# *Space lattices.*

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THE concept of a space lattice is fundamental in crystallography. A space lattice, or more simply a lattice, is an indefinitely extended regular array of points, in which the environment of each point is exactly the same. This implies that if the lattice is (1) translated parallel to itself, or (2) inverted about one of its points, or (3) rotated it will remain precisely the same as it was before such transformations. Such projective transformations as translation, inversion, or rotation are called symmetry operations. A lattice therefore may be said to be invariant in respect to certain specific symmetry operations. It is then said to possess certain symmetry elements. The fundamental symmetry operations are translations, inversions, and rotations. There is no symmetry element corresponding to translation, which is implicit in all lattices. Centres of symmetry correspond to inversion and axes of symmetry correspond to specific rotations. Points of mirror symmetry and lines of mirror symmetry may also be considered as fundamental elements of symmetry, but the plane of mirror symmetry is a composite element of symmetry, being the resultant of two-fold rotation followed by inversion.

There are in all twenty types of lattices, as defined by their symmetry element: one one-dimensional, five two-dimensional, and fourteen three-dimensional. All these lattices have an application in the study of material objects: one-dimensional lattice to the chain structural units of crystals, two-dimensional lattices to the sheet structural units of crystals, and three-dimensional lattices to the crystals themselves.

The number of lattices in a space of $n$-dimensions ($S_n$) is equal to the sum of squares of the first $n$ members, i.e.

$$S_n = 1^2+2^2+...+n^2 = \sum_{k=1}^{n} k^2.$$

This expression may be transformed into a polynomial of the third degree: $S_n = \frac{1}{3}n^3+\frac{1}{2}n^2+\frac{1}{6}n$, the solution of which for $n = 1, 2, 3$, is respectively 1, 5, 14.

This equation can only be verified for the spaces of one, two, and three dimensions, as space lattices in dimensions higher than three have not been as yet constructed.

Lattices are specified by their parameters. The one-dimensional lattice, or linear row of equally-spaced points, is specified by one parameter—by a vector length ($a$) of primitive translation; the two-dimensional lattice or net is specified by the two vector lengths ($a$, $b$) and the angle between them ($\gamma$); the three-dimensional lattice is specified by three vector lengths ($a$, $b$, $c$) and three angles between them ($\alpha$, $\beta$, $\gamma$). The vector lengths are also referred to as 'axes' and the angles as 'direction angles'. All parameters may vary in respect of their relative equality: all unequal; two equal; all three equal. In addition, angle parameters may assume fixed values of 90° and 60° and also stand in certain relation to linear parameters.

It is very important to remember that the choice of axes of reference for each array of points is arbitrary and that each array of points may have a number of alternative systems of parameters. On the other hand, the symmetry elements of a lattice are absolutely fixed. Thus lattices may be specified by their parameters, but lattice types are defined by their elements of symmetry. Thus in a triclinic lattice the six parameters may exhibit innumerable variations, including that of two clino-angles and one right angle, but a diclinic lattice does not exist alongside the triclinic and monoclinic lattices.

Each lattice type, or more simply lattice, is characterized by an assemblage of symmetry elements. All lattices are formed by translations, and all are characterized by inversion, so that the diagnostic symmetry operations are the rotation and mirror reflections. The diagnostic elements of symmetry are therefore the points or axes of symmetry ($A_2$, $A_3$, $A_4$, $A_6$), and the points, lines, and planes of mirror symmetry ($P$). The degree of symmetry of a lattice is expressed by the symmetry number. As originally defined by W. H. Bragg,[1] 'symmetry number' is the number of assymetrical molecules in the unit cell of a molecular compound. In the case of lattices this number corresponds to the number of points geherated by the operation of inversion, rotation, and reflection on one original point. For three-dimensional lattices the symmetry number is equal to the number of the general faces ($hkl$) or ($hk\bar{i}l$) of the holosymmetrical class of the corresponding system.

