

# Tabulated Data for the Examination of the 230 Space-Groups by **Homogeneous X-Rays**

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VI. Tabulated Data for the Examination of the 230 Space-Groups by Homogeneous X-Rays.

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[Plates 5-24.]

## General Introduction.

The object of the present paper is to express the conclusions of mathematical crystallography in a form which shall be immediately useful to workers using homogeneous X-rays for the analysis of crystal structures. The results are directly applicable to such methods as the Bragg ionisation method, the powder method, the rotating crystal method, etc., and summarise in as compact a form as possible what inferences may be made from the experimental observations, whichever one of the 230 possible space-groups may happen to be under examination.

It is only in certain cases that the spacings of crystal planes as determined by the aid of homogeneous X-rays agree with the values of those spacings which would be expected from ordinary crystallographic calculations. In the majority of cases the relative arrangement of the molecules in the unit cell leads to apparent anomalies in the experimental results, the observed spacings of certain planes or sets of planes being submultiples of the calculated spacings. The simplest case (fig. 8) of such an apparent anomaly is found in the space-group  $C_{2}^{2}$  of the monoclinic system, where the presence of a two-fold screw-axis, because it interleaves halfway the (010) planes by molecules which are exactly like those lying in the (010) planes, except that they have been rotated through 180°, leads to an observed periodicity which is half the periodicity to be inferred from the dimensions of the unit cell, that is, leads to an observed spacing for (010) which is half the calculated. All screw-axes produce similar results, and, in general, a p-fold screw-axis leads to an observed spacing for the plane perpendicular to it which is  $\frac{1}{2}$  th that to be inferred from the dimensions of the cell. Besides those produced by the screw-axes, other abnormalities arise out of the presence of glide-planes. The simplest case of this is shown by the space-group C<sub>2</sub> (fig. 4) of the monoclinic system, in which the second molecule is obtained from the first by a reflection in a plane parallel to (010) and half a primitive translation parallel to that plane. If we look along a direction perpendicular to this glide-plane, the projections of the two molecules on the (010) plane are indistinguishable except in position, which is equivalent to saying that, for the VOL. CCXXIV.—A 621. 2 H [Published August 20, 1924.

purposes of X-ray interference, certain planes perpendicular to this plane of projection are interleaved by an identical molecular distribution. Furthermore, since the translation associated with the glide-plane must always be half a primitive translation parallel to the glide-plane, we know that the interleaving is always a submultiple of the full spacing and the periodicity is again reduced in a corresponding manner. The use of this method for discriminating between the various space-groups of the monoclinic system was described by Sir Wm. Bragg in a lecture to the Chemical Society.\* In the present paper the method has been extended to the whole of the 230 space-groups possible to crystalline structures. In general, it may be said that if a crystal possesses a certain glide-plane, a certain set of planes lying in the zone whose axis is perpendicular to that glide-plane will have their periodicity reduced by one-half.

A more obvious way by which the periodicity of crystal planes may be reduced is by the interleaving of completely identical molecules such as occurs in those Bravais lattices which have similar and similarly orientated molecules at the face-centres or the bodycentre of the unit cell. In these cases the interleaving molecules are identical from all points of view and the periodicity of certain sets of general planes is reduced. In a lattice in which there is an identical molecule at the centre of the (001) face, the spacings of all planes  $\{hkl\}$  for which (h+k) is odd will be reduced by half, while for a bodycentred lattice the same is true for all planes  $\{hkl\}$  for which (h+k) is odd, and for a face-centred lattice all planes  $\{hkl\}$  for which (h+k) or (k+l) or (l+h) is odd. Such abnormalities are well known and must be allowed for in addition to those arising out of the screw-axes and glide-planes. Thus it is that we find certain glide-planes giving rise, not merely to halved spacings, but also to quartered spacings.

The conclusions to be drawn from such arguments as are given above hold for the space-groups whatever the material from which they are built up, whether it be ions, molecules or polymers of molecules. They are the conclusions arising out of the theory of mathematical crystallography which in the general case concerns itself, not with the nature of the ultimate asymmetric units of crystalline structures, but with the groups of operations by which infinite systems of such units may be brought into coincidence. Figs. 1-230 (Plates 5-24) are diagrams showing in as condensed a form as possible the arrangement of these ultimate units in the 230 possible cases. In the majority of crystals the ultimate units undoubtedly correspond in substance to single chemical molecules, and it is chiefly for the elucidation of such structures that the columns described "Possible Molecular Symmetry "will be found useful. The diagrams show the ways in which Nature, from completely asymmetric material, builds up crystals of highly symmetrical form and properties. The small arrows marked by the letters u and d represent asymmetric molecules, but it is clear that the theory is unaffected by the substitution of a molecule of p-fold symmetry for p asymmetric molecules of suitable relative orientations; in other words, instead of using n asymmetric molecules to build up a crystal we may use

<sup>\*</sup> Sir William Bragg, 'Trans. Chem. Soc.,' 1922, vol. 121, p. 2766.

n/p molecules each of symmetry p. It must be distinctly understood here that p refers to the molecular symmetry in the crystal. What relation this bears to the molecular symmetry in the non-crystalline state is another matter which has been discussed elsewhere.\* There is little doubt that the two are closely connected, and that the distortions involved in the passage from one state to the other are not at all of a high order.

The substitution of a molecule of p-fold symmetry for p asymmetric molecules can be represented diagrammatically by making the tails of p suitable small arrows coincide on an element of symmetry. A glance at the diagrams will make this process clear (cf. also fig. VII (a) and (b)), and at the same time show how the number and nature of the possible molecular symmetries are governed by the distribution of the symmetry elements. Such a process can be conceived to hold in all organic and most inorganic crystals, for in them the molecules preserve their identity and can be treated as distinct units.

The case of so-called "ionised" crystal-structures, e.g. the alkali halides, is rather different, since in them it is impossible to localise the molecules and treat them as separate entities built together with suitable relative orientations. The crystal is an equilibrium distribution of positive and negative parts and as such is best considered from the point of view of the theory of coincidence operations, that is, by aid of the symmetry elements alone. For instance, in rock-salt (supposing the structure possesses full, 48-fold, cubic symmetry), we cannot argue from the fact that there are four molecules in the face-centred unit cell that each molecule has 48-fold symmetry because, in the first place, the molecules cannot be localised and, in the second, if they could be localised they would clearly possess a much lower symmetry. But examination of fig. 225 will bring out how, in spite of this apparent anomaly, the whole structure is subject to the particular combination of symmetry elements  $(O_b^5)$  there depicted. Similarly we can readily see how ammonium chloride, with only one molecule of low symmetry per unit cube, gives rise to the highly symmetrical arrangement shown in fig. 207. The analytical results of the theory of space-groups have been worked out completely by Wyckoff† and expressed as the co-ordinates of equivalent points. tabulated co-ordinates of course include all cases of ionised structures and the method of using them is described in his book. But, by the aid of figs. 1-230, the case of ionised structures can be expressed diagrammatically and visualised in the same way as the case of molecular structures. In addition to bringing the tails of various small arrows to coincidence we have now also to bring the heads of certain arrows to coincidence. instance, fig. VII (printed after figs. 1-230) shows the relation between the various molecular and ionised structures based on the symmetry  $C_{2v}^{-1}$ . Figs. 16 and VII (a) and (b) are molecular, while fig. VII (c) (d) (e) and (f) are ionised on the basis of

<sup>\* &#</sup>x27;Chem. Soc. Annual Reports,' 1923—" Crystallography."

<sup>†</sup> R. W. G. WYCKOFF, "The Analytical Expression of the Results of the Theory of Space-Groups," 'Carnegie Institution of Washington,' October, 1922. Cf. also Niggli, 'Phys. Ztsch.,' 1918, vol. 19, p. 225; and 'Geometrische Krystallographie des Diskontinuums,' Leipzig, 1919.

one positive to one negative. It will be noticed that the results given in the column on "Abnormal Spacings" apply equally to the two cases.

## Description of Tables and Diagrams.

The numbers in the first column of the tables correspond to figs. 1–230. The second column gives the name of the space-group adopted in Hilton's "Mathematical Crystallography," the third the underlying Bravais lattice, the fourth the number of asymmetric molecules per cell, the fifth the abnormal spacings to be expected, and the sixth and seventh the possible molecular symmetry. If n per cell is the number of asymmetric molecules required to produce the symmetry of the structure, there will be required only n/p molecules of symmetry p. The explanation of the notation used in the seventh column is as follows: C, centre; P, plane; 2-A, dyad axis; 3-A, triad axis; 4-A, tetrad axis; 4a-A, tetrad alternating axis; 6-A, hexad axis.

Figs. 1-230 are in all cases projections on the basal plane {001}, {111} or {0001}. The development follows that given in Hilton's "Mathematical Crystallography." The asymmetric molecules are represented by the small arrows marked u and d, and these are grouped about the elements of symmetry which are used to define the unit cell. By this means the coalescence of a large number of asymmetric molecules into a much smaller number of symmetrical molecules is more readily visualised than if we think of the unit cell as defined by the repetition of a certain standard molecule placed at the corner of the cell. Molecules marked with the subscript, are enantiomorphous to those marked with the subscript, that is, either of the two can be obtained from the other by an operation involving a reflection. Molecules marked  $u_1$  can be obtained from molecules marked  $d_1$  by rotation about a dyad axis which is parallel to the plane of the paper. This nomenclature simply means that if we think of the molecule  $u_1$ as pointing up, the molecule  $d_1$  is obtained from it by a rotation through 180° (plus a possible translation parallel to the axis) and is therefore pointing down to a corresponding extent. Thick lines denote planes of symmetry perpendicular to the plane of the paper, dotted lines denote glide-planes of symmetry, while thin lines denote the boundaries of the cell where these do not coincide with elements of symmetry. Axes of symmetry perpendicular to the plane of the paper are represented as follows: dyad rotation-axis

•; dyad screw-axis, •; triad axis, •; triad screw-axis • or •; tetrad axis,  $\spadesuit$ ; tetrad screw-axis of translation  $\frac{c}{4}$   $\clubsuit$  or  $\clubsuit$ ; tetrad screw-axis of translation  $\frac{c}{2}$   $\Leftrightarrow$ ; tetrad alternating axis  $\Leftrightarrow$  or  $\Leftrightarrow$  according to the position of the plane of symmetry involved; hexad axis lacktriangle; hexad screw-axis of translation  $\frac{c}{6}$  $\stackrel{\longleftarrow}{\Longrightarrow}$  or  $\stackrel{\frown}{\Longrightarrow}$  ; hexad screw-axis of translation  $\frac{c}{3}$   $\stackrel{\longleftarrow}{\Longrightarrow}$  or  $\stackrel{\frown}{\Longrightarrow}$  ; hexad screw-axis of

translation  $\frac{c}{2}$  Centres of symmetry, indicated by crosses, are marked in the triclinic, monoclinic and orthorhombic systems only.

As mentioned above, the unit cell in these diagrams must be considered as defined by the elements of symmetry. Axes of symmetry actually lying in the top plane of the cell are then marked by thick arrows (e.g.,  $\longrightarrow$  for a dyad rotation-axis,  $\aleph$ for a dyad screw-axis, etc.), while those lying in a plane  $\frac{\tau_z}{2}(i.e.,\frac{e}{4})$  lower down are drawn with thin lines. Axes at other depths are shown dotted, and in most cases the depth is marked. If we now commence with a standard molecule, say  $u_1$ , near the top left-hand corner of the cell, it must be remembered that its position is arbitrary and it will not in general lie in the top plane of the cell as defined by the elements of symmetry. This standard molecule is drawn with full line, as are also all molecules derived from it by the symmetry elements lying in the top plane of the cell and those planes of pure reflection and axes of pure rotation which lie perpendicular to this plane. In the majority of figures 1-230 only two kinds of molecules will be observed, full and The full ones are as just described, while the dotted ones bear a similar relation to the plane half-way down the cell—that is, they can be obtained from the standard molecule by the operation of a symmetry element perpendicular to the plane of the paper and involving a translation of  $\frac{c}{2}(\tau_z)$ . In certain of the orthorhombic, tetragonal and cubic groups, four types of molecules will be noticed. These are shown by thick full arrows, thin full arrows, thick dotted arrows and thin dotted arrows. full arrows are as first described, while the thin full arrows are associated with a plane one-quarter of the way down the cell, that is, they can be derived from the standard molecule by the operation of a symmetry element perpendicular to the plane of the paper and involving a translation of  $\frac{c}{4}\left(\frac{\tau_z}{2}\right)$ . Similar remarks apply to the thick and thin dotted arrows, except that they are associated with planes half-way and threequarters of the way down the cell respectively. In the trigonal (rhombohedral) and hexagonal systems some groups will be observed with three types of arrows, full thick, full thin and dotted. The second and third of these are associated with translations one-third and two-thirds of the way down the cell respectively. In some hexagonal groups six types are used, and these will readily be seen to be related to the six translations  $\left(0,\frac{c}{6},\frac{c}{3},\frac{c}{2},\frac{2c}{3},\frac{5c}{6}\right)$  which are possible in a direction parallel to a hexad axis.

There is a peculiar difficulty involved in depicting the cubic (regular) system by a single diagram per group, because of the presence of the four triad axes which emerge from the corners of a cube. This difficulty has been partly surmounted by writing three molecules arranged round a triad axis as 3u or 3d. The arrow marked 3u or 3d

is then really the projection of part of the triad axis, and thus serves in addition to indicate the point of emergence of this triad axis. The axis passes through the centre of gravity of the three molecules arranged round it, but it must be clearly understood that they bear no other fixed relation to it whatsoever. By analogy with the development of the previous space-groups, the space-groups of the cubic system are developed from a standard set of three molecules arranged symmetrically but otherwise arbitrarily round a standard triad axis.

In those diagrams where two molecules or two or four sets of three molecules are drawn lying closely side by side it must be considered that in a true projection the arrows, though not necessarily the molecules themselves, would really cover one another. They are slightly separated in the diagrams in order to reveal the presence of molecules of different depths or to distinguish between complementary trios of molecules arranged round the same triad axis. In some of the later groups, in order to avoid excessive congestion, a few of the symmetry elements have been omitted, and a similar remark applies to the lettering omitted from figs. 225-229.

## Triclinic System.

Both the triclinic space-groups are based on the simple lattice  $\Gamma_{tr}$ , the most general of all the lattices, in which the primitive translations are all independent of one another in magnitude and direction. The only possible element of symmetry is a centre, hence no halvings occur, since the position of the second molecule (if any) in the unit cell is quite indefinite. An investigation of any triclinic crystal using the X-ray spectrometer cannot, therefore, show halvings that fix the position of the second molecule, but can only give the usual crystallographic data and the intensities of reflection from the different crystal planes.

The figs. 1 and 2 may be taken as representing the projection of the unit cell on any plane whatever.

# TRICLINIC SYSTEM.

## TRICLINIC HEMIHEDRY (PEDIAL).

No	s.   sG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.	
1	C <sub>1</sub>	$\Gamma_{tr}$	1	None		None.	

## TRICLINIC HOLOHEDRY (PINAKOIDAL).

No	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
2	C.1	$\Gamma_{tr}$	2	None	2	C.

## Monoclinic System.

The space-groups of the monoclinic system are based either on the simple monoclinic lattice  $\Gamma_m$ , or on the lattice  $\Gamma_m'$ . In the groups, such as  $C_s^3$ ,  $C_2^3$ , etc., based on  $\Gamma_m'$ , subdivisions (a), (b i), (b ii) and (c) have been made. This simply means that in the (a) sub-division  $\Gamma_{m}$  has been taken as the centred monoclinic lattice, in (b i) as the monoclinic lattice with points at the centres of the {100} faces, in (b ii) as the monoclinic lattice with points at the centres of the {001} faces, and in the (c) as the face-centred mono-That these are simply different aspects of the same lattice will be obvious from fig. I.

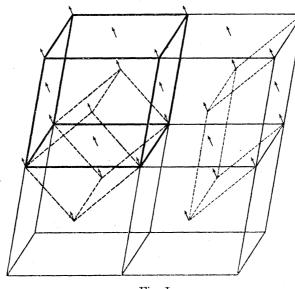


Fig. I.

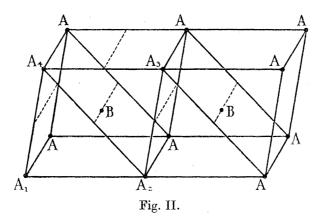
face-centred lattice. centred lattice.

lattice with one pair of opposite rectangular faces centred.

There are other ways of describing  $\Gamma_m$ , but these are the only aspects which introduce a lattice having one edge perpendicular to the other two.

In the groups  $C_s^2$ ,  $C_{2h}^4$ ,  $C_{2h}^5$ , there are three sub-divisions (a), (b) and (c). In  $C_s^2$  the unit cell contains two molecules, the second of which may be obtained from the first by a reflection plus a definite translation. Taking the position of any characteristic point of the first molecule as origin, the co-ordinates of the corresponding characteristic point of the second molecule referred to the crystallographic axes as axes of co-ordinates are either  $\left(\frac{a}{2}, v, 0\right)$  or  $\left(0, v, \frac{c}{2}\right)$  or  $\left(\frac{a}{2}, v, \frac{c}{2}\right)$ , where v is indeterminate. The particular position occupied simply depends on the choice of unit cell; all three arrangements really represent the same space-group, since a and c are interchangeable in the monoclinic The sub-division (a) gives the halvings if the second molecule B occupies the

position  $\left(\frac{a}{2}, v, 0\right)$ , (b) gives the halvings when B is at  $\left(0, v, \frac{c}{2}\right)$ , and (c) gives the halvings when B is at  $\left(\frac{a}{2}, v, \frac{c}{2}\right)$ , [cf. also groups  $C_{2h}^4$ ,  $C_{2h}^5$ , each of which have  $C_{\epsilon}^2$  as a sub-group]. Fig. II shows the equivalence of the three possible positions of B.



The co-ordinates of B, referred to the crystallographic cell A<sub>1</sub> A<sub>2</sub> A<sub>3</sub> A<sub>4</sub>, are Referred to the more oblique cell, they are  $\left(\frac{a}{2}, v, 0\right)$  or  $\left(0, v, \frac{c}{2}\right)$  according as to whether  $A_2$   $A_4$  is taken as a or as c.

According to conventional crystallography the axis of symmetry is always taken as the b axis and the plane of symmetry is therefore the (010). Hence in the column headed "Possible Molecular Symmetry," wherever the symbol 2-A occurs, the reader may automatically substitute 2-A  $\perp^r$  {010}, and similarly P should read P  $\parallel^t$  {010}. figures 3-15 show the projection of the unit cell on either  $\{100\}$  or  $\{001\}$ , since a and c are interchangeable in this system.

As the monoclinic system includes the simplest possible cases of glide-planes and screw-axes, it is especially suitable for illustrating the principles governing the occurrence of halvings, and it would be advisable for the reader to familiarise himself with the method of deducing the halvings by studying the figures 3-15 very carefully with reference to the tables before proceeding to the remaining systems.

This system is particularly important because of its frequent occurrence among the crystals of organic substances, the molecules of which are very often entirely asymmetric or possess only two-fold symmetry. It is obvious that the lower the symmetry of the molecule, the more likely it is to crystallise in a system of a low, rather than one of a high, order of symmetry.

It should be carefully noted that by X-ray investigation alone, it is not possible to distinguish between certain groups in different classes. For example, the halvings which occur in the group  $C_{2h}^{4}$  (holohedral class) are the same as those of the group  $C_{2h}^{2}$ (hemihedral class). If it is found that there are four molecules in the unit cell, it is not unreasonable to suppose that the crystal belongs to the  $C_{2h}$  class provided that the lattice

is  $\Gamma_m$ , but if there are only two molecules per cell then possibly, (a) the crystal is an example of the C<sub>2h</sub><sup>4</sup> group, each molecule possessing two-fold symmetry, either an axis or a centre, or else (b) the crystal belongs to the group C<sub>s</sub><sup>2</sup>, each molecule being entirely asymmetric.

If the external symmetry of the crystal indicates that it must belong to the holohedral group  $C_{2b}$  rather than to the hemihedral group  $C_s^2$  it is still not possible by X-ray methods to decide definitely whether the molecule possesses an axis or a centre of symmetry. The reader may easily multiply examples of this kind from the adjoining tables. in a limited number of cases is it possible to state absolutely the space group to which the crystal belongs and the symmetry of the molecule.

## MONOCLINIC SYSTEM.

## MONOCLINIC HEMIHEDRY (DOMATIC).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
3	C <sub>8</sub> 1	$\Gamma_m$	. 2	None	2	Р.
4	$C_s^2$	$\Gamma_m$	2	(a.) $\{hol\}$ halved if $h$ is odd (b.) $\{hol\}$ halved if $l$ is odd (c.) $\{hol\}$ halved if $(h+l)$ is odd		None.
5	$C_s^3$	$\Gamma_{m}'$ (cf. $\Gamma_{0}'''$ )	. 4	(a.) $\{hkl\}$ halved if $(h+k+l)$ is odd	2	P.
-		(cf. $\Gamma_0$ ')	4	$(b \text{ i.}) \{hkl\} \text{ halved if } (k+l)$ is odd		
	mananana wa	(cf. $\Gamma_0$ ')	4	$(b \text{ ii.}) \{hkl\} \text{ halved if } (h+k)$ is odd		
	*	(cf. $\Gamma_0^{\prime\prime}$ )	8	(c.) $\{hkl\}$ halved if $(h+k)$ or $(k+l)$ or $(l+h)$ is odd		
6	C <sub>s</sub> 4	$\Gamma_{m'}$	4	(a.) (bi.) (bii.) Same as C <sub>s</sub> <sup>3</sup> (a.) (bi.) (bii.) respectively; also all {hol} halved.	A-MARANTA -	None.
		i	8	(c.) Same as $C_s^3$ (c.); also $\{hol\}$ quartered if $(h+l)$ is odd, halved if even.		

