imately in a constant ratio. This can most simply be explained by the assumption of a difference in inclination of the chains along the edges of the concave angle; in this case formula 3·2·2·(4) applies.

3·6. *Discussion*

It is evident that the mechanism here proposed for *polysynthetic twinning* is in fact equivalent to the one for *polytypism*. It would as a consequence be justified, in a certain sense, to call the crystal of Fig. 5(*a*) a polytype. For the β-form of the *n*-alcohols the relation between twinning and polytypism (Part I) is even more striking: twin formation as well as polytypism are both direct consequences of the different stacking possibilities of successive bimolecular layers.

The author is grateful to Prof. W. Dekeyser for the stimulating interest taken in this work, which is part of a research programme (Centre pour l'étude de l'État Solide) supported by I. R. S. I. A. (Institut pour l'encouragement de la Recherche Scientifique dans l'Industrie et l'Agriculture).

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The Geometrical Basis of Crystal Chemistry. Part 6

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(*Received* 4 *July* 1955)

In Part 1 it was stated that the only three-dimensional 3-connected nets of the n^3 type are 8^3, 9^3 and 10^3, and that there are two different nets corresponding to the symbol 8^3 and similarly for 10^3. It is now shown that there are also nets 7^3, as well as further nets 8^3, 9^3 and 10^3. These new nets are derived in a systematic way and illustrated.

Three-dimensional 3-connected nets related to the regular solids

Part 1 (Wells, 1954*a*) dealt with the systematic derivation of periodic three-dimensional 3-connected nets containing 4 or 6 points in the repeat unit. It was noted that certain of these nets are related to the three regular solids which have three edges (faces) meeting at each vertex. The symbols 3^3 (tetrahedron), 4^3 (cube), and 5^3 (pentagonal dodecahedron) indicate that three 3-gons, 4-gons, or 5-gons respectively meet at each vertex. The next number of this n^3 series is the plane hexagonal net (6^3), and it was remarked that the series is continued by the three-dimensional nets 8^3, 9^3 and 10^3. Some of these were described and illustrated in Part 1, where it was stated: 'It would seem, though this point has not been proved, that the only nets of the n^3 type are 8^3, 9^3 and 10^3, and that there are two different nets corresponding to the symbol 8^3, and similarly for 10^3'. The purpose of the present paper is to show that, in fact, there are also nets 7^3, as well as further nets 8^3, 9^3 and 10^3, so that the series is complete from 3^3 to 10^3.

We shall require (1) that each point is connected to three others, and (2) that there must be a configuration of each net in which the distance between any pair of unconnected points is greater than the distance between any pair of connected points. Since we are interested in the three-dimensional 'homologues' of the 3-connected regular solids we shall also insist (3) that there must be a possible configuration of a net having all links equal in length. (This condition was not explicitly laid down in Part 1; it is related to (2) above, and it is possible that it has been implicitly assumed in Parts 1 and 2.)

In the systems 3^3, 4^3 and 5^3, and the strictly planar regular form of 6^3, it is sufficient to describe the polygons as equilateral *or* equiangular, since a regular plane polygon has both these properties, and all the polygons in a given system are congruent. In the three-dimensional nets we shall consider here the polygons are not plane, and it is possible to have configurations

Table 1. *Three-dimensional 3-connected n^3 nets*

Figure	n^3	All points equivalent	All n-gons congruent	All interbond angles 120°	Illustration
3(*a*); 4(*a*)	10^3	*	*	*	Part 1, Fig. 7 (Net 1)
2(*a*); 5(*a*), (*c*)	10^3	*	*	*	Part 1, Fig. 8 (Net 2)
3(*b*)	8^3	*	*	*	Part 1, Fig. 9 (Net 5)
3(*c*)	8^3	*	*	*	Part 1, Fig. 10 (Net 6)
2(*c*)	8^3	—	*	*	Fig. 8(*a*)
4(*b*); 5(*b*), (*d*)	10^3	*	—	—	Fig. 8(*b*)
6(*a*)	7^3	—	*	—	Fig. 8(*c*)
6(*d*)	7^3	—	*	—	Not illustrated
6(*b*)	8^3	—	*	—	Not illustrated
6(*e*)	8^3	—	*	—	Fig. 8(*d*)
5(*f*)	9^3	—	—	*	Part 1, Figs. 18 and 19
7(*c*)	9^3	—	—	—	Fig. 8(*e*)
6(*c*)	10^3	—	—	—	Fig. 8(*f*)

