Vertex-, face-, point-, Schläfli-, and Delaney-symbols in nets, polyhedra and tilings: recommended terminology

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We review the various kinds of symbols used to characterize the topology of vertices in 3-periodic nets, tiles and polyhedra, and symbols for tilings, making a recommendation for uniform nomenclature where there is some confusion and misapplication of terminology.

The recent explosion of interest in periodic nets and tilings as applied to the description of the topology of materials such as coordination polymers/networks and metal–organic frameworks (MOFs)[1] points to the need for clarification and agreement on the definition and terminology for certain commonly-used topological indices. Since the early work on coordination networks it has been evident there was need for a common terminology and software to examine the architectures observed and compared with the inorganic anologues (if any)[2] and many cases of wrong assignment of topology appeared in the literature (for example the confusion between NbO and $CdSO_4$ related topologies).[3] For recent applications derived from the geometrical study of periodic nets,[4] see the reticular chemistry approach[5] and many references reported in ref. 1.

In this highlight we review the various kinds of symbols used to characterize the topology of vertices in 3-periodic nets, tiles and polyhedra, and symbols for tilings. We make a recommendation for uniform nomenclature in this area wherever there is some confusion and misapplication of terminology. Some of the symbols in question rely on the identification of cycles and rings in the net so we first recall definitions in this area.[6]

An elementary *cycle* of a graph (net) is a sequence of vertices 1,2,3,…,*n*,1 of the graph such that (1,2), (2,3)…(*n*,1) are edges, and no vertex other than the beginning and ending one occurs more than once in the sequence.

The *sum* of two cycles is the set of edges (and their vertices) contained in just one or the other, but not both, cycles. A straightforward generalization is to the sum of a number of cycles as the set of all edges that occur only an odd number of times in the set of cycles.

A *ring* is a cycle that is not the sum of *two* smaller cycles. Rings have also been called fundamental circuits.[7]

A *strong ring* is not the sum of *any number* of smaller cycles and is necessarily also a ring.[8] See Fig. 1 for some examples from the graph of a cube.

It is appropriate to start with *Schläfli symbols* which have a long history in mathematics.[9] These are of the form {*p*,*q*,*r*…} and a symbol with *n* entries refers to a tiling of an *n*-dimensional space. {*p*} refers to tiling a 1-sphere

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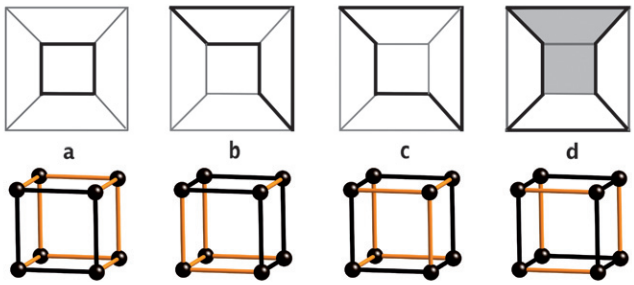

Fig. 1 Cycles, rings and strong rings in a cube shown on top as heavy lines on a Schlegel diagram and below as black edges. (a) a 4-cycle that is a strong ring, (b) a 6-cycle that is the sum of two 4-cycles and hence not a ring, (c) a 6-cycle that is the sum of three smaller cycles but not of two and is therefore a ring (but not a strong ring), (d) an 8-cycle that is the sum of two smaller cycles – a 6-cycle (shaded) and a 4-cycle and hence not a ring.

(a circle) with line segments and is a regular polygon with p sides. $\{p,q\}$ refers to a pattern in which q $\{p\}$'s meet at each vertex. Examples are the five Platonic solids: tetrahedron {3,3}, cube {4,3}, octahedron {3,4}, icosahedron {3,5} and dodecahedron {5,3}, which in this context are tilings of the 2-sphere. {6,3} refers to tiling the plane with hexagons in the familiar honeycomb pattern and {4,4} is the plane tiling by squares. A symbol such as {10,3} refers to tiling the hyperbolic plane by decagons.

A Schläfli symbol $\{p,q,r\}$ refers to a tiling of 3-D space in which r $\{p,q\}$'s meet at an edge. The familiar tiling of 3-D space with cubes has Schläfli symbol {4,3,4}, and {4,3,3} is the hypercube—a tiling of the 3-sphere which requires four dimensions for an embedding in Euclidean space just as a cube (tiling of the 2-sphere) requires 3-dimensions for an embedding in Euclidean space. {4,3,3,4} is a tiling of 4-D Euclidean space by hypercubes; and so it goes.