### MONOCLINIC HEMIMORPHY (SPHENOIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
7	C <sub>2</sub> 1	$\Gamma_m$	2	None	2	2-A.
8	C22	$\Gamma_m$	2	{010} halved	_	None.
9	C <sub>2</sub> <sup>3</sup>	$\Gamma_m{'}$	8	(a.) (bi.) (bii.) Same as C <sub>s</sub> <sup>3</sup> (a.) (bi.) (bii.) respectively. (c.) Same as C <sub>s</sub> <sup>3</sup> (c)	2	2-A.

## MONOCLINIC HOLOHEDRY (PRISMATIC).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
10	$C_{2h}^{1}$ $C_{2h}^{2}$	$\Gamma_m$ $\Gamma_m$	4	None	$egin{array}{c} 2 \ 4 \ 2 \end{array}$	$\begin{vmatrix} 2-A ; P. \\ 2-A & 1^r P. \\ P ; C. \end{vmatrix}$
12	C <sub>2h</sub> 3	$\Gamma_m{'}$	16	(a.) (bi.) (bii.) Same as C <sub>s</sub> <sup>3</sup> (a.) (bi.) (bii.) respectively (c.) Same as C <sub>s</sub> <sup>3</sup> (c.)	2 4	2-A; P; C. 2-A <b>1</b> <sup>r</sup> P.
13	C <sub>2h</sub> 4	$\Gamma_m$	4	(a.) (b.) (c.) Same as C <sub>s</sub> <sup>2</sup> (a.) (b.) (c.) respectively	2	2-A; C.
14	C <sub>2h</sub> <sup>5</sup>	$\Gamma_m$	4	(a.) (b.) (c.) Same as $C_s^2$ (a.) (b.) (c.) respectively; also	2	С.
15	C <sub>2h</sub> 6	$\Gamma_{m}{'}$		{010} halved. (a.) (bi.) (bii.) Same as $C_s^4$ (a.) (bi.) (bii.) respectively (c.) Same as $C_s^4$ (c.)	2	2-A; C.

## Orthorhombic System.

The orthorhombic space-groups are all based on one or other of four Bravais lattices:—

- (a) The simple rhombic lattice,  $\Gamma_0$ .
- (b) The rhombic lattice with points at the centres of one pair of opposite faces,  $\Gamma_0$ .
- (c) The face-centred rhombic lattice,  $\Gamma_0''$ .
- (d) The centred rhombic lattice,  $\Gamma_0^{\prime\prime\prime}$ .

The particular lattice involved must first be found, as usual, from an examination of the general planes  $\{hkl\}$ .

In the  $C_{\bullet n}$  class the c axis is taken parallel to the dyad axis and there are, therefore, planes or glide-planes parallel to {100} and {010}, but not to {001}. The figures 16-37 represent the projection of the unit cell on the {001} plane. Wherever the molecular symmetry "2-A" occurs, it will be understood that "2-A  $\perp$ " {001}" is meant, and that "2 P's intersecting in 2-A" means "2P's || {100} and {010} intersecting in 2-A  $\perp^r$  {001}." The a and b axes are interchangeable, since they are not conventionally fixed by symmetry considerations, as is the c axis. Thus in any group possessing, say, one plane and one glide-plane, the glide-plane may have been arbitrarily taken as parallel to  $\{100\}$ , as, for example, in  $C_{2v}^2$ ; here we have  $\{okl\}$ halved where l is odd, and the possible molecular symmetry is a plane parallel to  $\{010\}$ : but we might just as well have taken {010} as the glide-plane, and so we may substitute as an alternative in this group,  $\{hol\}$  halved where l is odd, the possible molecular symmetry then being a plane parallel to {100}. Similar alternatives could

be added in the groups  $C_{2v}^{4}$ ,  $C_{2v}^{5}$ ,  $C_{2v}^{6}$ ,  $C_{2v}^{7}$ ,  $C_{2v}^{9}$ ,  $C_{2v}^{12}$ , etc. If the X-ray worker, on examining a crystal, finds that the  $\{hol\}$  is halved where l is odd (say), instead of the  $\{okl\}$  where l is odd, that is given in the tables, then in order to see graphically the position of the molecules he must take the  $\{010\}$ , not the  $\{100\}$ , as the glideplane in fig. 17, and similarly for the other space-groups and their corresponding figures. In this class it will also be obvious that there are two possible cases of  $\Gamma_{0}'$ , one in which the pair of centred faces are  $\{001\}$ ,  $(C_{2v}^{11}$ , etc.), the other in which the pair of centred faces are the  $\{100\}$ ,  $(C_{2v}^{14}$ , etc.), or, alternatively, of course, the  $\{010\}$ .

In the Q and  $Q_h$  classes all three axes are interchangeable. Hence, where the table gives (for  $Q^3$ ): " $\{100\}$   $\{010\}$  halved; possible molecular symmetry, 2-A  $\perp^r$   $\{001\}$ ," the following are also possible alternatives in this group: " $\{100\}$   $\{001\}$  halved; 2-A  $\perp^r$   $\{010\}$ " or " $\{010\}$   $\{001\}$  halved; 2-A  $\perp^r$   $\{100\}$ ." The figures 38-74 represent the projection of the unit cell on the  $\{001\}$  plane, thus agreeing with the tables as they stand, but if the first alternative be adopted the corresponding figure 40 must be taken as representing the projection on  $\{010\}$ , and for the second alternative as the projection on  $\{100\}$ . It must be quite clear that if h and k (say) are interchanged in the list of abnormal spacings, then  $\{100\}$  and  $\{010\}$  must be interchanged in the list of possible molecular symmetry and in the corresponding diagram.

A reference to the tables for the orthorhombic system will show that, with the single exception of groups Q<sup>8</sup> and Q<sup>9</sup>, the halvings corresponding to the different space-groups in any given class are all different, and, therefore, given the class, the X-ray investigation will fix the space-group. In the case of Q<sup>8</sup> and Q<sup>9</sup>, the method fails to distinguish between these groups unless the unit cell is found to contain only two molecules, since the molecules in Q<sup>8</sup> can possess two-fold or four-fold symmetry, whereas in Q<sup>9</sup> they can only possess two-fold symmetry, not four-fold.

The tables also show, however, that quite frequently space-groups in different classes of the same system will have exactly the same halvings (cf.  $C_{2v}^{4}$ ,  $Q_{h}^{5}$ ;  $C_{2v}^{1}$ ,  $Q^{1}$ ,  $Q_{h}^{1}$ ; etc.). Here, as in the monoclinic system, the X-ray method alone will not definitely decide between such space-groups without the assistance of evidence derived from the external form and physical properties of the crystal.

For example, the X-ray method should distinguish crystals belonging to the Q class which have the spacings of the axial planes halved, but no other planes in the axial zones, and it can also distinguish those space-groups in the  $Q_h$  class which have spacings of planes in all three axial zones halved apart from those involved in the halvings of general planes  $\{hkl\}$ ; but it cannot distinguish any of the space-groups in the  $C_{2v}$  class from those in the  $Q_h$  class which have "identical halvings." The fundamental Bravais lattice can, of course, always be determined from the halvings found among the general planes  $\{hkl\}$ . In every case so far investigated (with some doubtful exceptions) the unit cell appears to contain the minimum number of molecules

rather than an integral multiple of that number. If we arbitrarily assume that this is always the case, then the molecular symmetry can also be determined but only to a somewhat limited extent. One of the most complicated examples is that of an orthorhombic crystal, of unknown class, in which all planes {hkl} are halved where (h+k+l) is odd.

Using the above-mentioned hypothesis, it is obvious that if the unit cell contains sixteen molecules, the space-group is  $Q_{h}^{25}$ , the molecules being asymmetric.

If the cell contains eight molecules only, the following are all possible arrangements:—

(a) Space-group  $Q_h^{25}$ ; molecular symmetry, a plane parallel to  $\{100\}$ ,  $\{010\}$  or  $\{001\}$ , or a centre.

X-ray measurements cannot absolutely decide between these two elements of symmetry, nor can they decide, in the case of the plane of symmetry, to which of the three axial planes this plane in the molecule itself is parallel.

- (b) Space-group Q<sup>8</sup>; molecule asymmetric.
- (c) Space-group Q<sup>9</sup>; molecule asymmetric.
- (d) Space-group  $C_{2\nu}^{20}$ ; molecule asymmetric.

If the cell contains four molecules only, the following arrangements are all possible:—

- (a) Space-group  $Q_h^{25}$ ; the molecule then must have four-fold symmetry, two planes parallel to any two axial planes intersecting in a dyad axis perpendicular to the third axial plane.
- (b) Space-group  $Q^3$ ; molecular symmetry, a dyad axis perpendicular to any one of the three axial planes.
- (c) Space-group  $Q^9$ ; the same molecular symmetry as in (b).
- (d) Space-group  $C_{2v}^{20}$ ; molecular symmetry, a plane parallel to  $\{100\}$  or  $\{010\}$ .

If the cell contains two molecules only, the possible arrangements are as follows:—

- (a) Space-group  $Q_{h}^{25}$ ; the molecule must have eight-fold symmetry, three planes parallel to {100}, {010} and {001} intersecting in three dyad axes.
- (b) Space-group Q<sup>8</sup>; the molecule has four-fold symmetry, three mutually perpendicular dyad axes.
- (c) Space-group  $C_{2v}^{20}$ ; the molecule has four-fold symmetry, two planes parallel to  $\{100\}$  and  $\{010\}$  intersecting in a dyad axis.

There cannot be only one molecule per cell in this case, as the fundamental Bravais lattice is  $\Gamma_0^{\prime\prime\prime}$ .

The limitations of the method are at once apparent, though the example taken above is certainly an extreme case, not likely to occur often.

# ORTHORHOMBIC SYSTEM. ORTHORHOMBIC HEMIMORPHY (PYRAMIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
16	C <sub>2v</sub> <sup>1</sup>	$\Gamma_0$	$oxed{4}$	None	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	P    $^{l}$ {100} or {010}. 2 P's intersecting in 2-A.
17	C <sub>2v</sub> <sup>2</sup>	$\Gamma_0$	4	$\{okl\}$ halved if $l$ is odd	2	$P \parallel^{l} \{010\}.$
18	C2v3	$\Gamma_0$	4	$\{hol\}$ halved if $l$ is odd; $\{okl\}$ halved if $l$ is odd	2	2-A.
19	C2v4	$\Gamma_{0}$	4	$\{hol\}$ halved if $h$ is odd	2	$2-A$ ; $P \parallel^{l} \{100\}$ .
20	$C_{2v}^{5}$	$\Gamma_0$	4.	$\{hol\}$ halved if $h$ is odd; $\{okl\}$ halved if $l$ is odd		None.
21	C2v	$\Gamma_0$	4	$\{bol\}$ halved if $(h+l)$ is odd; $\{okl\}$ halved if $l$ is	2	2-A.
22	C <sub>2v</sub> <sup>7</sup>	$\Gamma_0$	4	$\begin{array}{c} \operatorname{odd} \\ \{\mathit{hol}\} \end{array}$ halved if $(\mathit{h}+\mathit{l})$ is	2	P    {100}.
23	C208	$\Gamma_0$	4	odd $\{hol\}$ halved if $h$ is odd;	$^2$	2-A.
24	C2v9	$\Gamma_0$	4	$\{okl\}$ halved if $k$ is odd $\{hol\}$ halved if $h$ is odd; $\{okl\}$ halved if $(k+l)$ is		None.
25	C <sub>2v</sub> <sup>10</sup>	$\Gamma_0$	4	$egin{array}{lll}  ext{odd} \ \{  ext{\it hol} \} &  ext{halved if} & ( ext{\it h} + l) &  ext{is} \  ext{odd} \ ; & \{  ext{\it okl} \} &  ext{halved} &  ext{if} \end{array}$	2	2-A.
26	C2v11	$\Gamma_0{'}$	8	$egin{array}{ll} (k+l)  ext{ is odd} \ \{hkl\}  ext{ halved if } (h+k)  ext{ is odd} \end{array}$	2 4	2-A; P $\ ^{l}$ {100} or {010}. 2 P's intersecting in 2-A.
27	$C_{2v}^{-12}$	$\Gamma_0{'}$	8	Same as $C_{2v}^{11}$ ; also all $\{okl\}$ halved	2	$P \parallel^{l} \{010\}.$
28	$C_{2v}^{-13}$	$\Gamma_0{'}$	8	Same as $C_{2v}^{11}$ ; also all $\{okl\}$ , $\{hol\}$ halved	2	2-A.
29	C2v14	$\Gamma_0$	8	$\{hkl\}$ halved if $(k+l)$ is odd		Same as $C_{2v}^{-1}$ .
30	C2v15	$\Gamma_0{'}$	8	Same as $C_{2v}^{14}$ ; also all $\{okl\}$ halved	2	$2-A$ ; $P \parallel^l \{010\}$ .
31	C2v16	$\Gamma_0{'}$	8	Same as $C_{2v}^{14}$ ; also all $\{hol\}$	2	$2-A$ ; $P \parallel^{l} \{100\}$ .
32	$C_{2v}^{-17}$	$\Gamma_0$	8	halved Same as $C_{2v}^{14}$ ; also all $\{okl\}$ ,	2	2-A.
33	C2018	$\Gamma_0{''}$ .	16	$\{hol\}$ halved $\{hkl\}$ halved if $(h+k)$ or		Same as $C_{2v}^{11}$ .
34	C <sub>20</sub> 19	$\Gamma_0{}^{\prime\prime}$	16	(k + l) or $(l + h)$ is odd Same as $C_{2v}^{18}$ ; also $\{hol\}$ quartered if $(h + l)$ is odd, halved if even; $\{okl\}$ quartered if $(k + l)$	2	2-A.
35	$\mathrm{C}_{2v}^{-20}$	$\Gamma_0^{\prime\prime\prime}$	8	is odd, halved if even $\{hkl\}$ halved if $(h+k+l)$		Same as $C_{2v}^{-1}$ .
36	C2v21	$\Gamma_0^{\prime\prime\prime}$	8	is odd Same as $C_{2v^{-1}}$ ; also all $\{hol\}$ ,	2	2-A.
37	C <sub>2*</sub> <sup>22</sup>	$\Gamma_0^{\prime\prime\prime}$	8	$egin{array}{l} \{okl\} &  ext{ halved} \\  ext{Same as } \mathrm{C}_{2v}^{\ \ 2o} ; &  ext{also all } \{hol\} \\ &  ext{ halved} \end{array}$	2	2-A; P    <sup>l</sup> {100}.

## ORTHORHOMBIC ENANTIOMORPHY (BISPHENOIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
38	Q1	$\Gamma_0$	4	None	2	$2-A \perp^r \{100\}, \{010\} \text{ or } \{001\}.$
39	$\mathbf{Q^2}$	$\Gamma_0$	4	{001} halved	$\begin{vmatrix} 4\\2 \end{vmatrix}$	3 mutually $\hat{\mathbf{L}}^r$ 2–A's. 2–A $\hat{\mathbf{L}}^r$ {100} or {010}.
40	$Q_3$	$\Gamma_0$	4	{100}, {010} halved	2	$2-A \perp^r \{001\}.$
41	Q4	$\Gamma_0$	4	{100}, {010}, {001} halved		None.
42	$Q^5$	${\Gamma_0}'$	8	$\{hkl\}$ , halved if $(h+k)$ is odd; also $\{001\}$ halved.	2	2-A $\perp^r \{100\}$ or $\{010\}$ .
43	$Q^{6}$	$\Gamma_0{}'$	8	$\{hkl\}$ halved if $(h+k)$ is odd		Same as $Q^1$ .
44	$Q^7$	$\Gamma_0{}^{\prime\prime}$	16	$\{hkl\}$ halved if $(h+k)$ or $(k+l)$ or $(l+h)$ is odd		Same as $Q^1$ .
45	$Q_8$	$\Gamma_0^{\prime\prime\prime}$	8	$\{hkl\}$ halved if $(h+k+l)$ is odd		Same as $Q^1$ .
46	Q9	$\Gamma_0^{\prime\prime\prime}$	8	Same as $Q^8$	2	2–A $\perp^r$ {100}, {010} or {001}.

## ORTHORHOMBIC HOLOHEDRY (BIPYRAMIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
47	$Q_h^1$	$\Gamma_0$	8	None	$\begin{bmatrix} 2\\4\\8 \end{bmatrix}$	P    {100}, {010} or {001}. 2 P's intersecting in 2-A. 3 P's intersecting in 3 2-A's.
48	$Q_h^2$	$\Gamma_0$	8	$\{okl\}$ halved if $(k+l)$ is odd; $\{hol\}$ halved if $(l+h)$ is odd; $\{hko\}$ halved if $(h+k)$ is odd	2 4	2-A $\mathbf{L}^r$ {100}, {010} or {001}; C. 3 mutually $\mathbf{L}^r$ 2-A's.
49	$Q_h$ <sup>3</sup>	$\Gamma_0$	8	$\{okl\}$ halved if $l$ is odd; $\{hol\}$ halved if $l$ is odd	$\frac{2}{4}$	2-A $\mathbf{L}^r$ {100}, {010} or {001}; P $\parallel^r$ {001}. 2-A $\mathbf{L}^r$ P $\parallel^r$ {001}; 3 mutually $\mathbf{L}^r$ 2-A's.
50	$Q_h$	$\Gamma_0$	8	$\{okl\}$ halved if $k$ is odd; $\{hol\}$ halved if $h$ is odd; $\{hko\}$ halved if $(h+k)$ is odd		Same as $Q_h^2$ .
51	$Q_h^5$	$\Gamma_0$	8	$\{hol\}$ halved if $l$ is odd	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	2-A $\mathbf{L}^r$ {100}; P    $^t$ {100} or {001}. 2-A $\mathbf{L}^r$ P    $^t$ {100}; 2 P's    $^t$ {100} and {001} intersecting in 2-A.
52	$Q_h{}^6$	$\Gamma_{0}$	8	$\{okl\}$ halved if $(k+l)$ is odd; $\{hol\}$ halved if $h$ is odd; $\{hko\}$ halved if $(h+k)$ is odd	$2 \mid$	$2-A \perp^r \{100\} \text{ or } \{010\}; \text{ C.}$
53	$Q_h^7$	$\Gamma_0$	8	$\{hol\}$ halved if $(h+l)$ is odd; $\{hko\}$ halved if $h$ is odd	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	2–A $\perp^r \{100\}$ or $\{010\}$ ; P $\parallel^t \{100\}$ . 2–A $\perp^r$ P $\parallel^t \{100\}$ .
54	$Q_h^8$	$\Gamma_0$	8	$\{okl\}$ halved if $k$ is odd; $\{hol\}$ halved if $l$ is odd; $\{hko\}$ halved if $k$ is odd.		Same as $Q_h^6$ .

# ORTHORHOMBIC HOLOHEDRY (BIPYRAMIDAL)—continued.

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
55	$Q_h^{-9}$	$\Gamma_{0}$	8	$\{okl\}$ halved if $k$ is odd; $\{hol\}$ halved if $h$ is odd	2 4	2-A $\mathbf{L}^r \{001\}$ ; P $\parallel^l \{001\}$ . 2-A $\mathbf{L}^r$ P $\parallel^l \{001\}$ .
56	$Q_h^{10}$	$\Gamma_0$	8	$\{okl\}$ halved if $l$ is odd; $\{hol\}$ halved if $l$ is odd; $\{hko\}$ halved if $(h+k)$ is	2	2–A $\mathbf{L}^r$ {001}; C.
57	$Q_h^{-11}$	$\Gamma_0$	8	$egin{array}{ll}  ext{odd} \ \{  ext{hol} \} &  ext{halved if } h  ext{ is odd} \ \{  ext{hko} \} &  ext{halved if } k  ext{ is odd} \end{array}$	. 2	2–A $\perp^r \{001\}$ ; P $\parallel^l \{100\}$ ; C.
<b>5</b> 8	$Q_h^{12}$	$\Gamma_0$	8	$\{okl\}$ halved if $(k+l)$ is odd; $\{hol\}$ halved if		Same as $Q_h^9$ .
. 59	$Q_h^{13}$	$\Gamma_{0}$	8	$(h+l)$ is odd $\{hko\}$ halved if $(h+k)$ is odd	$\frac{2}{4}$	$P \parallel^{l} \{100\} \text{ or } \{010\} ; C.$ 2 P's $\parallel^{l} \{100\}$ and $\{010\}$ intersecting
60	Q,14	$\Gamma_{f 0}$	8	$\{okl\}$ halved if $l$ is odd; $\{hol\}$ halved if $(h+l)$ is odd; $\{hko\}$ halved if $k$ is odd		in 2–A. Same as $Q_h^{10}$ .
61	$Q_h^{15}$	$\Gamma_{0}$	8	$\{okl\}$ halved if $k$ is odd; $\{hol\}$ halved if $l$ is odd;	2	C.
62	$Q_h^{16}$	$\Gamma_0$	8	$\{hko\}$ halved if $h$ is odd $\{okl\}$ halved if $(k+l)$ is odd; $\{hol\}$ halved if $h$ is odd	2	P    <sup>z</sup> {001} ; C.
63	Q,17	$\Gamma_{0}{}'$	16	Same as $Q^6$ ; also all $\{hol\}$	2 4	2-A $\perp^r \{100\}$ ; P    $^l \{100\}$ or $\{001\}$ ; C. 2 P's    $^l \{100\}$ and $\{001\}$ intersecting
6 <b>4</b>	$Q_h^{18}$	$\Gamma_{f 0}{}'$	16	Same as $Q^6$ ; also all $\{hol\}$ and $\{hko\}$ halved	2	in 2-A; 2-A $\perp^r$ P    <sup>l</sup> {100}. 2-A $\perp^r$ {100} or {010}; P    <sup>l</sup> {100}; C.
65	$Q_h^{19}$	$\Gamma_{f 0}{}'$	16	Same as Q <sup>6</sup>	4 2	$2-A$ $L^r$ P $\parallel^l$ {100}. $2-A$ $L^r$ {001}; P $\parallel^l$ {100}, {010} or {001}.
					4	$\left \begin{array}{c} 2 \text{ P's intersecting in 2-A ; 2-A } \mathbf{L}^r \text{ P } \parallel^l \\ \{001\}. \end{array}\right $
66	$Q_h^{20}$	$\Gamma_{f 0}{}'$	16	Same as $Q^0$ ; also all $\{okl\}$ and $\{hol\}$ halved	8 2	3 P's intersecting in 3 2-A's. 2-A $\mathbf{L}^r$ {100}, {010} or {001}; P   ^l {001}.
67	$Q_h^{21}$	$\Gamma_{f o}{}'$	16	Same as $Q^6$ ; also all $\{hko\}$	4 2	3 mutually $\mathbf{L}^r$ 2-A's; 2-A $\mathbf{L}^r$ P $\ ^t$ {001}. 2-A $\mathbf{L}^r$ {100}, {010} or {001}; P $\ ^t$
0.	*	1 0	1.0	halved	4	$\begin{array}{ c c c c c }\hline \{100\} \text{ or } \{010\}. \\ 2 \text{ P's } \parallel^l \{100\} \text{ and } \{010\} \text{ intersecting } \end{array}$
		·				in 2-A; 3 mutually $\perp^r$ 2-A's; 2-A $\perp^r$ P $\parallel^l$ {100}; 2-A $\perp^r$ P $\parallel^l$ {010}.
68	Q,22	$\Gamma_{f 0}{}'$	16	Same as $Q^6$ ; also all $\{okl\}$ , $\{hol\}$ , $\{hko\}$ halved	$\frac{2}{4}$	$2-A \perp^r \{100\}, \{010\} \text{ or } \{001\}; C.$ 3 mutually $\perp^r 2-A$ 's.
69	$Q_h^{23}$	$\Gamma_0^{\prime\prime}$	32	Same as $Q^7$	$\frac{1}{2}$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$
					4	2 P's intersecting in 2-A; 2-A $\mathbf{L}^r$ P    $l^2$ {100}, {010} or {001}.
					8	3 P's intersecting in 3 2-A's.

