addition to the Petrie–Coxeter regular apeirohedra, there are three more with finite skew faces (in fact the skew polygons of Fig. 1). These are all tilings with vertex configurations {4,6}, {6,4} or {6,6} on infinite periodic surfaces. Although they are well characterized, I have not found a crystallographic description (space group and coordinates) or even, in some cases, an illustration of an embedding either of the polyhedra or of the nets they carry (the 1-skeleton) although the nets of some were identified by Grünbaum (1977).

These and related structures were identified by finding the possibilities for tilings $\{p,q\}$ of a surface in which the symmetry acts transitively on the vertices, edges and faces (this is a weaker requirement than that of flag transitivity). This is done using the Euler equation

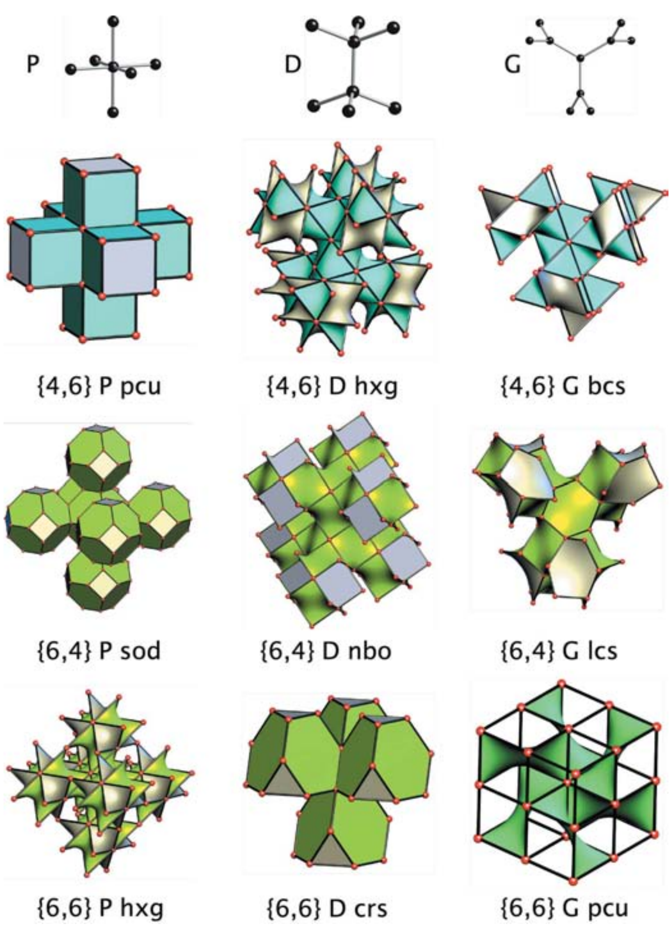

Figure 2
Fragments of the infinite polyhedra described in the text. The top row illustrates a part of the labyrinth graph of the *P*, *D*, *G* surfaces.

$$f - e + v = 2 - 2g, \qquad (1a)$$

where *f*, *e* and *v* are the number of faces, edges and vertices in a primitive cell of a tiling of a surface of genus *g* (also calculated for a primitive cell) combined with the conservation equations:

$$e = vq/2, \quad f = vq/p. \qquad (1b)$$

As the structure is to be periodic and vertex-, edge- and face-transitive, *v*, *e* and *f* must be compatible with crystallographic symmetry, *i.e.* must be dividers of 48, and solutions of equations (1) that satisfy these conditions are sought. As there has to be an axis of rotation at each vertex and in the center of each face, p, $q \le 6$ and pf, $qv \le 48$. Under these restrictions, there are only four positive integer solutions for (g, p, q, v), namely:

$$(g, p, q, v) = (3, 4, 6, 8), (3, 6, 4, 12), (3, 6, 6, 4), (5, 6, 6, 8). \qquad (2)$$

With p or q = 6, to have a 3-periodic structure there must be non-parallel sixfold axes (which in fact must be $\bar{3}$ axes) so the structures must be cubic. The three cubic minimal surfaces, *P*, *D* and *G*, with $g = 3$, are of course well known and known to be the only ones of this type (Fogden & Hyde, 1992*a*,*b*), and are discussed further below. It appears probable that there is no structure with $g = 5$, as a surface of this genus must have a labyrinth graph with the same genus and there is no known cubic vertex- and edge-transitive graph of this sort. Note that the object of this exercise is to find out where to look for the infinite polyhedra, which are already known to mathematicians. Note also that the conditions given above are necessary but not sufficient for a structure of the appropriate type to exist.

