Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Edge-transitive lattice nets

Olaf Delgado-Friedrichs[a,b] and Michael O'Keeffe[a]*

[a]Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287, USA, and [b]Supercomputer Facility, The Australian National University, Canberra, ACT 2600, Australia. Correspondence e-mail: mokeeffe@asu.edu

Received 26 May 2009
Accepted 6 July 2009

Lattice nets have one vertex in the topological unit cell. Some two- and three-periodic lattice nets with one kind of edge (edge-transitive) are described. Simple expressions for the topological density of the two-periodic nets are found empirically. Thirteen infinite families of three-periodic cubic lattice nets and hexagonal, trigonal and tetragonal families are identified.

1. Introduction

A lattice net is here defined as a periodic net that has just one vertex in the repeat unit so that in a maximum-symmetry embedding the vertices fall on a lattice. In the simplest cases the edges correspond to shortest lattice vectors. In other cases the edges may correspond to longer lattice vectors; a simple three-periodic example with RCSR symbol (O'Keeffe *et al.*, 2008) **ilc** was given by Delgado-Friedrichs & O'Keeffe (2005). Nets in which edges do not correspond to shortest distances between vertices are becoming increasingly important in crystal chemistry; see for example the net **tcb** (Delgado-Friedrichs *et al.*, 2005). In this paper attention is focused on lattice nets in which all edges are equivalent (edge-transitive); of course, in lattice nets all vertices are equivalent so these nets are semiregular in the classification of Delgado-Friedrichs *et al.* (2003).

Before considering the periodic structures it is instructive to look at a finite example. If we take a figure with vertices at the positions of the vertices of a regular dodecahedron and second-nearest-neighbor vectors as edges, we obtain a figure of five concentric cubes with each vertex common to two cubes (Fig. 1).[1] As each cube is a 4^3 tiling we could consider the structure as a fivefold 4^3 tiling of a sphere ($\mathbf{S}^2$) and write the two-dimensional vertex figure of the assembly as $(4^3)^2$. The structures we examine next correspond to analogous multiple tilings of the plane ($\mathbf{E}^2$).

2. Two-periodic nets

2.1. Square nets

We consider first nets based on the square lattice with symmetry $p4mm$ with edges from 0,0 to u,v with $u \leq v$. u,v = 0,1 corresponds to the familiar 4^4 net of the square lattice. For all the lattice points to be vertices of a unique net then it is easy to show (see Appendix *A*) that (*a*) u and v must be co-prime (have no common divider other than 1), (*b*) $u + v \neq 2n$ (where n is an integer), (*c*) $u < v$.

The net for $u = 1$, $v = 2$ corresponds to vertices arranged as the nodes of a square lattice and edges corresponding to a knight's moves on a chess board (every chess player knows that the knight can visit every square). It is illustrated in Fig. 2, which illustrates the structure as ten superimposed 4^4 tilings in

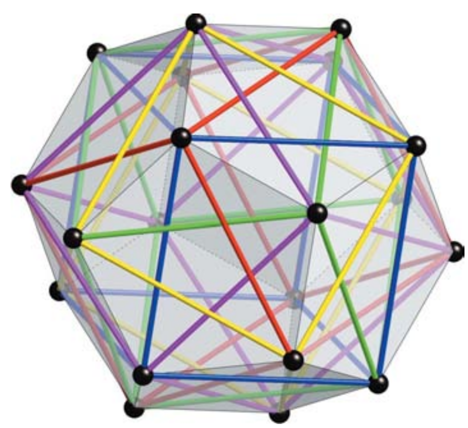

Figure 1
Five concentric cubes (each colored differently) with vertices at the positions of the vertices of a regular dodecahedron.