Table 2. *Details of the five most symmetrical n^3 nets*

Figure	n^3	Symmetry	Space group	Equivalent position	Conditions
3(*a*); 4(*a*)	10^3	Cubic	$I4_13$	8(*a*)	—
2(*a*)	10^3	Tetragonal	$I4_1/amd$	8(*e*)	$c/a = 2\sqrt{3}$; $z = 1/12$
3(*b*)	8^3	Rhombohedral	$R\bar{3}m$	6(*f*)	$c/a = \sqrt{6}/5$; $x = 2/5$ (for 18(*f*) in hexagonal cell)
3(*c*)	8^3	Hexagonal	$P6_222$	6(*i*)	$c/a = 3\sqrt{2}/5$; $x = 2/5$
2(*c*)	8^3	Hexagonal	$P6_3/mmc$	2(*c*)+6(*h*)	$c/a = 2/5$; $x = 7/15$

of a particular n-gon which are both equilateral and equiangular but not congruent (compare the 'chair' and 'boat' forms of cyclohexane). We may therefore expect to find three-dimensional nets in which the polygons, in addition to being equilateral, are *either* equiangular *or* congruent, or *both* equiangular *and* congruent. A further complication is the possibility that the polygons in a particular net are not congruent but enantiomorphic. When classifying the n^3 nets we shall for simplicity group together congruency and enantiomorphism. Finally, the points in each of 3^3, 4^3, 5^3 and 6^3 are all equivalent, being related by the symmetry elements of a point group or plane group. We shall find that the points of some of the three-dimensional nets are equivalent, i.e. the net is formed by connecting up one set of equivalent points of a particular space-group, whereas this is not so for other n^3 nets.

The most symmetrical three-dimensional n^3 nets we could hope to find would have an equilateral configuration in which

(*a*) all points are equivalent,
(*b*) all n-gons are congruent,
(*c*) the arrangement of links at each point is the most symmetrical possible, i.e. inter-bond angles of 120°.

It appears that only four nets satisfy all these conditions, namely, the 10^3 Nets 1 and 2 and the 8^3 Nets 5 and 6 of Part 1. One net has been found satisfying (*b*) and (*c*), and others satisfying only one of the conditions (*a*), (*b*) or (*c*). It is probable that the enumeration of nets n^3 in these groups is complete but this is not certain for the less 'regular' nets which do not satisfy any of the above conditions. The thirteen n^3 nets derived in this paper are listed in Table 1 and geometrical data for the first five are given in Table 2.

It seems fairly certain that the value of n in n^3 nets cannot exceed 10, though this point still awaits proof. The peculiar uncertainty as to the numbers of nets of the various types (and as to the maximum value of n) arises because there are no equations for three-dimensional nets comparable with the very simple equations for plane nets which relate to the proportions of polygons of different kinds. This may be compared with the fact that an infinite array n_∞ of points on a plane may be joined up to form $2n_\infty$ triangles whereas there is no corresponding expression for the number of tetrahedra formed from an infinite three-dimensional array of points (Laves, 1931).

The derivation of n^3 nets

In Part 1 periodic three-dimensional 3-connected nets were derived by introducing 2-connected points on the links of two-dimensional 3-connected nets and joining up the layers through these points which thereby become 3-connected. Here it will be convenient to adopt a different procedure since we are interested only in nets of a particular type (n^3) and not in nets containing assortments of polygons of many different kinds.