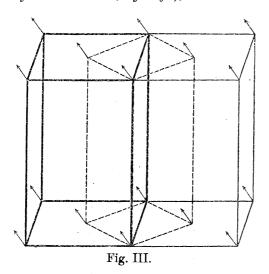
ORTHORHOMBIC HOLOHEDRY (BIPYRAMIDAL)—(continued).

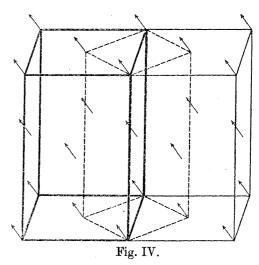
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No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
70	$Q_h^{24}$	$\Gamma_0$ "	32	Same as $Q^7$ ; also $\{okl\}$ quartered if $(k+l)$ is odd, halved if even; $\{hol\}$ quartered if $(h+l)$ is odd, halved if even; $\{hko\}$ quartered if $(h+k)$ is odd, halved if even	$\begin{vmatrix} 2 \\ 4 \end{vmatrix}$	2–A $\perp^r$ {100}, {010} or {001}; C. 3 mutually $\perp^r$ 2–A's.
71	$Q_h^{25}$	$\Gamma_0^{\prime\prime\prime}$	16	Same as $Q^8$	$\frac{2}{4}$	$P \parallel^{l} \{100\}, \{010\} \text{ or } \{001\}; C.$ 2 P's intersecting in 2-A.
			1.		8	3 P's intersecting in 3 2-A's.
72	$Q_h^{26}$	$\Gamma_0^{\prime\prime\prime}$	16	Same as $Q^8$ ; also all $\{okl\}$ , $\{hol\}$ halved	$^2$	$\begin{bmatrix} 2-A \perp^r \{100\}, \{010\} \text{ or } \{001\}; P \end{bmatrix}^l = \{001\}; C.$
					4	3 mutually $\mathbf{L}^r$ 2-A's; 2-A $\mathbf{L}^r$ P $\parallel^l$ {001}.
73	$Q_h^{27}$	$\Gamma_{0}^{\prime\prime\prime}$	16	Same as $Q^8$ ; also all $\{okl\}$ , $\{hko\}$ , $\{hko\}$ halved	2	$2-\vec{A} \perp r' \{100\}, \{010\} \text{ or } \{001\}; C.$
74	Q,28	$\Gamma_0^{\ \prime\prime\prime}$	16	Same as $Q^8$ ; also all $\{hko\}$ halved	2	2–A $\perp^r \{100\}$ or $\{010\}$ ; P $\parallel^l \{100\}$ or $\{010\}$ .
					4	2-A $\mathbf{L}^r \mathbf{P} \parallel^l \{100\}$ or $\{010\}$ ; 2 P's $\parallel^l \{100\}$ and $\{010\}$ intersecting in 2-A.

## Tetragonal System.

There are only two tetragonal lattices,  $\Gamma_t$  and  $\Gamma_t'$ . The first of these,  $\Gamma_t$ , may be regarded either as a simple tetragonal lattice (cf.  $\Gamma_0$ ) or as a lattice with the square This is clearly shown in fig. III, the simple lattice being outfaces centred (cf.  $\Gamma_0$ ). lined by dotted lines.

Similarly, fig. IV shows that  $\Gamma_t$  may be regarded either as a centred lattice (shown by dotted lines; cf.  $\Gamma_0'''$ ), or as a face-centred lattice (cf.  $\Gamma_0''$ ).





In each case crystallographers may adopt either alternative in describing the occurrence of various "forms," therefore both are given in all space-groups except those belonging to the hemihedral class  $D_{2d}$ . In this class the axial planes are always taken

as bisecting the angles between the symmetry planes of the crystal and so only one alternative is possible whether the lattice is  $\Gamma_t$  or  $\Gamma_t'$ . To avoid confusion, the orthorhombic lattice with which the actual tetragonal lattice may be compared is inserted in brackets under the Bravais lattice column. In classes C<sub>4</sub>, C<sub>4</sub>, C<sub>4</sub>, the possible molecular symmetry is the same for both the alternatives 1.) and 2.) in each space-group. In classes  $C_{4v}$ ,  $D_4$ ,  $D_{4h}$ , however, the possible molecular symmetry given refers only to 1.); in order to apply it to 2.) {100} must be changed throughout into {110} and {110} into {100}. In every class the diagrams given for the space-groups refer to 1.); the diagrams corresponding to 2.) may be obtained by interchanging the {110} and {100} as in the tables.

Another point to be noticed very carefully is that in the tetragonal system the form  $\{100\}$  includes both the (100) and (010) planes, similarly the  $\{okl\}$  includes both the (okl) and the (hol) planes, that is, the {100} and {010} are indistinguishable from each other. For example,  $C_{4v}^{4}$  1.) reads: " $\{okl\}$  halved if (k+l) is odd; possible molecular symmetry, 2-A  $\perp^r$  {001}, P  $\parallel^l$  {110}, or 2 P's  $\parallel^l$  {110} intersecting in 2-A." This means that not only are all planes in the  $\{okl\}$  zone halved if (k+l)is odd, but also all planes  $\{hol\}$  for which (h+l) is odd; also, corresponding to any molecule having in itself a plane of symmetry parallel to (110) there is a second molecule whose plane of symmetry is parallel to  $(1\overline{1}0)$ . If, in this group, the molecule has two planes of symmetry intersecting in a dyad axis, those planes will be parallel to (110) and (110) respectively.

Under the column "Possible Molecular Symmetry" will be found occasional references to a four-fold alternating axis. This is not a type of symmetry that is likely to occur often, but it should be kept in mind because of its probable existence in compounds such as  $C[(C.dXYZ)_2 (C.lXYZ)_2]$  and  $(CH.C.dXYZ)_2 (CH.C.lXYZ)_2$ . Another still more complicated type of symmetry, referred to in the  $D_{2d}$  and  $D_{4h}$  classes, is the full D<sub>2d</sub> symmetry. This consists of two perpendicular planes of symmetry intersecting in a four-fold alternating axis. This means that there will be also two two-fold axes of symmetry perpendicular to the four-fold alternating axis and bisecting the angles between the planes. In the  $D_{2d}$  class the planes must always be parallel to the  $\{110\}$ (by convention), but in the  $D_{4h}$  they may be parallel to the {110} or the {100}.

It should be noted that, in the three systems previously discussed, the triclinic, monoclinic and orthorhombic, there is only one type of Laue diagram given by "white" This is because X-rays automatically add a centre of symmetry to the symmetry already possessed by the crystal and thus give rise to fewer Laue diagrams than the thirty-two types would lead us to expect. In the tetragonal system adding a centre to the seven classes in turn reduces them to two only, one possessing full C<sub>4h</sub> symmetry and the other possessing full D<sub>4h</sub> symmetry. Consequently, by the additional aid of Laue diagrams we can readily discriminate between the  $C_4$ ,  $C_4$  and  $C_{4h}$  classes on the one hand, and the  $D_{2d}$ ,  $C_{4n}$ ,  $D_4$  and  $D_{4h}$  classes on the other. Such a partitioning of the seven classes may be found useful in those cases where the abnormal spacings are the same for certain space-groups in different classes.

# TETRAGONAL SYSTEM. TETRAGONAL TETARTOHEDRY OF THE SECOND SORT (BISPHENOIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
75	C' <sub>4</sub> <sup>1</sup>	$\begin{array}{c c} \Gamma_t \left( \Gamma_0 \right) \\ \left( \Gamma_0 \right) \end{array}$	4 8	1.) None	$\frac{2}{4}$	$\begin{vmatrix} 2-A & \mathbf{L}^r & \{001\}, \\ 4a-A & \mathbf{L}^r & \{001\}. \end{vmatrix}$
76	C'42	$\Gamma_t'(\Gamma_0'')$	16	1.) $\{hkl\}$ halved if $(h+k)$ or $(k+l)$ or $(l+h)$ is odd		Same as C' <sub>4</sub> <sup>1</sup> .
		$(\Gamma_{0'''})$	8	2.) $\{hkl\}$ halved if $(h+k+l)$ is odd		

## TETRAGONAL HEMIHEDRY OF THE SECOND SORT (SCALENOHEDRAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
77	$D_{2d}^{-1}$	$\Gamma_t (\Gamma_0)$	8	None	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$
					8	3 mutually $\mathbf{L}^r$ 2-A's. 2 P's $\parallel^l$ {110} intersecting in $4a$ -A $\mathbf{L}^r$ {001}.
78	$\mathbf{D_{2d}}^2$	$\Gamma_t (\Gamma_0)$	8	$\{hhl\}$ halved if $l$ is odd	$\begin{array}{ c c }\hline 2\\ 4 \end{array}$	2-A $\mathbf{L}^r$ {100} or {001}. 3 mutually $\mathbf{L}^r$ 2-A's; $4a$ A $\mathbf{L}^r$ {001}.
79	$\mathrm{D}_{2d}^{-3}$	$\Gamma_t(\Gamma_0)$	8	{100} halved	2 4	$ \begin{vmatrix} 2-A & L^r \\ 2 & P's \end{vmatrix}^l \{110\}, $ intersecting in 2-A;
80	$D_{2d}^{4}$	$\Gamma_t \left( \Gamma_0 \right)$	8	$\{100\}$ halved; $\{hhl\}$ halved if $l$ is odd.	2	$ \begin{array}{c c} 4a-A \ \mathbf{L}^r \ \{001\}. \\ 2-A \ \mathbf{L}^r \ \{001\}. \\ A \ A \ \mathbf{L}^r \ \{001\}. \end{array} $
81	$\mathrm{D}_{2d}^{5}$	$\Gamma_t (\Gamma_0')$	16	Same as $C'_4$ <sup>1</sup> 2.)	4 2 4	$egin{array}{lll} & \{a-A, L^r \{001\}, \\ P & \{110\}, \\ 2 & P's & \ ^l \{110\} & \text{intersecting in } 2-A. \end{array}$
			•		8	2 P's $\parallel^l$ {110} intersecting in $4a$ -A $\perp$ $\perp$ 4001}.
82	$D_{2d}^{6}$	$\Gamma_t (\Gamma_0')$	16	Same as $C'_4$ 2.); also $\{hhl\}$ halved if $l$ is odd		Same as $D_{2d}^{'2}$ .
83	$\mathrm{D}_{2d}^{7}$	$\Gamma_t (\Gamma_0')$	16	Same as $C'_4$ <sup>1</sup> 2.); also $\{hhl\}$ halved if $h$ is odd		Same as $D_{2d}^2$ .
84	$\mathrm{D}_{2d}^{-8}$	$\Gamma_t (\Gamma_0')$	16	Same as $C_4^{\prime 1}$ 2.); also $\{hhl\}$ halved if $(h+l)$ is odd		Same as $D_{2d}^{-2}$ .
85	$\mathrm{D}_{2d}{}^{9}$	$\Gamma_t'$ $(\Gamma_0'')$	32	Same as $C'_4^2$ 1.)	2 4 8	2-A $\mathbf{L}^r$ {100}; P    <sup>l</sup> {110}. 2 P's    <sup>l</sup> {110} intersecting in 2-A. 2 P's    <sup>l</sup> {110} intersecting in 4a-A $\mathbf{L}^r$
86	$\mathbf{D_{2d}^{10}}$	$\Gamma_t'$ $(\Gamma_0'')$	32	Same as $C_4^{\prime 2}$ 1.); also all		$\{001\}.$ Same as $\mathrm{D}_{2d}{}^2.$
87	$\mathrm{D}_{2d}^{-11}$	$\Gamma_{t}'$ $(\Gamma_{0}''')$	16	$\{hhl\}$ halved Same as $C'_{4}{}^{2}$ 2.)	$egin{array}{c} 2 \ 4 \end{array}$	2–A $\mathbf{L}^r$ {100} or {001}; P $\parallel^l$ {110}. 2 P's $\parallel^l$ {110} intersecting in 2–A; 3 mutually $\mathbf{L}^r$ 2–A's; $4a$ –A $\mathbf{L}^r$
, 1					8	$\{001\}$ . 2 P's $\parallel^l \{110\}$ intersecting in $4a$ -A $\perp^r$
88	$D_{2d}^{-12}$	$\Gamma_t'(\Gamma_0''')$	16	Same as $C_4^2$ 2.); also $\{hhl\}$ quartered if $l$ is odd, normal if $l = 2x$ , where $x$ is odd, halved if $l = 2x$ , where $x$ is even or zero	$egin{array}{c} 2 \\ 4 \end{array}$	$\{001\}.$ 2-A $\mathbf{L}^r \{100\}$ or $\{001\}.$ $4a$ -A $\mathbf{L}^r \{001\}.$

## TETRAGONAL TETARTOHEDRY (PYRAMIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
89	$C_{f 4}^{-1}$	$\Gamma_t(\Gamma_0)$	4 8	1.) None $\left\{\begin{array}{cccccccccccccccccccccccccccccccccccc$	2 4	2-A <b>L</b> <sup>r</sup> {001}. 4-A <b>L</b> <sup>r</sup> {001}.
90	C42	$ \begin{array}{c c} (\Gamma_{0'}) \\ \Gamma_{t} (\Gamma_{0}) \\ (\Gamma_{0'}) \end{array} $	4	1.) {001} quartered		None.
91	C <sub>4</sub> <sup>3</sup>	$\begin{array}{c c} \Gamma_t \left( \Gamma_0 \right) \\ \left( \Gamma_0 \right) \end{array}$	4 8	1.) {001} halved { 2.) Same as C' <sub>4</sub> <sup>1</sup> 2.); also { {001} halved	2	2-A <b>L</b> <sup>r</sup> {001}
92	C44	Same as C	42, bu	t in opposite rotatory sense,	there	fore identical data.
93	C45	$\Gamma_{t}'(\Gamma_{0}'')$	16	1.) Same as $C'_{4}^{2}$ 1.) { 2.) Same as $C'_{4}^{2}$ 2.) { 1.) Same as $C'_{4}^{2}$ 1.); also {	-	Same as C <sub>4</sub> <sup>1</sup> .
94	C46	$ \Gamma_t^{(1 \ 0)}(\Gamma_0^{"}) $ $ \Gamma_t^{(1 \ 0)}(\Gamma_0^{"}) $	l	1.) Same as $C_{4}^{2}$ 1.); also { $\{001\}$ quartered 2.) Same as $C_{4}^{2}$ 2.); also $\{001\}$ quartered	· <del>7 </del> ,	Same as C <sub>4</sub> <sup>3</sup> .

## TETRAGONAL PARAMORPHY (BIPYRAMIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
95	C4h1	$\Gamma_t (\Gamma_0) \atop (\Gamma_0')$	8 16	1.) None $\left\{\begin{array}{cccccccccccccccccccccccccccccccccccc$	2 4	$ \begin{vmatrix} 2-A & \mathbf{L}^r & \{001\} ; & P \parallel^l & \{001\} . \\ 4-A & \mathbf{L}^r & \{001\} ; & 2-A & \mathbf{L}^r & P \parallel^l & \{001\} . \end{vmatrix} $
96	C4h2	$\begin{array}{c} \Gamma_t \left( \Gamma_0 \right) \\ \left( \Gamma_0 ' \right) \end{array}$	8 . 16	1.) {001} halved { 2.) Same as C' <sub>4</sub> <sup>1</sup> 2.); also {	8 $2$ $4$	$ \begin{vmatrix} 4 - \mathbf{A} \ \mathbf{L}^r \ \mathbf{P} \ \ ^l \ \{001\}, \\ 2 - \mathbf{A} \ \mathbf{L}^r \ \{001\}; \ \mathbf{P} \ \ ^l \ \{001\}, \\ 2 - \mathbf{A} \ \mathbf{L}^r \ \mathbf{P} \ \ ^l \ \{001\}. $
97	C413	$\Gamma_t \ (\Gamma_0)$	8	$\{001\}$ halved $\{1.\}$ $\{hko\}$ halved if $(h+k)$ is odd	$\frac{2}{4}$	2-A $\mathbf{L}^r$ {001}; C. 4-A $\mathbf{L}^r$ {001}; 4a-A $\mathbf{L}^r$ {001}.
98	C 4	$(\Gamma_{0}')$ $\Gamma_{t}(\Gamma_{0})$	16 8	2.) Same as $C'_{4}^{1}$ 2.); also all $\{hko\}$ halved	2	$2-A \perp^r \{001\}$ ; C.
90	C <sub>4h</sub> 4	$(\Gamma_{0}')$	16	1.) $\{hko\}$ halved if $(h+k)$ is odd; $\{001\}$ halved 2.) Same as $C_{4}^{-1}$ 2.); also	4	$4a-A \mathbf{L}^r \{001\}.$
99	C <sub>4h</sub> 5	$\Gamma_{t\_}'(\Gamma_{0}'')$	32	all $\{hko\}$ and $\{001\}$ halved  1.) Same as $C'_4{}^2$ 1.) $\int$		Same as $C_{4h}^{-1}$ .
100	$C_{4h}^{6}$	$\Gamma_t'(\Gamma_0''')$	$\begin{array}{c c} 16 \\ 32 \end{array}$	2.) Same as $C'_{4}^{2}$ 2.)	-	Same as $C_{4h}^4$ .
				$\{hko\}$ quartered if $(h+k)$ is odd, halved if even; $\{001\}$ quartered		
		$(\Gamma_{0}^{\prime\prime\prime})$	16	2.) Same as $C_4^2$ 2.); also $\{hko\}$ all halved; $\{001\}$ quartered		