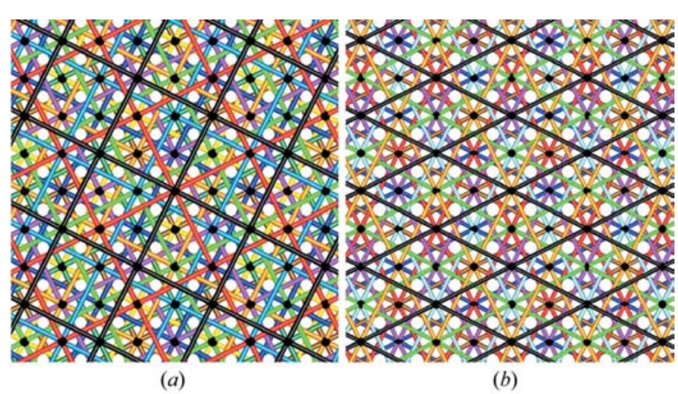

Figure 2
The square net with u,v = 1,2 edges, showing (*a*) square and (*b*) rhomboidal tiles. Separate tilings are outlined in different colors.

[1] For an alternative description of this figure as the uniform polyhedron 3/2 | 3 5, see Coxeter *et al.* (1954).

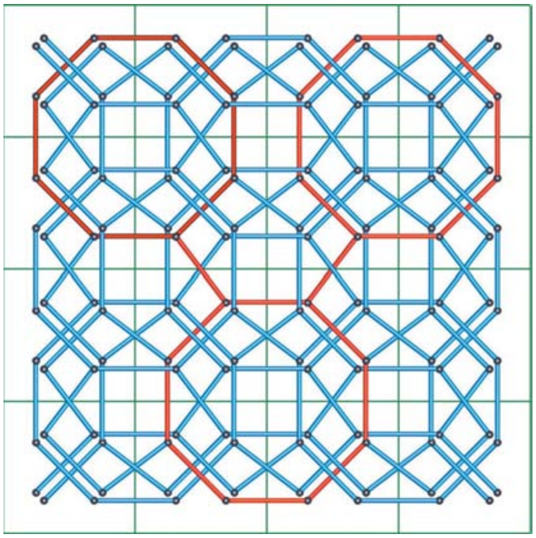

Figure 3
The augmented net of Fig. 2 with three linked octagons shown in red.

which the vertices and edges of the tiles are vertices and edges of the graph. Each vertex belongs to two tilings so the vertex symbol is written as $(4^4)^2$. The tiling is self-dual. Instead of ten square tilings, the same structure could be generated from a superposition of eight 4^4 tilings by rhombic tiles as also shown in Fig. 2. In general the u, v structure will require $2(u^2 + v^2)$ coverings by square 4^4 tilings. Note that the set of vertices and edges of all the tilings are the vertices and edges of just one net (by definition a connected graph).

Considered as a layer, the combinatorial symmetry of the nets is $p4mm$, but there is not a faithful embedding with this symmetry as all edges would be confined to one plane and would intersect. They are therefore examples of nets that are two-periodic but not planar (in the graph-theoretic sense).

Interest in edge- and vertex-transitive nets arises in part from an interest in ways of linking simple symmetrical geometrical shapes by one kind of linker (Delgado-Friedrichs *et al.*, 2007). In the present case, if the vertices are replaced by vertex figures (a process called augmentation; Delgado-Friedrichs *et al.*, 2003), one obtains ways of linking octagons by one kind of link; Fig. 3 shows a fragment of the augmented $u, v = 1,2$ structure. Considered as a three-dimensional structure, the vertex symbol is $8.12_4.12_5$ with the subscripts showing that there are four and five dodecagons that are the shortest rings at two of the angles; the fact that there are more than one indicates that the net is non-planar.

2.2. Hexagonal nets

An analogous family of 12-coordinated structures is based on the hexagonal lattice (3^6) and has symmetry $p6mm$ with edge from 0,0 to u, v. Now the conditions for every lattice point being on a unique single net are (*a*) u, v co-prime, (*b*) $u + v \neq 3n$ (where n is an integer), (*c*) $u < v - u$. A fragment of the net with $u, v = 1,3$ is shown in Fig. 4. The structure is derived from 14 superimposed 3^6 tilings, two of which are emphasized

