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ART. XVII.—*The Determination of the Space Group of a Cubic Crystal;* by RALPH W. G. WYCKOFF.

Introduction.

The theory of space groups presumably defines all of the ways in which elements of symmetry may be distributed in space so that their aggregates will possess crystallographic symmetry.[1] A knowledge of the space group to which a particular crystal should be assigned thus describes completely its characteristics of symmetry, and forms thereby one of the principal goals of descriptive crystallography. On the basis of direct experimental evidence it has hitherto been impossible to carry crystallographic description so far; only in a few isolated cases could the appropriate space groups be inferred.[2] Use of the diffraction effects resulting from the action of X-rays upon crystals offers, however, the opportunity in many cases of determining experimentally the space group corresponding to a crystal.

The crystal symmetry which is deduced by the use of X-ray methods of study is the symmetry of the arrangement of the atoms of which the crystal is composed. The identification of this *internal* symmetry with the *external* crystal symmetry, obtained from studies of face-development and the like, requires an assumption equivalent to one that states that the external symmetry of a crystal is consistent with the arrangement of its constituent atoms. Not only does it appear natural to relate them thus but the generally satisfactory agreement between the external symmetries and the symmetries of the crystal models of those crystals whose structures have thus far been studied with X-rays points to the correctness of this assumption.

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[1] A. Schoenflies, Krystallsysteme und Krystallstructur, Leipzig, 1891.

[2] For instance, C. Viola, Z. Kryst., 28, 225, 1897; L. Sohncke and E. Federov have made similar assignments.

The probable space groups corresponding to a few crystals have already been determined by showing that the structures assigned to them by the X-ray studies can be deduced from certain particular space groups.[3] It is the intention of the present paper, however, to show, by taking the cubic crystals as the simplest examples, how the space groups of many crystals can be uniquely determined in advance of a complete elucidation of their structures and to state criteria which serve to distinguish between the various cubic space groups where such a distinction is possible. Not only is such a knowledge of the space group of a crystal an ultimate aim of formal crystallography but it may be of great value in the problem of crystal structure study itself.

In the crystals whose structures have been determined all, or nearly all, of the atoms of which they are composed have been found to occupy positions within the unit cells whose coördinate values are limited and defined by symmetry considerations (the corners, center, centers of the edges and of the faces of a unit cube are such positions). Such very special structures can usually be deduced from more than one space group. Most cubic crystals, however, have one or more of their constituent atoms in positions so general that the symmetry requirements permit their x, y and z coördinates to have any values. Physical data concerning the mechanism of the scattering of X-rays by atoms are not yet sufficient for the complete determination of the structure of any crystal having one or more atoms in these general positions. A knowledge of the space group to which such a crystal should be assigned serves to determine the manner of arrangement of its atoms in many cases, even though the distances between some of these atoms cannot now be established with accuracy.

X-ray criteria for distinguishing between the different space groups are most simply and satisfactorily deduced for those crystals having some atoms of appreciable scattering power in general positions. For this reason and also because a knowledge of the space group of such crystals is valuable to the crystal analyst, the discussion which follows will be limited to cubic crystals having one or more atoms in general positions. Similar criteria

[3] A. Johnsen, Physikal. Z., 16, 269, 1915.

have been established for other than cubic crystals, although their application to specific instances is not so straightforward. Some discrimination among the special cases where one or more of the coördinates of position are defined by considerations of symmetry can likewise be made.

Means of distinguishing between cubic space groups as an aid to studies of crystal structure by reflection spectrum observations of the relative spacings against the (100), (110) and (111) faces have already been given.[4] For a variety of reasons, however, this method is of little certain value in actual practice.

A study of the Laue photographs taken in a single direction through a crystal distinguishes as far as possible between the various space groups. Because of the much larger mass of data with which they deal, space group determinations based upon Laue photographic studies are not open to the same measure of uncertainty as those derived from reflection spectrum measurements.