Lattices are also characterized, but not uniquely, by their degree of

[1] W. H. Bragg, The significance of crystal structure. Journ. Chem. Soc. London, 1922, vol. 121, pp. 2766–2787. [M.A. 2–328.]

freedom, which can be defined as the number of independent variable parameters which are needed to specify a lattice. The degree of freedom is equal to, or less than, the number of parameters. The degree of freedom is reduced when one or more parameters is given a fixed value such as equality to another parameter or, in the case of angle parameters, equality to 90° or 60°.

Figures relative to the two-dimensional and to the three-dimensional lattices are given in tables I and II. Symbols used for lattices are: $L$ (line) one-dimensional lattice; $N$ (net) two-dimensional lattices, bearing qualifying subscripts ($N_c$, $N_o$, &c.); $P$ primitive three-dimensional lattices, bearing qualifying subscripts; also $C$ ($c$-face-centred); $F$ (face-centred); and $I$ (body-centred).

A one-dimensional lattice, or a line lattice, is a row of equally-spaced points along a straight line of an indefinite length (geometrical lattices, in distinction to real crystals, have no boundary points). It has one degree of freedom—the linear parameter ($a$). Besides translation and inversion it is characterized by points of mirror symmetry (lattice points and half-way points). In virtue of its one-dimensionality it cannot possess either axes or planes of symmetry.

Two-dimensional lattices, plane-lattices or net lattices, can be postulated to be made of equally-spaced array of line lattices. In all, there are five two-dimensional lattices, particulars of which are given in table I.

TABLE I. Two-dimensional lattices.

| Symbol. | Mesh. | Parameters. Linear. | | Parameters. Angles. | Degree of freedom. | Points of rotation ($A_n$) and lines of mirror symmetry. | Symmetry number. |
|---|---|---|---|---|---|---|---|
| $N_c$ | Clino- | $a$ | $b$ | $\gamma$ | 3 | $A_2$ | 2 |
| $N_o$ | Ortho- | $a$ | $b$ | 90° | 2 | $A_2$, $2P$ | 4 |
| $N_r$ | Rhombo- | $a$ | $a$ | $\gamma$ | 2 | $A_2$, $2P$ | 4 |
| $N_t$ | Tetra- | $a$ | $a$ | 90° | 1 | $A_4$, $A_2$, $4P$ | 8 |
| $N_h$ | Hexa- | $a$ | $a$ | 60° | 1 | $A_6$, $A_3$, $A_2$, $6P$ | 12 |
| | | or | | | | | |
| | | $a$ | $b = a\sqrt{3}$ | 90° | | | |

The nomenclature followed, namely clino-mesh, ortho-mesh, rhombo-mesh, tetra-mesh, and hexa-mesh, is that proposed by W. L. Bond.[1] Besides translation and inversion these lattices possess rotation points

[1] W. L. Bond, The fourteen space lattice. Univ. Toronto Studies, Geol. Ser., 1947, no. 51 (for 1946), pp. 9–20. [M.A. 10–149.]

and lines of mirror symmetry. It is usual to divide two-dimensional lattices into four primitive ($N_c$, $N_o$, $N_t$, and $N_h$) and one compound ($N_r$) lattice. In accordance with this I have arranged the four primitive lattices along the cardinal points of a centred triangle and have placed the rhombo-lattice outside this triangle (fig. 1). As will be seen later,

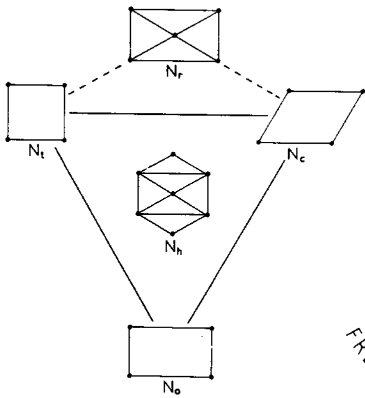


FIG. 1.