There are three regular two-dimensional nets, each having all points connected to the same number of others and having all polygons with the same number of sides (Fig. 1(*a*)–(*c*)). An operation involving translation perpendicular to the plane of the net may be introduced at some or all of the points of such a net. The operation used in crystallography is the screw axis n_m, and we shall indicate the heights of points as multiples of c/n where c is the repeat distance along the screw axis, as at (*d*) for 3_1. It is found that the only screw axes leading to 3-connected nets are 3_1 (or 3_2), 4_1 (or 4_3), 6_1 (or 6_5) and 6_2 (6_4). (The axes 4_2 and 6_3 give 5-connected nets.) It is, of course, necessary to consider combinations of left- and right-handed screw axes.

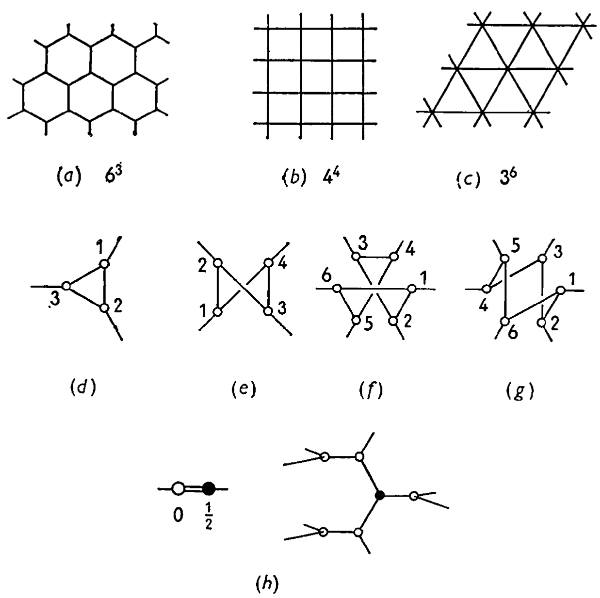

Fig. 1.

Instead of the screw axis 4_1 we could use the operation shown in Fig. 1(*e*), which may be written 4_{12}, and in addition to the normal sixfold screw axes there are operations of a similar kind, of which the simplest are the enantiomorphic pairs 6_{13} (and 6_{53}) and 6_{144} (and 6_{522})—see Fig. 1(*f*) and (*g*). These operations are mentioned because one particular n^3 net (Fig. 5(*f*)), which was derived in Part 1 by joining up layers, does not appear to arise in the systematic treatment based on screw axes. It does, however, arise if the operation 4_{12} is used, as shown later.

Instead of introducing screw axes at the points of the plane nets we may introduce 2_1 axes perpendicular to the plane of the net and passing through the mid-points of some or all of the links, as shown in plan and elevation in Fig. 1(*h*). The resulting three-dimensional net then contains the points of the original plane net, and therefore only 6^3 gives 3-connected three-dimensional nets when treated in this way. We may, however, introduce 2_1 axes in this way along the links of 4^4 or 3^6 *in addition to* 4_1 or 6_1 axes at the points of the net.

2_1 *axes only*

The plane 6^3 net arises by joining up sets of points generated by parallel 2_1 axes (Fig. 2(*a*)). Three-dimensional nets are formed if 2_1 axes are introduced at the mid-points of some or all of the links of 6^3, the direction of translation of the axis being perpendicular to the plane of the net. Of the three possibilities shown in Fig. 2 only (*a*) and (*c*) lead to n^3 nets. The net (*a*) is a system of 10-gons and is Net 2 of Figs. 6 and 8 of Part 1. (The net (*b*) consists of points $8^2.10$ and 8.10^2.) The net (*c*) is illustrated in Fig. 8(*a*).* Both the nets (*a*) and (*c*) have in their most symmetrical configurations congruent, equiangular, polygons, and may be built with inter-bond angles of 120°. The net (*a*) is one of the two simplest three-dimensional 3-connected nets, having only 4 points in the simplest unit cell. (The data in Table 2 refer to the most symmetrical configuration of the net.)

3_1 *axes and the plane net* 6^3

The simplest nets arise by erecting 3_1 axes at either one-half or all of the points (Fig. 3). In projection, the points generated by the 3_1 axes appear as triangles, as indicated in Fig. 1(*d*). The net (*a*) is the Net 1

* An asterisk indicates that the net is illustrated later by a pair of stereoscopic photographs.

