Acta Cryst. (1972). B**28**, 711

The Geometrical Basis of Crystal Chemistry. XI. Further Study of 3-Dimensional 3-Connected Nets

By A. F. Wells

Department of Chemistry and Institute of Materials Science, University of Connecticut, Storrs, Conn. 06268, *U.S.A.*

(*Received* 16 *March* 1971)

A new uniform 3-dimensional 3-connected net (10,3) with 6 points in the repeat unit, overlooked in a previous study of this family of nets, is described. It represents the basic topology of the crystal structure of the form of B_2O_3 stable under atmospheric pressure. A more detailed study of uniform (10,3) and (8,3) nets is reported.

In part I (Wells, 1954) the author derived and illustrated two 3-dimensional 3-connected nets having 4 points in the (topological) repeat unit and nineteen such nets with $Z_t=6$. Since no systematic way of deriving these nets is known it cannot be claimed that any compilation is exhaustive, but the existence of only two nets with $Z_t=4$ seems certain. Some further 3-connected nets of much greater complexity were added in parts V and VI (Wells, 1955, 1956).

It is convenient to illustrate a net in its most symmetrical configuration, that is, with equal links and with equal interbond angles if this is possible. The unit cell of such a configuration of the net contains Z_c points where Z_c may be, but is not necessarily, a multiple of Z_t. The most symmetrical forms of the two nets with $Z_t=4$ have respectively cubic and tetragonal symmetry, equal links, all interbond angles 120°, and in both cases $Z_c=8$. Both nets are of the type (10,3) or (10^3), that is, the shortest circuits including any pair of links from any pcint are 10-gons (uniform net). In order to characterize and to distinguish between nets with the same value of Z_t further, we may determine the values of x, the number of 10-gons to which each point belongs, and y, the number of 10-gons to which each link belongs. The ratio x/y is equal to $\frac{3}{2}$ for a 3-connected net. It is important to note that the condition for uniformity does not imply that all points are topologically equivalent or that all links are equivalent, as will be evident from the values of x and y in Table 1. For example, in the cubic (10,3) net all the points are equivalent and all the links are equivalent; the net is therefore described by one value of x (15) and one value of y (10). In the tetragonal (10,3) net the points are equivalent but the links are of two kinds, and it is therefore necessary to assign two different values of y. The relation $x/y=\frac{3}{2}$ still holds provided that y is now the weighted mean of the values for the two kinds of link, as noted in part VII (Wells, 1963). For one-third of the links $y_1=8$ and for the remainder $y_2=6$, whence $y_{\text{mean}}=6\frac{2}{3}$, consistent with $x=10$. In addition to these two uniform nets for which $Z_t=4$ three other uniform (10,3) nets will be described later which have $Z_t=8$, 12, and 20 respectively.

The publication of the crystal structure of the normal form of B_2O_3 (Strong & Kaplow, 1968)* has indicated the existence of a new 3-dimensional 3-connected net with $Z_t=6$ which was missed in the earlier derivation of the nineteen nets with $Z_t=6$. Moreover, the new net is a uniform (10,3) net. The structure of B_2O_3 consists of planar BO_3 groups sharing each 0 atom with one other similar group. It is therefore basically a 3-connected net of B atoms linked through O atoms which are simply 2-connected units situated between each bonded pair of B atoms; these O atoms may be omitted when considering the topology of the net. The most symmetrical configuration of the basic net has three equal coplanar links from each point and interbond angles of 120°. It has trigonal symmetry and 6 equivalent points in the unit cell (Fig. 1), so that for this particular net $Z_c=Z_t$. The net is fully described as follows:

Hexagonal axes, $c/a=(3\sqrt{3})/2$; $Z=6$; space group

* See also Strong, Wells & Kaplow (1971).

Table 1. *Uniform* (10,3) *nets*

Net	Z_t	x	$\sum a/y$	y	y_{mean}	Examples
Cubic	4	15	1	10	30/3	H_2O_2, $Hg_3S_2Cl_3$
Tetragonal	4	10	$\frac{3}{2}$	8, 6, 6	20/3	$ThSi_2$, P_2O_5, $La_2Be_2O_5$, $Zn_2Cl_5.H_5O_2$
Trigonal	6	5	3	4, 3, 3	10/3	B_2O_3
			x_{mean}			
Part VI, Fig. 4(*b*)	8	10		8, 6, 6	20/3	α and β resorcinol
Part VI, Fig. 8(*f*)	12	11, 9	10	8, 6, 6	20/3	
Part VII, dual of Fig. 20(*b*)	20	12		7, 8, 9	8	

$P3_212$ (No. 153) with points in 6(*c*), $x=\frac{1}{6}$, $y=\frac{5}{6}$, $z=\frac{1}{18}$. This is a uniform (10,3) net very closely related to the tetragonal (10,3) net, from which it differs in the way in which the zigzag chains are cross-linked. All the points are equivalent and each belongs to five 10-gons ($x=5$), and as in the tetragonal net the links are of two kinds. Those parallel to the *c* axis have $y_c=4$ while those in the zigzag chains have $y_a=3$. Since the former constitute one-third of the total the weighted mean value of y is $\frac{10}{3}$, consistent with $x=5$. This net is clearly the third member of the family of uniform (10,3) nets which have $x=15$, 10, and 5 respectively (Table 1). All 3-D uniform (10,3) nets, of which those in Table 1 are the simplest examples, represent the 3-D homologues of the unique 6-gon 3-connected plane net.