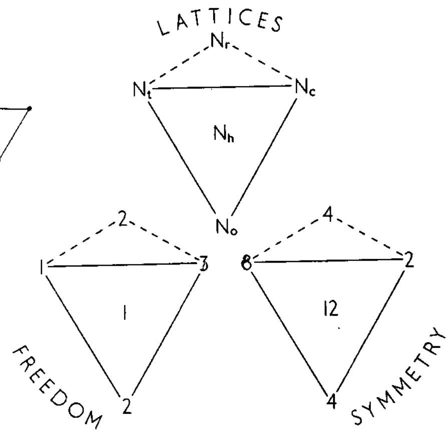


FIG. 2.

Two-dimensional lattices.

such a pattern has a direct relation to the pattern of the three-dimensional lattices. The double-triangle pattern of the two-dimensional lattices provides an arrangement in which there is a regular transition of the values of the degree of freedom and symmetry number of the lattices as shown graphically in fig. 2.

Other groupings are possible. For example, the rhombo-lattice may be called primitive and the ortho-lattice compound, as being derived by the combination of two $N_r$ lattices. In the same way, the hexa-lattice may be considered to be formed from the combination of two $N_o$ lattices. Such a principle of equivalence is a normal case among lattices and is constantly to be found among three-dimensional lattices. The choice of co-ordinate axes is also arbitrary. Thus the hexa-lattice can be referred to three axes of equal length at 120° to each other, or to two axes of equal length at 60° to each other, or to two axes $a$ and $b = a\sqrt{3}$ at 90° to each other. Rhombo-lattice may also be referred to two axes of equal length, or two axes at right angles to each other (ortho-axes).

Three-dimensional lattices are usually divided into seven primitive and seven compound lattices, the total number being fourteen. The principle of equivalence discussed above with regard to two-dimensional lattices may be applied to some of these lattices, such, for example, to the hexagonal lattice or to the rhombohedral lattice. The same applies to the freedom of choice of axes of reference. Particulars for the seven primitive lattices are given in table II. Compound lattices have the

TABLE II. Primitive three-dimensional lattices.

| Symbol. | Lattice. | Parameters. Linear. | | | Angles. | | | Degree of freedom. | Axes of rotation ($A_n$) and planes of mirror symmetry ($P$). | Symmetry number. |
|---|---|---|---|---|---|---|---|---|---|---|
| $P_{tr}$ | Triclinic | $a$ | $b$ | $c$ | $\alpha$ | $\beta$ | $\gamma$ | 6 | — | 2 |
| $P_m$ | Monoclinic | $a$ | $b$ | $c$ | 90° | $\beta$ | 90° | 4 | $A_2, P$ | 4 |
| $P_o$ | Orthorhombic | $a$ | $b$ | $c$ | 90° | 90° | 90° | 3 | $3A_2, 3P$ | 8 |
| $P_{te}$ | Tetragonal | $a$ | $a$ | $c$ | 90° | 90° | 90° | 2 | $A_4, 4A_2, 5P$ | 16 |
| $P_c$ | Cubic | $a$ | $a$ | $a$ | 90° | 90° | 90° | 1 | $3A_4, 4A_3, 6A_2, 9P$ | 48 |
| $P_r$ | Rhombohedral | $a$ | $a$ | $a$ | $\alpha$ | $\alpha$ | $\alpha$ | 2 | $A_3, 3A_2, 3P$ | 12 |
| $P_h$ | Hexagonal | $a$ | $(a\sqrt{3})$ | $c$ | 90° | 90° | 90° | 2 | $A_6, 6A_2, 7P$ | 24 |
| | | or | | | | | | | | |
| | | $a$ | $a$ | $c$ | 90° | 90° | 60° | | | |

same symmetry and degree of freedom as their mother primitive lattices. The hexagonal lattice, for the sake of uniformity, is referred to a three-axial system. This, however, does not replace the four-axial system used in crystal morphology, but is introduced so that the hexagonal lattice can be compared and contrasted with the two neighbouring lattices—rhombohedral and orthorhombic.