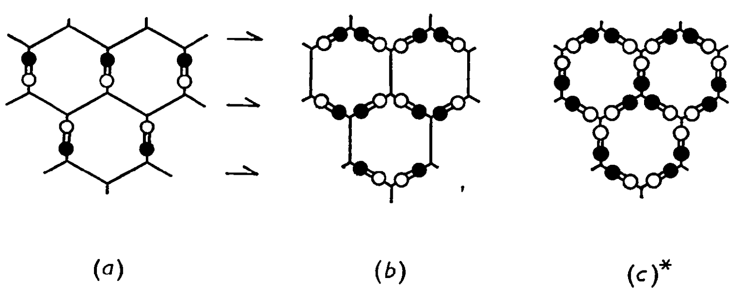

Fig. 2.

of Figs. 6 and 7 of Part 1 and contains congruent, equiangular 10-gons. It has only 4 points in the simplest unit cell and in its most symmetrical configura-

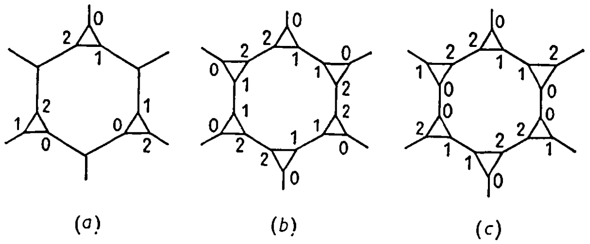

Fig. 3.

tion has cubic symmetry (see Table 2). When screw axes are erected at all points of 6^3 there are two possibilities, the axes being either alternately 3_1 and 3_2 or all 3_1 (or 3_2). In the latter case the net is enantiomorphic (Fig. 3(*c*)). Both of these 8^3 nets, which are Nets 5 and 6 of Figs. 9 and 10 in Part 1, can be realized with congruent, equiangular 8-gons.

4_1 *axes and the plane net* 4^4

The two simplest possibilities are shown in Fig. 4, the net (*a*) being the same as that of Fig. 3(*a*). The net of Fig. 4(*b*) is also an assembly of 10-gons, and has

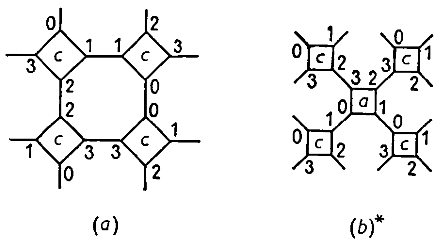

Fig. 4.

been illustrated in Fig. 15 of Part 1. It arises by joining up the equivalent positions 8(*e*) of the space group *Pnna*.

6_1 *axes and the plane net* 3^6

It is found impossible to construct nets analogous to those of Figs. 3 and 4 by erecting 6_1 axes at the points of the plane net 3^6, but 6_2 axes give the very interesting Net 21 of Figs. 4(*b*) and 13 of Part 1, in which the smallest polygons are 12-gons. However, this is not an n^3 net but has the symbol $12^2.14$; nets 12^3 are apparently not possible.

The use of the operation 4_{12}

This may be combined with any plane net containing 4-connected points, the simplest possibilities being those of Fig. 5(*a*) and (*b*). The first is the 10^3 net of Fig. 2(*a*); the second is the 10^3 net of Fig. 4(*b*).