# TETRAGONAL HEMIMORPHY (DITETRAGONAL PYRAMIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
101	$C_{4v}$	$\Gamma_t(\Gamma_0)$	8	1.) None	$\begin{array}{ c c } 2 \\ 4 \\ 8 \end{array}$	P    <sup>l</sup> {100} or {110}. 2 P's    <sup>l</sup> {100} intersecting in 2-A. 4 P's    <sup>l</sup> {100} and {110} intersecting
MA AND AND AND AND A SALE AND ASSAULT OF THE SALE AND		$(\Gamma_0')$	16	2.) Same as C' <sub>4</sub> <sup>1</sup> 2.) ]		in 4-A. Same as 1.), substituting {110} ₹ 100}. [and similarly throughout the
102	C <sub>4v</sub> <sup>2</sup>	$\Gamma_t \left( \Gamma_0  ight) \ \left( \Gamma_0'  ight)$	8 16	1.) $\{okl\}$ halved if $k$ is odd $\{a,b\}$ Same as $C'_{4}^{1}$ 2.); also $\{a,b\}$ halved if $b$ is odd $\{a,b\}$	$\frac{2}{4}$	classes $C_{4v}$ , $D_4$ , $D_{4h}$ ]. P    $^l$ {110}. 4-A $\mathbf{L}^r$ {001} ; 2 P's    $^l$ {110} intersecting in 2-A.
103	C <sub>4v</sub> <sup>3</sup>	$\Gamma_t(\Gamma_0) \ (\Gamma_0')$	8 16	1.) $\{okl\}$ halved if $l$ is odd $\{2.\}$ Same as $C'_4$ 2.); also $\{hhl\}$ halved if $l$ is odd	$egin{pmatrix} 2 \ 4 \end{bmatrix}$	$egin{array}{cccccccccccccccccccccccccccccccccccc$
104	C4v4	$\Gamma_{t}\left(\Gamma_{0} ight)$	8	1.) $\{okl\}$ halved if $(k+l)$ is odd	archaenna.	Same as $\mathrm{C}_{4^v}^3$ .
		$(\Gamma_0')$	16	2.) Same as $C'_{4}^{1}$ 2.); also $\{hhl\}$ halved if $(h+l)$ is odd		:
105	$C_{4v}^{5}$	$\Gamma_{t}\left(\Gamma_{0} ight)$	8	1.) $\{okl\}$ and $\{hhl\}$ halved if $l$ is odd	$\frac{2}{4}$	$2-A \mathbf{L}^r \{001\}.$ $4-A \mathbf{L}^r \{001\}.$
		$(\Gamma_0{}')$	16	2.) Same as $C'_4{}^1$ 2.); also all $\{okl\}$ halved; $\{hhl\}$ halved if $l$ is odd.		1 11 (001).
106	C <sub>4v</sub> 6	$\Gamma_t \ (\Gamma_0)$	8	1.) $\{okl\}$ halved if $(k+l)$ is odd; $\{hhl\}$ if $l$ is odd		Same as $C_{4v}^{5}$ .
	A	$(\Gamma_0')$	16	2.) Same as $C_{4}^{\prime 1}$ 2.); also $\{$ all $\{okl\}$ halved; $\{hhl\}$	-	
107	$\mathbf{C_{4}}_{v}$ 7	$\Gamma_t (\Gamma_0) \ (\Gamma_0')$	8 16	halved if $(h+l)$ is odd (1.) $\{hhl\}$ halved if $l$ is odd (2.) Same as $C'_4$ 2.); also (	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	$P \parallel^{l} \{100\}.$ 2 P's $\parallel^{l} \{100\}$ intersecting in 2-A.
108	$C_{4v}^{-8}$	$\Gamma_t (\Gamma_0)$	8	all $\{okl\}$ halved  1.) $\{okl\}$ halved if $k$ is	$\begin{bmatrix} 1 \\ 2 \end{bmatrix}$	2-A <b>1</b> <sup>r</sup> {001}.
	30	$(\Gamma_{0}')$	16	odd; $\{hhl\}$ if $l$ is odd 2.) Same as $C'_{4}^{1}$ 2.); also all $\{okl\}$ halved; $\{hhl\}$		
109	$C_{4v}^{9}$	$\Gamma_t'$ $(\Gamma_0'')$	32	halved if $h$ is odd 1.) Same as $C'_4{}^2$ 1.)	$_2$	$P \parallel^{l} \{100\} \text{ or } \{110\}.$
		$(\Gamma_0^{\prime\prime\prime\prime})$	16	2.) Same as $C'_{4}^{2}$ 2.)	8	2 P's $\parallel^l$ {110} intersecting in 2-A. 4 P's $\parallel^l$ {100} and {110} intersecting
110	C4v10	$\Gamma_t'$ $(\Gamma_0'')$	32	1.) Same as $C'_4{}^2$ 1.); also $\begin{cases} \\ \\ \\ \end{cases}$ all $\{hhl\}$ halved	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	in 4-A. P $\parallel^l$ {100}. 4-A $\perp^r$ {001}; 2 P's $\parallel^l$ {100} inter-
		$(\Gamma_0^{\ \prime\prime\prime})$	16	2.) Same as $C'_4{}^2$ 2.); also all $\{okl\}$ halved	4	secting in 2–A.
111	C <sub>4v</sub> <sup>11</sup>	$\Gamma_t'$ $(\Gamma_0'')$	32	1.) Same as $C'_4{}^2$ 1.); also $\{okl\}$ quartered if $(k+l)$	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	P $\parallel^l$ {110}. 2 P's $\parallel^l$ {110} intersecting in 2A.
		$(\Gamma_0^{\prime\prime\prime})$	16	is odd, halved if even 2.) Same as $C'_4{}^2$ 2.); also $\{hhl\}$ quartered if $l$ is odd, normal if $l = 2x$ , where $x$ is odd, halved if $l = 2x$ , where $x$ is		
	Ì	1		even or zero	ľ	

# TETRAGONAL HEMIMORPHY (DITETRAGONAL PYRAMIDAL)—(continued).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
112	C <sub>4v</sub> <sup>12</sup>	$\Gamma_t' \ (\Gamma_0'')$ $(\Gamma_0''')$	32	1.) Same as C' <sub>4</sub> <sup>2</sup> 1.); also {     {okl} quartered if (k+l)       is odd, halved if even;     all {hhl} halved 2.) Same as C' <sub>4</sub> <sup>2</sup> 2.); also all {okl} halved; {hhl} {     quartered if l is odd, normal if l = 2x, where x is odd, halved if l = 2x, where x is odd, halved if l = 2x, where x is even or zero		Same as $\mathrm{C}_{4v}^{-8}$ .

# TETRAGONAL ENANTIOMORPHY (TRAPEZOHEDRAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
113	$D_4^{-1}$	$\Gamma_t(\Gamma_{0}) \\ (\Gamma_{0}')$	8 16	1.) None	2 4 8	2-A L <sup>r</sup> {100}, {110} or {001}. 4-A L <sup>r</sup> {001}; 3 intersecting 2-A's L <sup>r</sup> {100} and {001}. 4 2-A's L <sup>r</sup> {100} and {110} inter-
114	$D_4^2$	$\begin{array}{c c} \Gamma_t(\Gamma_0) \\ (\Gamma_0') \end{array}$	8 16	1.) $\{100\}$ halved $\{2.\}$ Same as $C_{4}^{-1}$ 2.); also $\{110\}$ halved	$_{4}^{2}$	secting in $4$ –A $\perp^r$ {001}. 2–A $\perp^r$ {001} or {110}. 4–A $\perp^r$ {001}; 3 intersecting 2–A's $\perp^r$ {110} and {001}.
115	$D_4^{\ 3}$	$\begin{array}{c} \Gamma_t(\Gamma_0) \\ (\Gamma_0') \end{array}$	8 16	$\begin{bmatrix} 1.0 \\ 1.) \\ \{001\} \\ \text{quartered} \\ 2.) \\ \text{Same as } C'_{4}^{1} \\ 2.); \\ \text{also} \\ \end{bmatrix}$	2	$2-A \mathbf{L}^r \{100\} \text{ or } \{110\}.$
116	$D_4^4$	$\Gamma_t (\Gamma_0)$	8	1. $  100 $ halved; $  100$	2	$2-A \perp^r \{110\}.$
		$(\Gamma_0')$	16	quartered 2.) Same as $C_{4}^{\prime 1}$ 2.); also $\{110\}$ halved, $\{001\}$ quartered		
117	$D_4^{5}$	$\begin{array}{c c} \Gamma_t(\Gamma_{0}) \\ (\Gamma_{0}') \end{array}$	8 16	1.) $\{001\}$ halved $\{2.\}$ Same as $C'_{4}^{1}$ 2.); also $\{001\}$ halved	$\frac{2}{4}$	2-A $\perp^r$ {100}, {110} or {001}. 3 intersecting 2-A's, either $\perp^r$ {110} and {001}, or $\perp^r$ {100} and {001}.
118	$D_4^6$	$\Gamma_t(\Gamma_0)$	8	1.) {100} a n d {001} halved	$\frac{2}{4}$	2-A $\mathbf{L}^r$ {001} or {110}. 3 intersecting 2-A's, $\mathbf{L}^r$ {001} and
		$(\Gamma_{0}')$	16	2. Same as C' <sub>4</sub> <sup>1</sup> 2.); also (001) and (110) halved		{110}.
119	$D_4^7$	Same as D	<b>)<sub>4</sub>3</b> , bu	at in opposite rotatory sense,	there	fore identical data.
120	$D_4^8$	Same as I	<b>)<sub>4</sub>4</b> , bu	at in opposite rotatory sense,	heref	fore identical data.
121	$D_4^{9}$	$ \begin{vmatrix} \Gamma_t' (\Gamma_0'') \\ (\Gamma_0''') \end{vmatrix} $	32 16	1.) Same as $C'_{4}^{2}$ 1.)	$\frac{2}{4}$	2-A $\mathbf{L}^r$ {100}, {110} or {001}. 4-A $\mathbf{L}^r$ {001}; 3 intersecting 2-A's $\mathbf{L}^r$ {110} and {001}.
	-				8	4 2-A's $\mathbf{L}^r$ {100} and {110} intersecting in 4-A $\mathbf{L}^r$ {001}.
122	$D_4^{10}$	$\Gamma_{t'}(\Gamma_{0''})$	32	1.) Same as $C'_4{}^2$ 1.); also $\begin{cases} \\ 001 \end{cases}$ quartered	$\frac{2}{4}$	2-A $\mathbf{L}^r$ {100}, {110} or {001}. 3 intersecting 2-A's $\mathbf{L}^r$ {100} and
		$(\Gamma_0^{\prime\prime\prime})$	16	2.) Same as $C'_4{}^2$ 2.); also {001} quartered	1,	{001}.

TETRAGONAL HOLOHEDRY (DITETRAGONAL BIPYRAMIDAL).

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No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
123		$\begin{array}{c c} \Gamma_t(\Gamma_{0}) \\ (\Gamma_{0}') \end{array}$	16 32	1.) None	2 4	P    <sup>l</sup> {100}, {110} or {001}. 2 P's    <sup>l</sup> {100} intersecting in 2-A; 2 P's    <sup>l</sup> {001} and {100} intersecting in 2-A; 2 P's    <sup>l</sup> {001} and {100} and {110} intersecting in 2-A.
					8	3 P's    <sup>l</sup> {100} and {001} intersecting in 3 2-A's; 4 P's    <sup>l</sup> {100} and {110} intersecting in 4-A. 4 P's    <sup>l</sup> {100} and {110} intersecting
124	$D_{4h}^2$	$\Gamma_t (\Gamma_0)$	16	1.) $\{okl\}$ halved if $l$ is odd;	2	$\begin{bmatrix} \text{in } 4\text{-A} + P \parallel^{l} \{001\}, \\ 2\text{-A } 1^{r} \{100\}, \{110\} \text{ or } \{001\}; P \parallel^{l} \end{bmatrix}$
		$(\Gamma_0')$	32	$\{hhl\}$ halved if $l$ is odd $[2]$ . Same as $C'_4$ $[2]$ .; also all $\{ohl\}$ halved; $\{hhl\}$ halved if $l$ is odd	4	$\{001\}.$ 4-A $\perp^r \{001\}$ ; 3 intersecting 2-A's $\perp^r \{100\}$ and $\{001\}$ ; 2-A $\perp^r P \parallel^l \{001\}.$
	A T T A A A A A A A A A A A A A A A A A				8	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$
125	$D_{4h}$	$\Gamma_t (\Gamma_0)$	16	1.) $\{hko\}$ halved if $(h+k)$ is odd; $(okl)$ halved if $k$ is odd	2 4	$ \begin{vmatrix} 2-A & \mathbf{L}^{r} & \{100\} \text{ or } \{110\}; & P \parallel^{l} & \{110\}. \\ 4-A & \mathbf{L}^{r} & \{001\}; & 2 & P's \parallel^{l} & \{110\} \text{ intersecting in } 2-A; & 2-A & \mathbf{L}^{r} & P \parallel^{l} \end{vmatrix} $
	-	$(\Gamma_0')$	32	2.) Same as $C'_4$ 2.); also all $\{hko\}$ halved; $\{hhl\}$ halved if $h$ is odd	8	{110}. 4 2 A's $\mathbf{L}^r$ {110} and {100} intersecting in 4-A $\mathbf{L}^r$ {001}; full $\mathbf{D}_{2d}$
126	D <sub>4h</sub> <sup>4</sup>	$\Gamma_t (\Gamma_0)$	16	1.) $\{hko\}$ halved if $(h+k)$ is odd; $\{okl\}$ halved if $(k+l)$ is odd; $\{hhl\}$	2 4	symmetry (P    $^{l}$ {110}). 2-A $\mathbf{L}^{r}$ {100}, {110} or {001}; C. 4-A $\mathbf{L}^{r}$ {001}; 3 intersecting 2-A's $\mathbf{L}^{r}$ {100} and {001}; $4a$ -A $\mathbf{L}^{r}$
		$(\Gamma_0')$	32	halved if $l$ is odd 2.) Same as $C'_{4}^{1}$ 2.); also all $\{hko\}$ , $\{okl\}$ halved; $\{hkl\}$ halved if $(h+l)$ is odd	8	$\{001\}.$ $4 \ 2-A$ 's $\mathbf{L}^r \{100\}$ and $\{110\}$ intersecting in $4-A \ \mathbf{L}^r \{001\}.$
127	$D_{4h}^{5}$	$\Gamma_t (\Gamma_0)$	16	1.) $\{okl\}$ halved if $k$ is odd	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	$P \parallel^{l} \{110\} \text{ or } \{001\}.$ 4-A $L^{r} \{001\}$ ; 2 P's $\parallel^{l} \{110\}$ inter-
		$(\Gamma_0')$	32	2.) Same as $C'_4$ 2.); also $\{hhl\}$ halved if $h$ is odd	8	secting in 2-A; 2 P's $\parallel^{l}$ {001} and {110} intersecting in 2-A. 4-A $\perp^{r}$ P $\parallel^{l}$ {001}; 3 P's $\parallel^{l}$ {110}
128	$D_{4h}^{6}$	$\Gamma_t (\Gamma_0)$	16	1.) $\{okl\}$ halved if $(k+l)$ is odd; $\{hhl\}$ halved if $l$ is odd	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	and {001} intersecting in 3 2–A's. 2–A $\perp^r$ {110} or {001}; P $\parallel^l$ {001}. 4–A $\perp^r$ {001}; 3 intersecting 2–A's $\perp^r$ {110} and {001}; 2–A $\perp^r$ P $\parallel^l$
		$(\Gamma_{0}')$	32	2.) Same as $C'_4$ 2.); also all $\{okl\}$ halved; $\{hhl\}$ halved if $(h+l)$ is odd	8	{001}. 4-A <b>L</b> <sup>r</sup> P    <sup>l</sup> {001}.
129	$D_{4h}^7$	$\Gamma_t (\Gamma_0)$	16	1.) $\{hko\}$ halved if $(h+k)$ is odd	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	2-A $\perp^r$ {110}; P   <sup>l</sup> {100} or {110}. 2 P's    <sup>l</sup> {100} intersecting in 2-A;
		$(\Gamma_0')$	32	2.) Same as $C'_{4}$ 2.); also all $\{hko\}$ halved	8	2–A $\mathbf{L}^r$ P    $^l$ {110}. 4 P's    $^l$ {100} and {110} intersecting in 4–A; full $\mathbf{D}_{2d}$ symmetry (P   $^l$ {100}).
130	D <sub>4h</sub> <sup>8</sup>	$\Gamma_t (\Gamma_0)$	16	1.) $\{hko\}$ halved if $(h+k)$ is odd; $\{okl\}$ , $\{hhl\}$ halved if $l$ is odd		2-A $\perp^r$ {001} or {110}; C. 4-A $\perp^r$ {001}; 3 intersecting 2-A's $\perp^r$ {001} and {110}; 4a-A $\perp^r$
-		$(\Gamma_0')$	32	2.) Same as $C'_4$ 2.); also all $\{hko\}$ , $\{okl\}$ halved; $\{hkl\}$ halved if $l$ is odd	The second secon	{001}.

# TETRAGONAL HOLOHEDRY (DITETRAGONAL BIPYRAMIDAL)—(continued).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
131	D <sub>4h</sub> 9	$\Gamma_t \left( \Gamma_0 \right)$ $\left( \Gamma_0 \right)$	16 32	1.) $\{hhl\}$ halved if $l$ is odd 2.) Same as $C'_4$ 2.); also all $\{okl\}$ halved	2 4 8	2-A $\mathbf{L}^r$ {110}; P    $^l$ {100} or {001}. 2 P's    $^l$ {100} intersecting in 2-A; 2 P's    $^l$ {001} and {100} intersecting in 2-A. 3 P's    $^l$ {100} and {001} intersecting in 3 2-A's; full $D_{2d}$ symmetry
132	$D_{4h}^{10}$	$\Gamma_t(\Gamma_0) = \Gamma_t(\Gamma_0')$	16 32	1.) $\{okl\}$ halved if $l$ is odd 2.) Same as $C'_{\underline{4}}^1$ 2.); also $\{hhl\}$ halved if $l$ is odd	4 8	$ \begin{array}{c} (P \parallel^{l} \{100\}). \\ 2\text{-A} \ \ \mathbf{L}^{r} \ \{100\} \ \ \text{or} \ \{001\} \ ; \ P \parallel^{l} \{110\} \\ \text{or} \ \{001\}. \\ 2 \ P's \parallel^{l} \{110\} \ \ \text{intersecting in} \ \ 2\text{-A} \ ; \\ 2 \ P's \parallel^{l} \{001\} \ \ \text{and} \ \{110\} \ \ \text{intersecting} \\ \text{secting in} \ \ 2\text{-A} \ \ \mathbf{L}^{r} \ \ P \parallel^{l} \\ \{001\} \ ; \ \ 3 \ \ \text{intersecting} \ \ 2\text{-A's} \ \ \mathbf{L}^{r} \\ \{100\} \ \ \text{and} \ \{001\}. \\ 3 \ P's \parallel^{l} \{110\} \ \ \text{and} \ \{001\} \ ; \ \ \text{full} \ \ D_{2d} \\ \end{array} $
133	$D_{4h}^{-11}$	$\Gamma_t (\Gamma_0)$	16	1.) $\{hko\}$ halved if $(h+k)$ is odd; $\{okl\}$ halved if $k$ is odd; $\{hkl\}$ halved if $l$ is odd	$egin{bmatrix} 2 \ 4 \end{bmatrix}$	symmetry (P    $^{l}$ {110}). 2-A $\mathbf{L}^{r}$ {100}, {001} or {110}; C. 3 intersecting 2-A's $\mathbf{L}^{r}$ {100} and {001}; 3 intersecting 2-A's $\mathbf{L}^{r}$ {110} and {001}; $4a$ -A $\mathbf{L}^{r}$ {001}.
134	$\mathrm{D}_{4h}^{-12}$	$(\Gamma_0')$ $\Gamma_t (\Gamma_0)$ $(\Gamma_0')$	32 16 32	2.) Same as $C_{4}^{1}$ 2.); also all $\{hko\}$ , $\{okl\}$ halved; $\{hhl\}$ halved if $h$ is odd 1.) $\{hko\}$ halved if $(h+k)$ is odd; $\{okl\}$ halved if $\{k+l\}$ is odd 2.) Same as $C_{4}^{1}$ 2.); also all $\{hko\}$ halved; $\{hhl\}$ halved if $(h+l)$ is odd	2 4	2-A $L^r$ {100}, {001} or {110}; P   ^l {110}. 3 intersecting 2-A's $L^r$ {100} and {001}; 3 intersecting 2-A's $L^r$ {110} and {001}; 2 P's   ^l {110} intersecting in 2-A; 2-A $L^r$ P   ^l
135	$D_{4h}^{13}$	$\Gamma_t \left( \Gamma_{0} \right)$ $\left( \Gamma_{0} \right)$	16 32	1.) $\{okl\}$ halved if $k$ is odd; $\{hhl\}$ halved if $l$ is odd 2.) Same as $C'_{4}$ 2.); also all $\{okl\}$ halved; $\{hhl\}$	8 2 4	$ \begin{array}{c} \{110\}. \\ \text{Full } \mathrm{D}_{2d} \text{ symmetry } (\mathrm{P} \parallel^l \{110\}). \\ 2\text{-A } \mathbf{L}^r \{001\} \text{ or } \{110\} \text{ ; } \mathrm{P} \parallel^l \{001\}. \\ 3 \text{ intersecting } 2\text{-A's } \mathbf{L}^r \{110\} \text{ and } \\ \{001\} \text{ ; } 2\text{-A } \mathbf{L}^r \mathrm{P} \parallel^l \{001\} \text{ ; } 4a\text{-A} \\ \mathbf{L}^r \{001\}. \end{array} $
136	$D_{4h}^{-14}$	$\Gamma_t \left( \Gamma_0 \right)$ $\left( \Gamma_0 \right)$	16 32	halved if $h$ is odd  1.) $\{okl\}$ halved if $(k+l)$ is odd  2.) Same as $C'_{4}$ 2.); also $\{hkl\}$ halved if $(h+l)$ is odd	2 4 8	2-A $\mathbf{L}^r$ {001}; P    <sup>l</sup> {110} or {001}. 2 P's    <sup>l</sup> {110} intersecting in 2-A; 2 P's    <sup>l</sup> {001} and {110} intersecting in 2-A; 2 excipation 2-A; 2-A $\mathbf{L}^r$ P    <sup>l</sup> {001}; 4a-A $\mathbf{L}^r$ {001}. 3 P's    <sup>l</sup> {110} and {001} intersecting in 2-2 A'z
137	$D_{4h}^{-15}$	$\Gamma_t (\Gamma_0)$	16 32	1.) $\{hko\}$ halved if $(h+k)$ is odd; $\{hhl\}$ halved if $l$ is odd	2 4 8	in 3 2–A's. 2–A $\mathbf{L}^r$ {110}; P    <sup>l</sup> {100}; C. 2 P's    <sup>l</sup> {100} intersecting in 2–A. Full $D_{2d}$ symmetry (P    <sup>l</sup> {100}).
138 .	$D_{4h}^{16}$	$(\Gamma_{0}')$ $\Gamma_t (\Gamma_{0})$	16	2.) Same as $C'_4$ 2.); also all $\{hko\}$ , $\{okl\}$ halved 1.) $\{hko\}$ halved if $(h+k)$ is odd; $\{okl\}$ halved if $l$ is odd	$egin{bmatrix} 2 \\ 4 \end{bmatrix}$	2-A $\mathbf{L}^r$ {001} or {110}; P    <sup>l</sup> {110}. 3 intersecting 2-A's $\mathbf{L}^r$ {110} and {001}; 2 P's    <sup>l</sup> {110} intersecting
	-	$(\Gamma_0{}')$	32	2.) Same as $C_4^{-1}$ 2.); also all $\{hko\}$ halved; $\{hhl\}$ halved if $l$ is odd		in 2-A; 2-A $\perp^r P \parallel^l \{110\}$ ; 4a-A $\perp^r \{001\}$ .