Systematic generation of 3-periodic nets in Euclidean space is being carried out by suitable projections of the nets of hyperbolic tilings onto infinite periodic surfaces (Hyde *et al.*, 2006). The results are being recorded in EPINET (http://epinet.anu.edu.au); accordingly this is the place to look.

The genus 3 structures given in equation (2) are all identified in EPINET as projections on the *P*, *D* and *G* surfaces of the hyperbolic regular tilings {4,6}, {6,4} and {6,6} and the RCSR (http://rcsr.anu.edu.au) symbols of the nets they carry are given. It is known (Robins *et al.*, 2005) that achiral hyperbolic tilings have exactly one projection on each surface and it can readily be verified that the tilings of *P* and *D* are flag-1-transitive and the tilings of *G* are flag-2-transitive (but of course vertex-, edge- and face-transitive). Accordingly, the regular infinite polyhedra with finite faces are identified. The symmetry of the flag-2-transitive tilings of *G* is such that adjacent flags are in distinct orbits. Such structures are called 'chiral' in the mathematics literature (Schulte, 2004), but of course the term has a quite different meaning to crystallographers so I avoid its use in this context.

The nets are all either regular or semiregular in the classification of Delgado Friedrichs *et al.* (2003*a*,*b*) where they are all described.

3. Nets and crystallographic description

Units of the structures with finite faces are illustrated in Fig. 2 and some basic properties given in Table 1. Notice that the duals of {6,4} are {4,6} and that the {6,6} are self dual. The Petrials of the Petrie–Coxeter polyhedra have infinite (helical) faces with axes that intersect and are discussed further below. The Petrials of the regular polyhedra with finite skew faces are polyhedra of the same sort (see Table 1). The Petrials of the G tilings do not have regular faces. Also listed in the table is the *vf*-net which is the net obtained by linking the centers of the faces to the vertices of the face. I now comment on the individual structures.

{4,6}P. This is one of the Petrie–Coxeter polyhedra. Notice that the faces are only half the faces of a tiling of cubes, so the symmetry is lower ($\mathbf{a}' = 2\mathbf{a}$) than that of the net (**pcu**) it carries.

{4,6}D. This structure has faces that are Petrie polygons of tetrahedra. It, and the net it carries, have already been described by Schoen (1970). The polyhedron and the net have the same symmetry. The Petrial of this net is {6,6}P which therefore carries the same net and has the same symmetry.

{4,6}G. This structure and its net (**bcs**) were again described by Schoen (1970); I believe for the first time. The faces are skew quadrangles with angles of $\cos^{-1}(1/3) = 70.5°$.

{6,4}P. This is another Petrie–Coxeter polyhedron and consists of the hexagonal faces of the familiar sodalite structure; accordingly it has the net (**sod**) and symmetry of that structure.

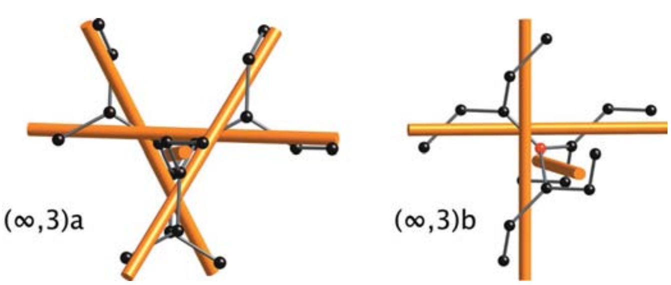

Figure 3
Fragments of the {∞,3} polyhedra. The faces shown are 3_2 and 4_1 helices with axes shown as cylinders. The net, **srs**, is the same in both cases.

Figure 4
Part of the $\{\infty,4\}_{\cdot,*3}$ polyhedron. The net is **nbo**.

Table 1
Data for some infinite polyhedra with finite faces.

Entries under 'Polyh.' such as {4,6}P indicate a tiling of the P surface by quadrangles with six meeting at each vertex. MS refers to the symbols of McMullen & Schulte (1997) and S.g. refers to the space group of the polyhedron. The coordinates refer to the origin on an inversion center. Edges correspond to shortest distances between vertices. The *vf*-net is the net of vertices and faces (see text).