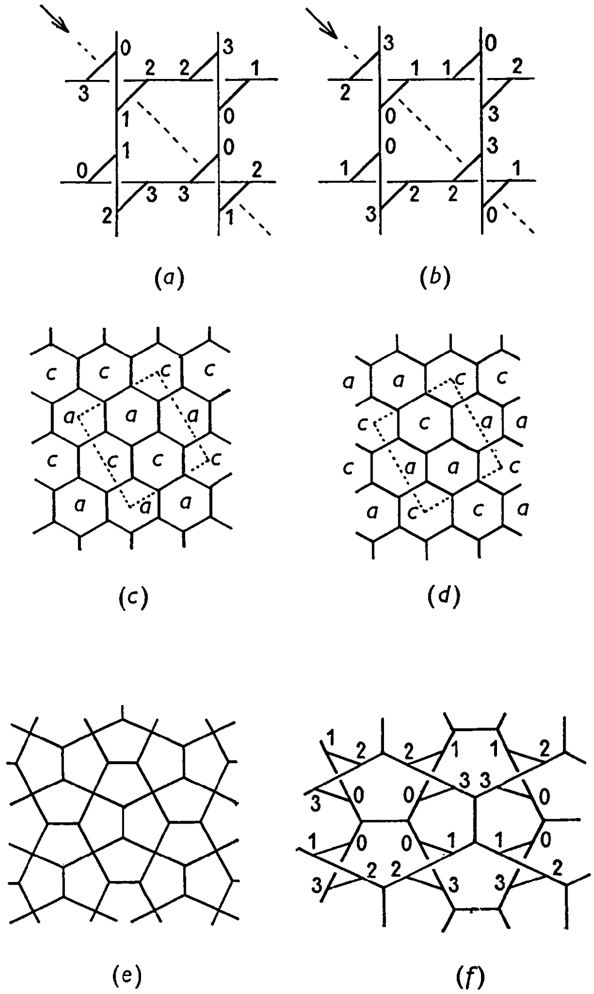

Fig. 5.

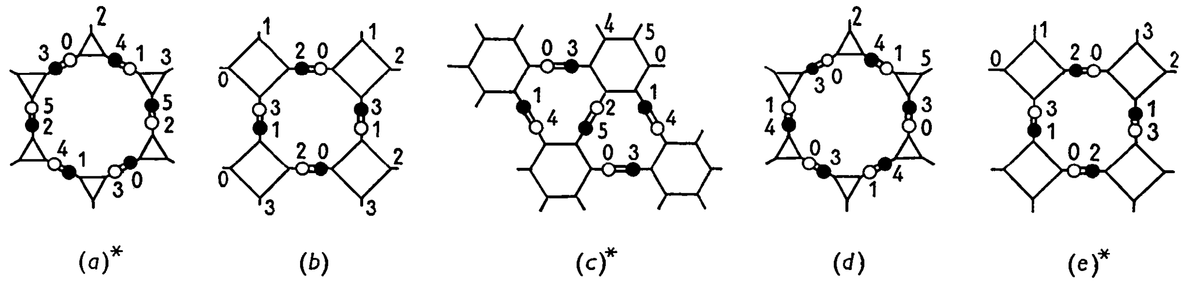

Fig. 6.