The values of $\sum(a/y)$ are included in the Table in order to draw attention to a remark in the Appendix to part VII which could be misleading, (a_1 *etc.* are the numbers of edges of each 10-gon which are shared between y_1 *etc.* 10-gons.) It is stated there that $\sum(a/y)$ for the tetragonal net is $\frac{3}{2}$, consistent with $p=3$, seeming to imply that $\sum(a/y)$ has this value for all 3-connected nets. In fact, $\sum(a/y)$ is equal to $pn/2x$ (here $15/x$) and its value is therefore different for the first three nets of Table 1.

Because of the remarkably simple relation between the three simplest uniform (10,3) nets and because models were available it seemed worth while to re-examine other uniform nets of this family, three of which are at present known. The first ($Z_t=8$) was illustrated in part I [Fig. 15(*f*)] and in projection in part VI [Fig. 4(*b*)]; it represents diagrammatically the structures of the two crystalline forms of resorcinol. All points in this net have $x=10$, one-third of the links have $y=8$, and the remainder $y=6$, these values being the same as for the simpler tetragonal net. The second of the three more complex uniform nets was illustrated in part VI [Fig. 8(*f*)]. This hexagonal net ($Z_t=12$) has equal numbers of points with $x=9$ and $x=11$, whence $x_{\text{mean}}=10$; it is the only known uniform (10,3) net in which points have different x values. The links have the same y values as those of the preceding net. The last net of Table 1 has not been previously described, but in part VII it was remarked that the duals (reciprocals) of the triangulated 3-D polyhedra (3,p) form a new family of 3-connected nets. The 3-D polyhedra arise by tessellating the surfaces resulting from 'inflating' the links of simple 3-D nets, and the dual of a tessellation having 10 triangles meeting at a point is a surface tessellation in which 3 10-gons meet at each point. Provided that no polygons with fewer than 10 edges arise in the dual (around the 'tunnels') the resulting net is a uniform (10,3) net. An example is the dual of the 6-tunnel (3,10) polyhedron of which a unit was illustrated in Fig. 20(*b*) of part VII. Since the (3,10) tessellation has 6 points in the (topological) repeat unit the (10,3) net has $Z_t=20$. In this complex net all points have $x=12$, but for the first time we find three kinds of link, equal numbers having $y=7$, 8, and 9 ($y_{\text{mean}}=8$).

It may be noted in passing that the relation $\sum y=2x$ is satisfied not only for the net as a whole but for each individual point; this is illustrated later for points in some of the (8,3) nets.

The known uniform nets (7,3), (8,3), (9,3), and (10,3) were summarized in Table 1 of part VI. To these may now be added the duals of certain (3,8) tessellations (3-D polyhedra) of part VII. It seemed worth while to make a further study of the models of the twelve known uniform (8,3) nets. The topological data are summarized in Table 2 and are amplified by the following notes.

(*a*) and (*b*) These are the two closely related nets 5 and 6 of part I. In (*a*) all points lie on 3_1 or 3_2 helices and have $x=4$. The links in the helices have $y=3$ and those joining the helices have $y=2$. In (*b*) all points lie on 3_1 helices, and the x and y values are the same as in (*a*).

(*c*) This net is a tessellation of 8-gons on the surfaces of an assembly of close-packed parallel hexagonal tunnels. It is illustrated in projection in Fig. 2(*c*) of part VI and stereoscopically in Fig. 8(*a*) of that paper. It is closely related to a simple 2-D tessellation and has values of x and y equal to twice those for a plane net.

(*d*) Reference to the projection [Fig. 6(*b*) of part VI] shows that there are 4 points in the 4_1 helix and 4 points in the zigzags joining the helices. For the former points $x=5$ and for the latter $x=3$. For the links in the helices $y=4$ and for the remainder $y=2$:

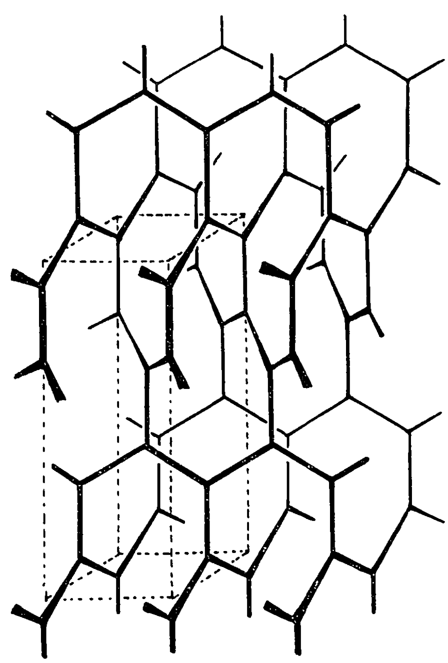


Fig. 1. Uniform (10,3) net; $Z=6$, $x=5$.