Polyh.	MS	Net	S.g.	Coords.	*vf*-net	Petrial
{4,6}P	{4,6|4}	**pcu**	$Im\bar{3}m$	1/4, 1/4, 1/4	**she**	$\{\infty,6\}_{4,4}$
{4,6}D	$\{4,6\}_6$	**hxg**	$Pn\bar{3}m$	0, 0, 0	**toc**	{6,6}P
{4,6}G	–	**bcs**	$Ia\bar{3}d$	0, 0, 0	**gar**	–
{6,4}P	{6,4|4}	**sod**	$Im\bar{3}m$	1/4, 0, 1/2	**she**	$\{\infty,4\}_{6,4}$
{6,4}D	$\{6,4\}_6$	**nbo**	$Pn\bar{3}m$	1/4, 1/4, 3/4	**toc**	Self
{6,4}G	–	**lcs**	$Ia\bar{3}d$	3/8, 0, 1/4	**gar**	–
{6,6}P	$\{6,6\}_4$	**hxg**	$Pn\bar{3}m$	0, 0, 0	**pcu-b**	{4,6}D
{6,6}D	{6,6|3}	**crs**	$Fd\bar{3}m$	0, 0, 0	**hxg-b**	$\{\infty,6\}_{6,3}$
{6,6}G	–	**pcu**	$Ia\bar{3}$	1/4, 1/4, 1/4	**bcs-b**	–

{6,4}D. This structure uses as faces one half of the 6-rings of the **nbo** net. Accordingly, the tiling has lower symmetry ($Pn\bar{3}m$) than that ($Im\bar{3}m$) of the net. It is self-Petrial as the Petrie operation simply interchanges the roles of the used and unused rings. The faces are congruent with the Petrie polygons of a cube.

{6,4}G. The net (**lcs**) of this structure is interesting from a number of aspects. The net of the structure contains only 6-rings, but they are of two kinds. Using one set produces an isohedral simple tiling of infinite tiles (Delgado Friedrichs *et al.*, 2002). {6,4}G uses the other set of 6-rings. The faces are skew hexagons with angles of $\cos^{-1}(-1/6) = 99.6°$.

{6,6}P. This structure was also described by Schoen (1970) – see the remarks on its Petrial {4,6}D above.

{6,6}D. This is a Petrie–Coxeter polyhedron and uses all the 6-rings of the **crs** net. The three-dimensional (rank 4)[1] tiling that carries this net is the familiar space filling by tetrahedra and truncated tetrahedra.

{6,6}G. The net of the structure is primitive cubic (**pcu**) with a doubled cell and the faces of the tiles are one quarter of the Petrie polygons. It is lower symmetry than the other G surface tilings. A fragment of the structure is illustrated by Schulte (2004).

4. Regular polyhedra with infinite faces

There are six 'pure' regular 3-periodic polyhedra with infinite faces. Three were identified in Table 1 as Petrials of polyhedra with finite faces. The Petrial pair {∞,3}a and {∞,3}b carry the chiral **srs** net (symmetry $I4_132$) and the faces are either threefold or fourfold helices as shown in Fig. 3. The faces do not intersect and their axes correspond to those of the chiral (in the crystallographic sense) invariant cylinder packings Σ and Π (O'Keeffe *et al.*, 2001), respectively.

[1] 'Rank 4' means that there are four kinds of element: vertices, edges, faces and tiles.

The final pure structure is $\{\infty,4\}_{\cdot,*3}$ in the notation of McMullen & Schulte (1997), who should be consulted for an explanation of the notation, and was first described by Dress (1981, 1985); see also Schulte (2005). This carries the achiral **nbo** net which, like all cubic structures, has 3_1 and 3_2 axes. Choosing as faces helices around axes of one hand produces the polyhedron with symmetry *I*432. The axes of the faces correspond to those of the chiral invariant cylinder packing with symbol Ω (O'Keeffe *et al.*, 2001) as shown in Fig. 4.

There are also six three-periodic polyhedra derived ('blended') from the two-periodic nets by replacing the polygons (triangles, squares or hexagons) by helices. In the notation of McMullen & Schulte (1997), this is indicated by appending $\#\{\infty\}$ to the symbol for the appropriate two-periodic structure. Thus from $\{3,6\}$ and its Petrial $\{\infty,6\}_3$, we get the Petrial pair $\{3,6\}\#\{\infty\}$ and $\{\infty,6\}_3\#\{\infty\}$. The structures are shown in projection in Fig. 5. Notice that the structures derived from $\{6,3\}$ are now six-coordinated. In $\{6,3\}\#\{\infty\}$, sets of six helical faces, three 6_1 and three 6_5, are co-axial as shown in Fig. 6. Each edge is common to a 6_1 face and a non-coaxial 6_5 face.

The symmetries and nets of all these structures are identified in Table 2. Notice that, as for polyhedra with finite faces, the symmetry of the nets is sometimes higher than the polyhedron that carries it. In particular, the nets of the blended polyhedra derived from $\{3,6\}$ and $\{4,4\}$ are actually cubic. The net of the latter is that of diamond (**dia**) and a fragment of $\{\infty,4\}_4\#\{\infty\}$ is shown in Fig. 7 to illustrate this point.