It will be seen from the criteria to be discussed that many of the space groups give diffraction effects which are different from those given by any other space group and thus a method is established for deducing completely and uniquely the (internal) symmetry of a crystal without recourse to methods of studying external symmetry, such as those of face-development and etch-figure formation.

These space group criteria have already been used upon a number of crystals of rather complicated chemical compositions. Of these, studies of nickel nitrate hexammonate[5] and of sodium hydrogen acetate[6] have either been published or are in the course of publication; the determination of the symmetry and structure of zinc bromate hexahydrate, published elsewhere in this Journal,[7] has been written primarily to serve as an illustration of the application of these criteria.

Methods of Distinguishing between the Cubic Space Groups.

The general characteristics of the diffraction effects to

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[4] P. Niggli, Geometrische Krystallographie des Discontinuums, p. 492, Leipzig, 1919.

[5] Ralph W. G. Wyckoff, Jour. Am. Chem. Soc., June, 1922.

[6] Ralph W. G. Wyckoff, see the third article in this number of this Journal.

[7] See the following article in this number.

be obtained from atoms arranged according to the general positions of any one of the space groups can be readily calculated with the aid of the customary intensity expression:

$$I \propto f\left(\frac{d_{\mathrm{hkl}}}{n}\right)[A^2+B^2], \text{ where}$$

$$A=\sum_m [\sigma_m \cos 2\pi n(hx_m+ky_m+lz_m)], \qquad [1]$$

and B is a similar sine term. In this expression[8] I is the intensity and n is the order of reflection from a plane whose Miller indices are (hkl); x_m, y_m, z_m are the coördinate positions of each of the m atoms (within the unit) over which the summation is to be extended and σ_m is the scattering power of the atom m. The value of

$$f\left(\frac{d_{\mathrm{hkl}}}{n}\right)$$

where d_{hkl} is the spacing of the plane (hkl), need not be evaluated for the present purposes. If these diffraction effects are calculated for each of the space groups it is found that for some of them reflections from certain classes of planes in some orders will be entirely absent. Such a complete absence of definite classes of planes, different for different space groups, makes it possible to distinguish between these groups.

As an example of the mode of procedure a common space group, T_h^6, the sixth group having paramorphic hemihedral (pyritohedral) symmetry, will be considered in detail. The coördinates of the most generally placed equivalent points within a unit cube for this space group are

$$xyz;\ x+\tfrac12,\ \tfrac12-y,\ \bar{z};\ \bar{x},\ y+\tfrac12.\ \tfrac12-z;\ \tfrac12-x,\ \bar{y},\ z+\tfrac12;$$
$$zxy;\ \bar{z},\ x+\tfrac12.\ \tfrac12-y;\ \tfrac12-z,\ \bar{x},\ y+\tfrac12;\ z+\tfrac12.\ \tfrac12-x,\ \bar{y};$$
$$yzx;\ \tfrac12-y,\ \bar{z},\ x+\tfrac12;\ y+\tfrac12,\ \tfrac12-z,\ \bar{x};\ \bar{y},\ z+\tfrac12,\ \tfrac12-x;$$
$$\bar{x}\bar{y}\bar{z};\ \tfrac12-x,\ y+\tfrac12,\ z;\ x,\ \tfrac12-y\ \ z+\tfrac12;\ x+\tfrac12,\ y,\ \tfrac12-z;$$
$$\bar{z}\bar{x}\bar{y};\ z,\ \tfrac12-x,\ y+\tfrac12;\ z+\tfrac12,\ x,\ \tfrac12-y;\ \tfrac12-z.\ x+\tfrac12.\ y;$$
$$\bar{y}\bar{z}\bar{x};\ y+\tfrac12,\ z,\ \tfrac12-x;\ \tfrac12-y.\ z+\tfrac12,\ x;\ y.\ \tfrac12-z,\ x+\tfrac12.$$

Taking for the present purposes the scattering power (σ) of atoms in these general positions as unity and divid-

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[8] Ralph W. G. Wyckoff, this Journal, 50, 317, 1920.