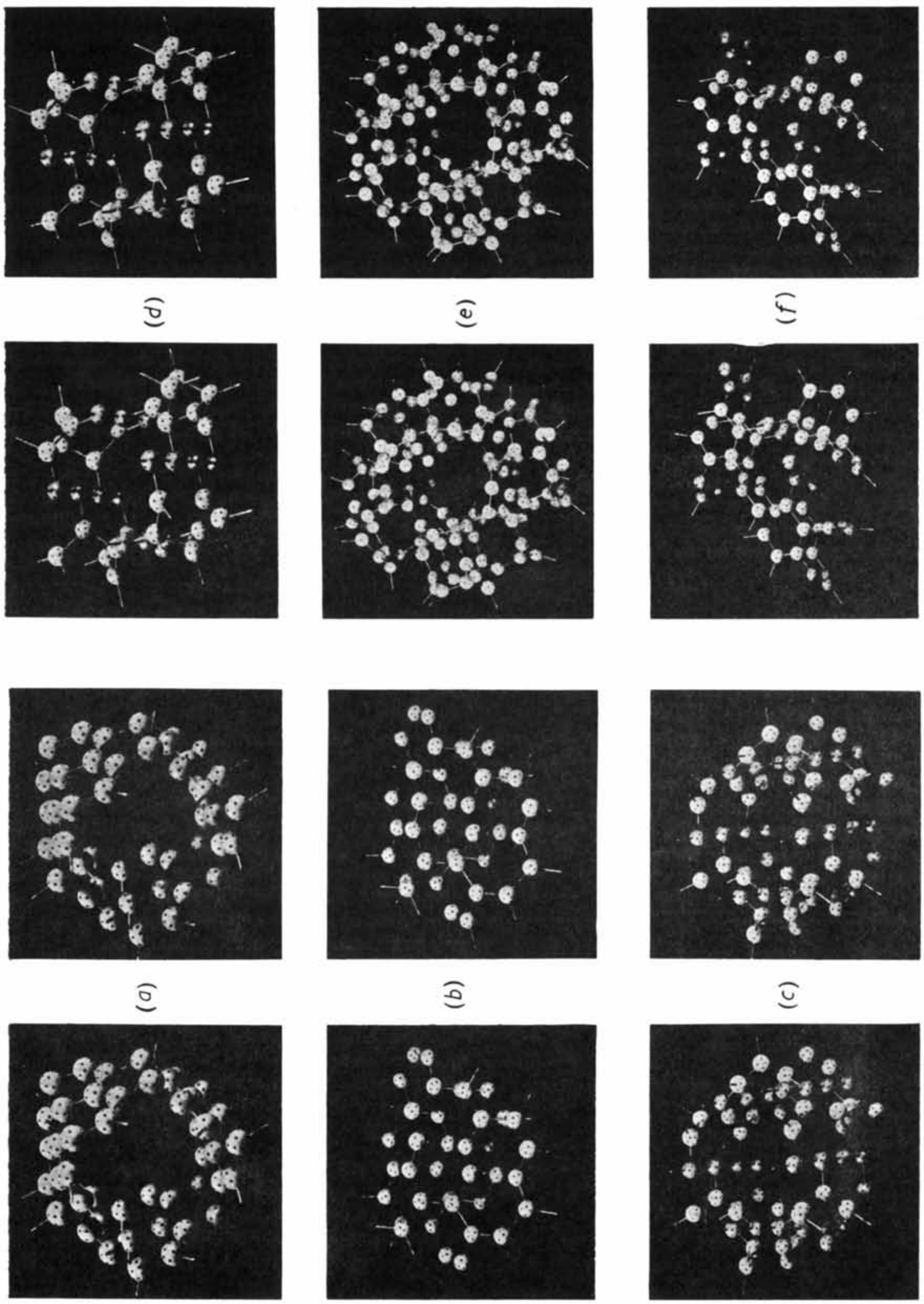

Fig. 8.

It is interesting that in addition to having the very similar projections of Fig. 5(*a*) and (*b*) these nets also project as the same plane net (6^3) along the directions of the arrows (Fig. 5(*c*) and (*d*)). No new n^3 nets arise by combining 4_{12} with the (3+4)-connected nets of Fig. 3(*a*), (*b*) and (*c*) of Part 2 (Wells, 1954*b*), but the plane pentagonal net of Fig. 5(*e*) gives the rhombohedral 9^3 net of Figs. 18 and 19 of Part 1, as shown in Fig. 5(*f*).

Combinations of 2_1 *with* 3_1, 4_1 *or* 6_1 *axes*

In addition to erecting 3_1, 4_1 or 6_1 axes at the points of the three regular plane nets we may also add 2_1 axes at the mid-points of the links, all the screw axes being parallel to one another and perpendicular to the plane of the 6^3, 4^4, or 3^6 net. Since the juxtaposition of two parallel screw axes n_1 and m_1 gives minimum circuits of n_1+m_1+2 we may expect to find nets with respectively 7-, 8- and 10-gon circuits. (The case, $n_1 = m_1 = 2_1$, corresponds to the plane hexagonal net, with 6-gon circuits.) The simplest possibilities are the enantiomorphic nets in which the axes at the points of the nets are all 3_1, all 4_1 or all 6_1 (Fig. 6(*a*), (*b*), (*c*)). Of these new nets, the first two have congruent 7-gons and 8-gons respectively, but the nets cannot be constructed with inter-bond angles of 120°. In the 10^3 net of Fig. 6(*c*) the polygons can neither be congruent nor have angles of 120°. In addition to these enantiomorphic nets, in which all the screw axes (other than 2_1) are either left- or right-handed, there are nets corresponding to the first two in which screw axes of opposite sense alternate (Fig. 6(*d*) and (*e*)). There is no net (corresponding to that of Fig. 6(*c*)) in which 6_1 and 6_5 alternate, because the polygon in the original plane net (3^6) has an odd number of sides.