5. Concluding remarks

There are two tasks of interest to the crystal chemist in connection with crystal nets which are special kinds of graph (Delgado-Friedrichs & O'Keeffe, 2005). The first is the systematic generation of structures, and in this endeavor the

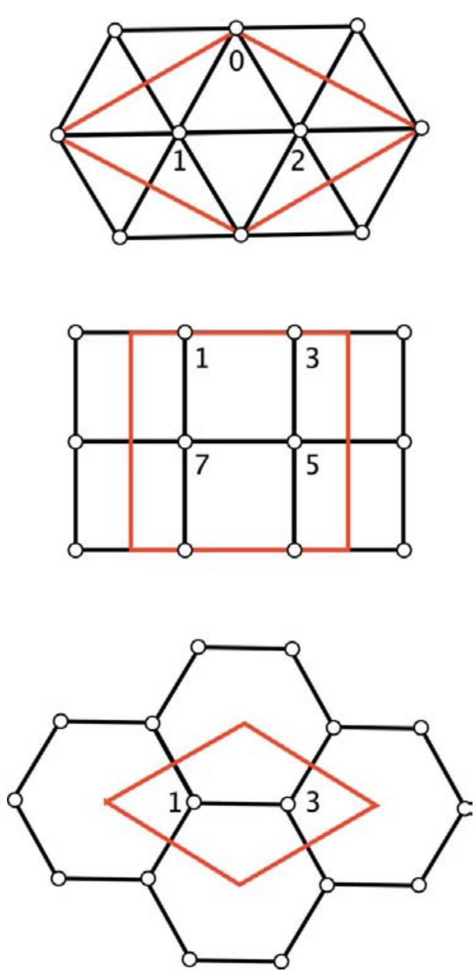

Figure 5
Projections of the blended polyhedra. Top $\{3,6\}\#\{\infty\}$: numbers are elevations in multiples of $\mathbf{c}/3$. Middle $\{4,4\}\#\{\infty\}$: numbers are elevations in multiples of $\mathbf{c}/8$. Bottom $\{6,3\}\#\{\infty\}$: numbers are elevations in multiples of $\mathbf{c}/4$.

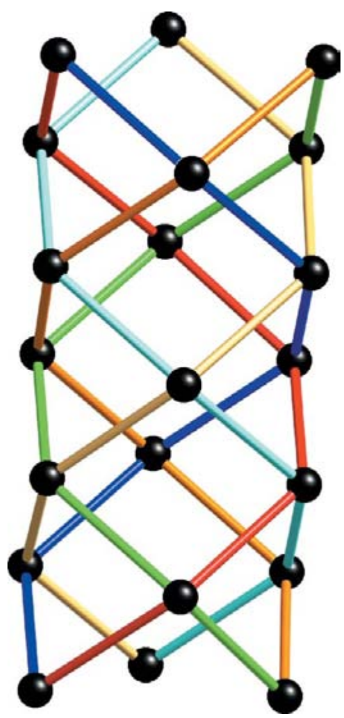

Figure 6
Part of one column of helical faces in $\{6,3\}\#\{\infty\}$. 6_5 red, orange and yellow. 6_1 blue and green.

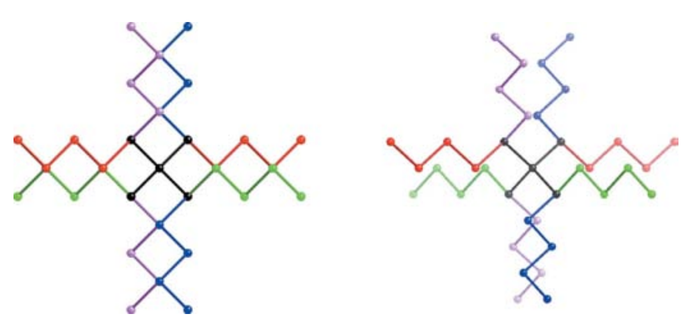

Figure 7
Four zigzag faces of $\{\infty,4\}_4\#\{\infty\}$ with a common vertex. Left: view down [001]. Right: the same tilted slightly off axis. Each black-colored edge is common to two zigzags.

Table 2
Data for some infinite polyhedra with infinite faces presented as in Table 1.

