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Three-Dimensional Nets and Polyhedra

A. F. Wells

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Foreword to the series

In the 1920's comparatively few people paid much attention to the branch of science known as crystallography, and the only journal devoted to it was circulated to a few hundred subscribers, mostly libraries. Scientists in the classical disciplines hardly recognized crystallography as a science, although each apparently regarded it as a small segment of his own field. No American university boasted a professor of crystallography and any instruction given was adjunct to mineralogy. Nevertheless, papers of interest to crystallographers appeared in journals of mineralogy, physics and chemistry, although not in large numbers. In those days one might claim to have an all-around acquaintance with crystallography because he was able to keep up with the literature.

This is no longer true. In the period between the first and second world wars, science flourished, and scientists not only published more papers, but an increasing proportion of them dealt with solid materials. It was inevitable that the chemists, metallurgists, physicists and ceramists should make increasing use of crystallographic theory and methods, that the journals of many fields should publish more papers of crystallographic interest, and that new journals devoted to crystallography and the "solid state" should arise. Soon the abstracting journals contained hundreds of titles of crystallographic interest with each issue, and now few of us can keep even reasonably well informed about the many aspects of the science of crystals, to say nothing of keeping abreast of the advances in all these aspects. Not only is it out of the question to keep up with the mass of literature that is turned out, but it is even a little difficult to maintain contact with all the advances in one's own specialty. Accordingly, we are tending to become parochial.

In the words of Warren Weaver ". . .the volume of the appreciated but not understood keeps getting larger and larger." In order to improve this condition to some extent we need the services of those who, having become authorities in some segments of our field, are willing to integrate their understandings of these limited regions. With such help many of us can gain a sufficient understanding of matters whose original literature we have neither the time nor the inclination to study. Such writings exist in several fields, but none, to date, in crystallography. It is to fill this need that the Wiley Monographs in Crystallography are offered.

MARTIN J. BUERGER

Preface

The following account represents an attempt to summarize the results of studies of three-dimensional systems of linked points, a subject that has interested the author during the past 20 years. Some of the results have been published as a series of papers in *Acta Crystallographica* entitled "The Geometrical Basis of Crystal Chemistry," Parts 1 to 12, 1954–1976. * During the past few years many new 3D nets and some new 3D polyhedra have been derived, but it has become obvious that the publication of further papers in this series is not a satisfactory way of describing the work. So many cross-references to earlier papers became necessary that the later papers tended to be unintelligible unless the reader had all the previous papers readily available and also had the patience to follow the sometimes devious lines of thought of the author. This book summarizes the earlier work and includes descriptions and illustrations of many new systems that have not been described.

The obvious and simple relation of much of this work to the Platonic solids and to simple Euclidean geometry makes it surprising that geometers have not explored this field during the past two thousand years or so. The reason is presumably that the study of *periodic* three-dimensional systems of points, lines, and volumes, seems to have been left for the most part to the crystallographer, despite notable contributions from a small number of mathematicians interested in three-dimensional geometry.

Apart from their intrinsic interest, and beauty, as examples of the logical extension of classical Euclidean geometry, three-dimensional systems of connected points are clearly very much a part of structural chemistry in its widest sense. The relation of the crystal structures of compounds such as zeolites and clathrate hydrates to space-filling arrangements of polyhedra is evident and has long been recognized; it is also well known that many silicates and aluminosilicates have structures based on vertex-sharing tetrahedra placed at the points of various 4-connected nets. The relation of 3-connected [and (3, 4)-connected] nets to a (smaller) number of crystal structures has

* "The Geometrical Basis of Crystal Chemistry," Parts 1–12, *Acta Crystallogr.*, pt. 1, 1954, **7**, 535; pt. 2, 1954, **7**, 545; pt. 3, 1954, **7**, 842; pt. 4, 1954, **7**, 849; pt. 5, 1955, **8**, 32; pt. 6, 1956, **9**, 23; pt. 7 (with R. R. Sharpe); 1963, **16**, 857; pt. 8, 1965, **18**, 894; pt. 9, 1968, **B24**, 50; pt. 10, 1969, **B25**, 1711; pt. 11, 1972, **B28**, 711, pt. 12, 1976, **B32**, 2619.

become apparent more recently. It is still unusual, however, for the crystallographer to describe a structure in terms of its basic topology. Such a description not only provides a simple and elegant way of representing the structure but it emphasizes relations between structures that are not always apparent from conventional descriptions in terms of space groups and sets of equivalent positions.

It has not been easy to write a connected account of this work, and some of the text may be difficult to follow when the reader is assisted only by line drawings and pairs of stereoscopic photographs. In this subject models are indispensable, and the author has had the advantage of studying models of most of the systems described. Models of many of the 3D polyhedra can be constructed quite easily from strips of thin card or plastic, and many 3D nets may be built from the plastic tubing and metal "valence clusters" that are commercially available.