A *flag* of a tiling of n-dimensional space is an assembly of contiguous 1, 2…n-dimensional components. Thus a flag of a 2-D tiling is the combination of a polygon, an edge of that polygon, and a vertex of that edge; for a 3-D tiling a flag is a polyhedron, a face of that polyhedron, an edge of that face, and a vertex of that edge (Fig. 2). If all flags of a tiling are related by symmetry (*flag transitive*), the tiling is said to be *regular*. Note that flag transitivity implies vertex-, edge- *etc.* transitivity. The Schläfli symbol as here described refers only to regular tilings; for other tilings a Delaney symbol ("extended Schläfli symbol") is needed as discussed below.

For vertices in polyhedra and 2-periodic tilings it is common to use a *vertex symbol* (sometimes also referred to as *vertex type* or *vertex configuration*) to describe the local topology of a vertex.[10] This denotes in cyclic order the size of the polygons meeting at a vertex and for an Archimedean polyhedron or plane tiling (one with one kind of vertex) is of the form *A.B.C*…. Thus the vertices of a cuboctahedron are 3.4.3.4 and those of a truncated tetrahedron are 3.6^2 (short for 3.6.6). Note that adherence to cyclic order is necessary to distinguish the nets of the 2-periodic tilings $3^3.4^2$ and $3^2.4.3.4$ (Fig. 3). Note also that subject to the constraint of cyclic order, smallest faces come first (3.4.3.4 not 4.3.4.3). In this symbolism the vertices of a cube are 4^3. This notation, with obvious extensions to structures with more than kind of vertex—thus a square pyramid is $(3^4)(3^2.4)_4$ giving also the ratio of different vertices—is almost universally used in crystal chemistry, but unfortunately in some influential books called Schläfli symbols.[11] A vertex symbol does not always describe a unique structure; thus there are two distinct polyhedra with vertex symbol 3.4^3 (Fig 4).[10c]

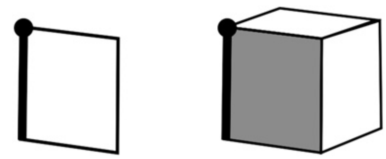

Fig. 2 Left, a flag of a 2-D tiling (a contiguous polygon, edge and vertex). Right a flag of a 3-D tiling (a contiguous polyhedron, polygon, edge and vertex).

O'Keeffe and Hyde[12] point out that the faces of a polyhedron or 2-periodic tiling are rings, and not necessarily shortest cycles. Consider, for example, the plane tiling 4.6.12 (Fig. 5). At the angle containing the 12-sided face there is a shorter 8-cycle that is the sum of a 4-cycle and a 6-cycle. Likewise in the polyhedron 4.6.10 (truncated icosidodecahedron **tid**) at the angle containing the 10-ring there is again a shorter 8-cycle.

But the faces of polyhedra may not be strong rings—consider for example the base quadrangle of a square pyramid which is the sum of four 3-rings (corresponding to the four triangular faces). So the numbers in vertex symbols refer to shortest rings, which in some instances may not be shortest cycles or strong rings—this is important in what follows.

We turn now to our main concern, 3-periodic nets. Wells[13] in his pioneering work placed special emphasis on *uniform* nets (which, unwisely we believe, he also called Platonic). In these the shortest cycle (necessarily also a strong ring in this case) at each angle at a vertex is of the same length. For a 3-coordinated net there are 3 angles at a vertex and for a net of this type, in which the shortest cycles at the angles are all of length p, Wells used the

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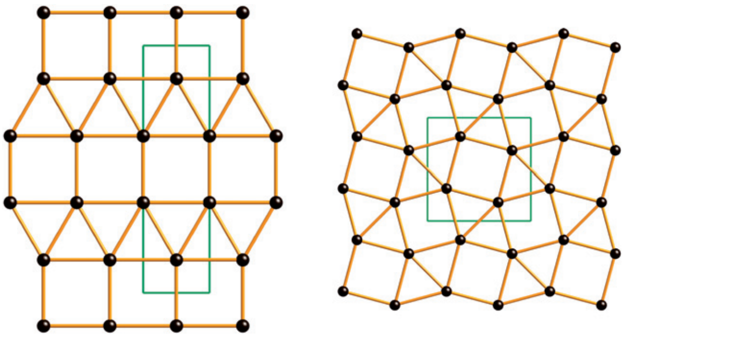

Fig. 3 Two 2-periodic nets of tilings by triangles and squares $3^3.4^2$ (left **cem**) and $3^2.4.3.4$ (right **tts**).