MS symbol	Net	S.g.	Coords.	Petrial
$\{\infty,6\}_{4,4}$	**pcu**	$Im\bar{3}m$	1/4, 1/4, 1/4	$\{4,6\|4\}$
$\{\infty,4\}_{6,4}$	**sod**	$Im\bar{3}m$	0, 1/2, 1/4	$\{6,4\|4\}$
$\{\infty,6\}_{6,3}$	**crs**	$Fd\bar{3}m$	0, 0, 0	$\{6,6\|3\}$
$\{\infty,3\}a$	**srs**	$I4_132$	1/8, 1/8, 1/8	$\{\infty,3\}b$
$\{\infty,3\}b$	**srs**	$I4_132$	1/8, 1/8, 1/8	$\{\infty,3\}a$
$\{\infty,4\}_{\cdot,*3}$	**nbo**	$I432$	0, 1/2, 1/2	
$\{3,6\}\#\{\infty\}$	**pcu**	$R\bar{3}m$	0, 0, 0	$\{\infty,6\}_3\#\{\infty\}$
$\{\infty,6\}_3\#\{\infty\}$	**pcu**	$R\bar{3}m$	0, 0, 0	$\{3,6\}\#\{\infty\}$
$\{4,4\}\#\{\infty\}$	**dia**	$I4_1/amd$	0, 3/4, 1/8	$\{\infty,4\}_4\#\{\infty\}$
$\{\infty,4\}_4\#\{\infty\}$	**dia**	$I4_1/amd$	0, 3/4, 1/8	$\{4,4\}\#\{\infty\}$
$\{6,3\}\#\{\infty\}$	**acs**	$P6_3/mmc$	1/3, 2/3, 1/4	$\{\infty,3\}_6\#\{\infty\}$
$\{\infty,3\}_6\#\{\infty\}$	**acs**	$P6_3/mmc$	1/3, 2/3, 1/4	$\{6,3\}\#\{\infty\}$

approach of starting from tilings, either of the hyperbolic plane as in EPINET or from tiling Euclidean space (Delgado-Friedrichs *et al.* 1999; Delgado-Friedrichs & Huson, 2000) has been particularly fruitful. One lesson to be learned from the present study is that nets can arise in, at first sight, surprising contexts; thus one finds **pcu** (the net of the primitive cubic lattice) carried by a tiling of the G surface (as in $\{6,6\}G$) and the harvest of EPINET turns out to be much richer than might have been supposed.

The second task is that of establishing a taxonomy of nets, and here it has been found again useful to consider nets as derived from rank-4 tilings of Euclidean space. But now we have to play by different rules, ones that lead to a unique description of a net (contrast the multiple structures carrying nets such as **pcu**, **hxg** and **srs** described above). One rule is that normally the only candidates for faces are cycles of the graph that are not the sums of smaller cycles. Depending on context, these are known as *relevant cycles* or *strong rings* (Delgado-Friedrichs & O'Keeffe, 2005). Notice that the Petrie polygons of Fig. 1 are not strong rings, nor are the infinite polygons in this paper. We also require the tiles to be finite and the tiling to have the same symmetry as the net. These rules lead to a unique (*natural*) tiling for the nets of the infinite polyhedra described here. For lower-symmetry nets, further rules may be necessary (Blatov *et al.*, 2007). Grünbaum (2003) has pointed out that, for generality, one should include *e.g.* structures with edges of zero length so that distinct vertices are represented by the same point. As atoms can never occupy the same point, such structures are probably less relevant to crystal chemistry.

In Table 3, I summarize the transitivity properties of the natural tilings carrying the nets of this paper. It may be seen that **pcu** is the only flag-transitive such tiling, and indeed it is easy to show that it is the only one in general. It is for this reason that the definition of *regularity* for nets was given a more relaxed condition which corresponded in fact to nets whose natural tilings were vertex-, edge-, face- and tile-transitive (Delgado Friedrichs *et al.*, 2003*a*).

Table 3
Symmetry and transitivity properties of some natural tilings of nets.

Net	Symmetry	Vertex	Edge	Face	Tile	Flag
pcu	$Pm\bar{3}m$	1	1	1	1	1
nbo	$Im\bar{3}m$	1	1	1	1	2
dia	$Fd\bar{3}m$	1	1	1	1	2
srs	$I4_132$	1	1	1	1	10
sod	$Im\bar{3}m$	1	1	2	1	3
hxg	$Pn\bar{3}m$	1	1	2	1	4
crs	$Fd\bar{3}m$	1	1	2	2	4
acs	$P6_3/mmc$	1	1	2	2	6
lcs	$Ia\bar{3}d$	1	1	2	2	10
bcs	$Ia\bar{3}d$	1	1	2	2	16

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