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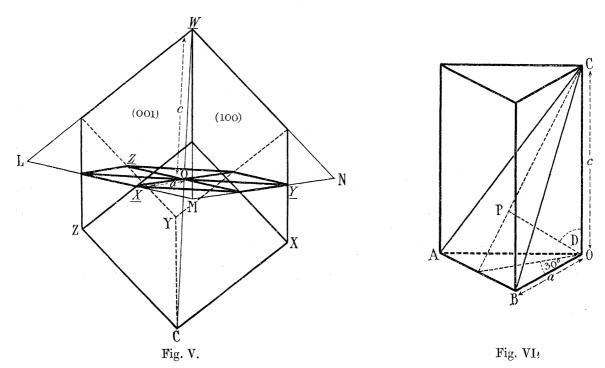
No.	SG.	B.L.	$n$ .	Abnormal Spacings.	p.	Possible Molecular Symmetry.
				j	l P	
139	$\mathrm{D}_{4h}^{-17}$	$ \begin{array}{c c} \Gamma_t'(\Gamma_0'') \\ (\Gamma_0''') \end{array} $	64 32	1.) Same as $C'_{4}^{2}$ 1.)	2 4	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$
					0	secting in 2-A; 2 P's $\parallel^l$ {001} and {110} intersecting in 2-A.
					8	3 P's $\parallel^l$ {110} and {001} intersecting in 3 2-A's; 4 P's $\parallel^l$ {100} and {110} intersecting in 4-A; full
					16	$\begin{array}{c c} D_{2d} \text{ symmetry } (P \parallel^{l} \{110\}). \\ 4 P's \parallel^{l} \{100\} \text{ and } \{110\} \text{ intersecting } \\ \vdots & A A + B \parallel^{l} \{001\} \end{array}$
140	$D_{4h}^{18}$	$\Gamma_t'(\Gamma_0'')$	64	1.) Same as $C_4^2$ 1.); also all $\{hhl\}$ halved	2	$\begin{array}{c c} & \text{in } 4\text{-}A + P \parallel^l \{001\}, \\ 2\text{-}A \perp^r \{100\} \text{ or } \{110\} \text{ ; } P \parallel^l \{100\} \text{ or } \{001\}. \end{array}$
		$(\Gamma_{0}''')$	32	2.) Same as $C'_4{}^2$ 2.); also all $\{okl\}$ halved	4	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$
					8	$egin{array}{cccccccccccccccccccccccccccccccccccc$
			0.000			$\{001\}$ intersecting in $3$ 2-A's; full $D_{2d}$ symmetry $\{P \mid l^2 \{100\}\}$ .
141	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	$\Gamma_{t}'(\Gamma_{0}'')$	64	1.) Same as $C'_4{}^2$ 1.); also $\{hko\}$ quartered if $(h+k)$ is odd, halved if even;	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	2–A $\mathbf{L}^r$ {100} or {110}; P    <sup>l</sup> {110}. 2–A $\mathbf{L}^r$ P    <sup>l</sup> {110}; 2 P's    <sup>l</sup> {110} intersecting in 2–A.
				$\{okl\}$ quartered if $(k+l)$ is odd, halved if even	8	Full $D_{2d}$ symmetry (P $\parallel^l$ {110}).
		$(\Gamma_{0}^{\prime\prime\prime\prime})$	32	2.) Same as $C'_4$ <sup>2</sup> 1.); also $\langle hko \rangle$ halved; $\langle hhl \rangle$		
				quartered if $l$ is odd, $ $ normal if $l = 2x$ , where $ $		
				$x \text{ is odd, halved if } l = 2x, \mid$ where $x \text{ is even or zero} \mid$	.	
142	$D_{4h}^{20}$	$\Gamma_t'$ $(\Gamma_0'')$	64	1.) Same as $C'_4^2$ 1.); also $\{hko\}$ quartered if $(h+k)$ is odd, halved	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	2-A $\mathbf{L}^r$ {100}, {001} or {110}; C. 3 intersecting 2-A's $\mathbf{L}^r$ {100} and {001}; $4a$ -A $\mathbf{L}^r$ {001}.
				if even; $\{okl\}$ quartered if $(k+l)$ is odd, halved if even; all $\{hhl\}$ halved		
		$(\Gamma_0^{\prime\prime\prime})$	32	2.) Same as $C'_4{}^2$ 2.); also all $\{hko\}$ , $\{okl\}$ halved;		
	Top control of			$\{hhl\}$ quartered if $l$ is odd, normal if $l = 2x$ , where $x$ is odd, halved		
a department				if $l = 2x$ , where $x$ is even or zero		

## Rhombohedral and Hexagonal Systems.

For the purposes of structure theory, it is convenient to discuss these two systems together because, though the hexagonal system is based solely on the hexagonal lattice, the rhombohedral system is based on both the rhombohedral and hexagonal lattices.

The hexagonal lattice  $\Gamma_h$  is identical with a simple orthorhombic diamond lattice (Γ<sub>0</sub>') of angle 120°, the hexad or triad axis being perpendicular to the diamond-shaped face. The rhombohedral lattice  $\Gamma_{rh}$  is a simple cube compressed or elongated in a direction parallel to a triad axis (which then becomes the unique triad axis of the system). It occurs as an alternative to the hexagonal lattice in the following classes: C<sub>3</sub>, C<sub>3i</sub>, C<sub>3i</sub>, C<sub>3i</sub>,  $D_3$  and  $D_{3d}$ . On this account a peculiar difficulty arises in the examination of crystals belonging to any of these five classes, for trigonal crystals, of whatever basic lattice, are usually referred to the rhombohedral crystal axes named after Miller. These crystal axes, being parallel to the edges of a rhombohedron, are not suitable for the description of crystals based on a hexagonal lattice, just as the Bravais-Miller hexagonal axes are not adapted to the requirements of true rhombohedral crystals. The obvious way out of the difficulty is to reserve exclusively the Miller axes for true rhombohedral crystals and the Bravais-Miller axes for all crystals based on the hexagonal lattice.

To do this it is necessary first to find out on which of the two lattices the crystal under examination is built. This is not completely possible by examination of the external form alone, though, in general, a crystal will tend to betray its basic lattice in its "habit." In trigonal crystals based on  $\Gamma_h$  we should expect simple trigonal prisms and pyramids, while in those based on  $\Gamma_{rh}$  the development of rhombohedra is more likely. Consider now a crystal developed as a simple trigonal pyramid only. A face of this pyramid would



be taken as parametral plane and for  $\Gamma_h$  would correspond to ABC in fig. VI. For  $\Gamma_{rh}$ it would correspond to an extended rhombohedron face such as WMN of fig. V. In the first case the ratio c/a = OC/OA and in the second c/a = OW/OX. If the lattice is  $\Gamma_h$ 

the crystallographic and experimental values of c/a will agree in the simplest case  $(C_{3}^{1}, say)$ , but should the lattice be really rhombohedral  $(C_{3}^{4})$  the observed ratio will be  $\frac{2}{3}c/2a = c/3a$ . Unfortunately, this is only the simplest case, and such a test would not distinguish immediately between  $C_3^2$  (or  $C_3^3$ ), in which there are screw-axes of translation  $2\tau_z/3$ , and  $C_3^4$  which is based on a simple rhombohedral lattice.

There are, however, always certain planes which can be used as an aid to identifying the underlying space-lattice. Such planes are the prism faces  $(1\overline{2}1)$  [or  $(10\overline{1}0)$ ] and  $(1\overline{1}0)$ [or  $(11\overline{2}0)$ ]. A glance at the tables shows that the spacings of these planes are unaffected by the dispositions of the molecules. Fig. V shows the relation between the rhombohedral axes (parallel to CX, CY, CZ) and the hexagonal axes (OX, OY, OZ, OW). The volume of the rhombohedron is  $4a^2c/\sqrt{3}$ , while the volume of the corresponding hexagonal cell is  $a^2c\sqrt{3}/2$ : the ratio between the two is 8/3. Thus the dimensions of a rhombohedron with 8/3 molecules per cell will correspond crystallographically to those of a hexagonal cell with one molecule per cell, that is, the dimensions in the two cases are based on the same values of c and a.

Suppose now in a given trigonal crystal the chosen parametral plane is the true parametral plane of either  $\Gamma_h$  or  $\Gamma_{rh}$ . The possible numbers (N, say) of molecules per cell can be obtained from the tables, and from the above we know that the dimensions of a rhombohedron containing 8N/3 molecules per cell will correspond to the dimensions of a hexagonal cell of N molecules per cell. Hence we can calculate and compare the corresponding spacings of these two corresponding cells. For the hexagonal cell,  $d_{10\bar{1}0}=a\sqrt{3/2}$  and  $d_{11\bar{2}0}=a/2$ , but for the corresponding rhombohedral cell,  $d_{1\bar{2}1}=a/\sqrt{3}$ and  $d_{110} = a$ . Thus in a trigonal crystal based on a hexagonal lattice, but referred by convention to rhombohedral axes, provided that the crystallographic parametral plane is the same as the parametral plane of the hexagonal lattice, we can detect the hexagonal lattice by testing the  $(1\bar{2}1)$  and the  $(1\bar{1}0)$  of a rhombohedron containing 8N/3 molecules per cell, where N is either equal to n, the number of asymmetric molecules given by the class, or to some sub-multiple of n. We shall find that the observed spacing of  $(1\overline{2}1)$  is  $\frac{3}{2}$  times the calculated, while for  $(1\overline{1}0)$  it is  $\frac{1}{2}$  the calculated. Additional information is afforded by (a) the (111), the observed spacing of which is normally \(\frac{3}{2}\) times the calculated, but which by a thirding or halving may be reduced to  $\frac{1}{2}$  or  $\frac{3}{4}$  times the calculated; and by (b) the (100), the observed spacing of which is normally  $\frac{1}{2}$  the calculated, but which by a halving may be reduced to  $\frac{1}{4}$  of the calculated.

If the above treatment leads to anomalous results, the inference is that the crystallographic parametral plane does not correspond to the true parametral plane of the lattice, in which case it is necessary to repeat the examination, using the face of another general form  $\{hkl\}$  as parametral plane and making the new "angular element"  $D = \angle (hkl)$  – (111). (N.B.  $c/a = \tan D \cos 30^{\circ}$ .) When agreement is found, the crystallographic nomenclature should be abandoned and the crystal referred to the true structural axes.

A method of detecting the underlying lattice, based on the study of LAUE diagrams has been suggested by Wyckoff.\*

Another difficulty, similar to the one discussed above, arises in the examination of crystals based on  $\Gamma_h$  from the frequent discrepancy between the conventional relations between crystallographic axes and elements of symmetry, and the true structural relations. For instance, in the  $C_{3v}$  and  $D_{3h}$  classes, the conventional crystallographic axes (rhombohedral, since the class is trigonal) lie in the symmetry planes, and the hexagonal axes derived from these are perpendicular to the symmetry planes. Thus these derived hexagonal axes correspond to the true structural axes in groups  $C_{3v}^{-1}$  and  $C_{3v}^{-3}$ , but are perpendicular to them in groups  $C_{3v}^{-2}$  and  $C_{3v}^{-4}$ . In the two last mentioned, the crystallographic angle  $D = \angle (100) - (111)$  is not the true structural angular element (D<sub>0</sub>, say). The two are connected by the equations  $c/a = \tan D_0 \cdot \cos 30^\circ = \tan D \cdot \sin 30^\circ$ , where c and a refer to the true structural values. It must be distinctly understood that all the figures, 1-230, and the tabulated data derived from them refer exclusively to the true structural axes, that is, to the edges of the true unit cell. If there is any discrepancy between the conventional and structural axes the worker must first localise this difficulty as far as is theoretically possible, and then apply the tabulated results. This sort of problem occurs in many of the crystal classes in addition to those belonging to this system,† and no general rules for guidance can be offered. With regard to other classes of the systems now being discussed it should be noticed that in the classes  $D_3$  and  $D_{3d}$  crystallographers always take the dyad axes as hexagonal axes, whereas the true structural axes may be parallel or perpendicular to the dyad axes. By referring to the tables it will be found that only in a very limited number of cases is it possible without complete examination to distinguish between groups in which the true structural hexagonal axes lie in the symmetry planes  $(C_{3v}^2, C_{3v}^4, D_{3h}^3, D_{3h}^4)$  and the corresponding groups in which they are perpendicular to the symmetry planes  $(C_{3v}^{-1}, C_{3v}^{-3}, D_{3h}^{-1}, D_{3h}^{-2})$ . For example, we can distinguish between  $C_{3v}^{-1}$  and  $C_{2v}^{-2}$  if there are two molecules only per cell, for then the molecule itself must possess a triad axis, and this is only possible in  $C_{3v}^2$ ; but the tables alone do not distinguish between them if there are one, three or six molecules per cell. Similar considerations hold with regard to the pairs of groups in which the true hexagonal axes are parallel and perpendicular respectively to the dyad axes of the structure  $(D_3^2 \text{ and } D_3^1; D_3^4 \text{ and } D_3^3; D_3^6 \text{ and } D_3^5; D_{3d}^3 \text{ and } D_{3d}^1; D_{3d}^4 \text{ and } D_{3d}^2).$ 

In Laue photographs of crystals belonging to these two systems classes C<sub>3</sub> and C<sub>3i</sub> appear as  $C_{3i}$ ;  $C_{3v}$ ,  $D_3$  and  $D_{3d}$  appear as  $D_{3d}$ ;  $C_{3h}$ ,  $C_6$  and  $C_{6h}$  appear as  $C_{6h}$ ;  $D_{3h}$ ,  $D_6$ ,  $C_{6v}$ , and  $D_{6h}$  appear as  $D_{6h}$ ; thus the twelve classes are reduced to four.

<sup>\*</sup> R. W. G. Wyckoff, 'Am. J. Soc,' 1920, vol. 50, p. 329

<sup>†</sup> Cf. 'Roy. Soc. Proc.,' A, 1923, vol. 104, p. 219.

# RHOMBOHEDRAL AND HEXAGONAL SYSTEMS.

## RHOMBOHEDRAL TETARTOHEDRY (TRIGONAL PYRAMIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.			
143	C <sub>3</sub> 1	$\Gamma_h$	3	None	3	$3$ -A $\perp^r \{0001\}$ .			
144	. C <sub>3</sub> <sup>2</sup>	$\Gamma_h$	3	{0001} thirded		None.			
145	$C_3^3$ Same as $C_3^2$ , but in opposite rotatory sense, therefore identical data.								
146	C <sub>3</sub> <sup>4</sup>	$\Gamma_{rh}$	3	None	3	3-A <b>Д</b> <sup>*</sup> {111}.			

# HEXAGONAL TETARTOHEDRY OF THE SECOND SORT (RHOMBOHEDRAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
147	$\mathbf{C_{3i}^1}$ $\mathbf{C_{3i}^2}$	$\Gamma_{n}$ $\Gamma_{nh}$	6	None	2 3 6 2 3 6	C. 3-A $\mathbf{L}^r$ {0001}. 3-A $\mathbf{L}^r$ {0001} + C. C. 3-A $\mathbf{L}^r$ {111}. 3-A $\mathbf{L}^r$ {111} + C.

## RHOMBOHEDRAL HEMIMORPHY (DITRIGONAL PYRAMIDAL).

No	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
149	C <sub>3v</sub> 1	$\Gamma_h$	6	None	$\frac{2}{6}$	$P \parallel^{l} \{11\overline{2}0\}.$ 3 P's $\parallel^{l} \{11\overline{2}0\}$ intersecting in 3–A.
150	$C_{3v}^{2}$	$\Gamma_h$	6	None	$\frac{2}{3}$	$ P  ^{l}$ {1010}. 3-A <b>L</b> <sup>r</sup> {0001}. 3 P's    <sup>l</sup> {1010} intersecting in 3-A.
151	C3v3	$\Gamma_h$	6	$\{mo\overline{m}l\}$ halved if $l$ is odd .	3	$3-A \perp^r \{0001\}.$
152	C3v4	$\Gamma_{h}$	6	$\{mm\overline{2m}l\}$ halved if $l$ is odd.	3	3-A \(\psi^r\) \(\left\) \(\left\) \(\left\) \(\left\).
153	C3,5	$\Gamma_{rh}$	6	None	$\frac{2}{6}$	$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$
154	C3v6	$\Gamma_{rh}$	6	$\{hhl\}$ halved if $l$ is odd	3	$3-A$ $\mathbf{L}^r$ {111}.

# THE EXAMINATION OF THE 230 SPACE-GROUPS BY HOMOGENEOUS X-RAYS. 249 RHOMBOHEDRAL ENANTIOMORPHY (TRAPEZOHEDRAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry
155	D <sub>3</sub> <sup>1</sup>	$\Gamma_h$	6	None	$\begin{bmatrix} 2 \\ 3 \\ 6 \end{bmatrix}$	$2-A \perp^r \{10\bar{1}0\}.$ $3-A \perp^r \{0001\}.$ $3  2-A$ 's $\perp^r \{10\bar{1}0\}$ intersecting in
156	$D_3^2$	$\Gamma_h$	6	None	2 3 6	$3-A \perp^r \{0001\}.$ $2-A \perp^r \{11\overline{2}0\}.$ $3-A \perp^r \{0001\}.$ $3 \ 2-A$ 's $\perp^r \{11\overline{2}0\}$ intersecting in
157-	$D_3^3$	$\Gamma_h$	6	{0001} thirded	2	$3-A \perp^r \{0001\}.$ $2-A \perp^r \{1010\}.$
158	D <sub>3</sub> <sup>4</sup>	$\Gamma_h$	6	{0001} thirded	2	2-A <b>L</b> * {1120}.
159	$D_3^{5}$	Same as I	) <sub>3</sub> 3, bi	it in opposite rotatory sense,	there	fore identical data.
160	$D_3^6$	Same as I	) <sub>3</sub> 4, bu	at in opposite rotatory sense,	$_{ m there}$	fore identical data.
161	D <sub>3</sub> <sup>7</sup>	$\Gamma_{rh}$	6	None	$\begin{bmatrix} 2 \\ 3 \\ 6 \end{bmatrix}$	$ \begin{vmatrix} 2-A \perp^r \{1\bar{1}0\}, \\ 3-A \perp^r \{111\}, \\ 3  2-A's \perp^r \{1\bar{1}0\} & \text{intersecting in} \\ 3-A \perp^r \{111\}. \end{vmatrix} $

## RHOMBOHEDRAL HOLOHEDRY (DITRIGONAL SCALENOHEDRAL).

	No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
	162	$D_{3d}^{-1}$	$\Gamma_h$	12	None	2	$2-A \perp^r \{10\bar{1}0\}; P \parallel^l \{10\bar{1}0\}.$
		*				8 4	$egin{array}{lll} 3-A & \mathbf{L}^r & \{0001\}, \\ 2-A & \mathbf{L}^r & P & \ ^l & \{10\overline{1}0\}. \end{array}$
						6	$3 \text{ P's } \parallel^l \{10\overline{10}\}\$ intersecting in 3-A;
							$3$ 2-A's $\perp^r$ {10\overline{10}} intersecting in
							$3-A \perp^r \{0001\}.$
			-		·	12	$ 3 \text{ P's}  ^{l} \{10\overline{1}0\} + 3 \text{ 2-A's } \mathbf{L}^{r} \{10\overline{1}0\} $
	1.00	T 0		1.0			all intersecting in 3-A $\perp^r$ {0001}.
	163	$D_{3d}^2$	$\Gamma_h$	12	$\{mm2ml\}$ halved if $l$ is odd	$\frac{2}{2}$	$2-A \perp^r \{10\bar{1}0\}$ ; C.
						3 6	$3-A \perp^r \{0001\}.$
l						0	3 2-A's $\hat{L}^r$ {1010} intersecting in 3-A
	164	$D_{3d}^3$	$\Gamma_h$	12	None	. 2	$\begin{array}{c c} \mathbf{L}^{r} \{0001\}; \ 3-\mathbf{A} \ \mathbf{L}^{r} \{0001\} + \mathbf{C}. \\ 2-\mathbf{A} \ \mathbf{L}^{r} \{11\overline{2}0\}; \ \mathbf{P} \parallel^{l} \{11\overline{2}0\}. \end{array}$
-		3a	- n			4	$2-A \perp^r P \parallel^l \{11\overline{2}0\}.$
			1			6	3 P's $\parallel^l$ {11 $\bar{2}$ 0} intersecting in 3-A.
						12	$ 3 \text{ P's}  ^{l} \{11\overline{2}0\} + 3 \text{ 2-A's } \mathbf{L}^{r} \{11\overline{2}0\}$
	105	D 4		10			all intersecting in 3-A $\perp^r$ {0001}.
	165	$-\mathrm{D}_{3d}^{-4}$	$\Gamma_h$	12	$\{moml\}$ halved if $l$ is odd.	2	$2-A \perp^r \{11\bar{2}0\}$ ; C.
ŀ		-				3 6	$3-A \perp^r \{0001\}$
						0	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$
	166	$D_{3d}^{5}$	$\Gamma_{rh}$	12	None	2	$2-A \perp^r \{110\}; P \parallel^l \{110\}.$
		- 30	- 471			4	$ 2-A \perp^r P ^l \{1\overline{10}\}.$
l						6	3 P's $\parallel^l$ {110} intersecting in 3-A.
				İ		12	$3 \text{ P's }   ^{l} \{1\overline{1}0\} + 3 \text{ 2A's } \mathbf{L}^{r} \{1\overline{1}0\} \text{ all }$
	1.05	D. C	П.	10	(77)		intersecting in 3-A $\perp$ r {111}.
-	167	$D_{3d}^{6}$	$\Gamma_{rh}$	12	$\{hhl\}$ halved if $l$ is odd	2	$2-A \perp^r \{110\}; C$
1						$\begin{vmatrix} 3 \\ 6 \end{vmatrix}$	3-A 1 <sup>r</sup> {111}.
						. 0	3 2-A's $\mathbf{L}^r$ {1\overline{1}0} intersecting in 3-A $\mathbf{L}^r$ {111}; 3-A $\mathbf{L}^r$ {111} + C.
_				1			

## TRIGONAL PARAMORPHY (TRIGONAL BIPYRAMIDAL).

N	Го.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
10	68	$\mathrm{C}_{3\hbar}^{-1}$	$\Gamma_h$	6	None	2 3 6	$P \parallel^{l} \{0001\}.$ 3-A $\mathbf{L}^{r} \{0001\}.$ 3-A $\mathbf{L}^{r} P \parallel^{l} \{0001\}.$

## TRIGONAL HOLOHEDRY (DITRIGONAL BIPYRAMIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
169	$D_{3h}^{1}$	$\Gamma_h$	12	None	2 4	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$
					$\begin{array}{ c c } & 6 \\ 12 & \end{array}$	3 P's $\parallel^l$ {1120} intersecting in 3-A. 3 P's $\parallel^l$ {1120} intersecting in 3-A.
170	$\mathrm{D}_{3h}^{-2}$	$\Gamma_h$	12	$\{mo\overline{m}l\}$ halved if $l$ is odd	2 3	$\mathbf{L}^r \mathbf{P} \parallel^l \{0001\}.$ 2-A $\mathbf{L}^r \{10\overline{1}0\}$ ; $\mathbf{P} \parallel^l \{0001\}.$ 3-A $\mathbf{L}^r \{0001\}.$
	-				6	3-A $\mathbf{L}^r P \parallel^r \{0001\}$ ; 3 2-A's $\mathbf{L}^r \{10\overline{1}0\}$ intersecting in 3-A $\mathbf{L}^r \{0001\}$ .
171	$D_{3h}^{3}$	$\Gamma_h$	12	None	$\begin{bmatrix} 2 \\ 3 \\ 4 \end{bmatrix}$	$P \parallel^{\tilde{t}} \{0001\} \text{ or } \{10\overline{1}0\}, \\ 3-A \perp^{t} \{0001\}. \\ 2 \text{ P's } \parallel^{\tilde{t}} \{0001\} \text{ and } \{10\overline{1}0\} \text{ inter-}$
	-		The second secon		6	secting in 2–A. 3–A $\mathbf{L}^r$ P    $^l$ {0001}; 3 P's    $^l$ {1010}
					12	intersecting in 3-A.  3 P's $\parallel^l$ {10\overline{10}} intersecting in 3-A $\perp^r$ P $\parallel^l$ {0001}.
172	$D_{3h}^4$	$\Gamma_h$	12	$\{mm2ml\}$ halved if $l$ is odd	$\begin{bmatrix} 2 \\ 3 \\ 6 \end{bmatrix}$	2–A $\mathbf{L}^r$ {11 $\overline{20}$ }; P    <sup>l</sup> {0001}. 3–A $\mathbf{L}^r$ {0001}. 3–A $\mathbf{L}^r$ P    <sup>l</sup> {0001}; 3 2–A's $\mathbf{L}^r$
						$\{11\overline{2}0\}$ intersecting in 3-A $\mathbf{L}^r$ $\{0001\}$ .