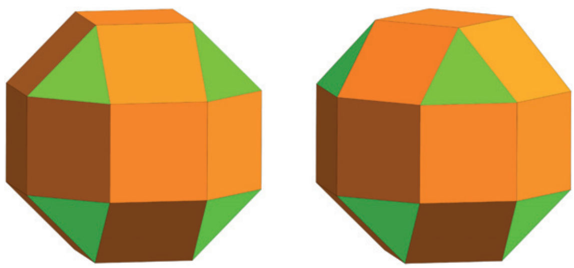

Fig. 4 Left: a rhombicuboctahedron **rco** with all vertices related by symmetry (symmetry O_h) and with vertex symbol 3.4^3 Right: a second polyhedron (symmetry D_{4d}) with two kinds of vertex, but both having symbol 3.4^3. Both polyhedra also have the same face symbol $[3^8.4^{18}]$.

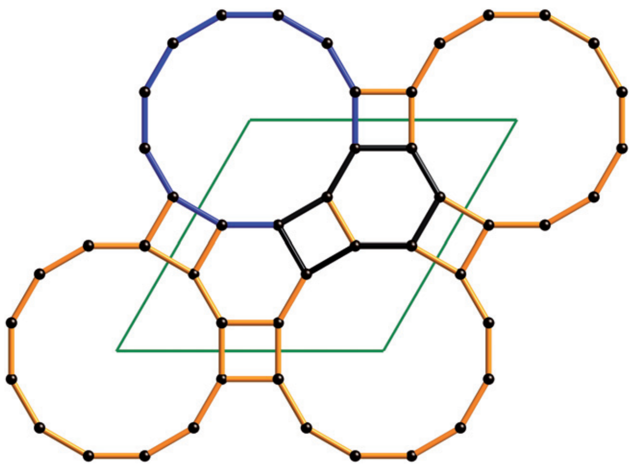

Fig. 5 Part of the vertex-transitive 2-periodic tiling **fxt** with vertex symbol 4.6.12. At an angle containing a 12-ring (blue) a shorter 8-cycle is indicated in black.

symbol (p,3). This was a unfortunate as these symbols have been confused with Schläfli symbols, although Wells himself appears not to have used that term. We emphasize that the Schläfli symbol {10,3} refers to tiling of the hyperbolic plane in which three 10-gons meet at each vertex. The Wells symbol (10,3) refers to a 3-periodic net in which the shortest ring at each angle of the net is a 10-ring. There are several nets known of this type; the one Wells called (10,3)-*a* has fifteen 10-rings meeting at a vertex as Wells was well aware.

For other than uniform nets Wells used a symbol, that he called a *point symbol*, which has superficial resemblance to a vertex symbol, but is really rather different. First we note that for an n-coordinated vertex in a 3-D net there are $n(n-1)/2$ angles and the shortest *cycle* at each angle was identified. The point symbol then was of the form $A^a.B^b\ldots$ indicating that there are a angles with shortest cycles that are A-cycles, b angles with shortest cycles that are B-cycles, *etc.* with $A < B, < \ldots$ and $a + b + \ldots = n(n-1)/2$. So net (10,3)-*a* has point symbol 10^3.

Unfortunately point symbols also became called Schläfli symbols in important papers by Smith[14] although in later work he called them circuit symbols[15] and finally vertex symbols.[16] The description of point symbols as Schläfli symbols has been misused in about 300 articles from RSC and ACS journals since year 2000 (searching the words "Schläfli symbol" as text search from the web pages of the two chemical societies) and persists in recent comprehensive accounts[17–19] and tutorial reviews.[20]

Smith[14] did remark that instead of using point symbols (which, as we have seen, he called Schläfli symbols) it would be better to use symbols involving shortest rings but did not implement that suggestion. O'Keeffe[21] appears to be the first to implement Smith's suggestion and he defined a symbol using shortest rings, which he called "fundamental circuits" as in some earlier practice.[7] This symbol was unfortunately called an "extended Schläfli symbol", or "long Schläfli symbol"[21] although later a *vertex symbol*.[22] These symbols (described next) are also called vertex symbols in the zeolite framework type[23] and RCSR[24] databases and we recommend that that name be adopted.