The seven primitive three-dimensional lattices are arranged in a classificatory pattern which has the form of a centred hexagon (fig. 3). The seven compound lattices are arranged in places adjoining their mother lattices (fig. 4). The relation of this pattern to the patterns of the degrees of freedom and symmetry numbers of the seven primitive lattices is shown by means of a special diagram (fig. 5). It will be seen from this diagram that an attempt has been made to arrange lattices in such a way that, with some exceptions, the transition from one lattice into another is effected with a minimum change in the degree of freedom and symmetry number. According to their symmetry the seven lattices can be divided into three classes, which in the diagram form three distinct zones: high symmetry ($P_c$, $P_h$); medium symmetry ($P_{te}$, $P_r$); and low symmetry ($P_o$, $P_m$, $P_{tr}$).

In the hexagonal pattern the hexagonal circuit ($P_{tr}$, $P_m$, $P_o$, $P_{te}$, $P_c$, $P_r$) must be distinguished from the vertical diagonal traverse, in which all the four lattices can be referred to the same system of orthorhombic

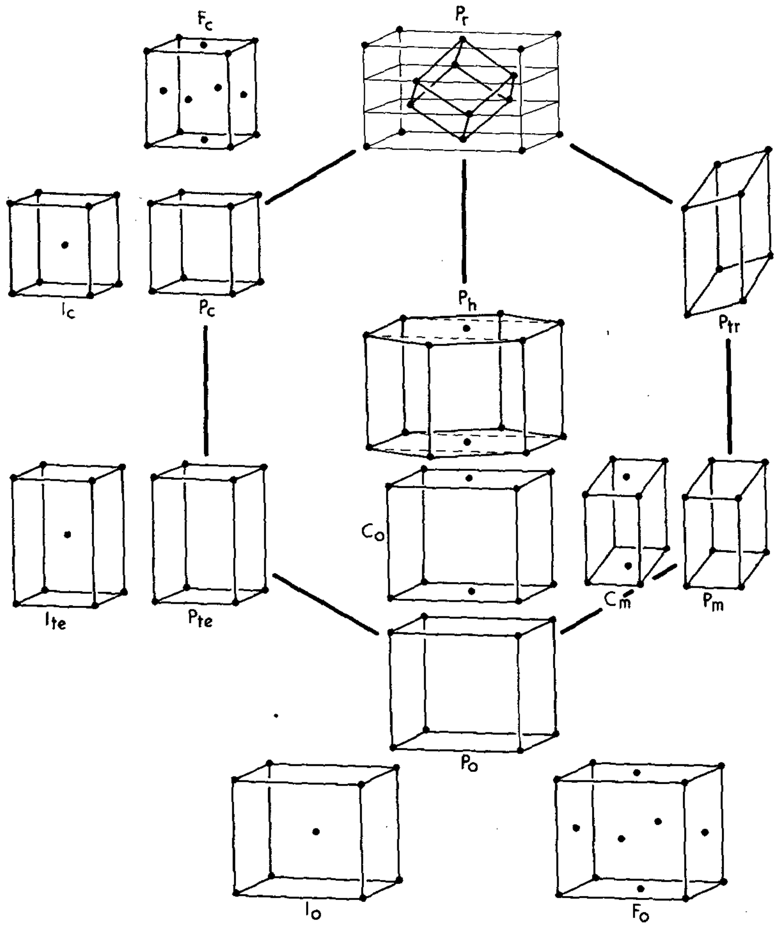

FIG. 3. Three-dimensional lattices.

axes, and can all be postulated to be modifications of the primitive orthorhombic lattice, in the following way:

$$C_o = 2P_o;\ P_h = C_o\ (\text{at}\ b = a\sqrt{3});\ P_r = 3P_h,$$

with co-ordinate points (0, 0, 0), (0, 1/3, −1/3), (0, −1/3, 1/3); and $c \neq a\sqrt{3}/2$ (at $c = a\sqrt{3}/2$, $P_r$ becomes $P_c$).