ing all reflecting planes into three classes having indices that are (1) two even and one odd, (2) two odd and one even and (3) all odd, the A and B terms of expression [1] are found to be as follows for the first order region of the spectrum (which can be distinguished in Laue photographic data from cubic crystals without any uncertainty):

(1) When the indices are two even and one odd, and p, q, and r are any integers: $B = 0$, and

$$\begin{array}{llll}
A=2\cos & 2\pi[2px+2qy+(2r+1)z] & +2\cos & 2\pi[-2px+2qy-(2r+1)z+\tfrac{1}{2}] \\
+2 & \text{``}\quad [2pz+2qx+(2r+1)y] & +2 & \text{``}\quad [-2pz+2qx-(2r+1)y+\tfrac{1}{2}] \\
+2 & \text{``}\quad [2py+2qz+(2r+1)x] & +2 & \text{``}\quad [-2py+2qz-(2r+1)x+\tfrac{1}{2}] \\
+2 & \text{``}\quad [2px-2qy-(2r+1)z] & +2 & \text{``}\quad [-2px-2qy+(2r+1)z+\tfrac{1}{2}] \\
+2 & \text{``}\quad [2pz-2qx-(2r+1)y] & +2 & \text{``}\quad [-2pz-2qx+(2r+1)y+\tfrac{1}{2}] \\
+2 & \text{``}\quad [2py-2qz-(2r+1)x] & +2 & \text{``}\quad [-2py-2qz+(2r+1)x+\tfrac{1}{2}]
\end{array}$$

(2) When the indices are two odd and one even: $B = 0$ and

$$\begin{array}{llll}
A=2\cos & 2\pi[2px+(2q+1)y+(2r+1)z] & +2\cos & 2\pi[2px-(2q+1)y-(2r+1)z+\tfrac{1}{2}] \\
+2 & \text{``}\quad [2pz+(2q+1)x+(2r+1)y] & +2 & \text{``}\quad [2pz-(2q+1)x-(2r+1)y+\tfrac{1}{2}] \\
+2 & \text{``}\quad [2py+(2q+1)z+(2r+1)x] & +2 & \text{``}\quad [2py-(2q+1)z-(2r+1)x+\tfrac{1}{2}] \\
+2 & \text{``}\quad [-2px+(2q+1)y-(2r+1)z] & +2 & \text{``}\quad [-2px-(2q+1)y+(2r+1)z+\tfrac{1}{2}] \\
+2 & \text{``}\quad [-2pz+(2q+1)x-(2r+1)y] & +2 & \text{``}\quad [-2pz-(2q+1)x+(2r+1)y-\tfrac{1}{2}] \\
+2 & \text{``}\quad [-2py+(2q+1)z-(2r+1)x] & +2 & \text{``}\quad [-2py-(2q+1)z+(2r+1)x+\tfrac{1}{4}]
\end{array}$$

(3) When the indices are all odd: $B = 0$, and

$$\begin{array}{llll}
A=2\cos & 2\pi[(2p+1)x+(2q+1)y+(2r+1)z] & +2\cos & 2\pi[-(2p+1)x+(2q+1)y-(2r+1)z] \\
+2 & \text{``}\quad [(2p+1)z+(2q+1)x+(2r+1)y] & +2 & \text{``}\quad [-(2p+1)z+(2q+1)x-(2r+1)y] \\
+2 & \text{``}\quad [(2p+1)y+(2q+1)z+(2r+1)x] & +2 & \text{``}\quad [-(2p+1)y+(2q+1)z-(2r+1)x] \\
+2 & \text{``}\quad [(2p+1)x-(2q+1)y-(2r+1)z] & +2 & \text{``}\quad [-(2p+1)x-(2q+1)y+(2r+1)z] \\
+2 & \text{``}\quad [(2p+1)z-(2q+1)x-(2r+1)y] & +2 & \text{``}\quad [-(2p+1)z-(2q+1)x+(2r+1)y] \\
+2 & \text{``}\quad [(2p+1)y-(2q+1)z-(2r+1)x] & +2 & \text{``}\quad [-(2p+1)y-(2q+1)z+(2r+1)x]
\end{array}$$