# HEXAGONAL TETARTOHEDRY (HEXAGONAL PYRAMIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.		
173	C <sub>6</sub> <sup>1</sup>	$\Gamma_h$	6	None	$\frac{2}{3}$	2-A <b>L</b> <sup>r</sup> {0001}. 3-A <b>L</b> <sup>*</sup> {0001}.		
174	C <sub>6</sub> <sup>2</sup>	$\Gamma_h$		{0001} sixthed	6	$6-A \perp^r \{0001\}.$		
175	$C_6^3$	Same as C	Same as $C_6^2$ , but in opposite rotatory sense, therefore identical data.					
176	C <sub>6</sub> <sup>4</sup>	$\Gamma_h$	6	{0001} thirded	2	$2-A \perp^r \{0001\}.$		
177	C <sub>6</sub> <sup>5</sup>	Same as C	Same as $C_6^4$ , but in opposite rotatory sense, therefore identical data.					
178	C <sub>6</sub>	$\Gamma_h$	6	{0001} halved	$_3$	3-A L <sup>r</sup> {0001}.		

HEXAGONAL PARAMORPHY (HEXAGONAL BIPYRAMIDAL).

No	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
179	C <sub>6h</sub> 1	$\Gamma_h$	12	None	$\begin{array}{c} 2\\ 3\\ 4\\ 6 \end{array}$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$
180	C <sub>6h</sub> <sup>2</sup>	$\Gamma_h$	12	{0001} halved	$\begin{array}{c} 12 \\ 2 \\ 3 \\ 6 \end{array}$	6-A $\mathbf{L}^{r}$ P    <sup>t</sup> {0001}. P    <sup>t</sup> {0001}; C. 3-A $\mathbf{L}^{r}$ {0001}. 3-A $\mathbf{L}^{r}$ P    <sup>t</sup> {0001}; 3-A $\mathbf{L}^{r}$ {0001} + C.

# HEXAGONAL HEMIMORPHY (DIHEXAGONAL PYRAMIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
181	$C_{6v}^{-1}$	$\Gamma_h$	12	None	2 4	$P \parallel^{l} \{10\overline{1}0\} \text{ or } \{11\overline{2}0\}.$ 2 P's $\parallel^{l} \{10\overline{1}0\}$ and $\{11\overline{2}0\}$ intersecting in 2-A.
					$\frac{6}{12}$	[3 P's $  ^{l}$ {1120} intersecting in 3–A. 6 P's $  ^{l}$ {1120} and {1010} intersecting in 6– $\Lambda$ .
182	$C_{6v}^{2}$	$\Gamma_h$	12	$\{mo\overline{n}l\}$ and $\{mm\overline{2m}l\}$ . halved if $l$ is odd	$\frac{2}{3}$	$2-A \perp^r \{0001\}.$ $3-A \perp^r \{0001\}.$ $6-A \perp^r \{0001\}.$
183	$C_{6v}^{3}$	$\Gamma_h$	12	$\{mo\overline{m}l\}$ halved if $l$ is odd .	$\frac{2}{3}$	$egin{array}{c c} \mathrm{P} \parallel^l \{10\dot{1}0\}. \ 3-\mathrm{A} \ \mathbf{L}^r \{0001\}. \end{array}$
184	$\mathrm{C}_{\epsilon v}^{4}$	$\Gamma_h$	12	$\{mm\overline{2m}l\}$ halved if $l$ is odd	$\begin{bmatrix} 6 \\ 2 \\ 6 \end{bmatrix}$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$

## HEXAGONAL ENANTIOMORPHY (TRAPEZOHEDRAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
185	$D_6^1$	$\Gamma_h$	12	None	$\begin{bmatrix} 2\\3\\4\\6 \end{bmatrix}$	2-A $\mathbf{L}^r$ {0001}, {10 $\overline{1}$ 0} or {11 $\overline{2}$ 0}. 3-A $\mathbf{L}^r$ {0001}. 3 mutually $\mathbf{L}^r$ 2-A's. 6-A $\mathbf{L}^r$ {0001}; 3 2-A's $\mathbf{L}^r$ {10 $\overline{1}$ 0}
4.00	T 9	F	10	(0001)	12	intersecting in 3-A $L^r$ {0001}. 6 2-A's $L^r$ {1010} and {1120} intersecting in 6-A $L^r$ {0001}.
186	$\begin{array}{c c} D_6^2 \\ D_6^3 \end{array}$		i	{0001} sixthed	1.	2-A $\mathbf{L}^r$ {10 $\overline{1}$ 0} or {11 $\overline{2}$ 0}.
188	D <sub>6</sub> <sup>4</sup>		•			2-A $\mathbf{L}^r$ {0001}, {10 $\bar{1}$ 0} or {11 $\bar{2}$ 0}. 3 mutually $\mathbf{L}^r$ 2-A's.
189	$D_6^5$	Same as I	) <sub>6</sub> 4, b	at in opposite rotatory sense,	$_{ m there}$	fore identical data.
190	$D_6^6$	$\Gamma_h$	12	{0001} halved	$\begin{vmatrix} 2\\3\\6 \end{vmatrix}$	2-A $\mathbf{L}^r$ {1010} or {11 $\bar{2}$ 0}. 3-A $\mathbf{L}^r$ {0001}. 3 2-A's $\mathbf{L}^r$ {1010} intersecting in 3-A $\mathbf{L}^r$ {0001}; 3 2-A's $\mathbf{L}^r$ {11 $\bar{2}$ 0} intersecting in 3-A $\mathbf{L}^r$ {0001}.

## HEXAGONAL HOLOHEDRY (DIHEXAGONAL BIPYRAMIDAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
191	$D_{6h}^{-1}$	$\Gamma_h$	24	None	$\begin{vmatrix} 2 \\ 4 \end{vmatrix}$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$
					$\begin{bmatrix} 6 \\ 8 \end{bmatrix}$	secting in 2-A.  3 P's $\parallel^l$ {11 $\bar{2}0$ } intersecting in 3-A.  3 mutually $\perp^r$ P's $\parallel^l$ {0001}, {10 $\bar{1}0$ } and {11 $\bar{2}0$ } intersecting in 3 2-A's.  3 P's $\parallel^l$ {1120} intersecting in 3-A
		- -			24	L' P    <sup>l</sup> {0001}; 6 P's    <sup>l</sup> {10 $\overline{1}$ 0} and {11 $\overline{2}$ 0} intersecting in 6-A. 6 P's    <sup>l</sup> {10 $\overline{1}$ 0} and {11 $\overline{2}$ 0} and {11 $\overline{2}$ 0} intersecting in 6-A. L' P    <sup>l</sup> {0001}.
192	$D_{6h}^{2}$	$\Gamma_h$	24	$\{moml\}$ and $\{mm\overline{2m}l\}$ halved if $l$ is odd	2 3	$egin{array}{llllllllllllllllllllllllllllllllllll$
	The property of the second sec				4 6	3 mutually $\mathbf{L}^r$ 2-A's; 2-A $\mathbf{L}^r$ P $\parallel^t$ {0001}. 6-A $\mathbf{L}^r$ {0001}; 3-A $\mathbf{L}^r$ P $\parallel^t$ {0001}; 3 2-A's $\mathbf{L}^r$ {10 $\overline{1}$ 0} intersecting in 3-A $\mathbf{L}^r$ {0001}.
					12	6-A $\mathbf{L}^r$ P    $^l$ {0001}; 6-2-A's $\mathbf{L}^r$ {10\overline{10}} and {11\overline{20}} intersecting in 3-A $\mathbf{L}^r$ {0001}.
193	D <sub>6h</sub> <sup>3</sup>	$\Gamma_{h}$	24	$\{mo\overline{m}l\}$ halved if $l$ is odd .	$egin{array}{c} 2 \\ 3 \\ 4 \end{array}$	2-A $\mathbf{L}^r$ {10 $\overline{10}$ }; $\overset{\cdot}{\mathbf{P}} \parallel^l$ {0001} or {10 $\overline{10}$ }. 3-A $\mathbf{L}^r$ {0001}. 2 $\overset{\cdot}{\mathbf{P}}$ 's $\parallel^l$ {0001} and {10 $\overline{10}$ } intersect-
					6	ing in 2-A; 2-A $\mathbf{L}^r$ P $\parallel^l$ {10 $\overline{1}$ 0}. 3-A $\mathbf{L}^r$ P $\parallel^l$ {0001}; 3 P's $\parallel^l$ {10 $\overline{1}$ 0} intersecting in 3-A. 3 P's $\parallel^l$ {10 $\overline{1}$ 0} intersecting in 3-A
				. <del>.</del>		$\mathbf{L}^r \ \mathbf{P} \parallel^l \{0001\}; \ 3 \ \mathbf{P's} \parallel^l \{10\overline{1}0\} \\ + 3 \ 2-\mathbf{A's} \ \mathbf{L}^r \{10\overline{1}0\} \ \text{all intersecting in } 3-\mathbf{A} \ \mathbf{L}^r \{0001\}.$
194	D <sub>6h</sub> <sup>4</sup>	$\Gamma_h$	$\begin{vmatrix} 24 \\ \end{vmatrix}$	$\{mm2ml\}$ halved if $l$ is odd	$egin{array}{c c} 2 & & \\ 4 & & \\ \end{array}$	2–A $\mathbf{L}^r$ {11 $\overline{2}0$ }; P $\parallel^l$ {0001} or {11 $\overline{2}0$ } 2 P's $\parallel^l$ {0001} and {11 $\overline{2}0$ } intersecting in 2–A; 2–A $\mathbf{L}^r$ P $\parallel^l$ {11 $\overline{2}0$ }.
					$\begin{bmatrix} 6 \\ 12 \end{bmatrix}$	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$
						ing in 3-A <b>L</b> <sup>r</sup> {0001}.

# Regular System.

Belonging to the regular or cubic system there are three Bravais lattices only. The first of these,  $\Gamma_r$ , is the simple cubic lattice similar to  $\Gamma_0$  but with all its edges equal in length. Then there are the face-centred cubic lattice  $\Gamma_r'$  (cf.  $\Gamma_0''$ ) and the centred

cubic lattice  $\Gamma_r''$  ( $\Gamma_0'''$ ). There is no lattice in the regular system corresponding to  $\Gamma_0'$ , because it is not possible for one pair of opposite faces of the cubic lattice to be centred and not the other two pairs, since every cubic crystal possesses triad rotationaxes perpendicular to the  $\{111\}$ . Moreover throughout the regular system the a, b, caxes are not only equal in length, but absolutely indistinguishable. The figures 195— 230 may, therefore, be taken as representing the projection on any of the cube faces. The form  $\{hko\}$  includes all the three axial zones, just as the form  $\{100\}$  includes all the axial planes. This must be remembered in referring to the adjoining tables, for where we read, as in  $T_h^2$  "  $\{hko\}$  halved if (h+k) is odd; possible molecular symmetry 2-A  $\perp^r$  {100}, etc.," the abnormal spacings will include those of the planes (120) (012) (20 $\overline{1}$ ) (010) (001), etc., that is, the spacing of any plane in an axial zone will be halved if the sum of the indices of the plane is odd. Also if the molecule itself has a dyad axis then for each molecule whose axis is perpendicular to the (100), say, there will be two other molecules whose axes are perpendicular to (010) and (001) respectively. In the group  $T_h^6$  the spacings of the planes  $\{hko\}$  are halved if h is odd; this includes the

> (hko) if h is odd (okl) if k is odd (hol) if l is odd,

care being taken to preserve the cyclic order.

In the case in which the possible molecular symmetry is stated to be "2 P's || {100} and  $\{110\}$  intersecting in 2-A  $\perp^r \{110\}$ ," then any one molecule might have, for example, two planes parallel to (100) and  $(0\overline{1}1)$  intersecting in a dyad axis perpendicular to (011), in which case there would be two other molecules the direction of whose symmetry elements could be found by rotation through  $2\pi/3$  and  $4\pi/3$  respectively about a triad axis perpendicular to {111}; but no molecule can exist whose two planes are parallel to (100) and (101), say, since these two planes would intersect in a dyad axis perpendicular to  $\{100\}$  not  $\{110\}$ .

In the cubic system two types of LAUE diagrams can be obtained by using "white" X-rays, because adding a centre of symmetry to each of the five classes in turn reduces them to two only, the one possessing full  $T_h$  symmetry and the other full  $O_h$  symmetry. Thus, by the aid of Laue diagrams we can distinguish between the T and  $T_h$  classes on the one hand and the  $T_d$ , O and  $O_h$  classes on the other. No X-ray methods alone, however, can distinguish between, say, the  $T^1$  and the  $T_h^1$ , etc., if there are 12 or 6 molecules per cell, nor can X-rays, unaided, distinguish between the  $T_d^1$ ,  $O^1$ ,  $O_h^1$ , etc., if there are only 24, 12 or 6 molecules in the unit cell.

## REGULAR SYSTEM.

## REGULAR TETARTOHEDRY (TETRAGONAL PENTAGONAL DODECAHEDRAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
195	T1	$\Gamma_r$	12	None	$\begin{bmatrix} 2\\3\\12 \end{bmatrix}$	2-A $\perp^r$ {100}. 3-A $\perp^r$ {111}. 3 2-A's $\perp^r$ {100} intersecting in 3-A $\perp^r$ {111} ( <i>i.e.</i> full symmetry of
196	${ m T}^2$	$\Gamma_r{'}$	48	$\{hkl\}$ halved if $(h+k)$ or $(k+l)$ or $(l+h)$ is odd		class T). Same as T <sup>1</sup> .
197	$T^3$	$\Gamma_{r}^{\;\prime\prime}$	24	$(k+l)$ or $(l+h)$ is odd $\{hkl\}$ halved if $(h+k+l)$ is odd		Same as T <sup>1</sup> .
198	$T^4$	$\Gamma_r$	12	{100} halved	3	3-A <b>L</b> <sup>r</sup> {111}.
199	T <sup>5</sup>	$\Gamma_{r}^{\;\prime\prime}$	24	Same as T <sup>3</sup>	2 3	2-A <b>1</b> <sup>r</sup> {100}. 3-A <b>1</b> <sup>r</sup> {111}.

## REGULAR PARAMORPHY (DYAKISDODECAHEDRAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
200	$T_h^{-1}$	$\Gamma_r$	24	None	$\begin{vmatrix} 2\\ 3 \end{vmatrix}$	$P \parallel^{l} \{100\}, \ 3-A \perp^{r} \{111\}.$
					$\begin{vmatrix} 4\\24 \end{vmatrix}$	2 P's    <sup>l</sup> {100} intersecting in 2-A. 3 mutually $\mathbf{L}^r$ P's    <sup>l</sup> {100} with 4 3-A's $\mathbf{L}^r$ {111} passing through point of intersection ( <i>i.e.</i> full symmetry of
201	$T_h^2$	$\Gamma_r$	24	$\{hko\}$ halved if $(h+k)$ is odd	$\begin{bmatrix} 2 \\ 3 \\ 6 \end{bmatrix}$	class $T_h$ ) 2-A $\mathbf{L}^r$ {100}. 3-A $\mathbf{L}^r$ {111}. 3-A $\mathbf{L}^r$ {111} + C.
202	$T_h^3$	$\Gamma_{r}{'}$	96	Same as $T^2$	$\begin{bmatrix} 12 \\ 2 \\ 3 \\ 4 \end{bmatrix}$	Full symmetry of class T. 2-A $\mathbf{L}^r$ {100}; P    <sup>l</sup> {100}. 3-A $\mathbf{L}^r$ {111}. 2 P's    <sup>l</sup> {100} intersecting in 2-A.
203	$\mathrm{T}_h^{4}$	$\Gamma_r{'}$	96	Same as $T^2$ ; also $\{hko\}$ quartered if $(h+k)$ is	24	Full symmetry of class $T_h$ . Same as $T_h^2$ .
204	$T_h^{5}$	$\Gamma_{r}^{\prime\prime}$	48	odd, halved if even Same as T <sup>3</sup>	$egin{array}{c} 2 \ 3 \ 4 \end{array}$	$P \parallel^{l} \{100\}.$ 3-A $L^{r} \{111\}.$ 2 P's $\parallel^{l} \{100\}$ intersecting in 2-A.
205	$T_h^6$	$\Gamma_r$	24	$\{hko\}$ halved if $h$ is odd .	$\begin{array}{c} 6 \\ 24 \\ 3 \end{array}$	3-A $\mathbf{L}^r$ {111} + C. Full symmetry of class $\mathbf{T}_h$ . 3-A $\mathbf{L}^r$ {111}.
206	$\begin{bmatrix} T_h \\ T_h^7 \end{bmatrix}$	$\Gamma_{r}^{\prime\prime}$	48	Same as $T^3$ ; also all $\{hko\}$ halved	$\begin{array}{c c} 6 \\ 2 \\ 3 \\ 6 \end{array}$	3-A L <sup>r</sup> {111} + C. 2-A L <sup>r</sup> {100}. 3-A L <sup>r</sup> {111} + C. 3-A L <sup>r</sup> {111} + C.
					O	0-A <b>⊥</b> {111} + 0.

## REGULAR HEMIMORPHY (HEXAKISTETRAHEDRAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
207	$\mathrm{T}_d^{-1}$	$\Gamma_r$	24	None	$\frac{2}{4}$	$P \parallel^{l} \{110\}.$ 2 P's $\parallel^{l} \{110\}$ intersecting in 2-A. 3 P's $\parallel^{l} \{110\}$ intersecting in 3-A $\bot$ <sup>r</sup> $\{111\}.$
					24	6 P's    <sup>t</sup> {110} intersecting in 4 3-A's $\bot^r$ {111} + 3 2-A's $\bot^r$ {100} all intersecting in same point (i.e. full symmetry of class $T_d$ ).
208	$T_d^{2}$	$\Gamma_r{'}$	96	Same as T <sup>2</sup>		Same as $T_d^1$ .
209	$T_d^{\ 3}$	$\Gamma_r^{\prime\prime}$	48	Same as T <sup>3</sup>		Same as $T_d^{-1}$ .
210	$T_d^4$	$\Gamma_r$	24	$\{hhl\}$ halved if $l$ is odd	$\begin{bmatrix} 2\\3\\12 \end{bmatrix}$	2-A $\mathbf{L}^r$ {100}. 3-A $\mathbf{L}^r$ {111}. Full symmetry of class T.
211	$T_d^{5}$	$\Gamma_{r'}$	96	Same as T <sup>2</sup> ; also all {hhl} halved.		Same as $T_d^4$ .
212	$T_d^{6}$	$\Gamma_r^{\prime\prime}$	48	Same as $T^3$ ; also $\{hhl\}$ quartered if $l$ is odd, normal if $l=2x$ , where $x$ is odd, halved if $l=2x$ , where $x$ is even or zero.	3	2-A $\mathbf{L}^r$ {100}. 3-A $\mathbf{L}^r$ {111}.

## REGULAR ENANTIOMORPHY (PENTAGONAL-ICOSITETRAHEDRAL).

No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.		
213	O1	$\Gamma_r$	24	None	$\begin{array}{c}2\\3\\4\\24\end{array}$	2-A L <sup>r</sup> {110}. 3-A L <sup>r</sup> {111}. 4-A L <sup>r</sup> {100}. 6 2-A's L <sup>r</sup> {110} + 3 4-A's L <sup>r</sup> {100} all intersecting in a point through which pass 4 3-A's L <sup>r</sup> {111} (i.e.		
214	O2	$\Gamma_r$	24	{100} halved	$\begin{array}{c} 2\\3\\12\end{array}$	full symmetry of class O). 2-A $\mathbf{L}^r$ {100} or {110}. 3-A $\mathbf{L}^r$ {111}. Full symmetry of class T.		
215	$O_3$	$\Gamma_{r}{'}$	96	Same as $T^2$		Same as $O^1$ .		
216	O4	$\Gamma_{r}{'}$	96	Same as T <sup>2</sup> ; also {100} quartered.		Same as O <sup>2</sup> .		
217	$O^5$	$\Gamma_{r}^{\prime\prime}$	48	Same as 13	-	Same as O <sup>1</sup> .		
218	Oe	$\Gamma_r$	24	{100} quartered	$\begin{vmatrix} 2\\ 3 \end{vmatrix}$	2-A 1 <sup>r</sup> {110}. 2-A 1 <sup>r</sup> {111}.		
219	$O^7$	Same as C	Same as O <sup>6</sup> , but in opposite rotatory sense, therefore identical data.					
220	O <sub>8</sub>	$\Gamma_r^{\prime\prime}$ .	48	Same as T <sup>3</sup> ; also {100}   quartered	$\begin{vmatrix} 2\\3 \end{vmatrix}$	$\begin{bmatrix} 2-A & \mathbf{L}^r & \{100\} & \text{or} & \{110\} \\ 3-A & \mathbf{L}^r & \{111\} \end{bmatrix}$ .		