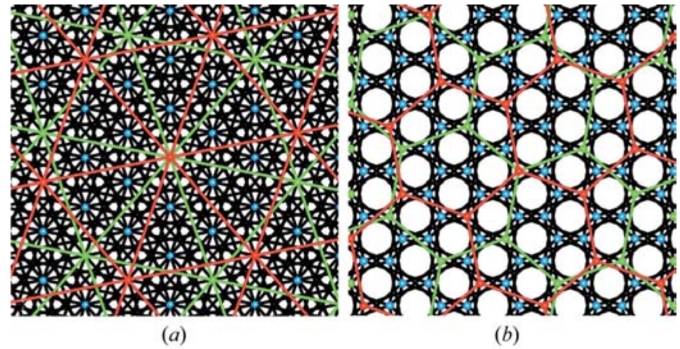

Figure 4
(*a*) The hexagonal net with $u, v = 1,3$ edges. Two sets of triangular tiles are shown in red and green. (*b*) The net dual to that in (*a*) with two sets of hexagonal tiles shown in red and green.

in the figure. In the general case there are $2(u^2 - uv + v^2)$ superimposed tilings with each vertex common to two tilings, so the vertex symbol can be expressed as $(3^6)^2$.

The duals of the hexagonal structures have two vertices in the unit cell and are derived from a superposition of multiple honeycomb (6^3) nets. The dual of the net with $u, v = 1,3$ is also shown in Fig. 4. Each vertex is six-coordinated and belongs to two tilings by regular hexagons; accordingly, the vertex symbol for this net can be written $(6^3)^2$. These are not lattice nets as there are two vertices in the primitive unit cell.

2.3. Coordination sequences

Coordination sequences have been determined for all square lattice nets with $v \leq 15$. It is found in every case that after a certain number, m, of shells the number in the kth shell is given by $n_k = ak + b$ (where a and b are fixed integers), with m generally increasing with the magnitude of u and v (for $u, v = 14,15$, $m = 53$). The cumulative number of topological neighbors of a vertex approaches $ak^2/2$ as $k \rightarrow \infty$; $a/2$ is known as the topological density of the net (O'Keeffe, 1991).

The value of a is of some interest. First it is noted that an elementary result in number theory (*e.g.* Tattersall, 1999) is that u and v, restricted as indicated above, lead directly to the integral solutions of $r^2 + s^2 = t^2$, giving the sides, r, s and t, of primitive Pythagorean triangles. Specifically, $r = v^2 - u^2$, $s = 2uv$, $t = v^2 + u^2$. What is of interest in the present connection is that it is found, by inspection, in every case that $a/4 = r + s = v^2 + 2uv - u^2$.

These last numbers ($a/4$) are also of interest as they are the numbers with prime factors $\pm 1 \pmod 8$ (see *e.g.* http://www.research.att.com/~njas/sequences/A058529).

As for square nets, after a certain number of shells the coordination sequence for hexagonal lattice nets settles down to a linear expression, $n_k = ak + b$. Again there is a connection with triangles with integral edges. If, instead of considering triangles with a 90° angle, Pythagoras had investigated triangles with a 120° angle, he would have found that the length of the longest side, t, is related to the lengths of the shorter sides, r and s, by $r^2 + rs + s^2 = t^2$. Primitive integral solutions of this equation with r, s, t positive are now given in terms of u and v

restricted as in (*a*)–(*c*) above as $r = v^2 - 2uv$, $s = 2uv - u^2$, $t = u^2 + v^2 - uv$.[2] It is found, again by inspection, that $a/6 = r + s = v^2 - u^2$. More than one triangle exists for a given *r*, *s* or *t* but a particular $r + s$ appears to only occur for one u,v so each net appears to have a unique topological density ($a/2$).

These numbers ($a/6$) are also known as the sequence of sides of a primitive equilateral triangle bearing at least one integral cevian that partitions an edge into at least two integral sections (http://www.research.att.com/~njas/sequences/A089025).

3. Three-periodic nets

3.1. Cubic

Clearly, as there is only one vertex in the unit cell, the only possible cubic symmetries are those of the six centrosymmetric symmorphic groups. Consider first a primitive cubic lattice with points that are all possible triplets of integers. Now consider edges from 0,0,0 to u,v,w and their symmetry-related counterparts. For a unique structure, *u*, *v* and *w* must be coprime, and for convenience $u \leq v \leq w$. Then there are three possibilities for the parities of *u*, *v* and *w*:

(*a*) One odd. All lattice points are on the structure which is therefore *P*.

(*b*) Two odd. Only lattice points whose coordinates add up to an even number are selected and these fall on an *F* lattice.