It is thus seen that in general all three groups will appear in the first order region of the spectrum. The following procedure will, however, serve to determine whether there may not be classes of planes within these groups which will show a different behavior.

$$\cos 2\pi(\alpha) = -\cos 2\pi(\beta), \text{ when } \alpha = (\pm\beta\pm\tfrac{1}{2})$$

Consequently any and all values of p, q, and r which will make $A = 0$ for the region $n = 1$ can be found by equating the *revolutions* of the first term of A, $[2px+2qy+(2r+1)z]$, to the revolutions of each of the other terms of A plus $\frac{1}{2}$ (and any integer s) and solving the resultant expressions for any possible integral values of p, q, and r. Thus,

$$2px+2qy+(2r+1)z=\pm[2pz+2qx+(2r+1)y+\tfrac{1}{2}+s],$$

$$2px+2qy+(2r+1)z=\pm[2py+2qz+(2r+1)x+\tfrac{1}{2}+s],$$

etc.

$$2px+2qy+(2r+1)z=\pm[2px-2qy-(2r+1)z+\tfrac{1}{2}+s],$$

etc.

It is readily shown that all of the solutions to any of these equations are comprehended by making $p=0$ and letting q and r have any values. A similar set of equations can be set up for the second and for each succeeding term of A and values of p, q and r which will make $A=0$ can be selected from those solutions which are common to all of these sets of equations. Because of the simplicity of these expressions this detailed procedure can be materially shortened in actual practice.

If the B term were not invariably equal to zero, a similar procedure would have to be followed and solutions common to it and to the A term chosen. Since

$$\sin 2\pi(\alpha) = -\sin 2\pi(\beta)$$

both when $\alpha = -\beta$ and when $\alpha = (\beta \pm \frac{1}{2})$, two sets of expressions somewhat different from those of the A terms must be established.

The carrying out of this procedure for each of the three groups of planes shows that

(1) When the indices are two even and one odd, $A = 0$ if $2p = h$, $2q = k = 0$, $(2r+1) = l$;

(2) When the indices are two odd and one even, $A = 0$ if $2p = h = 0$, $(2q+1) = k$, $(2r+1) = l$;

(3) When the indices are all odd, A is never equal to zero. This absence in the first order of planes of the class $h0l$, where h is even, and of the class $0kl$, where both k and l are odd, will then be a universal characteristic of the defraction effects from all crystals having the symmetry of the space group T_h^6. Since a further study of all of the space groups shows that there is no other one for which these classes of planes and no others are absent, a unique method is thus provided for determining from a study of its Laue photographs whether or not a crystal has the symmetry of the space group T_h^6.

By extending the typical treatment applied here to each of the cubic space groups, a series of criteria can be established for distinguishing in so far as is possible between them. Since in tetartohedral and paramorphic hemihedral (pyritohedral) crystals the plane *hkl* belongs to a different form from *khl* (for instance 041 is distinct from 401) the Laue photographs to which these crystals give rise will possess less symmetry than photographs of those belonging to one of the other classes of cubic symmetry. On the basis of an observed hemihedry or holohedry in the symmetry of the Laue photographs, crystals of the classes T or T^h can always be distinguished from crystals of the classes T^d,O or O^h.

Crystals corresponding to space groups based upon Γ_c, the simple cubic lattice, will in general like T_h^6 give reflections in the first order from planes of all three groups; those based upon the face-centered lattice, Γ_c', will give first (or any odd numbered) order reflections only from planes all of whose indices are odd; and those developed from the body-centered lattice, Γ_c'', will reflect in the first (or any odd numbered) order only planes having two indices that are odd and one even. Upon the observed symmetry of the corresponding Laue photographs and the nature of the underlying lattice, the cubic space groups can be given the following preliminary arrangement:

Γ_c: all kinds of planes in all orders,
Hemihedral Laue Photographs:
$T^1,T^4,T_h^1,T_h^2,T_h^6$;
Holohedral Laue Photographs:
$T_d^1,T_d^4,O^1,O^2,O^6,O^7,O_h^1,O_h^2,O_h^3,O_h^4$.