Table 2. *Uniform* (8,3) *nets*

	Net		Z_t	x	x_{mean}	y	y_{mean}
(*a*)	Part I,	Fig. 9	6	4		3, 3, 2	$2\frac{2}{3}$
(*b*)		Fig. 10	6	4		3, 3, 2	$2\frac{2}{3}$
(*c*)	Part VI,	Fig. 8(*a*)	6	6		4	4
(*d*)		Fig. 6(*b*)	8	} 3, 5	4	{ 2, 2, 2 and 2, 4, 4	$2\frac{2}{3}$
(*e*)		Fig. 8(*d*)	8				
(*f*)	Part VII,	Fig. 10(*a*) (dual)	8	4, 5	$4\frac{1}{2}$	2, 3, 4	3
(*g*)		Fig. 25	8	6, 7, 8, 9	$7\frac{1}{2}$	3, 4, 5, 6, 7	5
(*h*)		Fig. 26	16	3		2	2
(*i*)		Fig. 27	16	4		3, 3, 2	$2\frac{2}{3}$
(*j*)		Fig. 28	32	3, 4	$3\frac{3}{4}$	2, 2, 2 and 3, 3, 2	$2\frac{1}{2}$
(*k*)		Fig. 29	32	3		2	2
(*l*)		Fig. 30	48	4, 5, 6	5	2, 3, 4, 5	$3\frac{1}{3}$

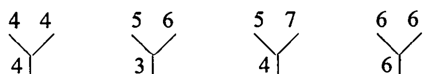
(*e*) This net is very closely related to the preceding one, the x and y values being the same for the two nets; instead of alternate *d* and *l* helices all the helices are of one kind.

The remaining nets of Table 2 are, like the last net of Table 1, duals of surface tessellations (3-D polyhedra) derived in part VII. Their x values range from the lowest possible value (3), the value for a 2-D tessellation, to the highest value ($7\frac{1}{2}$) found for a (8,3) net.

(*f*) The 3-D polyhedral surface on which this tessellation is inscribed corresponds to the tetragonal (10,3) net of Table 1. Additional 8-gons around the tunnels result in equal numbers of points having $x=4$ and 5, whence $x_{mean}=4\frac{1}{2}$. The y values for links meeting at the two kinds of point are

$x=4$ $x=5$

(*g*) This net is closely related to (*f*), being derived from the cubic (10,3) net by inflating the links and inscribing the tessellation on the surface so formed. In contrast to (*f*) there are numerous 8-gons around the tunnels in addition to those on the surface. In fact this net is, from the topological standpoint, the most complex one yet studied. Of the 8 points in the (topological) repeat unit, one has $x=6$, three have $x=7$, three have $x=8$, and one has $x=9$, giving $7\frac{1}{2}$ as the weighted mean. The y values associated with the four kinds of non-equivalent point are:



$x=6$ $x=7$ $x=8$ $x=9$

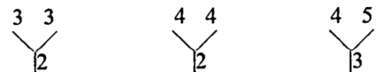
(*h*) The nets (*h*) and (*k*) are of special interest as having values of x and y the same as for a plane tessellation, namely, 3 and 2. In the duals of the 3-D polyhedra of part VII this arises if there are no 8-gon circuits around the tunnels. In this net there are numerous 9-gons but no 8-gons other than those on the surfaces of the tunnels.

(*i*) This net is derived from a 3-D polyhedron in which four coplanar tunnels meet at each point of the underlying net. In the derived (8,3) net all points have $x=4$.

(*j*)This and the succeeding net are derived from 6-tunnel 3-D polyhedra. In (*j*) 8 points in the repeat unit have $x=3$ and the other 24 have $x=4$, whence $x_{mean}=3\frac{3}{4}$. One half of the links have $y=2$ and the remainder have $y=3$.

(*k*) In this net, as in (*h*), there are no 8-gons other than those on the surface of the original polyhedron, and therefore $x=3$.

(*l*) Of the 48 points in the topological repeat unit 8 have $x=4$, 32 have $x=5$, and 8 have $x=6$, giving a weighted mean value of x equal to 5:



$x=4$ $x=5$ $x=6$

References

Strong, S. L. & Kaplow, R. (1968). *Acta Cryst.* **B24**, 1032.
Strong, S. L., Wells, A. F. & Kaplow, R. (1971). *Acta Cryst.* **B27**, 1662.
Wells, A. F. (1954). *Acta Cryst.* **7**, 535.
Wells, A. F. (1955). *Acta Cryst.* **8**, 32.
Wells, A. F. (1956). *Acta Cryst.* **9**, 23.
Wells, A. F. (1963). *Acta Cryst.* **16**, 857.