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## REGULAR HOLOHEDRY (HEXAKISOCTAHEDRAL).

	No.	SG.	B.L.	n.	Abnormal Spacings.	p.	Possible Molecular Symmetry.
	221	O <sub>h</sub> 1	$\Gamma_{r}$	48	None	$\begin{vmatrix} 2\\4 \end{vmatrix}$	$P \parallel^{l} \{100\}$ or $\{110\}$ . 2 P's $\parallel^{l} \{100\}$ and $\{110\}$ intersecting in 2-A $\mathbf{L}^{r} \{110\}$ .
						6	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$
						8	4 P's    <sup>l</sup> {100} and {110} intersecting in 4-A L <sup>r</sup> {100}.
					•	48	Full symmetry of class $O + C$ at point of intersection of axes (i.e. full symmetry of class $O_h$ ).
	222	O <sub>h</sub> 2	$\Gamma_r$	48	$\{hko\}$ halved if $(h+k)$ is odd; $\{hhl\}$ halved if $l$ -is odd	$\begin{bmatrix} 2\\ 3\\ 4 \end{bmatrix}$	$2-A \mathbf{L}^r \{110\}.$ $3-A \mathbf{L}^r \{111\}.$ $4-A \mathbf{L}^r \{100\}.$
A CONTRACTOR AND ADDRESS OF THE PERSON NAMED IN COLUMN 1				A children of the children of	·	$\begin{bmatrix} \frac{1}{6} \\ 24 \end{bmatrix}$	$3-A$ $L^r$ $\{111\} + C$ . Full symmetry of class O.
	223	$O_h^3$	Γ,	48	$\{hhl\}$ halved if $l$ is odd	$\begin{bmatrix} 2\\3\\4 \end{bmatrix}$	$\begin{vmatrix} 2-A & \mathbf{L}^r & \{110\} & P & \ ^l & \{100\} & \\ 3-A & \mathbf{L}^r & \{111\} & \end{vmatrix}$
AND DESCRIPTION OF PERSONS ASSESSED.	224	$O_h^4$	$\Gamma_r$	48	$\{hko\}$ halved if $(h+k)$ is	24 $2$	2-P's $\parallel^l$ {100} intersecting in 2-A. Full symmetry of class $T_h$ . P $\parallel^l$ {110}.
		h	- r		odd	$\frac{4}{6}$	$ \begin{vmatrix} 2 \text{ P's } \end{vmatrix}^l \{110\} \text{ intersecting in 2-A. }                                   $
The second of the Second second						12	3 P's $\ ^{l}$ {111}. 4 The section of the section
	225	O <sub>h</sub> 5	$\Gamma_{r}{'}$	192	Same as T <sup>2</sup>	24	Full symmetry of class $T_d$ . Same as $O_h^{-1}$ .
	226	$O_h^{-6}$	$\Gamma_r{'}$	192	Same as $T^2$ ; also all $\{hhl\}$ halved	$\begin{bmatrix} 2 \\ 3 \\ 4 \end{bmatrix}$	2-A $\mathbf{L}^r$ {110}; P    <sup>l</sup> {100}. 3-A $\mathbf{L}^r$ {111}. 4-A $\mathbf{L}^r$ {100}; 2 P's    <sup>l</sup> {100} inter-
						24	secting in 2–A. Full symmetry of class O; full sym-
-	227	O <sub>h</sub> 7	$\Gamma_{r}{'}$	192	Same as $T^2$ ; also $\{hko\}$ quartered if $(h+k)$ is odd,		metry of class $T_h$ . Same as $O_h^4$ .
	228	O <sub>h</sub> 8	$\Gamma_{r}'$	192	halved if even Same as $T^2$ ; also all $\{hhl\}$ halved; $\{hko\}$ quartered	$\begin{bmatrix} 2 \\ 3 \end{bmatrix}$	2-A <b>L</b> <sup>r</sup> {100} or {110}. 3-A <b>L</b> <sup>r</sup> {111}.
-	000	0.9	т.,,	0.0	if $(h+k)$ is odd, halved if even	$\begin{vmatrix} 6 \\ 12 \end{vmatrix}$	3-A 1' {111} + C. Full symmetry of class T.
	229	O <sub>h</sub> 9	1 ,	96	Same as T <sup>3</sup>	$\begin{bmatrix} 2 \\ 4 \end{bmatrix}$	P    <sup>l</sup> {100} or {110}. 2 P's    <sup>l</sup> {100} and {110} intersecting in 2-A $L^r$ {110}.
The same of the sa							3 P's $\parallel^l$ {110} intersecting in 3-A $\perp^r$ {111}.
				v homospanis de mais de			4 P's $  ^{7}$ {100} and {110} intersecting in 4-A L' {100}.
						12 48	3 P's    <sup>l</sup> {110} intersecting in 3-A $\Delta^r$ {111} + C. Full symmetry of class $O_h$ .
	230	O <sub>h</sub> 10	$\Gamma_{r}^{\prime\prime}$	96	Same as $T^3$ ; also all $\{hko\}$ halved; $\{hhl\}$ quartered	$\begin{bmatrix} 2 \\ 3 \end{bmatrix}$	2–A $\mathbf{L}^r$ {100} or {110}. 3–A $\mathbf{L}^r$ {111}.
			•		if $l$ is odd, normal if $l = 2x$ , where $x$ is odd, halved if $l = 2x$ , where	6	3-A $L^r$ {111} + C.
		.			x is even or zero	.	

## THE EXAMINATION OF THE 230 SPACE-GROUPS BY HOMOGENEOUS X-RAYS. 257

Appended below are a few examples of crystals which have been examined by X-rays and found to be based on the space-groups indicated. This list is in no sense intended to be exhaustive, but is given merely to add a touch of reality to the foregoing Tables.

C.1—CuO; racemic acid.  $D_3^3$  or  $D_3^4$  (and  $D_3^5$  or  $D_3^6$ )—Quartz. C<sub>2</sub>-Tartaric acid. D<sub>3d</sub> Calcite; corundum. T<sup>4</sup>—NaClO<sub>3</sub>; cobaltite.  $C_{2h}^2$ —Succinic acid.  $T_h^6$ —FeS<sub>2</sub>; Alums;  $N_2H_4$ .2HCl:  $C_{2h}^{5}$ —Naphthalene; anthracene. C<sub>20</sub>10—Resorcinol.  $T_d^1$ —NH<sub>4</sub>Cl.  $T_d^2$ —Zinc blende.  $Q_h^1$ —Succinimide.  $Q_h^{16}$ —Aragonite.  $T_d^3$ —Hexamethylene tetramine.  $\mathbf{D}_{2d}$ —Urea. O,1—CsCl, etc. C<sub>4,9</sub>—Penta-erythritol. O<sub>h</sub> - NaCl, etc. O<sub>h</sub><sup>7</sup>—Diamond; As<sub>4</sub>O<sub>6</sub>.  $D_{4h}^{1}$ — $R'_{2}X''Cl_{4}$ .  $D_{4h}^{19}$ —White tin.

Summary.

Given a crystal belonging to a particular system and class, the X-ray worker can, with two exceptions, determine to which space-group the crystal belongs, by means of the number of molecules per unit cell and the abnormal spacings found.

In order to facilitate this work, diagrams are given, one for each of the 230 space-groups, showing the distribution of symmetry elements and the relative positions and orientations of the molecules in the unit cell; and accompanying these diagrams are tables giving the fundamental Bravais lattice, the number of asymmetric molecules per cell, the abnormal spacings to be expected and the possible molecular symmetry for each space-group.

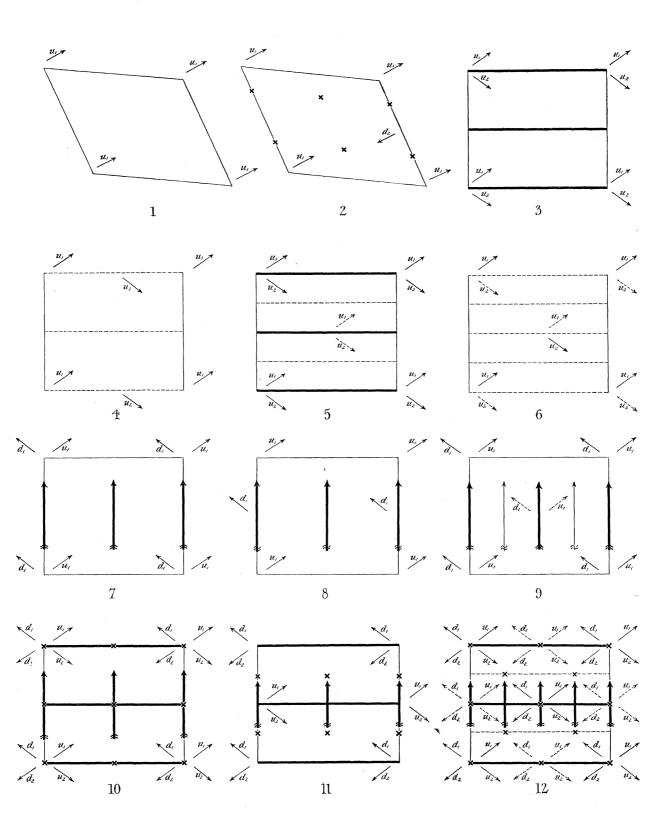
The general introduction gives an account of the usefulness of such tabulated data and explains the abbreviated notation used in the tables and the symbols adopted in the diagrams. To each system there is a special introduction, describing the Bravais lattices on which the space-groups in that system are based, and giving any information which concerns only that particular system and which may be of use in applying the data given to any special case.

Under certain circumstances X-ray methods alone can also reveal the class to which a crystal belongs, and such particulars are given as will enable the worker to decide when and how this may be done. In general, however, X-ray examination alone fails to determine the class of the crystal, and the limitations of the method are clearly indicated in the paper.

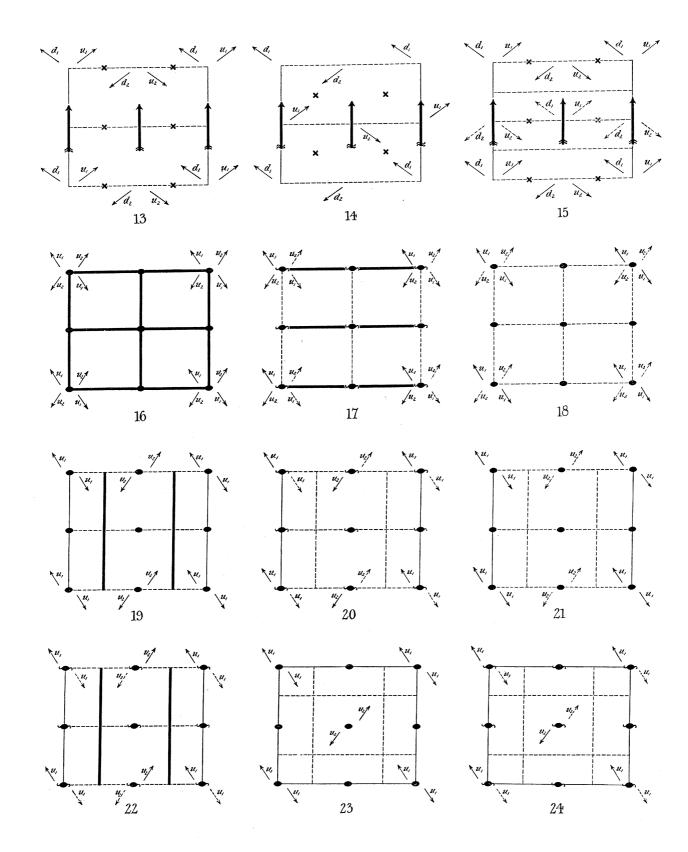
A few examples are given of some of the crystals the structures of which have already been determined, these being referred to their particular space-groups.

In conclusion, the authors wish to express once more their indebtedness to Sir Wm. Bragg for his unfailing encouragement and advice, and also to the Department of Scientific and Industrial Research and the Royal Institution for supplying the financial and laboratory necessities for the research.

Phil. Trans., A, vol. 224, Plate 5.



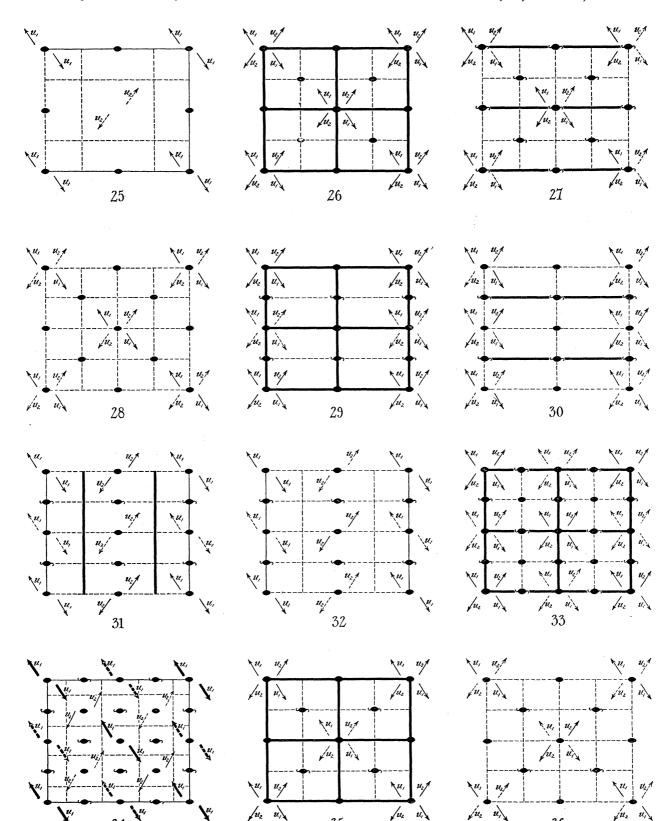
Phil. Trans., A, vol. 224, Plate 6.



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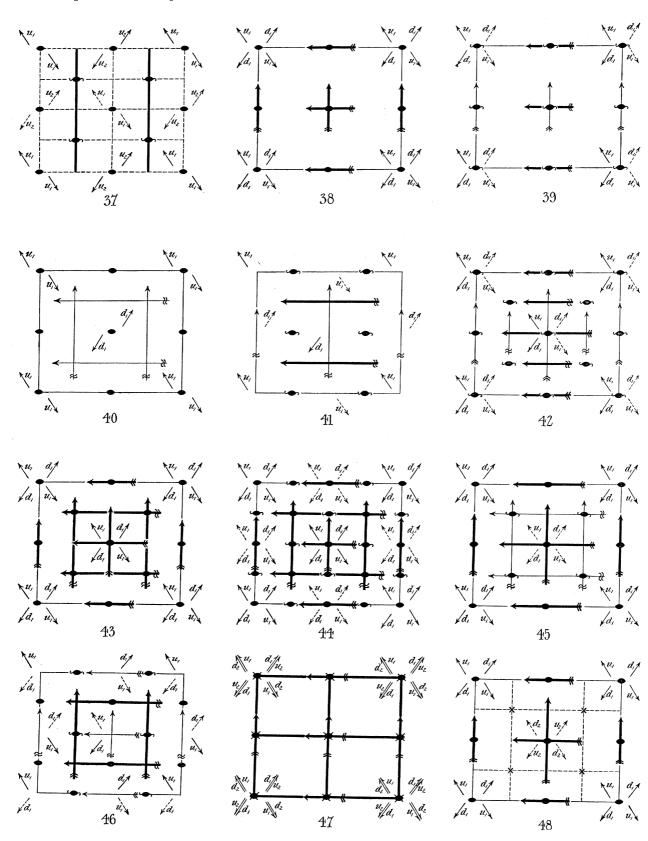
Phil. Trans., A, vol. 224, Plate 7.

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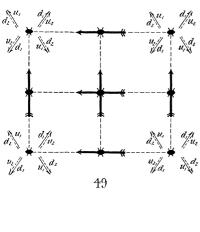


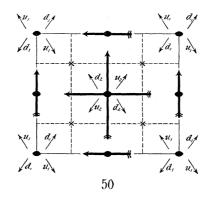
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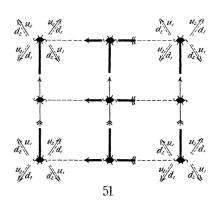
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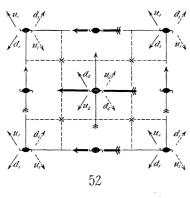


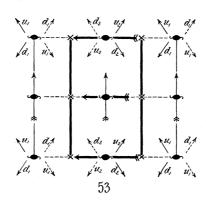
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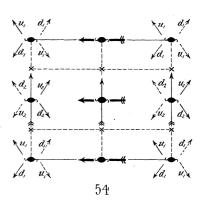