The vertex symbol devised by O'Keeffe was an attempt to extend the vertex symbol as used for 2-D structures to 3-D ones; hence the use of shortest rings rather than either shortest cycles or strong rings to be consistent with the usage for 2-dimensions. For 3-coordinated vertices with three angles it is of the form $A_a.B_b.C_c$ indicating that there are a shortest rings that are A-rings at the first angle, b shortest rings that are B-rings at the next angle, *etc.* Thus Wells' net (10,3)-*a* has vertex symbol $10_5.10_5.10_5$. To avoid subscripts and superscripts in the computer output of programs like TOPOS[25] this net has point symbol expressed as {10^3} and vertex symbol as [10(5).10(5).10(5)]. If there is only one shortest ring the subscript is suppressed.

In the case of 4-coordinated nets with six angles it was proposed[21] to group the angles in three pairs of opposite angles (those without a common edge). One advantage of this is that then the vertex symbol gives also the information embedded in loop configuration (a graphic symbol commonly used in the

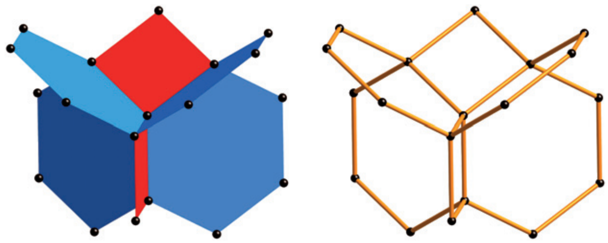

Fig. 6 Two views of the rings meeting at a vertex in the **sod** net.

description of zeolite net topology).[22,23] Subject to this pairing the symbol is written in lexicographic order (smallest numbers first). This is illustrated (Fig. 6) for a vertex of the net **sod** (the symbol is the RCSR symbol[24]), zeolite code[23] **SOD**. Here the vertex symbol is 4.4.6.6.6.6; notice that the first two 4's indicate that the 4-rings are contained in opposite angles. In this case the rings are also shortest cycles so the point symbol is $4^2.6^4$. Sometimes there is no ring contained in an angle and this is indicated by "*". For example, for the important **cds** net the vertex symbol is $6.6.6.6.6_2.*$. However there are always shortest cycles and the point symbol for this net is $6^5.8$. The net of the feldspar framework, RCSR symbol **fel**, has two kinds of vertex, both with point symbol $4^2.6^3.8$; here the vertex symbols are $4.6.4.6.8_2.10_{10}$ and $4.6_2.4.8.6.6_2$. Notice that we can immediately see that the 4-rings share edges.

For higher coordination, no simple grouping of angles is possible and the vertex symbol is such that the smaller rings come first, with angles with the same ring size sorted so that smaller subscripts come first. Thus for the 6-coordinated net with RCSR symbol **pcu-m** the vertex symbol is $3.3.3.3.4.4.4.8_2.8_2.8_3.9_2.9_3.9_4.9_5.9_6$.

Why should we use both point symbols and vertex symbols when vertex symbols are more informative and more in accord with long practice? The answer is, at least in part, that vertex symbols become very cumbersome for nets of high coordination numbers and we suggest they not be used, at least not in a printed form (they can be useful in electronic databases), when coordination numbers exceed 6. The current record for a MOF is 24-coordinated in a structure based on the **rht** topology.[26] The net is 24,3-coordinated and it would take quite a few lines of text to write down the vertex symbol for the 24-coordinated vertex which has $24 \times 23/2 = 276$ angles. However the point symbol for the net is very compact: $(4^3)_8(4^{72}.6^{132}.8^{72})$. A second difficulty with vertex symbols is that they can be tricky to compute for some nets. The problem is that there may be no ring at some angles and one does not know *a priori* the maximum size of cycle to use for testing for the presence of a ring, and a large maximum can lead to very long computing times. On the other hand point symbols, such as the one given above for **rht**, are computed essentially "instantly" with a program such as TOPOS.[25]

For polyhedra and tiles (which may be generalized polyhedra or *cages*) it is generally more informative to use a *face symbol* which is of the form $[A^a.B^b\ldots]$ indicating that there are *a* faces that are *A*-rings, *b* faces that are *B*-rings, *etc.* We suggest using the brackets to avoid possible confusion with point symbols. Most nets admit a *natural tiling*[27] which may consist of tilings by several kinds of tile; here one can give a *signature* (as reported by the program 3dt[28] and TOPOS[25]) that gives the ratio of numbers of tiles. Thus for tilings by tetrahedra and octahedra in which the tiles are in the ratio 2 : 1 the signature may be written $[3^4]_2[3^8]$. Because of the inconvenience of having subscripts and superscripts in computer output, 3dt and TOPOS would write this as 2[3^4] + [3^8].