(*c*) Three odd. Only lattice points whose coordinates are all odd or all even are selected and these fall on an *I* lattice.

In the last two cases, using conventional centered cubic cells, the edges are from 0,0,0 to $u/2, v/2, w/2$, and coordinates of points are multiples of 1/2.

Special cases are 0,0,1 → **pcu**, 0,1,1 → **fcu**, 1,1,1 → **bcu** (edges corresponding to shortest vectors of the primitive, face-centered and body-centered cubic lattices, respectively). Apart from these there are 13 different infinite families, listed in Table 1.

As in the two-periodic case, the structures can be considered as being derived from multiple tilings of space, now by parallelepipeds as suggested by Fig. 5. The vertices of the 12-, 24- and 48-coordinated structures belong to 2, 4 or 8 tilings, respectively. Note, however, that, in contrast to the two-periodic case, the tiles cannot be regular (cubes).

The augmented nets provide ways of linking polyhedra by one kind of link. Fig. 6 shows the case of the augmented $Pm\bar{3}m$ 0,1,2 structure (for all edges unity, $a = 1.8614$, $x = 0$, $y = 0.37987$, $z = 2y$) in which truncated octahedra are so linked.

3.2. Hexagonal

There is an infinite family of 24-coordinated edge-transitive lattice nets with symmetry *P*6/*mmm*. Edges are from 0,0,0 to $u,v,1$ where *u* and *v* are subject to the same constraints as for the two-periodic hexagonal nets. There is a special case of a 12-coordinated net with $u = 0$, $v = 1$. These nets have not been investigated in any detail.

[2] Presumably this is a well known result but it has not been found given explicitly.

Table 1
The 13 possibilities for cubic lattice nets by crystal class.

Point group	Edges	Coordination	Lattices
$m\bar{3}m$	$0,v,w$	24	*P*, *F*
	u,u,w	24	*P*, *F*, *I*
	u,v,w	48	*P*, *F*, *I*
$\bar{3}m$	$0,u,w$	12	*P*, *F*
	u,v,w	24	*P*, *F*, *I*

3.3. Trigonal

There is an infinite family of 12-coordinated edge-transitive lattice nets with symmetry $P\bar{3}m1$. Edges are from 0,0,0 to $u,v,1$, where *u* and *v* are subject to the same constraints as for the two-periodic hexagonal nets. The special case of $u = 0$, $v = 1$ is the *P*6/*mmm* net mentioned above.

There is also an infinite family of 12-coordinated edge-transitive lattice nets with symmetry $R\bar{3}m$. Edges are from 0,0,0, to $n + 2/3, 1/3, 1/3$ (*R*-centered hexagonal cell), where *n* is an integer. Again these nets have not been investigated in any detail.

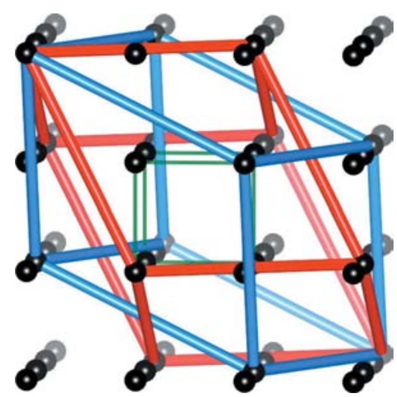

Figure 5
Two tiles (outlined in red and blue) of the $Pm\bar{3}m$ 012 net.

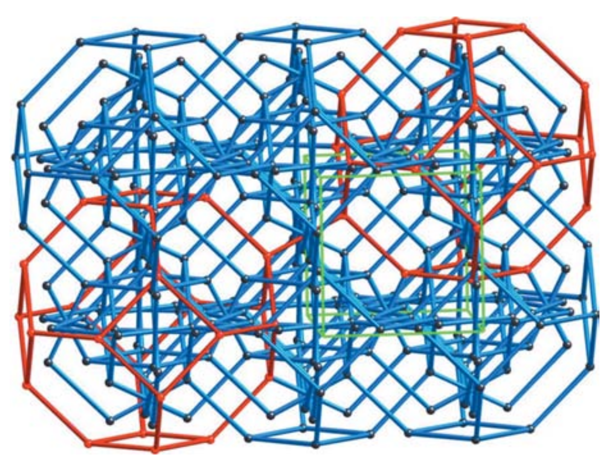

Figure 6
The augmented $Pm\bar{3}m$ $u,v,w = 0,1,2$ net.