A. F. WELLS

Storrs, Connecticut
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I acknowledge the contribution to the earlier work on 3D polyhedra of R. R. Sharpe (who also constructed some of the models of 3-connected nets) and the help received from my colleagues Profs. M. J. Buerger, B. L. Chamberland, and R. Schor at the University of Connecticut. I also wish to express my gratitude to the University of Connecticut Research Foundation for a grant that together with much practical assistance from Dr. J. Haberfeld made possible the stereoscopic photography of many new models.

A. F. W.

Three-dimensional nets and polyhedra

Contents

PART I

Three-dimensional nets

1

Introductory

The present study began by attempting to answer two questions. Only five simple convex polyhedra (n, p) have all their faces of the same kind (n-gons) and the same number (p) meeting at each vertex:

		p $\longrightarrow$		
	(3, 3) Tetrahedron	(3, 4) Octahedron	(3, 5) Icosahedron	(3, 6)
n	(4, 3) Cube	(4, 4)		
	(5, 3) Pentagonal dodecahedron	Plane nets		
	(6, 3)			

The tetrahedron is the first member of the family (3, 3), (4, 3), and (5, 3); in all members three edges meet at each vertex (3-connected), and the shortest circuits (n-gons) have 3, 4, or 5 edges. The next member of this family is the plane hexagonal net (6, 3), which has the property that the shortest circuit including any two of the three links meeting at any point is a 6-gon. Our first question concerns the nature of 3-connected nets $(n, 3)$ in which n is greater than 6. Such nets, in which the shortest circuit including any pair of links from any point is an n-gon, are called *uniform 3-connected nets*; evidently they contain no circuits smaller than n-gons.

Alternatively we may focus our attention on the circuits (polygons) that form the surface of the polyhedron. All the faces of three of these polyhedra, tetrahedron, octahedron, and icosahedron, are triangles (which are equilateral in the most regular forms of the solids), and the numbers of triangles meeting at each vertex are respectively 3, 4, and 5. If six triangles meet at each point, a closed convex polyhedron is no longer possible, and (3, 6) is a tessellation on an infinite two-dimensional (2D) surface and is the regular plane net (3, 6) on the Euclidean plane if the triangles are equilateral, or on an infinite (open-ended) cylindrical surface. If now we make a tessellation in which seven or more triangles meet at each point and make it from narrow strips of paper or plastic, which in the simplest case are made equal in length, we find that the surface buckles and eventually joins up in a complex way. Our second question concerns the nature of the surfaces on which tessellations (3, *p*) can be drawn when *p* exceeds the value (6) for a plane net. We refer to such surfaces as the surfaces of 3*D polyhedra.*

These two families, 3-connected nets (*n*, 3) and 3D polyhedra (3, *p*), form only part of the whole problem (Table 1.1), which includes all systems (*n*, *p*) having *n* and/or *p* greater than the values permissible for plane nets. Since we derive separately the uniform 3D nets (and also some other nets which are not uniform nets) and 3D polyhedra, and since systems of both types appear in Table 1.1, it is necessary to discuss the relation between them. A closely

Table 1.1 Systems (*n*, *p*) of connected points

	p						
n	3	4	5	6	7	8	. . .
3	*t*	*o*	*i*	(3, 6)			
4	*c*	(4, 4)					
5	*d*						
6	(6, 3)				3D Polyhedra and 3D nets		
7							
8							
⋮							

related question is the dual relation between pairs such as (3, 8) and (8, 3). However it is not feasible to consider such basic questions until we have described some 3D nets and polyhedra, and discussion of these matters is therefore deferred.

There are only five convex polyhedra having all faces of the same kind and the same number of faces meeting at each vertex, and there are only three plane nets having all polygons of the same kind and the same number of polygons meeting at each point. Moreover, there are two ways of accounting for these circumstances. The *topological* proof is concerned only with the number (n) of edges of the faces or polygons and with the connectedness (p) of the vertices (points), that is, the number of edges (links) meeting at each vertex (point). For a (finite) convex polyhedron or a plane net, this number p is the same as the number of n-gons meeting at a point, since two edges of each polygon meet at a given point and each edge is common to two polygons. For a finite convex polyhedron (n, p) with Z vertices, it follows directly from Euler's relation (which itself is purely topological) that

$$Z = \frac{4n}{4 - (n-2)(p-2)} \tag{1.1}$$

For finite values of Z,

$$(n-2)(p-2) < 4 \tag{1.2}$$

which is satisfied by only five integral combinations of n and p, namely:

(n, p)	Z	
(3, 3)	4	tetrahedron
(3, 4)	6	octahedron
(3, 5)	20	icosahedron
(4, 3)	8	hexahedron
(5, 3)	12	dodecahedron

The solutions for $Z = \infty$, that is, of

$$(n-2)(p-2) = 4 \tag{1.3}$$

correspond to the plane nets (n, p), that is, (3, 6), (4, 4), and (6, 3) (Fig. 1.1*a*).

Equation (1.1) also gives Z for the Archimedean and Catalan (semiregular) solids if the *mean* value of n or p is used. The 13 Archimedean solids have