If we want a symbol to describe tilings in general in the same way as the Schläfli symbol describes regular tilings, there is an *extended Schläfli symbol* available named a *Delaney symbol* by its inventor Andreas Dress, but also known as a *Delaney–Dress symbol* or just a *D-symbol*.[29] In generating a D-symbol, tiles are first dissected into *chambers.* In two dimensions a chamber is a triangle with vertices at the center of a tile, at the center of an edge of that tile, and at a vertex on that edge. In three dimensions a chamber is a tetrahedron with vertices at the center of a tile, at the center of a face of that tile, at the center of an edge of that face, and at a vertex of that edge. Fig. 7 illustrates a tile of the diamond (**dia**) net dissected into chambers. The D-symbol specifies how these chambers are interconnected. The details of deriving and interpreting D-symbols would take us too far afield here. We remark however that their power in systematically enumerating tilings, and hence the nets they carry, has been amply demonstrated.[29] 2-D D-symbols are used extensively by Conway *et al.*[30] (who call them extended Schläfli symbols) and by Ramsden *et al.*[31] The number of different kinds of chamber in a tiling is called the *complexity* by 3dt and reported as *D-size* by RCSR; this is in fact the same as the flag transitivity *i.e.* the number of non-equivalent flags. The only 3-D tiling with D-size equal to 1 is the regular tiling by cubes {4,3,4}.

In conclusion we remark that with the signs of awakening interest of mathematicians in periodic graphs,[32] it is important to use terminology that is as far as possible consistent with long-established mathematical usage. In particular we should reserve the term "*Schläfli symbol*" to its mathematical sense, and refer to the symbols for local topology of vertices in 3-periodic nets as "*point symbols*" (using shortest cycles) and "*vertex symbols*" (using shortest rings) as appropriate. Fig. 8 summarizes these recommendations; note particularly the difference between Schläfli, point, and vertex symbol for **pcu**.

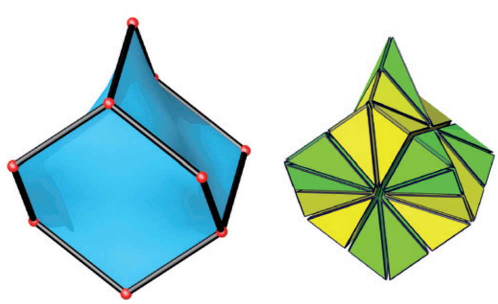

Fig. 7 A tile of the diamond structure (left) dissected into chambers (right).

recommended term	**other terms used (not recommended)**	**applied to**	**comments**	**examples from RCSR**
2-D				
Schläfli symbol		regular tilings		**sql**: {4,4}, **hcb**: {6,3)
Vertex symbol (**VS**)	vertex type	polyhedra and 2-periodic nets	uses shortest rings	**rco**: 3.4^3, **sql**: 4^4, **hcb**: 6^3, **cem**: $3^3.4^2$
Delaney symbol or D-symbol	extended Schläfli symbol	all tilings		
3-D				
Schläfli symbol		regular tilings		**pcu**: {4,3,4}
Vertex symbol (**VS**)	extended Schläfli symbol long Schläfli symbol	3-periodic nets	uses shortest rings	**pts**: $(4.4.8_2.8_2.8_8.8_8)(4.4.8_7.8_7.8_7.8_7)$ **pcu**: 4.4.4.4.4.4.4.4.4.4.4.4.*.*.*
Point symbol (**PS**)	Schläfli symbol circuit symbol vertex symbol	3-periodic nets	uses shortest cycles	**pts**: $4^2.8^4$ **pcu**: $4^{12}.6^3$
Face symbol		polyhedra and cages (tiles)		**rco**: $[3^8.4^{18}]$, **pts**: $[4^2.8^2]+[8^4]$, **pcu**: $[4^6]$
Delaney symbol or D-symbol	extended Schläfli symbol	all tilings		

Fig. 8 Recommended definitions and use of topological indices

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