Γ_c': only all odd planes in odd orders,
Hemihedral Laue Photographs:
T^2,T_h^3,T_h^4;
Holohedral Laue Photographs:
$T_d^2,T_d^5,O^3,O^4,O_h^5,O_h^6,O_h^7,O_h^8$.

Γ_c'': only two odd and one even planes in odd orders,
Hemihedral Laue Photographs:
T^3,T^5,T_h^5,T_h^7;
Holohedral Laue Photographs:
$T_d^3,T_d^6,O^5,O^8,O_h^9,O_h^{10}$.

Distinctions between most of the space groups of any one of these divisions are possible in the first order region of the spectrum (see page 183). By calculating the A and B terms of the intensity expression [1] for the second-order region for various space groups, using the same procedure previously employed, a few more distinctions between space groups can also be made. A final classification of all of the cubic space groups on the basis of the diffraction effects produced by corresponding crystals can be written as follows. In this table indistinguishable space groups are placed together on one line.

$$\Gamma_c: \qquad \left.\begin{array}{r} T^1, T_h^1; \\ T^4; \end{array}\right\} \text{uncertain} \qquad \Bigg\Vert \qquad \begin{array}{l} T_h^2; \\ T_h^6; \end{array}$$

$$\left.\begin{array}{r} T_d^1, O^1, \\ O^2; \\ O^6, O^7; \end{array}\right\} \begin{array}{l} O_h^1; \\ \text{uncertain} \\ \end{array} \qquad \Bigg\Vert \qquad \begin{array}{l} T_d^4, O_h^3; \\ O_h^2; \\ O_h^4. \end{array}$$

$$\Gamma_c': \qquad \left.\begin{array}{r} T^2, T_h^3; \\ T_h^4; \end{array}\right\} \text{second order region}$$

$$\left.\begin{array}{r} T_d^2, O^3, \\ O^4, \end{array}\right\} \begin{array}{l} \text{second order region,} \\ \text{uncertain,} \end{array} \qquad \left.\begin{array}{r} O_h^5; \\ O_h^7; \end{array}\right\} \begin{array}{l} \text{second order} \\ \text{region} \end{array}$$

$$\left.\begin{array}{r} T_d^5, O_h^6; \\ O_h^8. \end{array}\right\} \text{second order region}$$

$$\Gamma_c'': \qquad \begin{array}{r} T^3, T^5, T_h^5; \\ T_h^7; \end{array}$$

$$\left.\begin{array}{r} T_d^3, O^5; \\ O^8; \end{array}\right\} \begin{array}{l} \text{second order region,} \\ \text{uncertain,} \end{array} \qquad O_h^9;$$

$$\begin{array}{r} T_d^6; \\ O_h^{10}. \end{array}$$

Except where definitely stated as lying in the second-order region, the distinguishing characteristics are to be understood as being first-order effects. If it is assumed, as may or may not be the case, that studies of face development as commonly carried out upon crystals invariably indicate the symmetry of the arrangement of their atoms, then it will be seen that means are at hand for distinguishing between all of the various space groups except the two pairs T^3 and T^5 and O^6 and O^7. Those distinctions which involve the absence of planes of a single form (the {100} planes) can, however, be used if at all with only the greatest caution because it may readily happen that the scattering powers and relative positions of different atoms in a crystal will be such as to make the reflections from planes of this form so weak as not to be observed under the ordinary conditions of experimentation. Distinctions of this sort have consequently been designated as uncertain in the preceding classification.