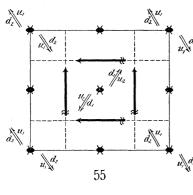


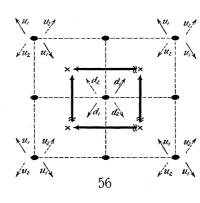


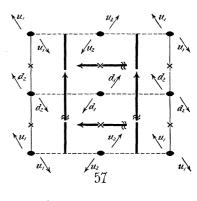


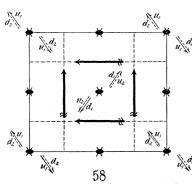


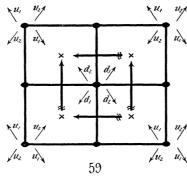


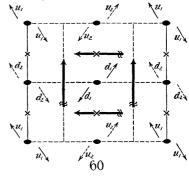




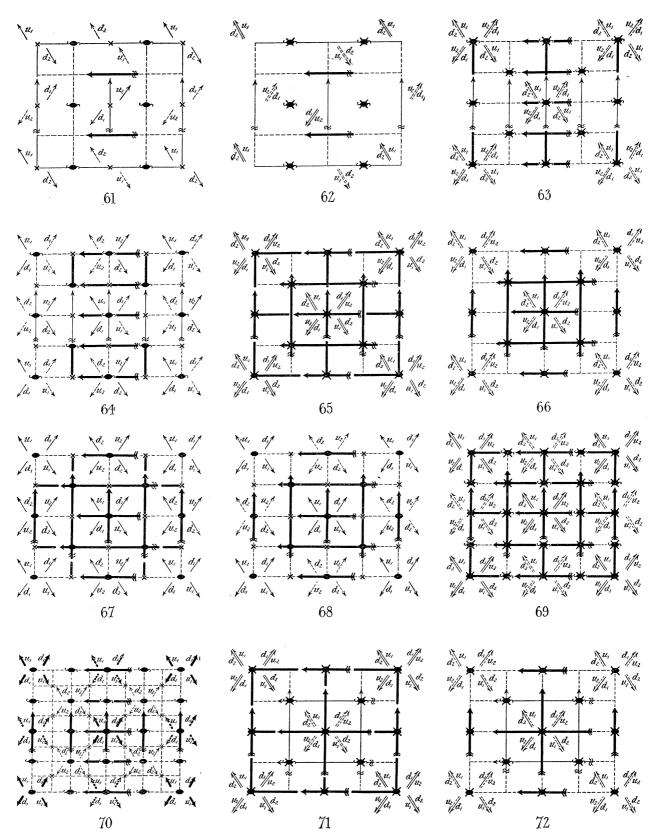




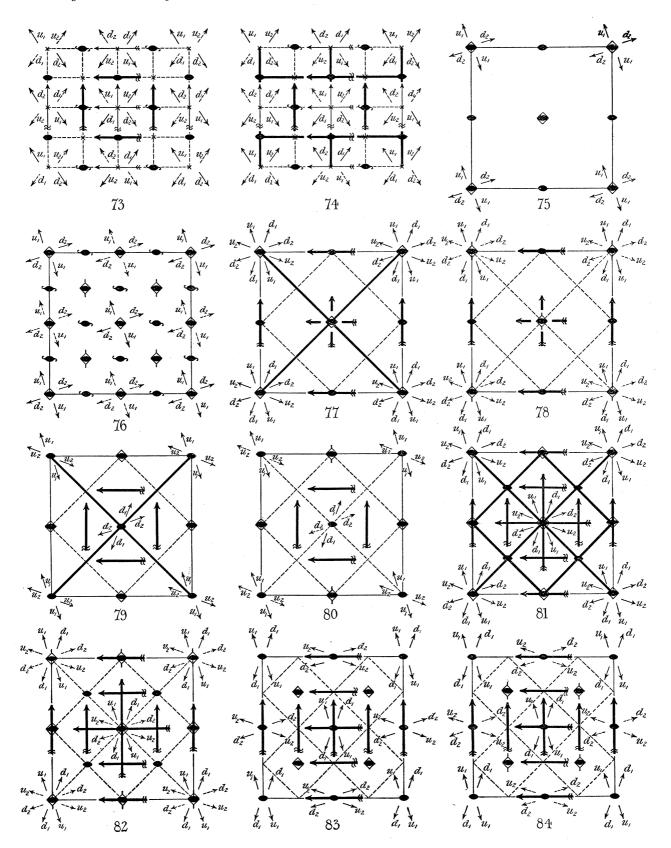




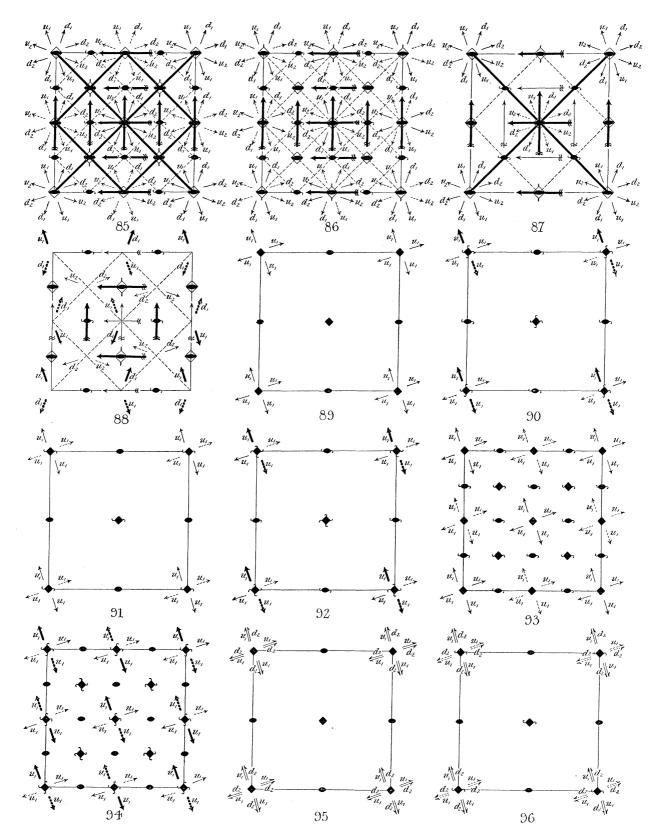
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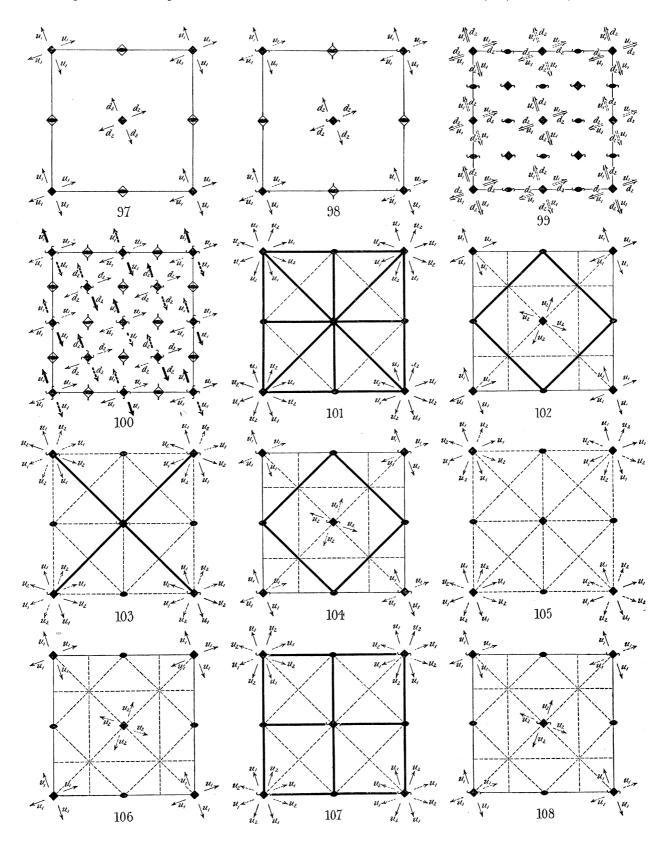
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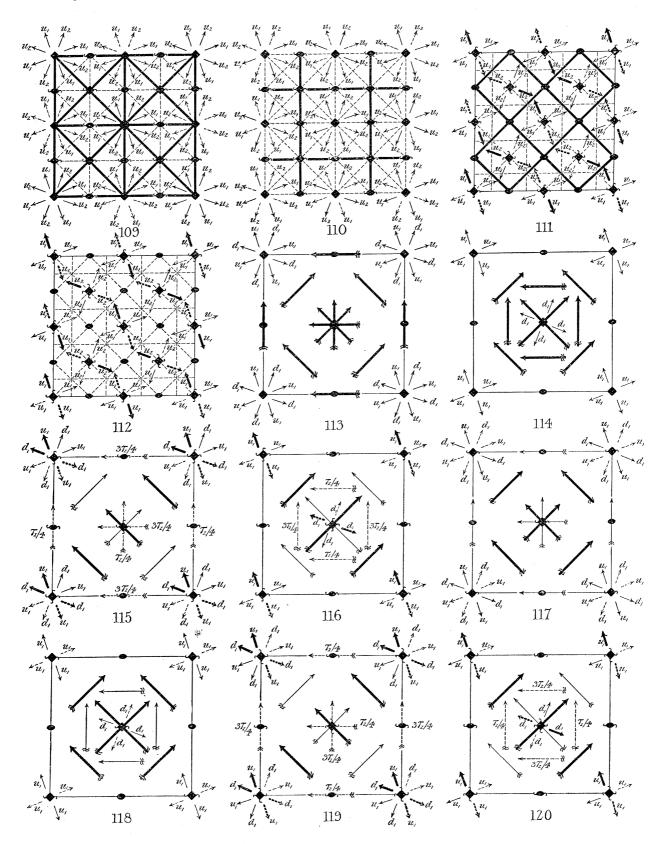
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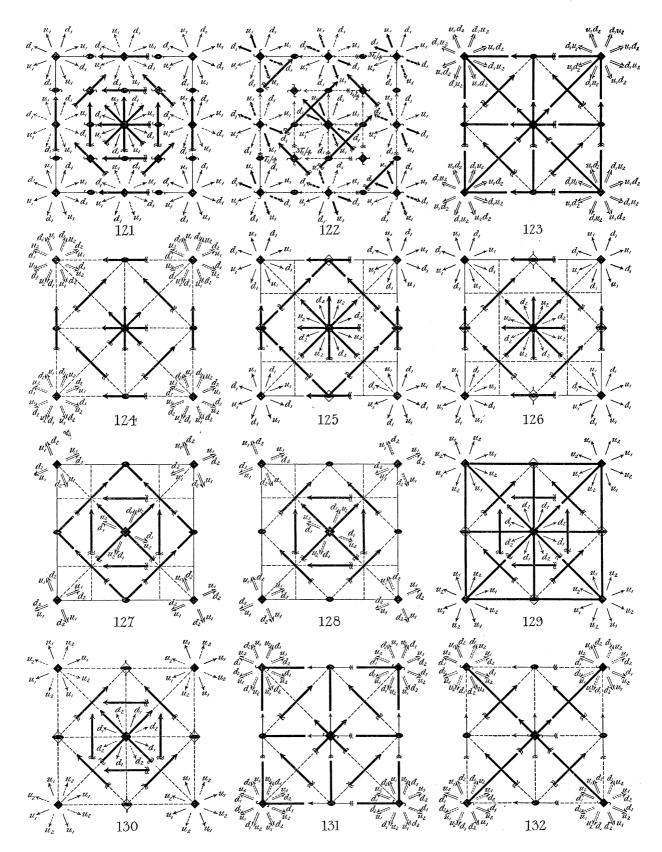
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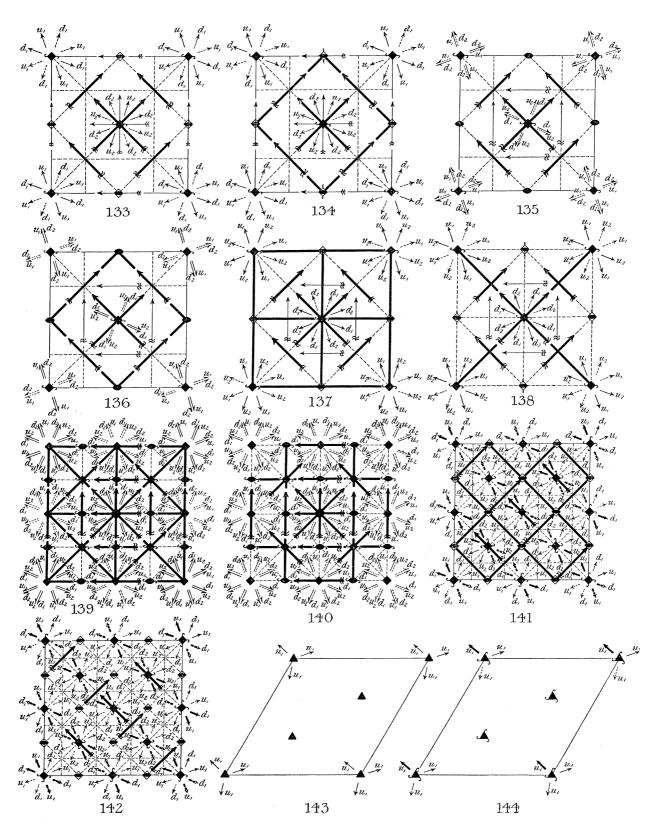
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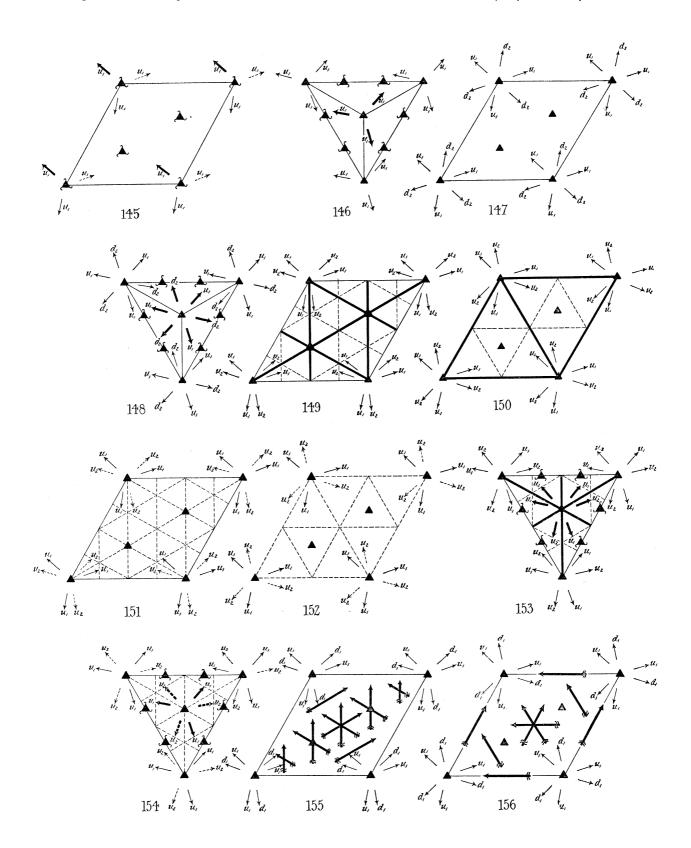
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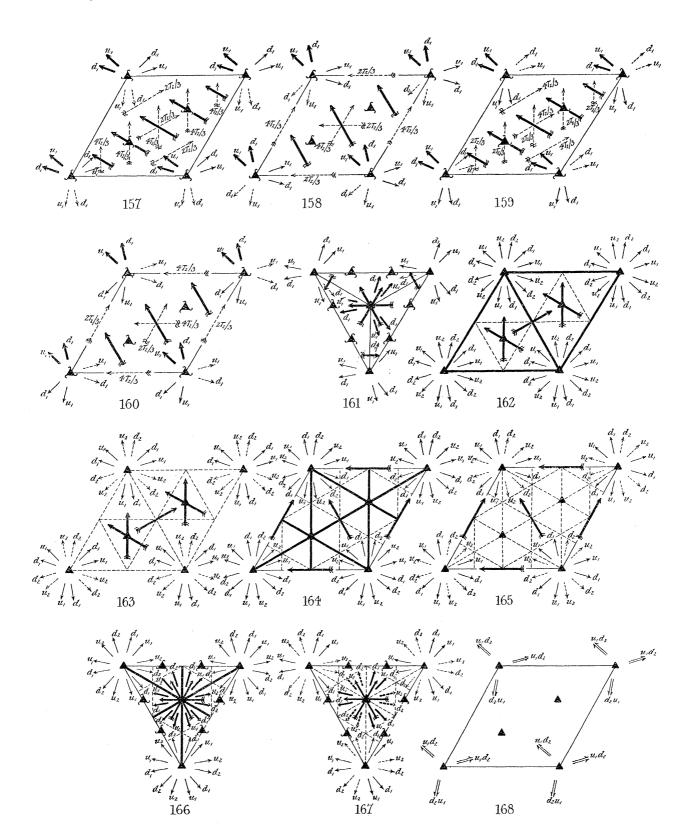
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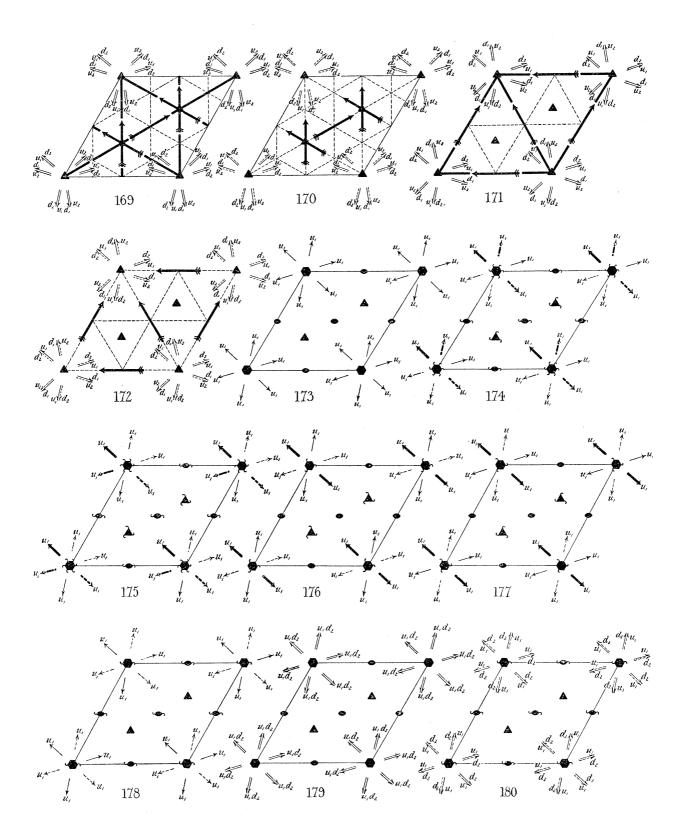
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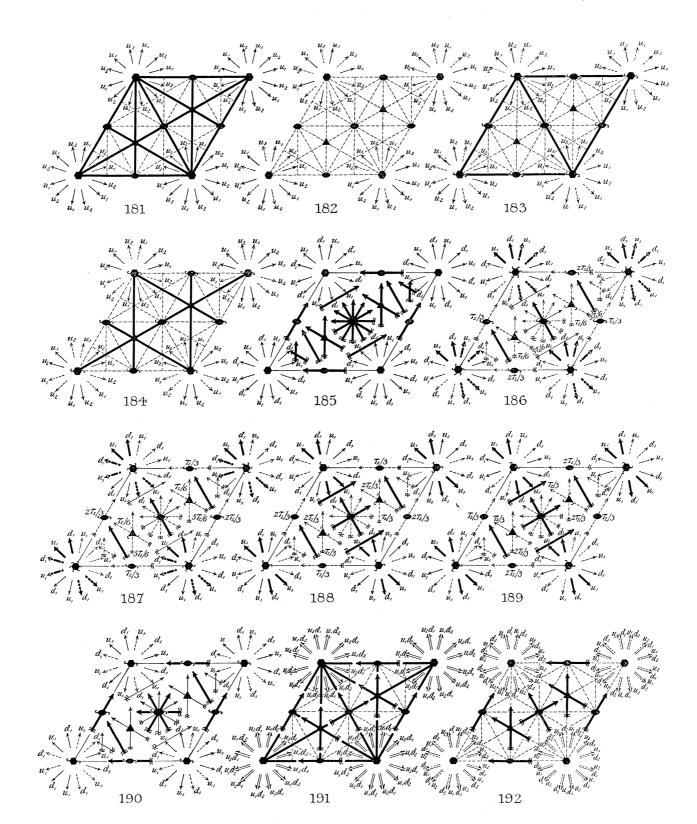
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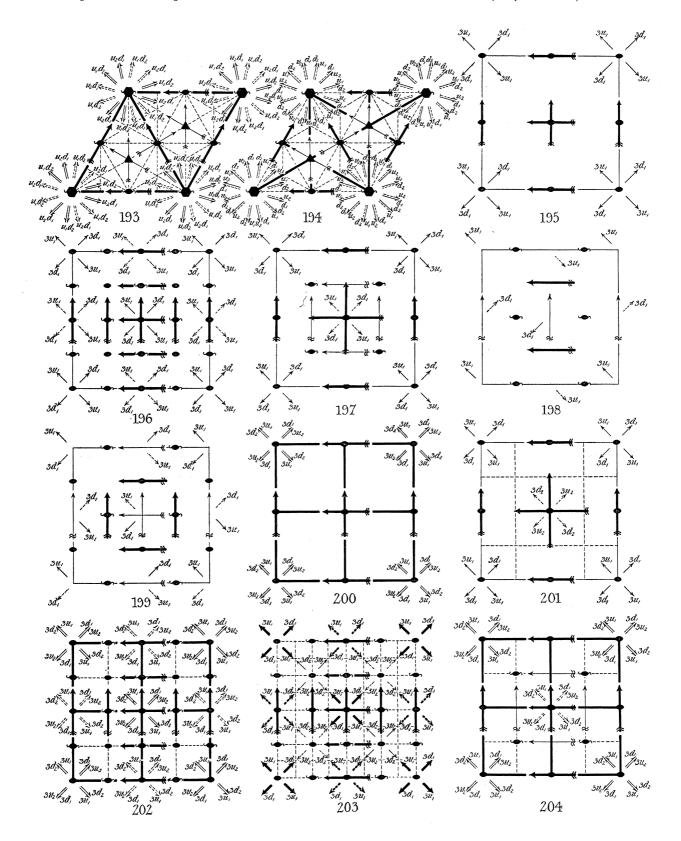
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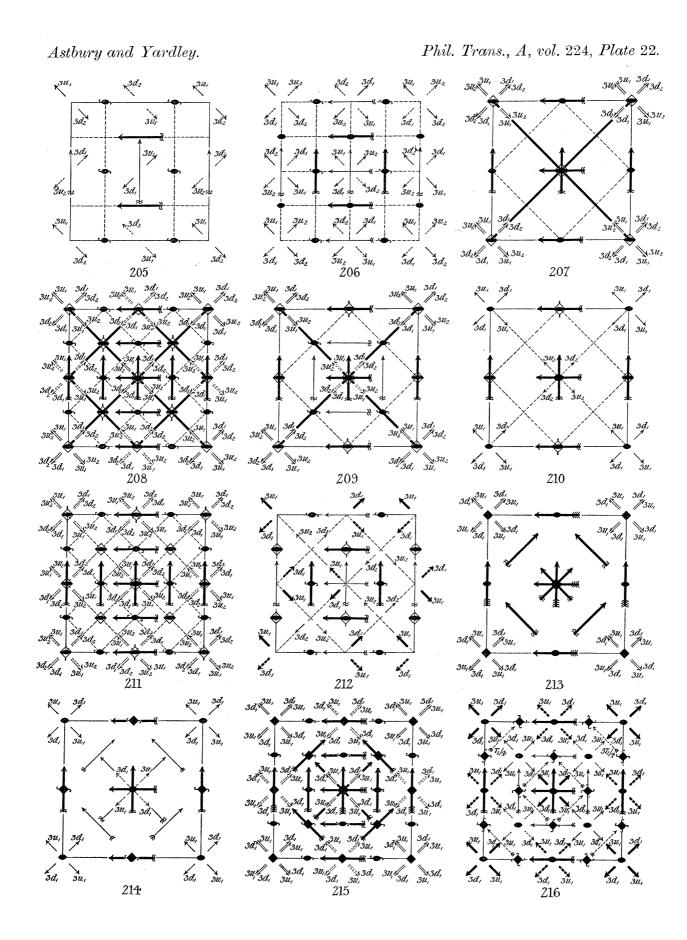
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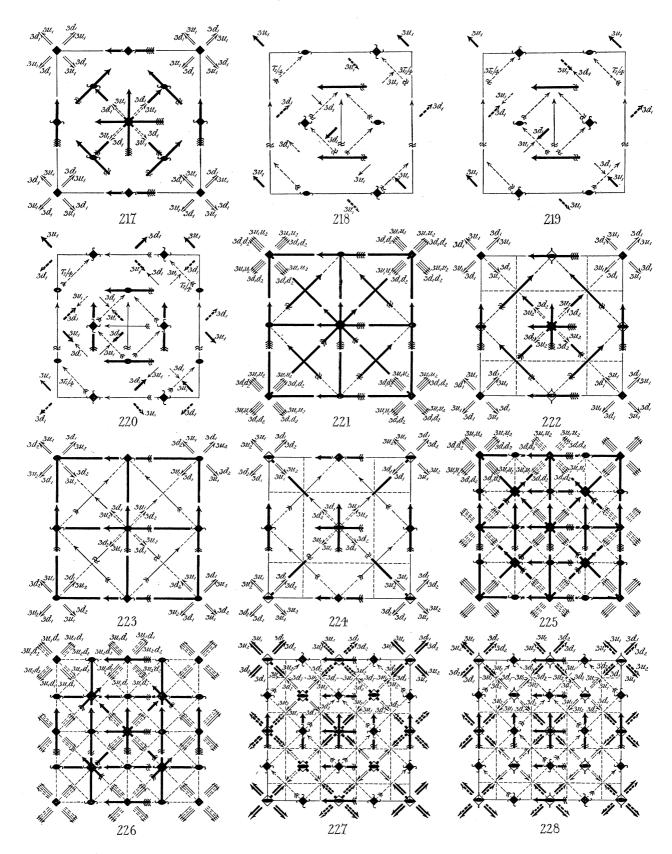
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Phil. Trans., A, vol. 224, Plate 24.