3.4. Tetragonal

In contrast to the hexagonal case there appear to be no edge-transitive lattice nets with *P*4/*mmm* symmetry. This is because with primitive tetragonal nets and edge vectors of the type $u, v, 1$ and symmetry equivalents, a path from 0,0,0 to 0,1,0 cannot be produced. This is a direct consequence of the fact that, in the two-periodic square case, to go from 0,0 to 0,1 by a sequence of steps u, v and symmetry equivalents always requires an odd number of steps.

There is, however, a family of 16-coordinated edge-transitive lattice nets with symmetry *I*4/*mmm*. With the conventional (centered) cell the edge vectors are from 0,0,0 to $u/2, v/2, 1/2$ with u and v both odd and $u > v$. Again these nets have not been investigated in any detail.

4. Concluding remarks

This paper calls attention to the fact that there are infinite families of edge- and vertex-transitive nets. We do not claim that the listing here is complete, but we mention that the existence of nets of the types cited have been verified using the program *Systre* (Delgado-Friedrichs & O'Keeffe, 2003; program available at http://www.gavrog.org/). We have focused on lattice nets, but, as the example of $(6^3)^2$ in §2 showed, there are also other families of vertex- and edge-transitive nets. There are in fact two three-periodic edge- and vertex-transitive nets identified in RCSR other than the semiregular nets of Delgado-Friedrichs *et al.* (2003). These are **lcx** and **lcz**; the edges correspond to second-neighbor distances in the most symmetrical embeddings of nets **lcw** and **lcy**, respectively. Clearly there are many more, and one can confidently predict that some at least will become important in crystal chemistry in the future.

APPENDIX *A*
Conditions for *u* and *v* in §2.1

Here we show that the conditions in §2.1 are sufficient to produce a connected graph. One of u, v is odd; for the moment, let u be odd. Now consider the path starting at 0,0.

First step u, v.

Then p pairs of steps u, v; $u, -v$.

Then q pairs of steps $-v, u$; $-v, -u$.

Then $(u-1)/2$ pairs of steps u, v; $-u, v$.

Then $v/2$ pairs of steps $v, -u$; $-v, -u$.

The finishing point is $x, y = (2p+1)u - 2qv, 0$. As u, v are co-prime there are always integers p and q such that $x = 1$ (Tattersall, 1999). If there is a path to 1,0, by symmetry there is a path to 0,1 and there is a path to all lattice points. If v is odd, interchange u and v in the above.

Work on nets and tilings at ASU is supported by the US National Science Foundation (grant number DMR 0804828).

References

Coxeter, H. S. M., Longuet-Higgins, M. S. & Miller, J. C. P. (1954). *Philos. Trans. R. Soc. A*, **246**, 401–450.

Delgado-Friedrichs, O., Foster, M. D., O'Keeffe, M., Proserpio, D. M., Treacy, M. M. J. & Yaghi, O. M. (2005). *J. Solid State Chem.* **178**, 2533–2554.

Delgado-Friedrichs, O. & O'Keeffe, M. (2003). *Acta Cryst.* A**59**, 351–360.

Delgado-Friedrichs, O. & O'Keeffe, M. (2005). *J. Solid State Chem.* **178**, 2480–2485.

Delgado Friedrichs, O., O'Keeffe, M. & Yaghi, O. M. (2003). *Acta Cryst.* A**59**, 515–525.

Delgado-Friedrichs, O., O'Keeffe, M. & Yaghi, O. M. (2007). *Phys. Chem. Chem. Phys.* **9**, 1035–1043.

O'Keeffe, M. (1991). *Z. Kristallogr.* **196**, 21–37.

O'Keeffe, M., Peskov, M. A., Ramsden, S. J. & Yaghi, O. M. (2008). *Acc. Chem. Res.* **41**, 1782–1789.

Tattersall, J. J. (1999). *Elementary Number Theory in Nine Chapters.* Cambridge University Press.