The characteristics serving to distinguish between each of the space groups can be stated as follows:

Space Groups based upon a *Simple Cubic Lattice,* in general all three kinds of planes appearing in all orders:

Hemihedral Photographs:

T^1 and T_h^1: No classes of planes absent;

T^4: Planes of the form {100} absent in odd orders;

T_h^2: Planes of the form $\{okl\}$, where k and l are one even and the other odd, are absent in odd orders;

T_h^6: Planes of the form $\{hol\}$, where h is even and l is odd, and of the form $\{okl\}$, where k and l are both odd, are absent in the odd orders.

Holohedral Photographs:

T_d^1, O^1, and O_h^1: No classes of planes absent.

T_d^4 and O_h^3: Planes of the form $\{hkl\}$, where $h = \pm k$ and either h is even and l is odd or both h and l are odd, are absent in odd orders;

O^2: Planes of the form {100} are absent in odd orders;

O^6 and O^7: Planes of the form {100} are absent in all but the fourth, eighth, etc., orders;

O_h^2: Planes of the form $\{okl\}$, where k is even and l is odd, and of the form $\{hhl\}$, where either h is even and l odd or both h and l are odd, are absent in odd orders.

O_h^4: Planes of the form $\{okl\}$, where k is even and l is odd, are absent in the odd orders.

Space Groups based upon a *Face Centered Cubic Lattice,* in general planes having all odd indices appearing in odd orders:

Hemihedral Photographs:

T^2, T_h^3, and T_h^4: No classes of all odd planes are absent in the first order. Second order reflections are absent from T_h^4 for planes of the forms $\{0hl\}$ and $\{h0l\}$, where h is even and l is odd.

Holohedral Photographs:

T_d^2, O^3, O^4, O_h^5, and O_h^7: No classes of all odd planes are absent in odd orders. From O^4 only fourth, eighth, etc., orders from planes of the form {100} are present. Second order reflections from O_h^7 are absent for planes of the form $\{0kl\}$ where k is even and l is odd;

T_d^5, O_h^6, and O_h^8: Planes with all odd indices are present in odd orders except those of the form $\{hkl\}$, where $h = \pm k$. Second order reflections from O_h^8 of planes of the form $\{0kl\}$, where k is even and l odd, are absent.

Space Groups based upon a *Body Centered Cubic Lattice,* in general planes having two odd and one even indices appearing in odd orders:

Hemihedral Photographs:

T^3, T^5, and T_h^5: No classes of two odd and one even planes are absent;

T_h^7: Planes of the form $\{0kl\}$, where k and l are both odd, are absent from odd orders.

Holohedal Photographs:

T_d^3, O^5, O^8 and O_h^9: No classes of two odd and one even planes are absent in the first order. Reflections in the second order from planes of the form {100} are absent for O^8.

T_d^6: Planes of the forms $\{hll\}$ where $\frac{1}{2}h$ is even and l odd are absent in odd orders. In the second order, planes of the forms $\{hhl\}$, where either h is even and l odd, or both h and l are odd, are absent.

O_h^{10}: Planes of the form $\{0kl\}$, where k and l are odd, and of the form $\{hll\}$, where $\frac{1}{2}h$ is even and l is odd, are absent in the first order. Reflections in the second order are absent for planes of the forms $\{hhl\}$ where either h is even and l odd or both h and l are odd.

It will be observed that a number of space groups give rise to diffraction effects which are different from those resulting from any other space group. These unique space groups are T_h^2,T_h^6,O_h^2,O_h^4,T_h^4,O_h^7,O_h^8,T_h^7,T_d^6,O_h^{10}; and, less certainly because they depend upon the presence or absence of planes of the single form 100; T^4,O^2,O^6 and O^7,O^4,O^8. The symmetry of a crystal corresponding to any one of these space groups can consequently be determined with complete certainty without any reference to face development, etch-figure symmetry or any other of the customary methods of crystallography. A possible experimental method is thus furnished for finding out what relations exist between the symmetry assigned to a crystal by studies of its external appearance and the symmetry of the arrangement of its atoms.