Combinations of 3_1+4_1, 3_1+6_1, *and* 4_1+6_1

The juxtaposition of these axes in parallel orientation might be expected to give three-dimensional nets with 9-, 11- and 12-gon circuits. Since it is necessary that two similar screw axes should never be adjacent (for this combination would give a different polygon) the plane nets required are those formed by connecting up *p*- and *q*-connected points (*p* and *q* being two of the numbers 3, 4 and 6) so that each *p*-connected point is connected only to *q*-connected points, each of the latter being connected only to *p*-connected points. The required (3+4)- and (3+6)-connected plane nets are shown in Fig. 7(*a*) and (*b*) and the projections of the three-dimensional nets in Fig. 7(*c*) and (*d*). There is no corresponding (4+6)-connected plane net. (For the maximum ratio of links to points in a plane net the polygons should clearly have the minimum number of sides, as in 6^3, built of triangles. To avoid adjacent points of the same kind in a mixed (*p*+*q*)-connected net the polygons must have even numbers of sides, so that the minimum is 4. This is reached in Fig. 7(*b*), with an average of 2 links per point, whence it follows that a (4+6)-connected net of this kind is impossible. An interesting corollary is that a compound A_2X_3 in which A is to be 6-coordinated and X 4-coordinated cannot have a simple layer structure; examples of *three-dimensional* (4+6)-connected nets are the structures of α-Al_2O_3, Mg_3P_2 and cubic Mn_2O_3.)

In Fig. 7(*c*) it is necessary that the three- and four-fold screw axes are all left- or all right-handed in order to avoid 8-gons. In this 9^3 net there are non-congruent 9-gons, and these polygons cannot have

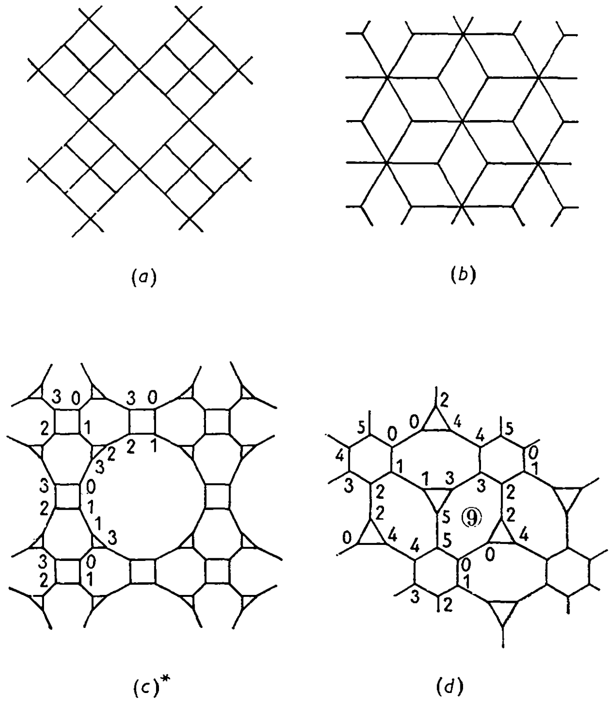

Fig. 7.

angles of 120°. When we attempt to build an 11^3 net from (*b*), as at (*d*), we find that it is impossible to avoid 9-gons, and the net is not of the n^3 type. Although the circuit involving 6_1 and 3_1 is necessarily an 11-gon it is possible to avoid the 6_1 in the circuit marked ⑨. It seems safe to assume that for a similar reason it will be impossible to find a net 12^3.

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