The triangular pattern of the two-dimensional lattices and the hexagonal pattern of the three-dimensional lattices provide two simple schemes of classification of these lattices on the basis of axes of refer-

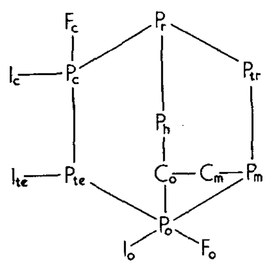


FIG. 4. Three-dimensional lattices.

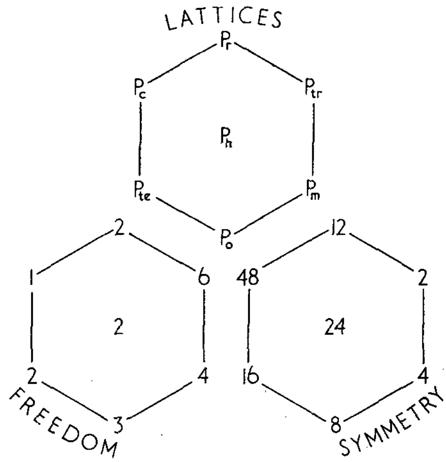


FIG. 5. Three-dimensional lattices.

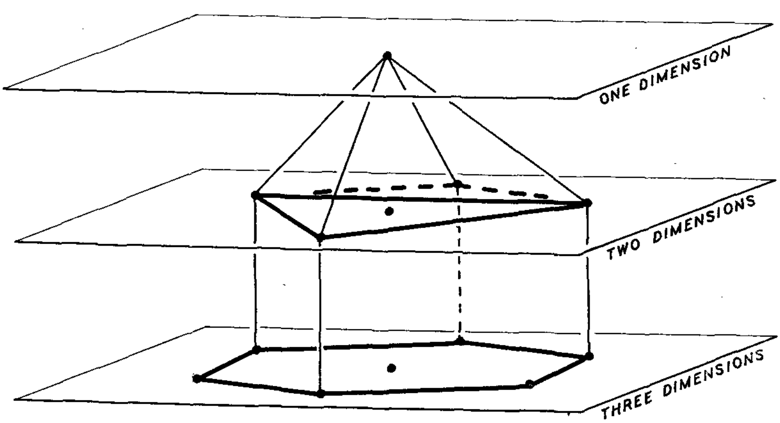


FIG. 6. Point relationship of 1-, 2-, and 3-dimensional lattices.

ence, degree of freedom, and symmetry number. But the net lattices are generated by the line lattices, and the three-dimensional lattices are generated by the net lattices. This means that all the twenty lattices can be brought together into one scheme of classification. This can be done by means of three horizontal parallel planes (fig. 6). The upper plane contains one point only, corresponding to one line lattice. The middle plane contains five points corresponding to the net lattices arranged in a double triangle pattern. The lower plane contains the fourteen three-dimensional lattices arranged about the hexagonal pattern. Remembering that $P_{tr}$ is generated by three $N_c$; $P_o$ by three $N_o$; $P_c$ by three $N_t$; $P_r$ by three $N_r$; and $P_h$ by one $N_h$ and two $N_o$; we can place the generating net lattices above the generated three-dimensional lattices, $N_c$ above $P_{tr}$; $N_o$ above $P_o$; $N_t$ above $P_c$; $N_r$ above $P_r$; and $N_h$ above $P_h$. This diagram is a graphical representation of the twenty lattices in their genetic relationships and in a general way it summarizes our knowledge of all lattices.

The whole scheme can be easily remembered; point, triangle, hexagon corresponding respectively to one-, two-, three-dimensions. It is a harmonious and interconnected system of lattices.

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