The experimental establishment of the space group of a particular crystal is simple and can be carried out by the procedure common in crystal structure determination of taking one or more Laue photographs about some convenient orientation, determining the indices of the various diffraction spots by the usual methods of projection and finding the wave-lengths of the X-rays producing these spots with the aid of a measurement of the dimensions of the unit cell through a reflection spectrum measurement from some convenient crystal face.[9] Then if the voltage applied to the X-ray tube in producing the photographs is known, the range of the spectrum in which there will be only first-order reflections can immediately be told. It happens that in all cases where it is necessary to go to the second-order region to distinguish between space groups, first-order reflections from the planes involved are also missing. No ambiguity is therefore introduced concerning the order of reflection of diffraction spots lying in the region of strong second-order effects. Reflections from faces of the form {100} are as a rule more readily obtained by reflection spectrum measurements than from Laue photographs. It is desirable to reëmphasize that, for the reasons already given, only the appearance and not the absence of {100} reflections can necessarily furnish conclusive evidence upon which to base assignments to particular space groups.

In certain of the cases where the diffraction data are

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[9] Ralph W. G. Wyckoff, this Journal, 50, 317, 1920.

insufficient, a knowledge of the numbers of chemical molecules to be associated with the unit cube, such as arises immediately from the density and the dimension of the unit, can be of service. For instance suppose that the diffraction data from a certain crystal assigned it to the two indistinguishable space groups T^3 and T^5, and suppose that the determination of the number of chemical molecules within the unit cube requires but two chemically like atoms within the unit cell, then since only T^3 contains as a special case two equivalent positions, the crystal may be assigned to it, rather than to T^5. In view of the present lack of definite knowledge as to what it is that conditions chemical equivalence in the crystalline state, such information must obviously be used with great caution.

There naturally arises a question of whether even with atoms in the most general equivalent positions coördinate values may not exist such that the diffraction results may simulate those corresponding to some space group other than the one to which it really belongs. Any such coördinates for a space group can readily be found by practically the same procedure which has already been employed in determining the reflection characteristics of planes in different orders. In this process, however, the sets of equations are to be solved for x, y and z rather than for h, k and l.

The space group T_h^6 will again serve as an illustration. The previously established set of equations, [2], must now be solved for x, y and z which can have any values between zero and unity, including the former, instead of for integral values of p, q and r. For the present purpose care must of course be taken to avoid such values of x, y and z as yield special cases with fewer than the maximum number of equivalent positions within the unit cell. By solving these sets of expressions in a manner analogous to that previously used it can be shown for instance that when $x = u$, $y = 0$ and $z = 0$, or when $x = \frac{1}{2}$, $y = \frac{1}{2}$ and $z = 0$, only all odd planes are to be found in the first order region. When attempting to ascertain the space group to which a crystal should be assigned, it is important to take into consideration the possibility of atoms occupying exactly or nearly such positions as these. It must likewise be borne in mind that atoms in special positions may not give diffraction effects in certain orders; so that in cases where most of the heavy atoms are in such positions, the characteristic effects upon which a choice of space groups is made may some of them be relatively weak. Especially in view of this possibility of atoms occupying in some instances coördinate positions which may alter the qualitative character of the resulting diffraction effects, it is necessary to emphasize the fact that though these criteria are not ambiguous when used properly they cannot be applied blindly.

Summary.

Criteria, which are valid for crystals which have any atoms of appreciable scattering power in general positions, are established for determining from studies of Laue photographs the space group to which a cubic crystal should be assigned. This knowledge is of value to the crystal analyst because it is thus possible to tell how the atoms in many chemically complicated crystals are arranged, even though existing methods are not sufficient to locate these atoms with accuracy, and because an assignment of a crystal to a particular space group defines completely the positions of all of its elements of symmetry. Many of the space groups give diffraction effects which are different from those given by any other groups and hence a method is provided, in the cases of crystals assignable to any of these unique space groups, of defining completely crystal symmetry without making use of the older methods such as face development and the like.

Geophysical Laboratory,
April, 1922.